



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:08 PM GMT

PDB ID : 4V8H
Title : Crystal structure of HPF bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

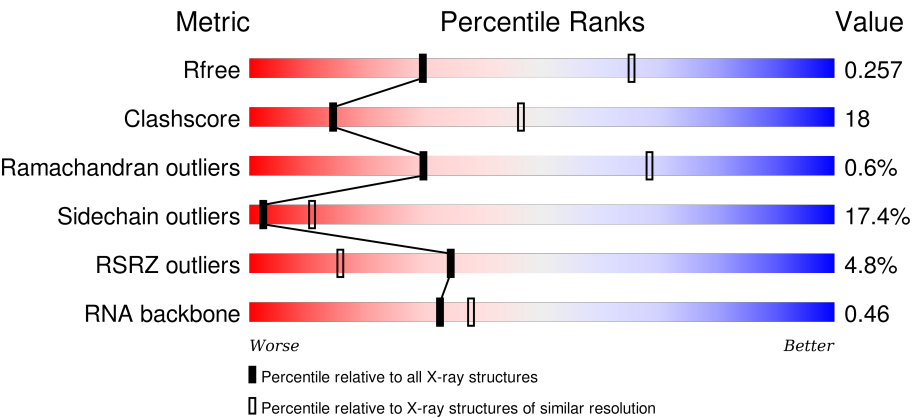
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1114 (3.14-3.06) |
| Clashscore | 102246 | 1222 (3.14-3.06) |
| Ramachandran outliers | 100387 | 1174 (3.14-3.06) |
| Sidechain outliers | 100360 | 1174 (3.14-3.06) |
| RSRZ outliers | 91569 | 1119 (3.14-3.06) |
| RNA backbone | 2183 | 1010 (3.52-2.68) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AA | 1522 | <div><div>4%</div><div>23%45%24%7%</div></div> |
| 1 | CA | 1522 | <div><div>4%</div><div>23%45%23%7%</div></div> |
| 2 | AB | 256 | <div><div>4%</div><div>37%40%13%10%</div></div> |
| 2 | CB | 256 | <div><div>5%</div><div>35%41%13%11%</div></div> |



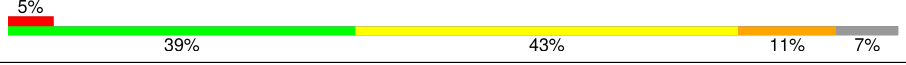
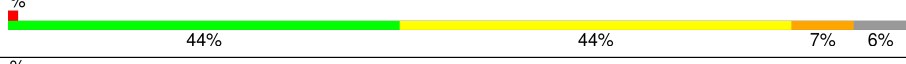
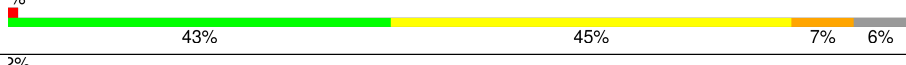
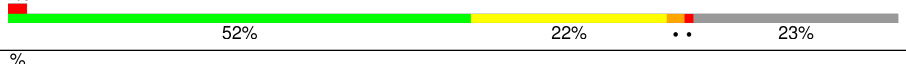
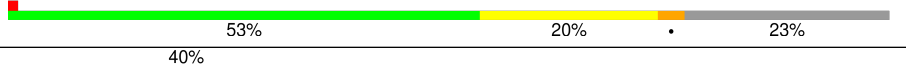


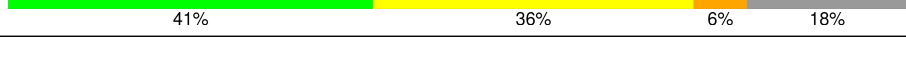

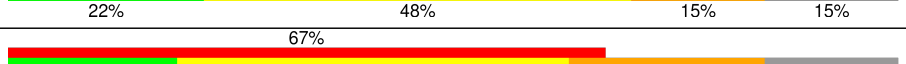
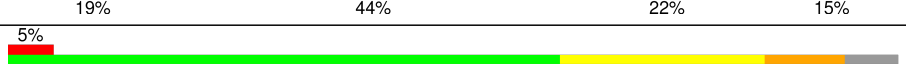
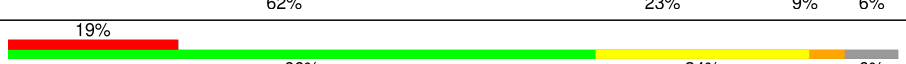
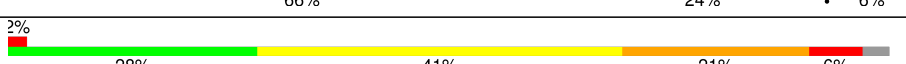
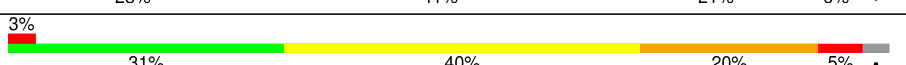
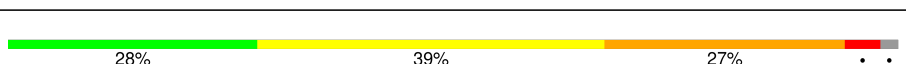
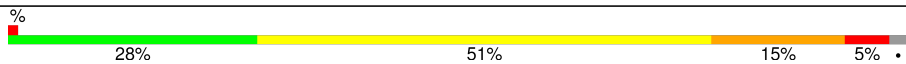
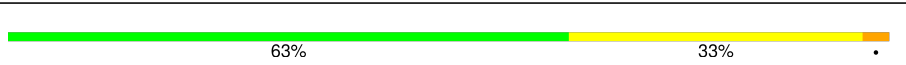


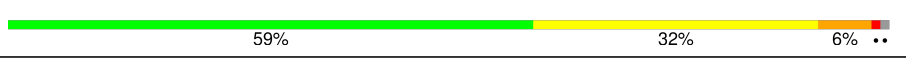
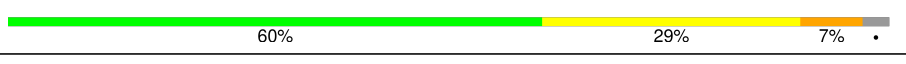


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 239 | |
| 3 | CC | 239 | |
| 4 | AD | 209 | |
| 4 | CD | 209 | |
| 5 | AE | 162 | |
| 5 | CE | 162 | |
| 6 | AF | 101 | |
| 6 | CF | 101 | |
| 7 | AG | 156 | |
| 7 | CG | 156 | |
| 8 | AH | 138 | |
| 8 | CH | 138 | |
| 9 | AI | 128 | |
| 9 | CI | 128 | |
| 10 | AJ | 105 | |
| 10 | CJ | 105 | |
| 11 | AK | 129 | |
| 11 | CK | 129 | |
| 12 | AL | 132 | |
| 12 | CL | 132 | |
| 13 | AM | 126 | |
| 13 | CM | 126 | |
| 14 | AN | 61 | |
| 14 | CN | 61 | |
| 15 | AO | 89 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | CO | 89 |  |
| 16 | AP | 88 |  |
| 16 | CP | 88 |  |
| 17 | AQ | 105 |  |
| 17 | CQ | 105 |  |
| 18 | AR | 88 |  |
| 18 | CR | 88 |  |
| 19 | AS | 93 |  |
| 19 | CS | 93 |  |
| 20 | AT | 106 |  |
| 20 | CT | 106 |  |
| 21 | AU | 27 |  |
| 21 | CU | 27 |  |
| 22 | AX | 101 |  |
| 22 | CX | 101 |  |
| 23 | BA | 2913 |  |
| 23 | DA | 2913 |  |
| 24 | BB | 122 |  |
| 24 | DB | 122 |  |
| 25 | BD | 276 |  |
| 25 | DD | 276 |  |
| 26 | BE | 206 |  |
| 26 | DE | 206 |  |
| 27 | BF | 210 |  |
| 27 | DF | 210 |  |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | BG | 182 | |
| 28 | DG | 182 | |
| 29 | BH | 180 | |
| 29 | DH | 180 | |
| 30 | BI | 148 | |
| 30 | DI | 148 | |
| 31 | BN | 140 | |
| 31 | DN | 140 | |
| 32 | BO | 122 | |
| 32 | DO | 122 | |
| 33 | BP | 150 | |
| 33 | DP | 150 | |
| 34 | BQ | 141 | |
| 34 | DQ | 141 | |
| 35 | BR | 118 | |
| 35 | DR | 118 | |
| 36 | BS | 112 | |
| 36 | DS | 112 | |
| 37 | BT | 146 | |
| 37 | DT | 146 | |
| 38 | BU | 118 | |
| 38 | DU | 118 | |
| 39 | BV | 101 | |
| 39 | DV | 101 | |
| 40 | BW | 113 | |



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 40 | DW | 113 |  |
| 41 | BX | 96 |  |
| 41 | DX | 96 |  |
| 42 | BY | 110 |  |
| 42 | DY | 110 |  |
| 43 | BZ | 206 |  |
| 43 | DZ | 206 |  |
| 44 | B0 | 85 |  |
| 44 | D0 | 85 |  |
| 45 | B1 | 98 |  |
| 45 | D1 | 98 |  |
| 46 | B2 | 72 |  |
| 46 | D2 | 72 |  |
| 47 | B3 | 60 |  |
| 47 | D3 | 60 |  |
| 48 | B4 | 71 |  |
| 48 | D4 | 71 |  |
| 49 | B5 | 60 |  |
| 49 | D5 | 60 |  |
| 50 | B6 | 54 |  |
| 50 | D6 | 54 |  |
| 51 | B7 | 49 |  |
| 51 | D7 | 49 |  |
| 52 | B8 | 65 |  |
| 52 | D8 | 65 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 53 | B9 | 37 |  |
| 53 | D9 | 37 |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | AA | 1610 | - | - | - | X |
| 54 | MG | AA | 1612 | - | - | - | X |
| 54 | MG | AA | 1618 | - | - | - | X |
| 54 | MG | AA | 1619 | - | - | - | X |
| 54 | MG | AA | 1624 | - | - | - | X |
| 54 | MG | AA | 1629 | - | - | - | X |
| 54 | MG | AA | 1633 | - | - | - | X |
| 54 | MG | AA | 1639 | - | - | - | X |
| 54 | MG | AA | 1650 | - | - | - | X |
| 54 | MG | AA | 1659 | - | - | - | X |
| 54 | MG | AA | 1660 | - | - | - | X |
| 54 | MG | AA | 1668 | - | - | - | X |
| 54 | MG | AA | 1671 | - | - | - | X |
| 54 | MG | AA | 1672 | - | - | - | X |
| 54 | MG | AA | 1680 | - | - | - | X |
| 54 | MG | AA | 1684 | - | - | - | X |
| 54 | MG | AA | 1711 | - | - | - | X |
| 54 | MG | AA | 1712 | - | - | - | X |
| 54 | MG | AD | 302 | - | - | - | X |
| 54 | MG | B3 | 101 | - | - | - | X |
| 54 | MG | BA | 3006 | - | - | - | X |
| 54 | MG | BA | 3011 | - | - | - | X |
| 54 | MG | BA | 3015 | - | - | - | X |
| 54 | MG | BA | 3019 | - | - | - | X |
| 54 | MG | BA | 3026 | - | - | - | X |
| 54 | MG | BA | 3031 | - | - | - | X |
| 54 | MG | BA | 3037 | - | - | - | X |
| 54 | MG | BA | 3040 | - | - | - | X |
| 54 | MG | BA | 3042 | - | - | - | X |
| 54 | MG | BA | 3046 | - | - | - | X |
| 54 | MG | BA | 3050 | - | - | - | X |
| 54 | MG | BA | 3061 | - | - | - | X |
| 54 | MG | BA | 3064 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | BA | 3065 | - | - | - | X |
| 54 | MG | BA | 3069 | - | - | - | X |
| 54 | MG | BA | 3089 | - | - | - | X |
| 54 | MG | BA | 3102 | - | - | - | X |
| 54 | MG | BA | 3103 | - | - | - | X |
| 54 | MG | BA | 3105 | - | - | - | X |
| 54 | MG | BA | 3109 | - | - | - | X |
| 54 | MG | BA | 3127 | - | - | - | X |
| 54 | MG | BA | 3129 | - | - | - | X |
| 54 | MG | BA | 3130 | - | - | - | X |
| 54 | MG | BA | 3145 | - | - | - | X |
| 54 | MG | BA | 3154 | - | - | - | X |
| 54 | MG | BA | 3157 | - | - | - | X |
| 54 | MG | BA | 3159 | - | - | - | X |
| 54 | MG | BA | 3167 | - | - | - | X |
| 54 | MG | BA | 3170 | - | - | - | X |
| 54 | MG | BA | 3172 | - | - | - | X |
| 54 | MG | BA | 3188 | - | - | - | X |
| 54 | MG | BA | 3189 | - | - | - | X |
| 54 | MG | BA | 3194 | - | - | - | X |
| 54 | MG | BA | 3212 | - | - | - | X |
| 54 | MG | BA | 3226 | - | - | - | X |
| 54 | MG | BA | 3245 | - | - | - | X |
| 54 | MG | BA | 3246 | - | - | - | X |
| 54 | MG | BA | 3247 | - | - | - | X |
| 54 | MG | BA | 3248 | - | - | - | X |
| 54 | MG | BA | 3249 | - | - | - | X |
| 54 | MG | BA | 3250 | - | - | - | X |
| 54 | MG | BA | 3251 | - | - | - | X |
| 54 | MG | BA | 3252 | - | - | - | X |
| 54 | MG | BA | 3253 | - | - | - | X |
| 54 | MG | BA | 3255 | - | - | - | X |
| 54 | MG | BA | 3256 | - | - | - | X |
| 54 | MG | BA | 3257 | - | - | - | X |
| 54 | MG | BA | 3259 | - | - | - | X |
| 54 | MG | BA | 3262 | - | - | - | X |
| 54 | MG | BA | 3264 | - | - | - | X |
| 54 | MG | BA | 3265 | - | - | - | X |
| 54 | MG | BA | 3270 | - | - | - | X |
| 54 | MG | BA | 3273 | - | - | - | X |
| 54 | MG | BA | 3278 | - | - | - | X |
| 54 | MG | BA | 3279 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | BA | 3282 | - | - | - | X |
| 54 | MG | BA | 3284 | - | - | - | X |
| 54 | MG | BA | 3333 | - | - | - | X |
| 54 | MG | BA | 3337 | - | - | - | X |
| 54 | MG | BA | 3368 | - | - | - | X |
| 54 | MG | BA | 3397 | - | - | - | X |
| 54 | MG | BA | 3419 | - | - | - | X |
| 54 | MG | BA | 3424 | - | - | - | X |
| 54 | MG | BA | 3451 | - | - | - | X |
| 54 | MG | BA | 3455 | - | - | - | X |
| 54 | MG | BA | 3456 | - | - | - | X |
| 54 | MG | BA | 3467 | - | - | - | X |
| 54 | MG | BA | 3473 | - | - | - | X |
| 54 | MG | BA | 3484 | - | - | - | X |
| 54 | MG | BA | 3492 | - | - | - | X |
| 54 | MG | BA | 3502 | - | - | - | X |
| 54 | MG | BA | 3574 | - | - | - | X |
| 54 | MG | BA | 3590 | - | - | - | X |
| 54 | MG | BA | 3595 | - | - | - | X |
| 54 | MG | BB | 206 | - | - | - | X |
| 54 | MG | BB | 212 | - | - | - | X |
| 54 | MG | BB | 220 | - | - | - | X |
| 54 | MG | BD | 301 | - | - | - | X |
| 54 | MG | BE | 301 | - | - | - | X |
| 54 | MG | CA | 1607 | - | - | - | X |
| 54 | MG | CA | 1611 | - | - | - | X |
| 54 | MG | CA | 1613 | - | - | - | X |
| 54 | MG | CA | 1619 | - | - | - | X |
| 54 | MG | CA | 1645 | - | - | - | X |
| 54 | MG | CA | 1685 | - | - | - | X |
| 54 | MG | CA | 1689 | - | - | - | X |
| 54 | MG | CA | 1690 | - | - | - | X |
| 54 | MG | CA | 1741 | - | - | - | X |
| 54 | MG | CA | 1749 | - | - | - | X |
| 54 | MG | CA | 1751 | - | - | - | X |
| 54 | MG | CQ | 201 | - | - | - | X |
| 54 | MG | DA | 3006 | - | - | - | X |
| 54 | MG | DA | 3008 | - | - | - | X |
| 54 | MG | DA | 3010 | - | - | - | X |
| 54 | MG | DA | 3011 | - | - | - | X |
| 54 | MG | DA | 3014 | - | - | - | X |
| 54 | MG | DA | 3017 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | DA | 3029 | - | - | - | X |
| 54 | MG | DA | 3039 | - | - | - | X |
| 54 | MG | DA | 3040 | - | - | - | X |
| 54 | MG | DA | 3041 | - | - | - | X |
| 54 | MG | DA | 3042 | - | - | - | X |
| 54 | MG | DA | 3044 | - | - | - | X |
| 54 | MG | DA | 3052 | - | - | - | X |
| 54 | MG | DA | 3063 | - | - | - | X |
| 54 | MG | DA | 3069 | - | - | - | X |
| 54 | MG | DA | 3083 | - | - | - | X |
| 54 | MG | DA | 3091 | - | - | - | X |
| 54 | MG | DA | 3092 | - | - | - | X |
| 54 | MG | DA | 3096 | - | - | - | X |
| 54 | MG | DA | 3100 | - | - | - | X |
| 54 | MG | DA | 3123 | - | - | - | X |
| 54 | MG | DA | 3125 | - | - | - | X |
| 54 | MG | DA | 3128 | - | - | - | X |
| 54 | MG | DA | 3130 | - | - | - | X |
| 54 | MG | DA | 3131 | - | - | - | X |
| 54 | MG | DA | 3133 | - | - | - | X |
| 54 | MG | DA | 3146 | - | - | - | X |
| 54 | MG | DA | 3150 | - | - | - | X |
| 54 | MG | DA | 3156 | - | - | - | X |
| 54 | MG | DA | 3157 | - | - | - | X |
| 54 | MG | DA | 3162 | - | - | - | X |
| 54 | MG | DA | 3163 | - | - | - | X |
| 54 | MG | DA | 3164 | - | - | - | X |
| 54 | MG | DA | 3167 | - | - | - | X |
| 54 | MG | DA | 3178 | - | - | - | X |
| 54 | MG | DA | 3182 | - | - | - | X |
| 54 | MG | DA | 3183 | - | - | - | X |
| 54 | MG | DA | 3196 | - | - | - | X |
| 54 | MG | DA | 3197 | - | - | - | X |
| 54 | MG | DA | 3203 | - | - | - | X |
| 54 | MG | DA | 3205 | - | - | - | X |
| 54 | MG | DA | 3209 | - | - | - | X |
| 54 | MG | DA | 3219 | - | - | - | X |
| 54 | MG | DA | 3221 | - | - | - | X |
| 54 | MG | DA | 3224 | - | - | - | X |
| 54 | MG | DA | 3229 | - | - | - | X |
| 54 | MG | DA | 3230 | - | - | - | X |
| 54 | MG | DA | 3231 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | DA | 3232 | - | - | - | X |
| 54 | MG | DA | 3241 | - | - | - | X |
| 54 | MG | DA | 3242 | - | - | - | X |
| 54 | MG | DA | 3244 | - | - | - | X |
| 54 | MG | DA | 3247 | - | - | - | X |
| 54 | MG | DA | 3257 | - | - | - | X |
| 54 | MG | DA | 3266 | - | - | - | X |
| 54 | MG | DA | 3269 | - | - | - | X |
| 54 | MG | DA | 3272 | - | - | - | X |
| 54 | MG | DA | 3276 | - | - | - | X |
| 54 | MG | DA | 3284 | - | - | - | X |
| 54 | MG | DA | 3293 | - | - | - | X |
| 54 | MG | DA | 3302 | - | - | - | X |
| 54 | MG | DA | 3303 | - | - | - | X |
| 54 | MG | DA | 3304 | - | - | - | X |
| 54 | MG | DA | 3305 | - | - | - | X |
| 54 | MG | DA | 3307 | - | - | - | X |
| 54 | MG | DA | 3308 | - | - | - | X |
| 54 | MG | DA | 3309 | - | - | - | X |
| 54 | MG | DA | 3311 | - | - | - | X |
| 54 | MG | DA | 3321 | - | - | - | X |
| 54 | MG | DA | 3337 | - | - | - | X |
| 54 | MG | DA | 3338 | - | - | - | X |
| 54 | MG | DA | 3345 | - | - | - | X |
| 54 | MG | DA | 3353 | - | - | - | X |
| 54 | MG | DA | 3366 | - | - | - | X |
| 54 | MG | DA | 3373 | - | - | - | X |
| 54 | MG | DA | 3374 | - | - | - | X |
| 54 | MG | DA | 3382 | - | - | - | X |
| 54 | MG | DA | 3414 | - | - | - | X |
| 54 | MG | DA | 3420 | - | - | - | X |
| 54 | MG | DA | 3441 | - | - | - | X |
| 54 | MG | DA | 3449 | - | - | - | X |
| 54 | MG | DA | 3473 | - | - | - | X |
| 54 | MG | DA | 3491 | - | - | - | X |
| 54 | MG | DA | 3514 | - | - | - | X |
| 54 | MG | DA | 3549 | - | - | - | X |
| 54 | MG | DA | 3570 | - | - | - | X |
| 54 | MG | DA | 3573 | - | - | - | X |
| 54 | MG | DA | 3578 | - | - | - | X |
| 54 | MG | DB | 201 | - | - | - | X |
| 54 | MG | DD | 302 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 54 | MG | DF | 301 | - | - | - | X |
| 54 | MG | DR | 202 | - | - | - | X |
| 54 | MG | DR | 203 | - | - | - | X |

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286308 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1501 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32270 | 14362 | 5983 | 10424 | 1501 | | | |
| 1 | CA | 1497 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32185 | 14324 | 5968 | 10396 | 1497 | | | |

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 230 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1787 | 1141 | 319 | 322 | 5 | | | |
| 2 | CB | 229 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1775 | 1132 | 318 | 320 | 5 | | | |

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1450 | 906 | 279 | 264 | 1 | | | |
| 3 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1450 | 906 | 279 | 264 | 1 | | | |

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | AD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1526 | 963 | 283 | 274 | 6 | | | |
| 4 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1526 | 963 | 283 | 274 | 6 | | | |

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 699 | 204 | 198 | 4 | | | |
| 5 | CE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 699 | 204 | 198 | 4 | | | |

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 777 | 493 | 137 | 144 | 3 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 777 | 493 | 137 | 144 | 3 | | | |

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1164 | 726 | 224 | 208 | 6 | | | |
| 7 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1164 | 726 | 224 | 208 | 6 | | | |

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 665 | 188 | 190 | 2 | | | |
| 8 | CH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 665 | 188 | 190 | 2 | | | |

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | AI | 125 | Total | C | N | O | 0 | 0 | 0 |
| | | | 852 | 533 | 163 | 156 | | | |
| 9 | CI | 125 | Total | C | N | O | 0 | 0 | 0 |
| | | | 852 | 533 | 163 | 156 | | | |

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10 | AJ | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 663 | 410 | 132 | 121 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10 | CJ | 96 | Total | C | N | O | | | |
| | | | 663 | 410 | 132 | 121 | 0 | 0 | 0 |

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 114 | Total | C | N | O | S | | | |
| | | | 828 | 516 | 155 | 154 | 3 | 0 | 0 | 0 |
| 11 | CK | 114 | Total | C | N | O | S | | | |
| | | | 828 | 516 | 155 | 154 | 3 | 0 | 0 | 0 |

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 122 | Total | C | N | O | S | | | |
| | | | 905 | 567 | 178 | 159 | 1 | 0 | 0 | 0 |
| 12 | CL | 122 | Total | C | N | O | S | | | |
| | | | 905 | 567 | 178 | 159 | 1 | 0 | 0 | 0 |

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 114 | Total | C | N | O | S | | | |
| | | | 804 | 497 | 164 | 142 | 1 | 0 | 0 | 0 |
| 13 | CM | 114 | Total | C | N | O | S | | | |
| | | | 804 | 497 | 164 | 142 | 1 | 0 | 0 | 0 |

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | AN | 60 | Total | C | N | O | S | | | |
| | | | 478 | 303 | 99 | 72 | 4 | 0 | 0 | 0 |
| 14 | CN | 60 | Total | C | N | O | S | | | |
| | | | 478 | 303 | 99 | 72 | 4 | 0 | 0 | 0 |

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | | | |
| | | | 724 | 453 | 143 | 126 | 2 | 0 | 0 | 0 |
| 15 | CO | 88 | Total | C | N | O | S | | | |
| | | | 724 | 453 | 143 | 126 | 2 | 0 | 0 | 0 |

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 651 | 416 | 123 | 111 | 1 | | | |
| 16 | CP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 651 | 416 | 123 | 111 | 1 | | | |

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |
| 17 | CQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | AR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 514 | 329 | 98 | 87 | | | |
| 18 | CR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 514 | 329 | 98 | 87 | | | |

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 19 | AS | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 560 | 351 | 108 | 99 | 2 | | | |
| 19 | CS | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 560 | 351 | 108 | 99 | 2 | | | |

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 87 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 410 | 142 | 111 | 2 | | | |
| 20 | CT | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 713 | 438 | 152 | 121 | 2 | | | |

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |
| 21 | CU | 23 | Total | C | N | O | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | |

- Molecule 22 is a protein called Probable sigma(54) modulation protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | AX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 631 | 396 | 116 | 118 | 1 | | | |
| 22 | CX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 601 | 378 | 108 | 114 | 1 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| AX | 96 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| AX | 97 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| AX | 98 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| AX | 99 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| AX | 100 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| AX | 101 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| CX | 96 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| CX | 97 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| CX | 98 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| CX | 99 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| CX | 100 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |
| CX | 101 | HIS | - | EXPRESSION TAG | UNP P0AFX0 |

- Molecule 23 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23 | BA | 2837 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61112 | 27197 | 11440 | 19639 | 2836 | | | |
| 23 | DA | 2814 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60621 | 26978 | 11351 | 19479 | 2813 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| BA | ? | - | U | DELETION | GB AP008226.1 |
| BA | ? | - | U | DELETION | GB AP008226.1 |
| DA | ? | - | U | DELETION | GB AP008226.1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| DA | ? | - | U | DELETION | GB AP008226.1 |

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 24 | BB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |
| 24 | DB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2135 | 1349 | 422 | 361 | 3 | | | |
| 25 | DD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | BE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |
| 26 | DE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1555 | 982 | 297 | 270 | 6 | | | |

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27 | BF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 298 | 273 | 2 | | | |
| 27 | DF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 298 | 273 | 2 | | | |

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1368 | 879 | 242 | 244 | 3 | | | |
| 28 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1368 | 879 | 242 | 244 | 3 | | | |

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |
| 29 | DH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1317 | 837 | 243 | 236 | 1 | | | |

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | BI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1037 | 666 | 180 | 190 | 1 | | | |
| 30 | DI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 953 | 608 | 168 | 176 | 1 | | | |

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |
| 31 | DN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 717 | 207 | 184 | 4 | | | |

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |
| 32 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 923 | 583 | 168 | 168 | 4 | | | |

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 703 | 229 | 196 | 3 | | | |
| 33 | DP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 703 | 229 | 196 | 3 | | | |

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 34 | DQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 35 | DR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36 | BS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 865 | 544 | 172 | 149 | | | |
| 36 | DS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 865 | 544 | 172 | 149 | | | |

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1063 | 666 | 213 | 183 | 1 | | | |
| 37 | DT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1063 | 666 | 213 | 183 | 1 | | | |

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 38 | DU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 554 | 172 | 153 | 2 | | | |
| 40 | DW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 881 | 554 | 172 | 153 | 2 | | | |

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 483 | 134 | 124 | 1 | | | |
| 41 | DX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 742 | 483 | 134 | 124 | 1 | | | |

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 503 | 145 | 131 | 6 | | | |
| 42 | DY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 503 | 145 | 131 | 6 | | | |

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BZ | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1536 | 980 | 272 | 282 | 2 | | | |
| 43 | DZ | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1522 | 972 | 269 | 279 | 2 | | | |

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | B0 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 594 | 368 | 125 | 100 | 1 | | | |
| 44 | D0 | 76 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 594 | 368 | 125 | 100 | 1 | | | |

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | B1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |
| 45 | D1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 745 | 469 | 144 | 131 | 1 | | | |

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | B2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |
| 46 | D2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 47 | B3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 458 | 293 | 87 | 78 | | | |
| 47 | D3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 458 | 293 | 87 | 78 | | | |

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48 | B4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |
| 48 | D4 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 349 | 223 | 57 | 64 | 5 | | | |

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 286 | 90 | 74 | 5 | | | |
| 49 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 286 | 90 | 74 | 5 | | | |

- Molecule 50 is a protein called 50S Ribosomal Protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 90 | 77 | 4 | | | |
| 50 | D6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 278 | 90 | 77 | 4 | | | |

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 51 | D7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |
| 52 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 326 | 99 | 82 | 2 | | | |

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | B9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 297 | 182 | 66 | 46 | 3 | | | |
| 53 | D9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 297 | 182 | 66 | 46 | 3 | | | |

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54 | BA | 660 | Total | Mg | 0 | 0 |
| | | | 660 | 660 | | |
| 54 | CA | 162 | Total | Mg | 0 | 0 |
| | | | 162 | 162 | | |
| 54 | DQ | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | DF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | B8 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54 | BE | 5 | Total 5 | Mg 5 | 0 | 0 |
| 54 | B1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | B5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | BB | 23 | Total 23 | Mg 23 | 0 | 0 |
| 54 | BT | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | D8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | B9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BF | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | DR | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | B2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | AA | 135 | Total 135 | Mg 135 | 0 | 0 |
| 54 | BQ | 4 | Total 4 | Mg 4 | 0 | 0 |
| 54 | CQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | AD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | DD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | D0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | BG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | B3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | DA | 598 | Total 598 | Mg 598 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 54 | DP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | DO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | DE | 4 | Total 4 | Mg 4 | 0 | 0 |
| 54 | AQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | D1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | AC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BS | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | D5 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BD | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | B0 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | CE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | BW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | AF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | DB | 8 | Total 8 | Mg 8 | 0 | 0 |

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 55 | B5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | B4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | AD | 1 | Total 1 | Zn 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 55 | CD | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | B9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | BY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | DY | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | D5 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | D4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | AN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | CN | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | D6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 55 | B6 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 56 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 56 | AA | 268 | Total 268 | O 268 | 0 | 0 |
| 56 | AE | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | AL | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | AO | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | AP | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | AT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | AX | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BA | 1694 | Total 1694 | O 1694 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 56 | BB | 57 | Total 57 | O 57 | 0 | 0 |
| 56 | BD | 20 | Total 20 | O 20 | 0 | 0 |
| 56 | BE | 11 | Total 11 | O 11 | 0 | 0 |
| 56 | BF | 6 | Total 6 | O 6 | 0 | 0 |
| 56 | BH | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BN | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | BO | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | BP | 11 | Total 11 | O 11 | 0 | 0 |
| 56 | BQ | 5 | Total 5 | O 5 | 0 | 0 |
| 56 | BR | 6 | Total 6 | O 6 | 0 | 0 |
| 56 | BT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BU | 3 | Total 3 | O 3 | 0 | 0 |
| 56 | BV | 3 | Total 3 | O 3 | 0 | 0 |
| 56 | BW | 3 | Total 3 | O 3 | 0 | 0 |
| 56 | BX | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | BY | 4 | Total 4 | O 4 | 0 | 0 |
| 56 | B0 | 8 | Total 8 | O 8 | 0 | 0 |
| 56 | B1 | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | B3 | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | B5 | 3 | Total 3 | O 3 | 0 | 0 |
| 56 | B6 | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 56 | B7 | 5 | Total 5 | O 5 | 0 | 0 |
| 56 | B8 | 10 | Total 10 | O 10 | 0 | 0 |
| 56 | B9 | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CA | 265 | Total 265 | O 265 | 0 | 0 |
| 56 | CC | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CD | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CE | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CL | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | CN | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CP | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CQ | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CX | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | DA | 1174 | Total 1174 | O 1174 | 0 | 0 |
| 56 | DB | 17 | Total 17 | O 17 | 0 | 0 |
| 56 | DD | 8 | Total 8 | O 8 | 0 | 0 |
| 56 | DE | 11 | Total 11 | O 11 | 0 | 0 |
| 56 | DF | 7 | Total 7 | O 7 | 0 | 0 |
| 56 | DN | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | DO | 5 | Total 5 | O 5 | 0 | 0 |

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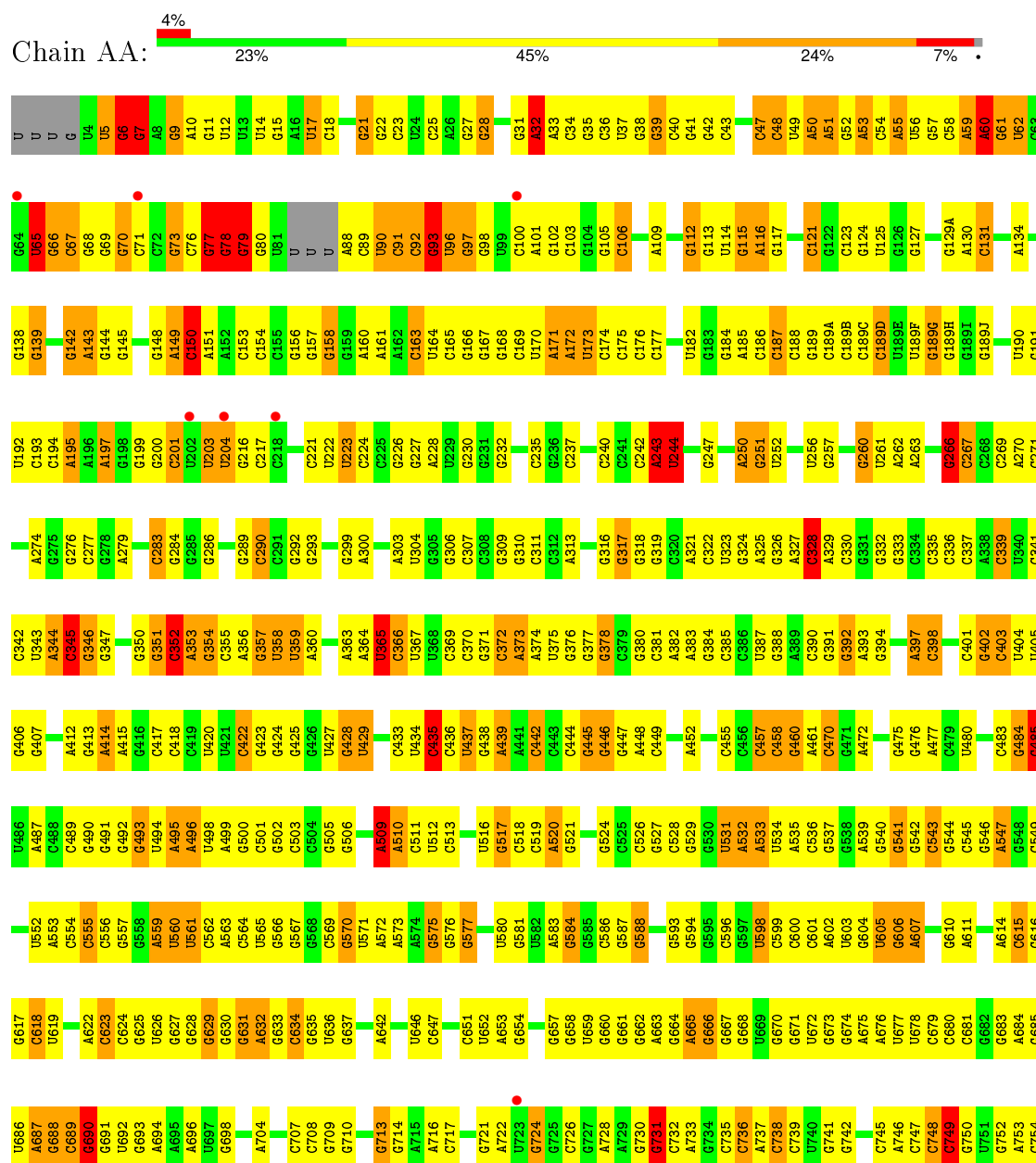
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | DP | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 56 | DQ | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | DR | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | DT | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | DU | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | DV | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | DW | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | DX | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DY | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | D0 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | D1 | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | D3 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | D4 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | D7 | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | D8 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

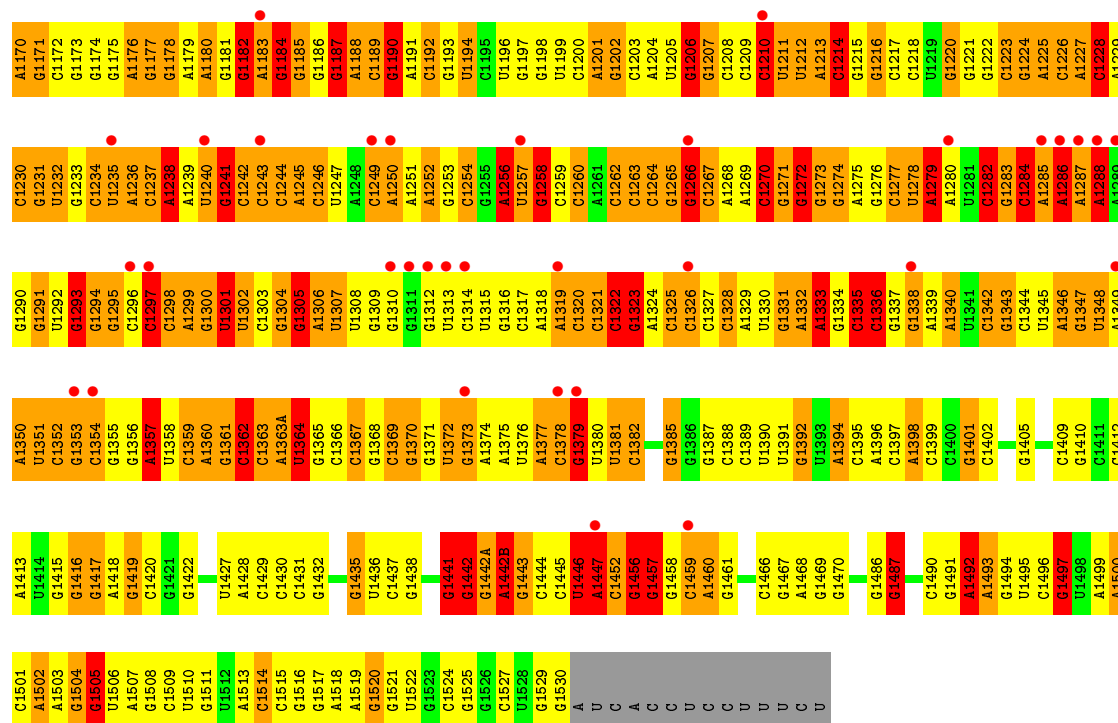
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

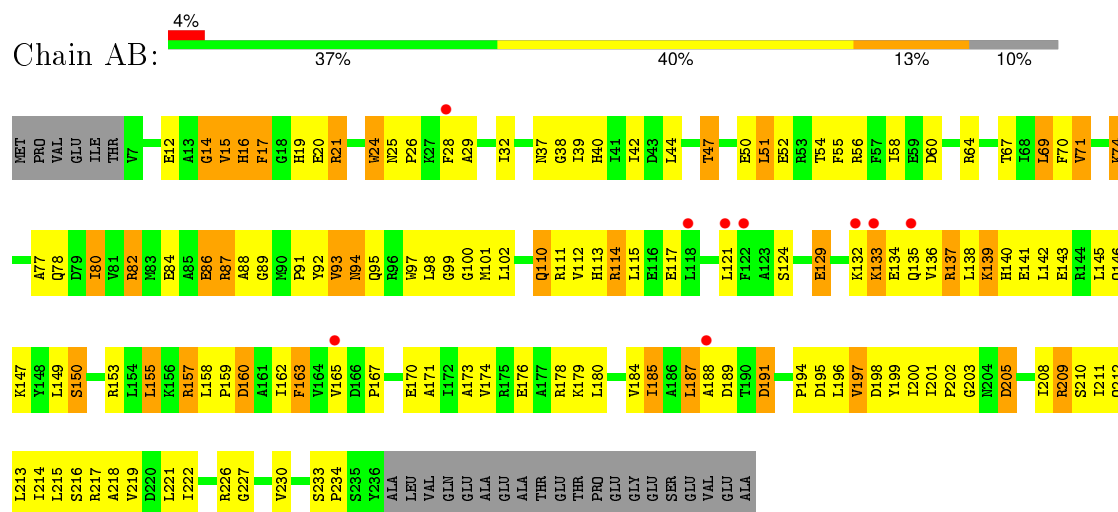
• Molecule 1: 16S Ribosomal RNA



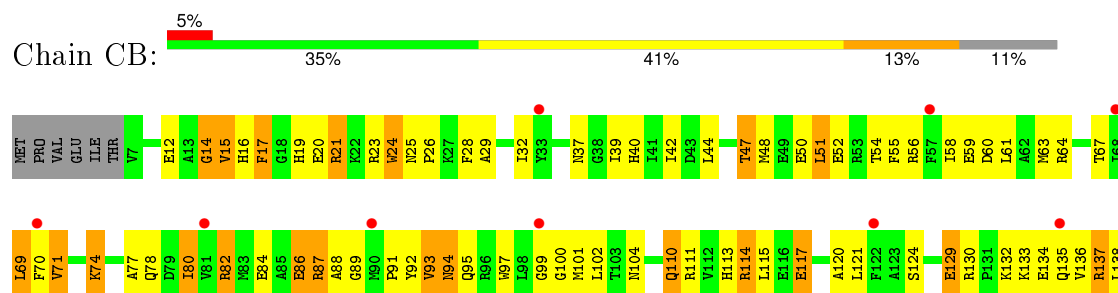
| | | | | | | | | | | | | | | | |
|-------|-------|--------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| C1109 | U1049 | A994 | C934 | C856 | A782 | G710 | U636 | C569 | G504 | G425 | A360 | C290 | A197 | A143 | U85 |
| A1110 | G1050 | C995 | A935 | C857 | C783 | G713 | G637 | C569 | G505 | G426 | A361 | C291 | A197 | G144 | G66 |
| A1111 | C1051 | A996 | C936 | G858 | C784 | G714 | G638 | U570 | A509 | G427 | U365 | C292 | C201 | G145 | C67 |
| C1112 | U1052 | A997 | A937 | G859 | C785 | G715 | A642 | A571 | A510 | G428 | C366 | G293 | U202 | G146 | G68 |
| C1113 | G1053 | C998 | A938 | A860 | C786 | G716 | A643 | A572 | C511 | G429 | U367 | U294 | U203 | G147 | G69 |
| C1114 | C1054 | C999 | G939 | G861 | A787 | C717 | U646 | A573 | C512 | A430 | U368 | U295 | U204 | G148 | G70 |
| C1115 | U1055 | U1000 | C940 | G862 | G791 | C718 | C647 | A574 | C513 | A431 | U369 | U296 | G216 | G149 | C71 |
| C1116 | A1056 | A1001 | G941 | A865 | G792 | G721 | G647 | G575 | C514 | C432 | C370 | A297 | C221 | C150 | C72 |
| G1117 | G1057 | G1001A | G942 | C866 | A792 | A722 | G650 | G576 | C515 | C433 | C371 | A298 | U222 | A151 | G73 |
| C1118 | U1058 | G1002 | U943 | C867 | C793 | U723 | G651 | G577 | G516 | C434 | C372 | A300 | U223 | A152 | C76 |
| C1119 | G1059 | G1003 | G944 | C868 | A794 | G724 | U652 | G578 | U517 | C435 | C373 | A301 | U224 | G77 | G78 |
| G1120 | C1060 | A1004 | G945 | G869 | C795 | G725 | U653 | U580 | C518 | U437 | A373 | C224 | C225 | G79 | G79 |
| G1121 | G1061 | A1005 | A946 | U870 | C796 | C726 | A653 | G581 | C519 | G438 | A374 | A303 | G226 | G | |
| U1122 | U1062 | C1006 | G947 | U871 | C797 | G727 | A654 | U582 | G520 | A439 | U375 | U804 | G227 | U | |
| A1123 | C1063 | C1007 | C948 | A872 | A802 | A729 | G657 | A583 | G521 | A441 | G376 | C307 | G227 | U | |
| G1124 | G1064 | C1008 | A873 | A873 | G803 | G730 | G658 | G584 | C522 | C442 | G377 | C308 | G232 | U | |
| U1125 | U1065 | G1009 | U950 | C874 | U804 | G731 | U659 | G585 | G523 | C443 | G378 | G309 | G233 | U | |
| U1126 | C1066 | G1010 | G951 | C875 | C805 | G732 | G660 | C586 | G524 | C444 | C379 | G310 | G234 | A | |
| G1127 | A1067 | G1011 | U952 | C876 | C806 | G733 | G661 | G587 | C525 | G445 | C380 | G311 | G235 | C | |
| C1128 | G1068 | U1012 | G953 | C877 | A807 | C734 | G662 | G588 | G526 | G446 | C381 | G312 | G236 | | |
| C1129 | C1069 | G1013 | G954 | C878 | C808 | C735 | G663 | C589 | G527 | G447 | C382 | G313 | G237 | | |
| U1130 | U1070 | A1014 | U955 | C879 | G809 | A737 | G664 | C590 | C528 | A448 | A383 | G314 | C240 | | |
| G1131 | C1071 | A1015 | U956 | C880 | C810 | G738 | A665 | G591 | C529 | C449 | A384 | G315 | C241 | | |
| C1132 | G1072 | A1016 | U957 | C881 | C811 | C739 | G666 | U598 | G530 | G450 | C385 | G316 | C242 | | |
| G1133 | U1073 | G1017 | A958 | C882 | C812 | U740 | G667 | C599 | G531 | A451 | C386 | G317 | C243 | | |
| G1134 | G1074 | C1018 | A959 | C883 | U813 | G741 | G668 | C600 | A532 | A452 | U387 | A321 | U244 | | |
| U1135 | C1075 | G1019 | U960 | U884 | A814 | G742 | G669 | C601 | A533 | A453 | G388 | C322 | G247 | | |
| U1136 | G1076 | U1020 | U961 | A815 | U815 | G743 | G670 | A602 | C534 | C454 | A389 | U323 | G248 | | |
| G1137 | G1077 | G1021 | G962 | G888 | A816 | C745 | U672 | U603 | C535 | C455 | C390 | G324 | G249 | | |
| C1138 | U1078 | G1022 | G963 | C889 | C817 | A746 | G673 | G604 | C536 | C456 | G391 | A325 | G251 | | |
| G1139 | G1079 | G1023 | A964 | C893 | G818 | C747 | G674 | U605 | C537 | C457 | G392 | G326 | U252 | | |
| C1140 | A1080 | G1024 | A965 | C894 | A819 | C748 | A675 | G606 | G538 | C458 | A393 | A327 | U253 | | |
| G1141 | U1081 | U1025 | G966 | C896 | U820 | C749 | A676 | A607 | C539 | G460 | C396 | C328 | G254 | | |
| G1142 | G1082 | G1026 | C967 | A900 | G821 | G750 | U677 | A608 | G540 | A461 | C397 | C330 | U256 | | |
| G1143 | U1083 | C1027 | A968 | A901 | C822 | U751 | G678 | A609 | G541 | C470 | C398 | G331 | G257 | | |
| G1144 | A1084 | A969 | G970 | G902 | G823 | G752 | G679 | G610 | C542 | G471 | C399 | G332 | G258 | | |
| C1145 | U1085 | C1028 | C971 | G903 | C826 | G753 | C680 | A611 | C543 | A472 | C401 | G333 | G259 | | |
| A1146 | U1086 | G1030 | G972 | G904 | U827 | G754 | C681 | A612 | C544 | G475 | G402 | G334 | G260 | | |
| C1147 | G1087 | U1030A | C973 | A909 | G827 | G755 | G682 | C615 | C545 | G476 | C403 | C335 | U261 | | |
| U1148 | U1088 | C1030B | G974 | C910 | A828 | C756 | G683 | G616 | C546 | G477 | C404 | C336 | A262 | | |
| C1149 | G1089 | G1030C | A975 | G911 | G829 | U757 | A684 | G617 | C547 | G478 | U405 | C337 | A263 | | |
| U1150 | U1090 | A1030D | A976 | G912 | G830 | G758 | G685 | G618 | C548 | G479 | U406 | C338 | G264 | | |
| A1151 | U1091 | G1031 | G976 | A913 | U831 | A759 | U686 | C619 | C549 | G480 | G407 | C339 | G265 | | |
| A1152 | A1092 | G1032 | A977 | A914 | C832 | G760 | A687 | C620 | C550 | U481 | G408 | C340 | G266 | | |
| C1153 | A1093 | G1033 | A978 | A915 | U833 | G761 | G688 | C621 | U551 | C482 | A409 | C341 | C267 | | |
| G1154 | G1094 | A1034 | C979 | A916 | C834 | G762 | C689 | A622 | U552 | C483 | A410 | C342 | C268 | | |
| G1155 | U1095 | A1035 | C980 | A917 | U835 | C763 | G690 | A623 | C553 | C484 | A411 | C343 | C269 | | |
| G1156 | C1096 | G1036 | U981 | U920 | G836 | G764 | G691 | G624 | C554 | G490 | G412 | C344 | A270 | | |
| A1157 | G1097 | G1037 | U982 | U921 | G837 | A766 | U692 | C625 | C555 | G491 | G413 | C345 | C271 | | |
| C1158 | U1098 | C1038 | A983 | G922 | G838 | A767 | G693 | G626 | C556 | G492 | A414 | C346 | G276 | | |
| U1159 | G1099 | C1039 | C984 | G923 | U839 | A768 | A694 | U627 | C557 | G493 | A415 | G350 | G277 | | |
| G1160 | C1100 | U1040 | C985 | G924 | C840 | G769 | G695 | G628 | G558 | U494 | G416 | G351 | C278 | | |
| C1161 | A1101 | A1041 | A986 | G925 | U841 | C770 | U697 | G629 | C559 | A495 | C417 | C352 | A279 | | |
| C1162 | G1042 | G1043 | G987 | G926 | C848 | G771 | U705 | G630 | U560 | A496 | C418 | A353 | G283 | | |
| C1163 | C1043 | C1044 | G988 | G927 | C849 | G772 | A706 | G631 | U561 | U497 | C419 | C354 | G284 | | |
| G1164 | G1104 | A1044 | G989 | G928 | U850 | G773 | U707 | G632 | U562 | A498 | U420 | C355 | G285 | | |
| C1165 | A1105 | C1045 | C990 | C930 | G851 | G774 | A708 | A632 | C563 | G500 | U421 | A356 | G286 | | |
| G1166 | G1106 | A1046 | U991 | C931 | G852 | G775 | C707 | G633 | C564 | G501 | C422 | U358 | G287 | | |
| U1167 | C1107 | U1047 | C992 | C932 | G853 | A777 | C708 | G634 | U565 | G502 | G423 | U359 | A195 | | |
| A1169 | G1108 | G1048 | G993 | G933 | G854 | G778 | G709 | G635 | C566 | C503 | G424 | | G289 | | |

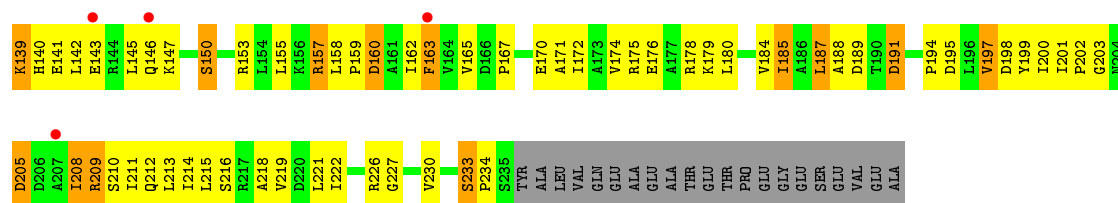


• Molecule 2: 30S Ribosomal Protein S2

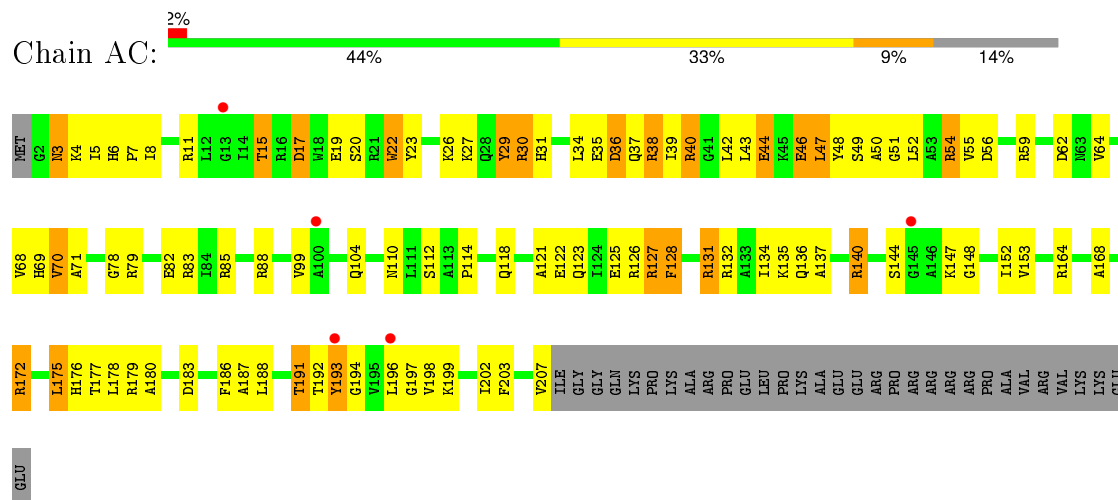


• Molecule 2: 30S Ribosomal Protein S2

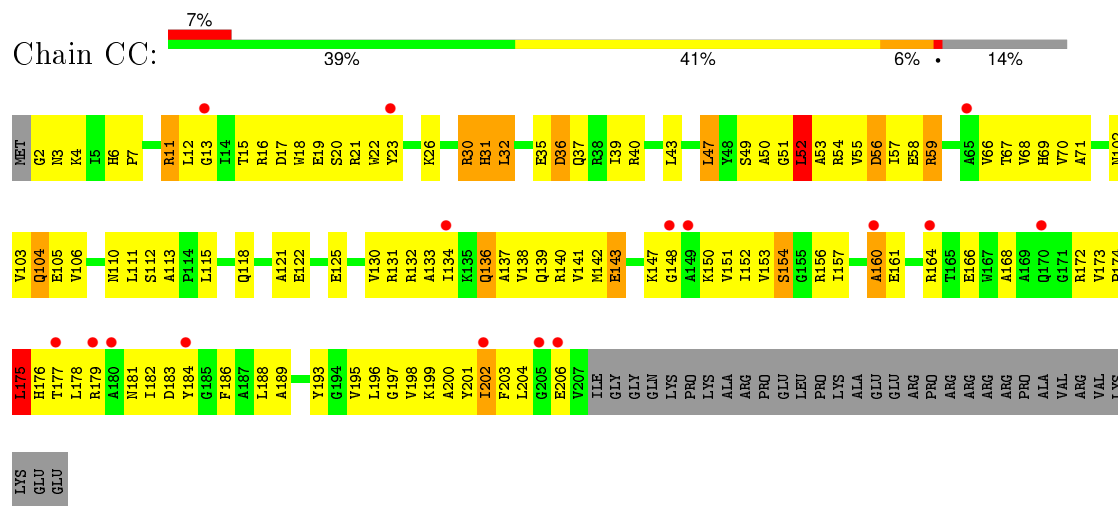




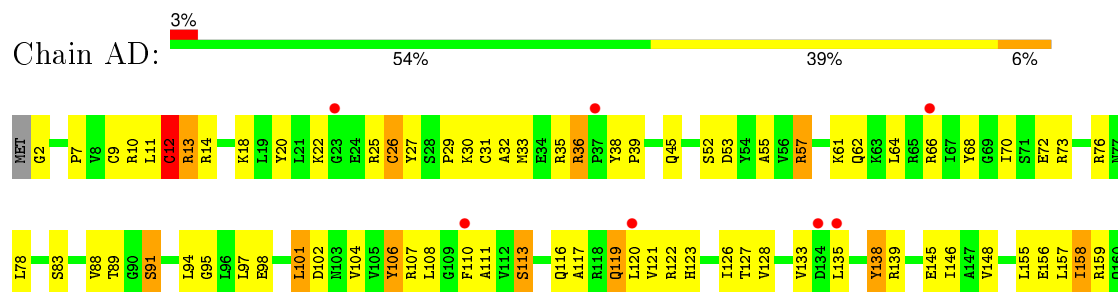
• Molecule 3: 30S Ribosomal Protein S3



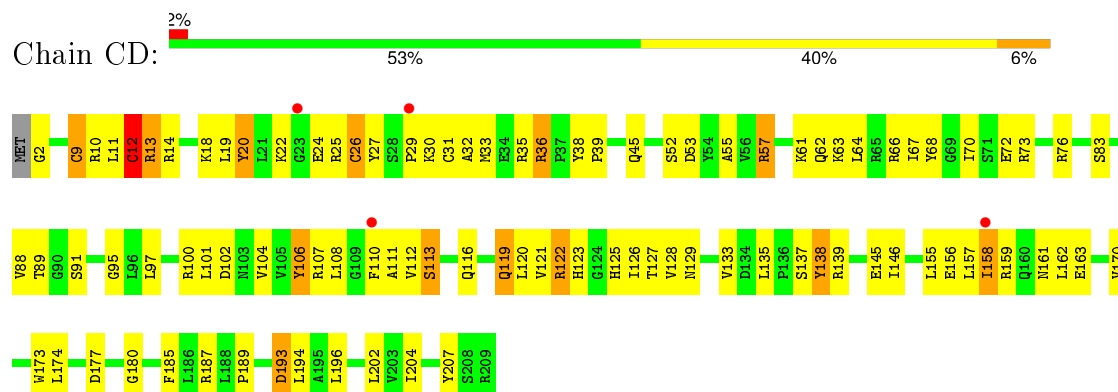
• Molecule 3: 30S Ribosomal Protein S3



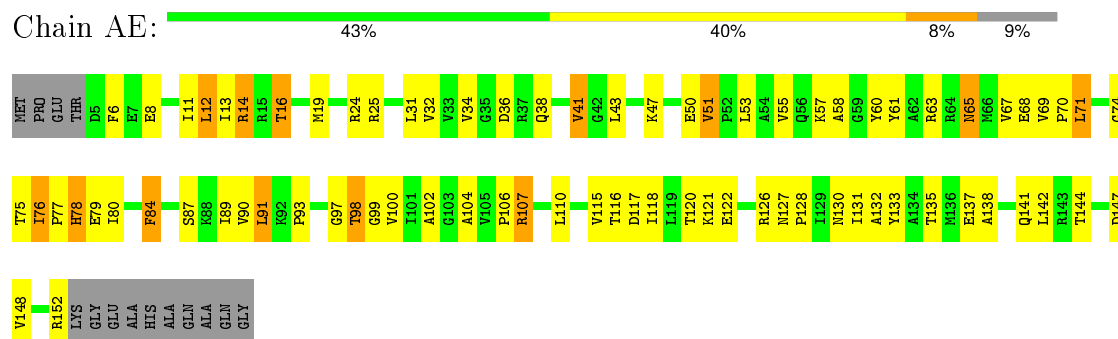
• Molecule 4: 30S Ribosomal Protein S4



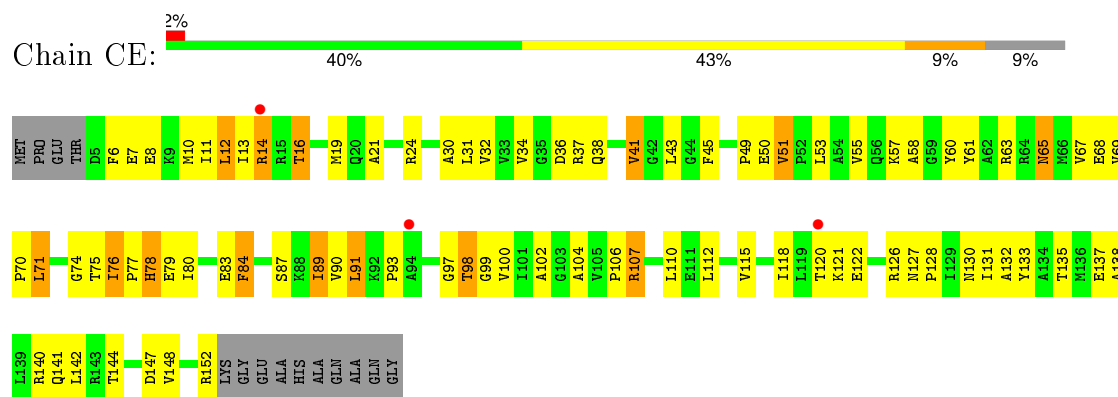
- Molecule 4: 30S Ribosomal Protein S4



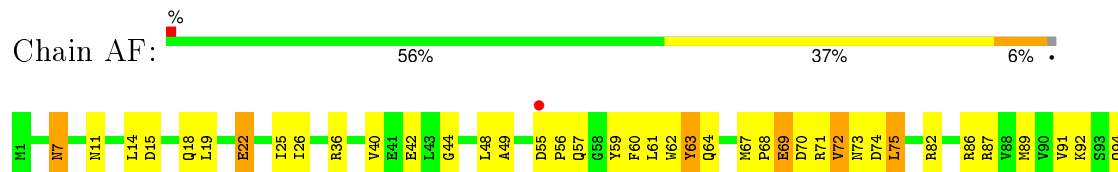
- Molecule 5: 30S Ribosomal Protein S5

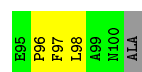


- Molecule 5: 30S Ribosomal Protein S5

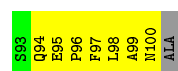
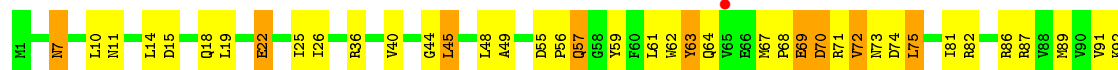


- Molecule 6: 30S Ribosomal Protein S6

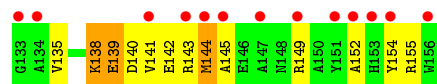
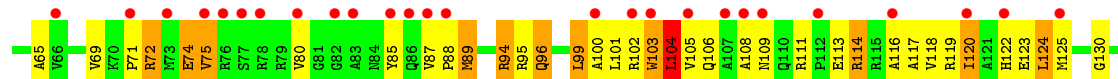
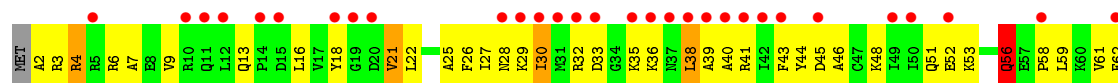
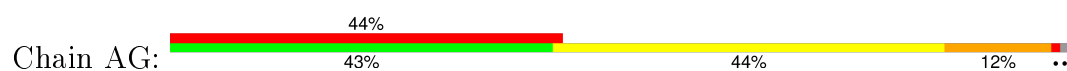




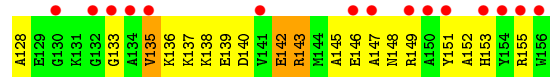
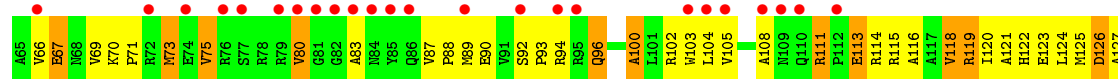
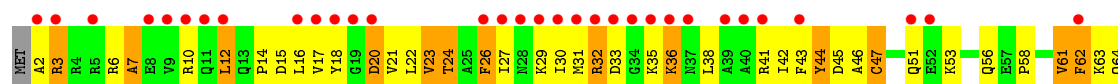
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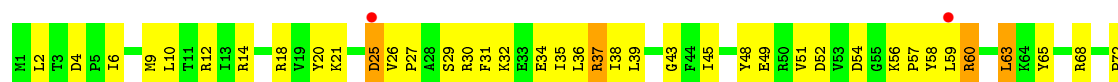
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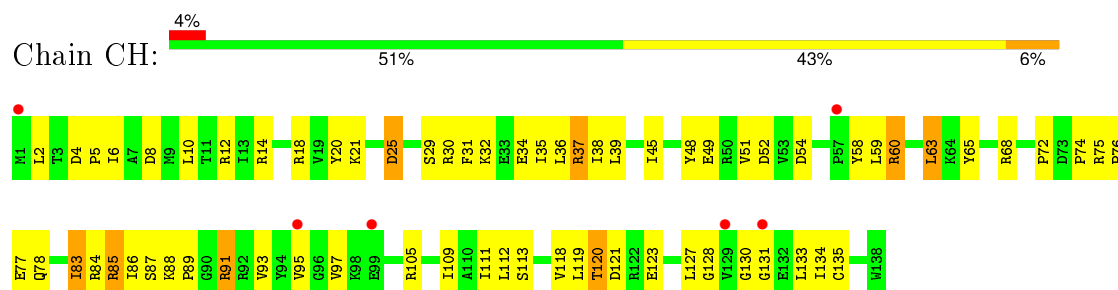
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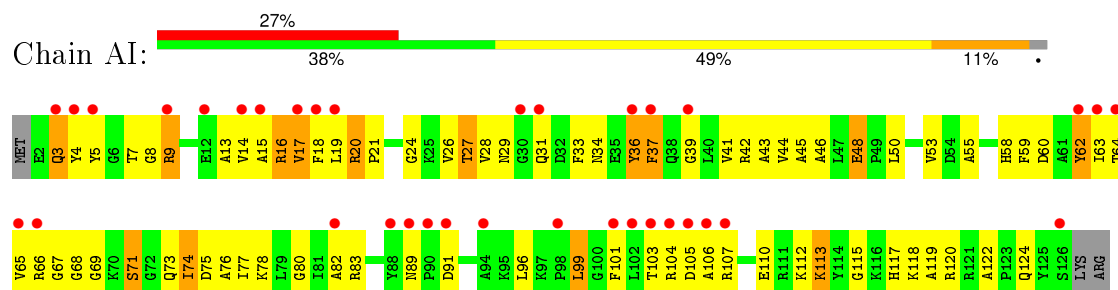
• Molecule 8: 30S Ribosomal Protein S8



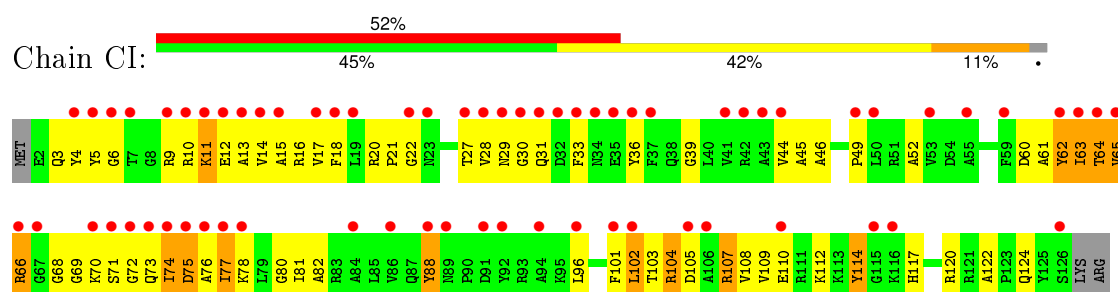
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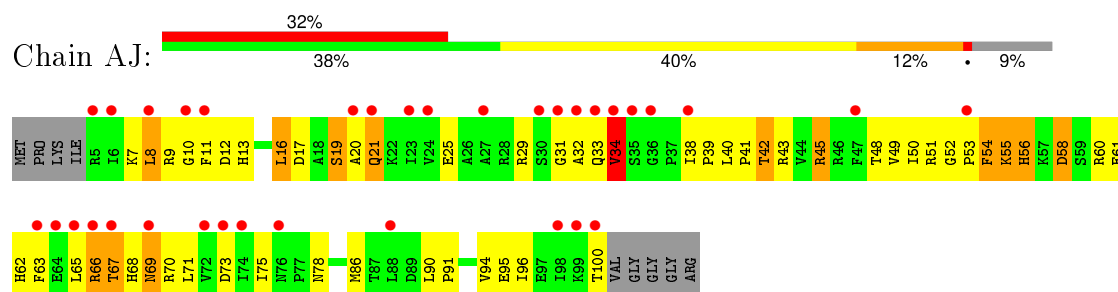
- Molecule 9: 30S Ribosomal Protein S9



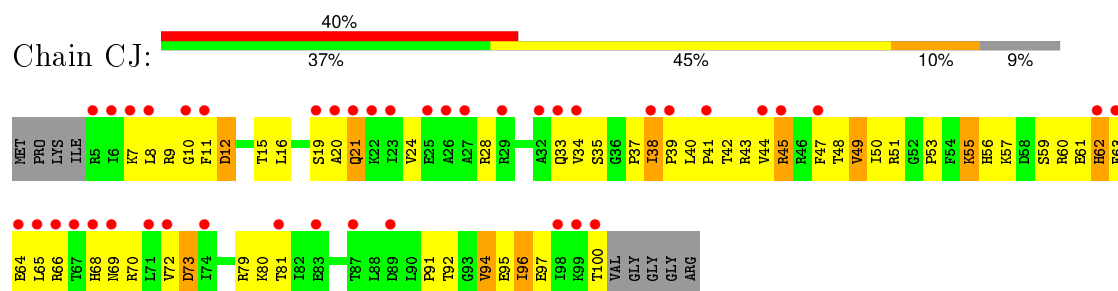
- Molecule 9: 30S Ribosomal Protein S9



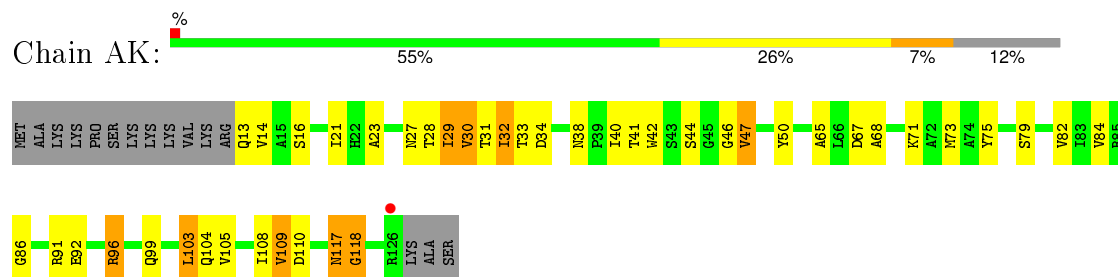
- Molecule 10: 30S Ribosomal Protein S10



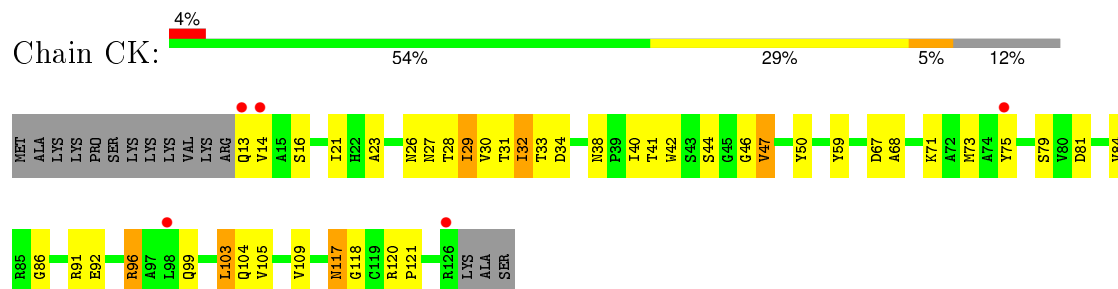
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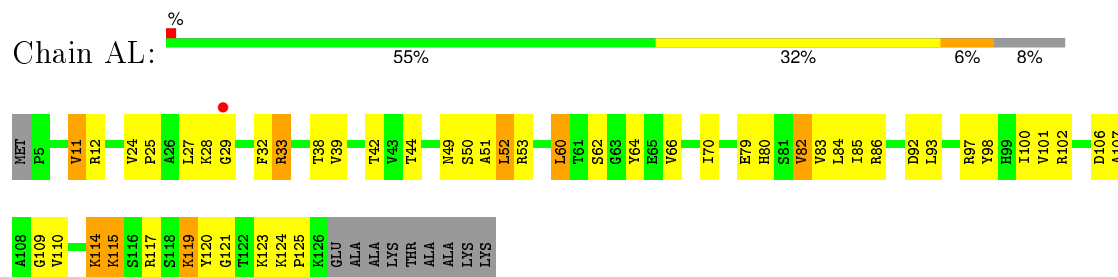
- Molecule 11: 30S Ribosomal Protein S11



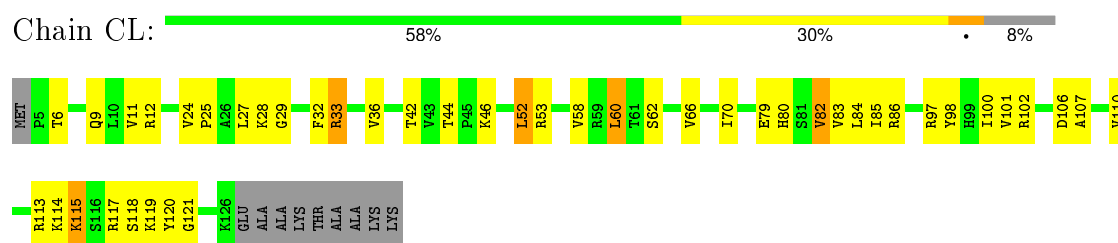
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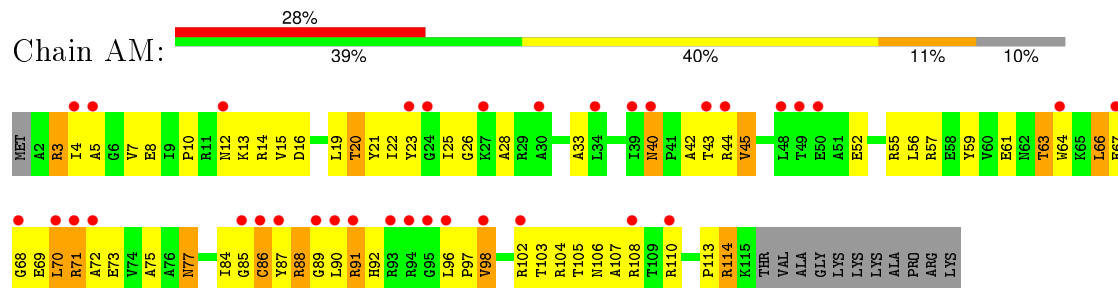
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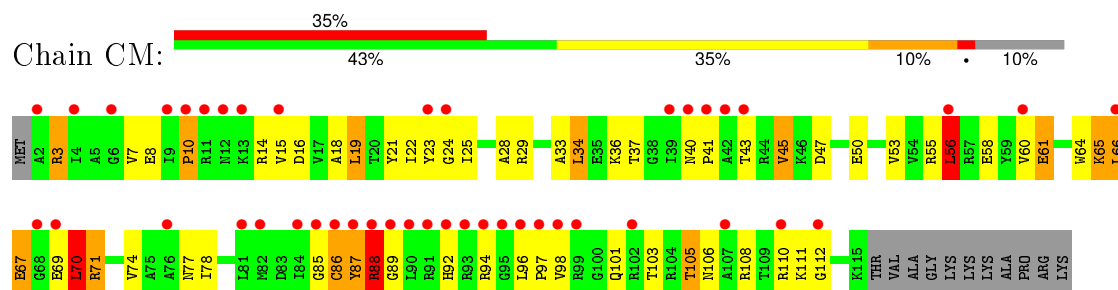
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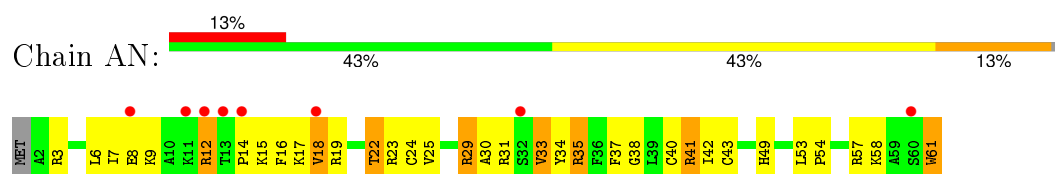
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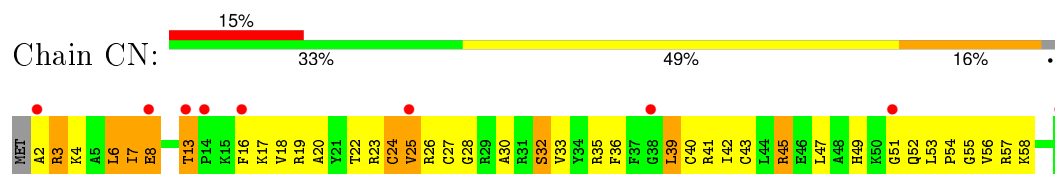
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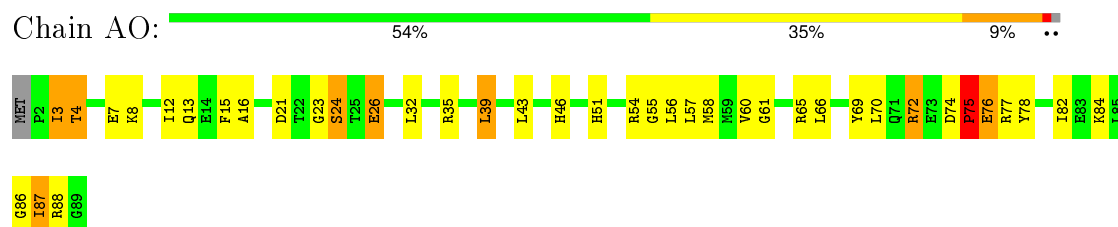
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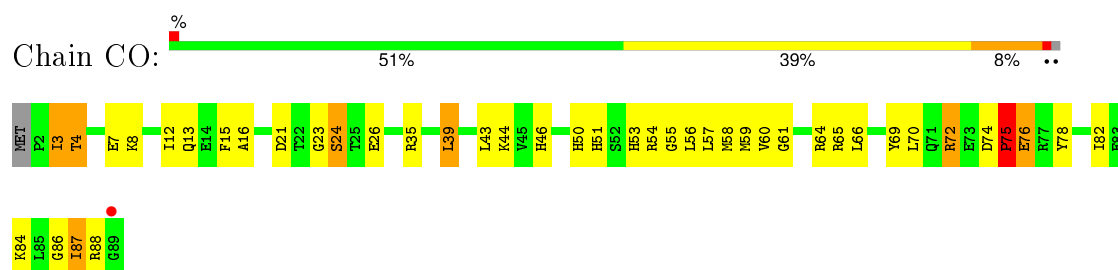
- Molecule 14: 30S Ribosomal Protein S14



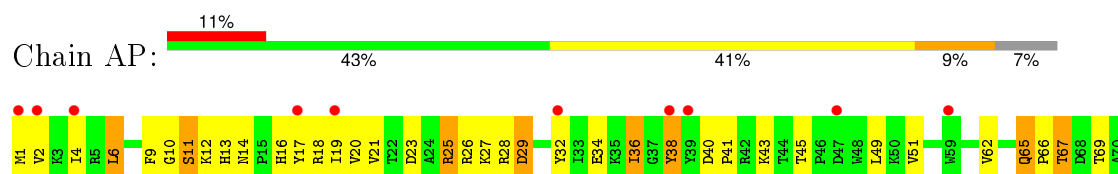
- Molecule 15: 30S Ribosomal Protein S15

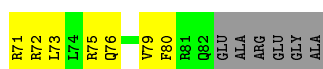


- Molecule 15: 30S Ribosomal Protein S15

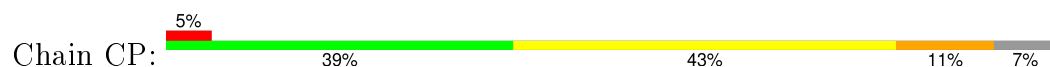


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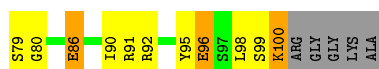
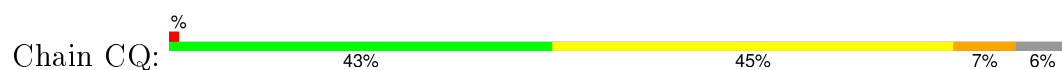
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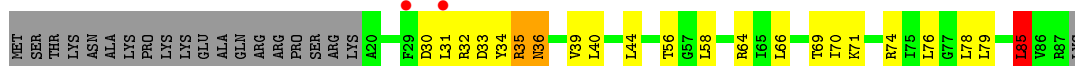
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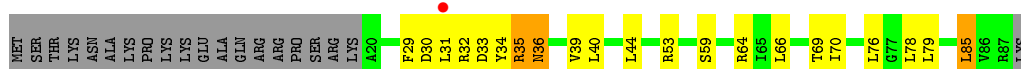
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• Molecule 18: 30S Ribosomal Protein S18

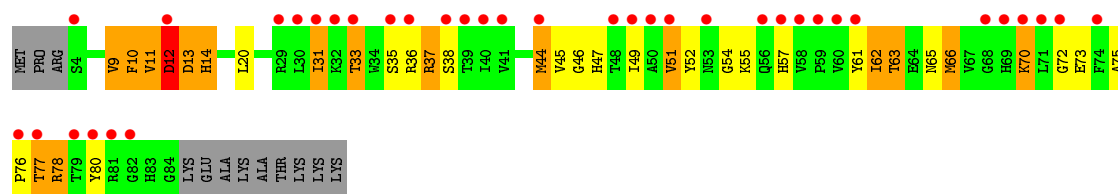


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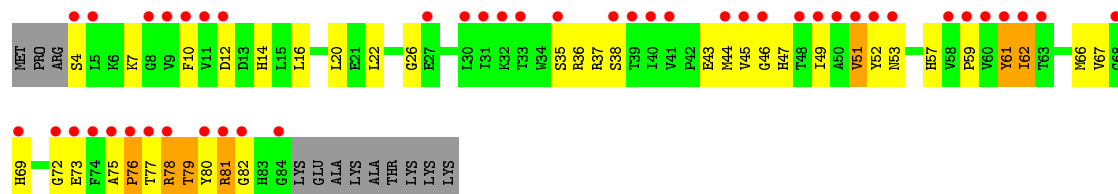


• Molecule 19: 30S Ribosomal Protein S19

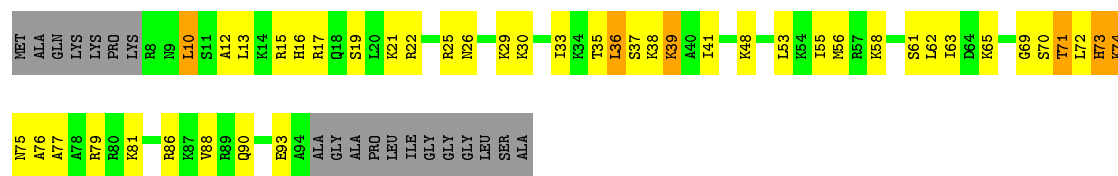




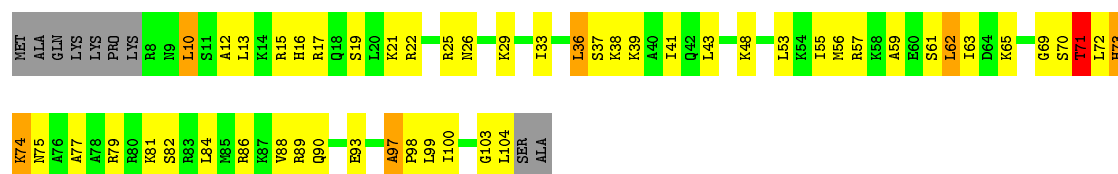
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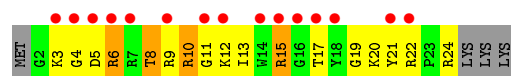
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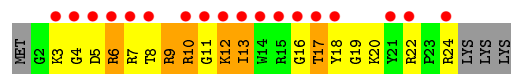
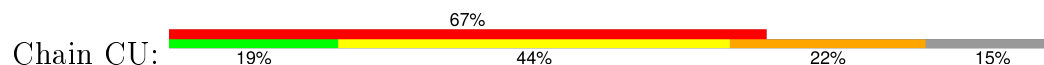
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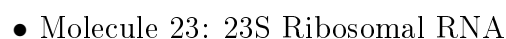
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX



• Molecule 22: Probable sigma(54) modulation protein



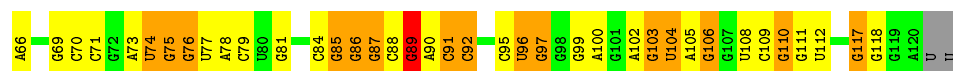
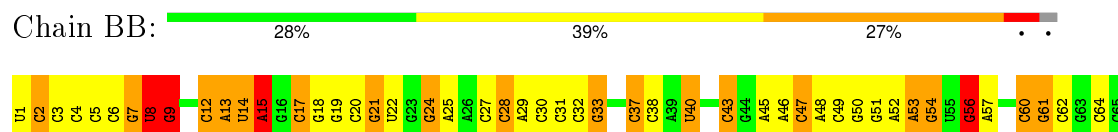
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| A1617 | G1482 | G1418 | U1340 | A1275 | A1210 | U1141 | U | G1017 | G949 | G881 | U811 | A751 | G686 |
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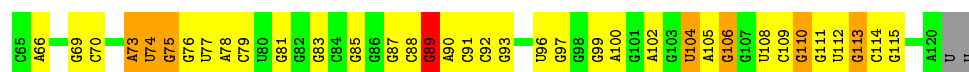
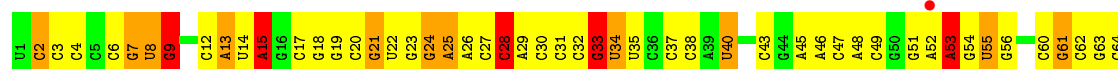


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| G1816 | G1752 | G1653 | C1582 | C1509 | U1430 | U1357 | G1289 | G1219 | A1139 | A | C1018 | A819 | C753 |
| A1817 | C1753 | A1654 | A1583 | A1509A | U1431 | U1358 | C1290 | A1220 | C1140 | U | U1019 | A820 | C754 |
| G1818 | A1755 | C1655 | C1584 | A1509B | G1432 | C1358 | U1291 | G1221 | U1141 | C | U1020 | A821 | C755 |
| A1819 | G1756 | C1656 | A1586 | G1510 | U1433 | A1359 | U1292 | C1222 | U1142 | C | A1021 | U822 | C756 |
| U1820 | U1757 | C1657 | A1587 | G1511 | U1434 | A1360 | C1293 | G1223 | A1142A | U | G1022 | G823 | U757 |
| A1821 | G1758 | C1658 | A1588 | U1512 | G1435 | C1361 | G1296 | G1223 | C1153 | U | U1023 | A824 | C758 |
| G1822 | A1759 | G1659 | G1593 | U1513 | C1436 | A1362 | C1297 | G1225 | C1154 | U | G1024 | C825 | G759 |
| G1823 | C1761 | C1663 | G1594 | U1514 | U1438 | A1366 | C1298 | G1226 | A1155 | A | U1026 | U826 | A760 |
| G1826 | A1762 | C1668 | G1595 | U1518 | G1439 | A1367 | C1299 | C1230 | C1156 | G | A1027 | U828 | U762 |
| C1827 | G1763 | A1668 | A1596 | G1519 | G1440 | G1368 | C1300 | G1231 | U1159 | A | A1028 | A829 | G763 |
| A1828 | C1764 | A1669 | A1597 | G1520 | G1441 | C1369 | A1301 | G1236 | G1160 | G | A1029 | G830 | A764 |
| A1829 | U1765 | C1670 | C1598 | G1521 | G1442 | U1370 | A1302 | A1237 | C1161 | U | G1030 | G831 | C765 |
| C1830 | C1767 | U1671 | G1525 | G1526 | A1445 | G1371 | G1303 | G1238 | G1162 | C | U1031 | U832 | G766 |
| U1833 | G1772 | G1674 | G1601 | G1526 | G1446 | U1372 | C1304 | G1239 | G1163 | C | A1032 | G | U767 |
| U1834 | A1773 | C1675 | U1602 | G1529 | G1448 | A1373 | C1305 | G1240 | G1164 | G | U1033 | U839 | G768 |
| G1835 | C1774 | A1676 | C1603 | C1530 | A1449 | G1375 | A1308 | U1241 | U1165 | U | G1034 | C840 | G770 |
| C1836 | U1775 | A1677 | C1604 | C1531 | G1450 | C1376 | G1309 | A1242 | G1166 | A | U1035 | A841 | G771 |
| G1837 | G1776 | C1685 | G1605 | C1532 | G1451 | G1377 | G1310 | G1243 | G1169 | A | G1036 | G842 | C772 |
| C1838 | U1777 | U1685 | G1606 | G | U1452 | A1378 | G1311 | G1244 | G1170 | U | G1037 | G843 | U773 |
| G1839 | U1778 | U1686 | A1608 | U | U1453 | A1379 | U1312 | A1247 | G1171 | A | C1038 | C844 | A774 |
| G1840 | U1779 | U1688 | A1609 | A | G1455 | A1380 | U1313 | G1248 | G | C | G1039 | C845 | G776 |
| C1843 | A1780 | A1689 | C1610 | C | G1456 | G1381 | C1314 | G1249 | A | U | A1041 | C846 | G776 |
| G1844 | C1781 | U1692 | C1611 | G1537 | G1459 | C1382 | C1315 | U1249 | U | C | G1042 | U847 | A777 |
| G1845 | G1782 | U1693 | G1612 | G1538 | G1460 | C1383 | U1316 | G1250 | A981 | C | C1043 | G848 | A781 |
| A1846 | A1783 | C1694 | G1613 | G1539 | C1464 | A1384 | A1317 | G1251 | G982 | C | A1044 | A849 | A782 |
| A1847 | U1784 | U1540 | A1614 | U1540 | G1465 | C1385 | C1318 | G1252 | A983 | U | A1045 | C850 | A783 |
| G1848 | A1785 | G1695 | C1615 | G1541 | G1466 | C1386 | G1319 | A1253 | C1178 | G1106 | A1046 | G853 | A784 |
| G1849 | U1786 | G1696 | A1616 | A1542 | C1467 | C1387 | C1320 | A1254 | C1179 | U1107 | G1047 | G | A785 |
| G1850 | A1787 | C1697 | C1617 | C1543 | G1467 | G1388 | A1321 | U1255 | C1180 | U1108 | A1048 | C856 | C786 |
| G1851 | C1788 | A1698 | A1618 | A1544 | G1470 | G1388 | A1322 | G1256 | C1181 | C1109 | A1049 | C857 | U787 |
| G1852 | A1789 | G1699 | A1619 | A1545 | A1471 | U1391 | A1322 | G1257 | C1185 | G1110 | A1050 | U858 | A788 |
| G1853 | C1790 | A1700 | C1546 | C1545 | A1472 | U1394 | G1325 | C1258 | C1186 | A1111 | G1051 | C859 | A789 |
| U1863 | A1791 | G1699 | C1547 | C1548 | A1477 | A1395 | U1326 | C1261 | C1187 | G1112 | C1052 | U860 | C790 |
| G1864 | C1792 | G1702 | C1548 | C1548 | G1478 | U1396 | C1327 | C1261 | U1188 | U1113 | C | A861 | C791 |
| G1865 | C1793 | G1703 | G1627 | A1553 | U1481 | C1403 | G1328 | G1264 | A1189 | A | A | G862 | G792 |
| C1866 | G1794 | G1704 | G1628 | A1554 | U1482 | C1404 | U1329 | A1265 | G1190 | G | G | A863 | A793 |
| A1876 | C1795 | U1709 | U1629 | C1557 | G1483 | U1405 | C1330 | G1266 | G1191 | G | A | G864 | G794 |
| A1877 | U1796 | C1710 | U1629 | C1557 | G1484 | U1406 | G1332 | U1267 | G1192 | A | G | C865 | C795 |
| G1878 | C1797 | C1711 | U1629 | A1558 | G1485 | U1407 | C1333 | C1268 | C1193 | G | G | A866 | C796 |
| U1798 | U1798 | C1712 | G1635 | A1559 | G1486 | C1408 | C1333 | A1268 | U1199 | G1120 | G | C867 | C797 |
| C1881 | G1799 | C1712 | G1635 | G1559 | G1487 | C1408 | A1336 | A1269 | U1199 | C1121 | U | U868 | A802 |
| G1882 | A1800 | U1713 | G1636 | G1560 | U1489 | C1408 | G1337 | C1270 | C1201 | G1122 | U | A870 | U803 |
| G1883 | G1801 | G1714 | C1637 | A1490 | U1490 | U1415 | G1338 | G1271 | C1202 | C1123 | G | G873 | A804 |
| A1884 | A1802 | G1717 | C1638 | C1564 | C1493 | G1416 | G1339 | A1272 | G1203 | G1125 | C | G874 | G805 |
| A1889 | A1803 | G1718 | C1639 | C1565 | C1494 | G1417 | G1340 | U1273 | A1204 | A1126 | U | G875 | C806 |
| A1890 | U1804 | G1721 | U1640 | A1567 | A1495 | G1418 | U1341 | A1276 | U1205 | A1127 | U | U807 | G806 |
| G1891 | C1806 | A1722 | A1641 | G1568 | A1495 | A1419 | A1342 | G1277 | G1206 | A1128 | A | A878 | G808 |

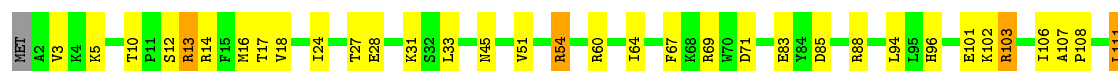
- Molecule 24: 5S Ribosomal RNA



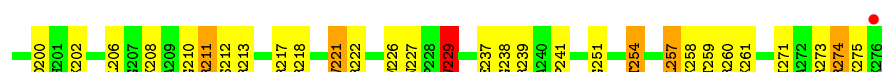
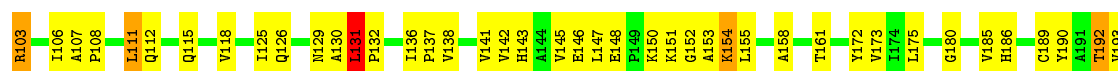
• Molecule 24: 5S Ribosomal RNA



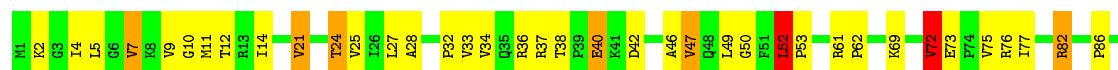
• Molecule 25: 50S Ribosomal Protein L2

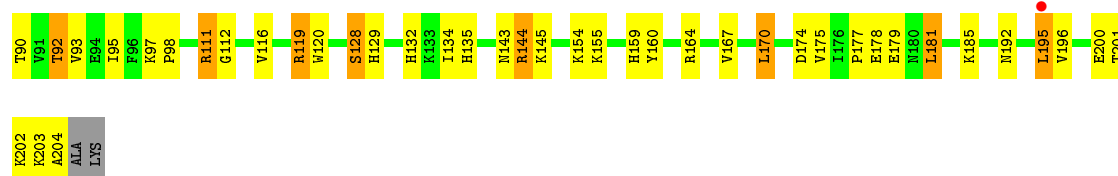


• Molecule 25: 50S Ribosomal Protein L2



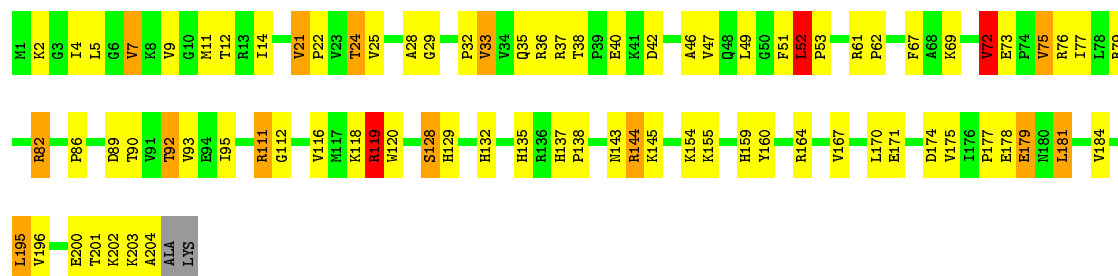
• Molecule 26: 50S Ribosomal Protein L3





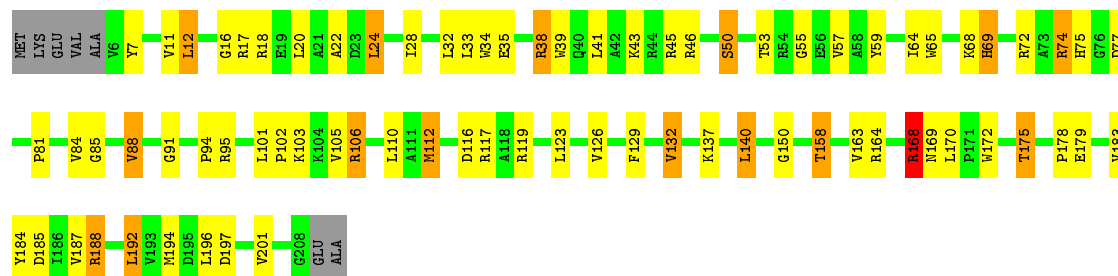
• Molecule 26: 50S Ribosomal Protein L3

Chain DE: 59% 32% 6% 2%



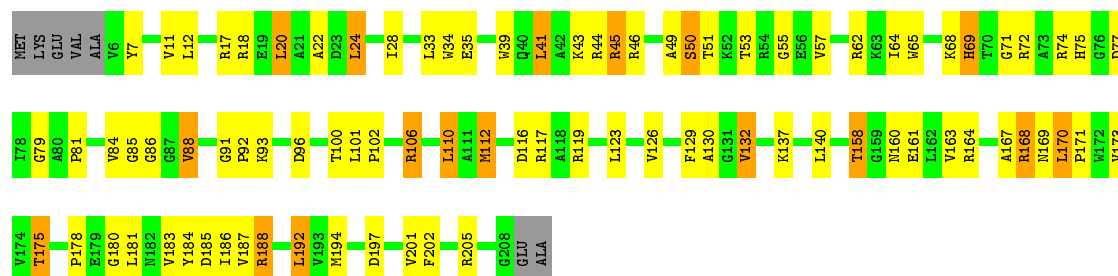
• Molecule 27: 50S Ribosomal Protein L4

Chain BF: 60% 29% 7% 1%



• Molecule 27: 50S Ribosomal Protein L4

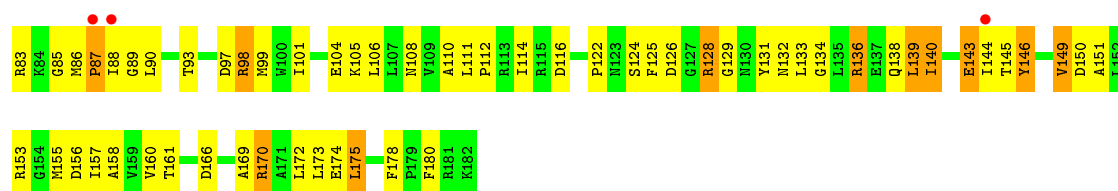
Chain DF: 55% 33% 8% 1%



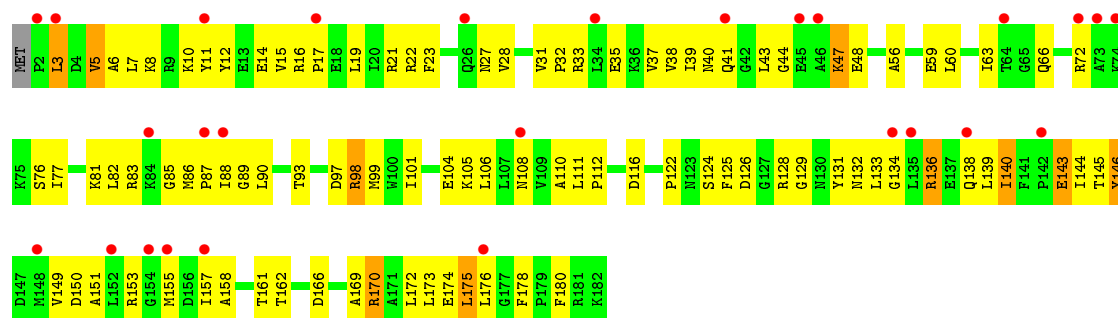
• Molecule 28: 50S Ribosomal Protein L5

Chain BG: 4% 46% 46% 8% 1%

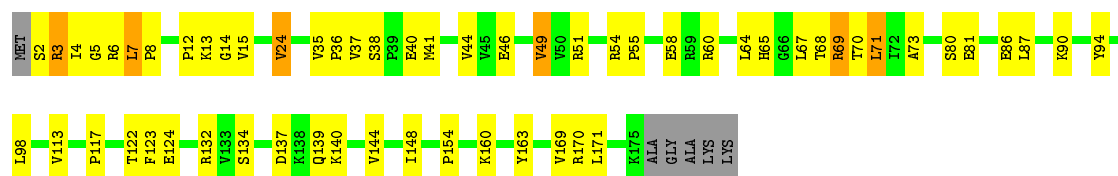




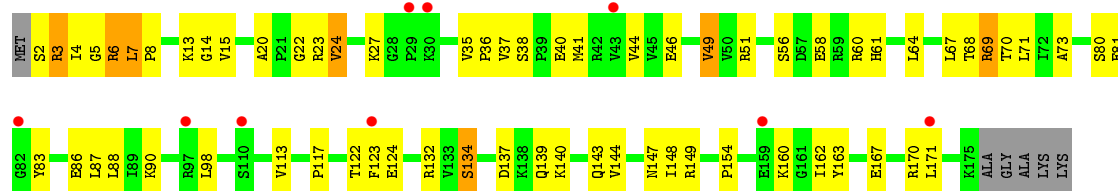
• Molecule 28: 50S Ribosomal Protein L5



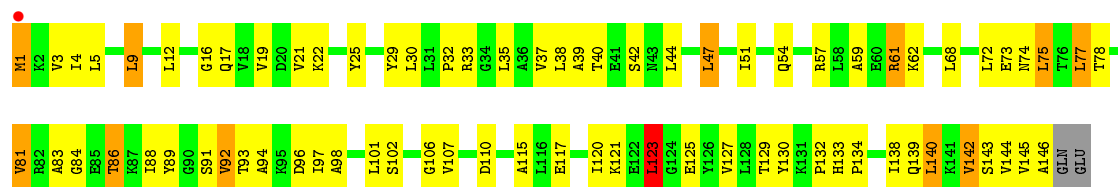
• Molecule 29: 50S Ribosomal Protein L6



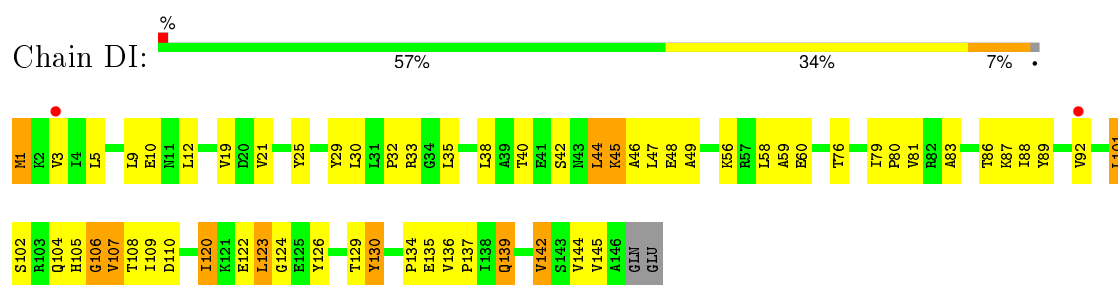
• Molecule 29: 50S Ribosomal Protein L6



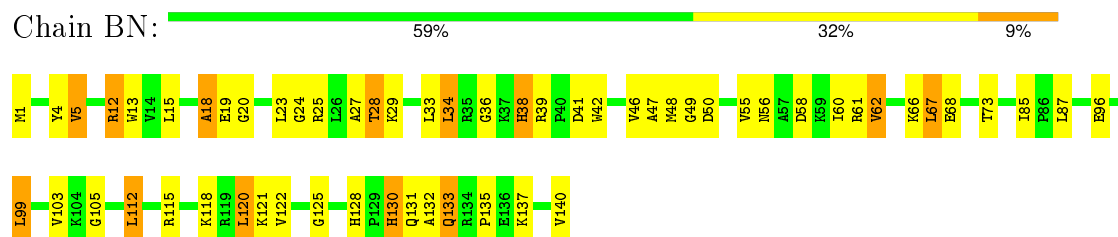
• Molecule 30: 50S Ribosomal Protein L9



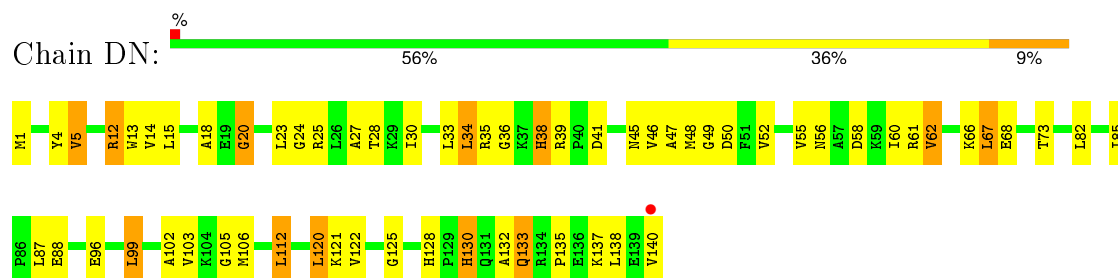
• Molecule 30: 50S Ribosomal Protein L9



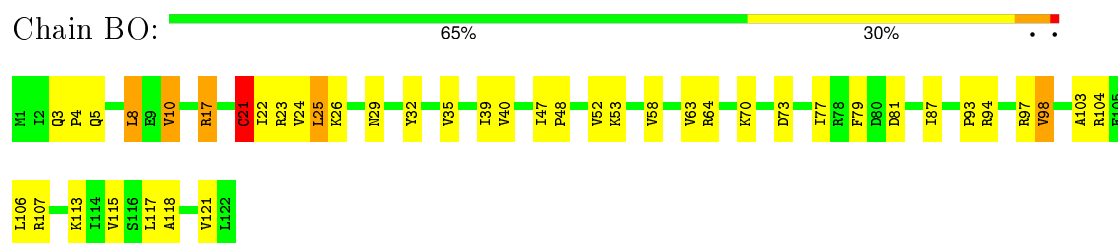
• Molecule 31: 50S Ribosomal Protein L13



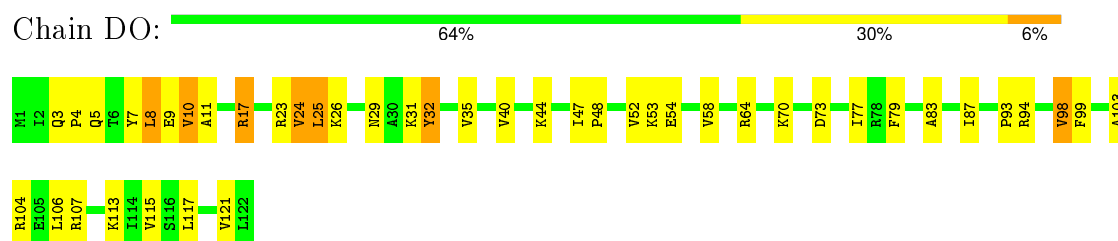
• Molecule 31: 50S Ribosomal Protein L13



• Molecule 32: 50S Ribosomal Protein L14

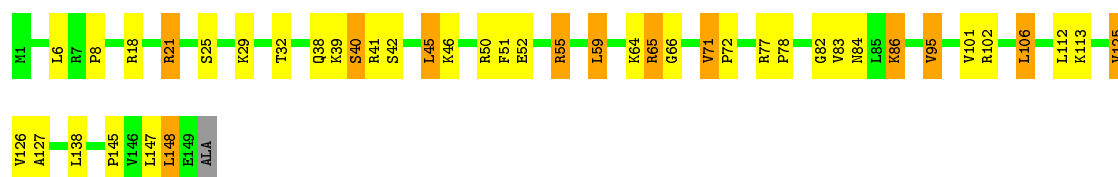


• Molecule 32: 50S Ribosomal Protein L14

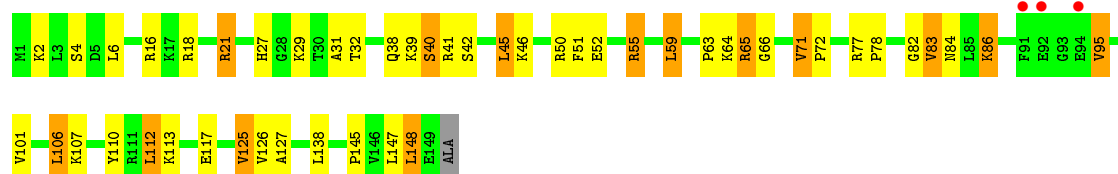


• Molecule 33: 50S Ribosomal Protein L15

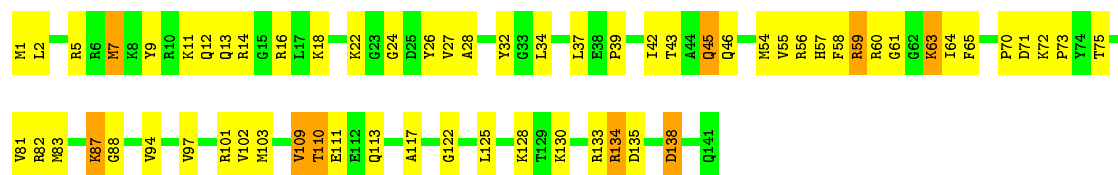




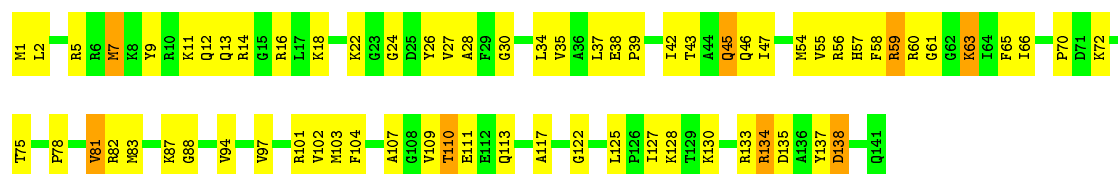
- Molecule 33: 50S Ribosomal Protein L15



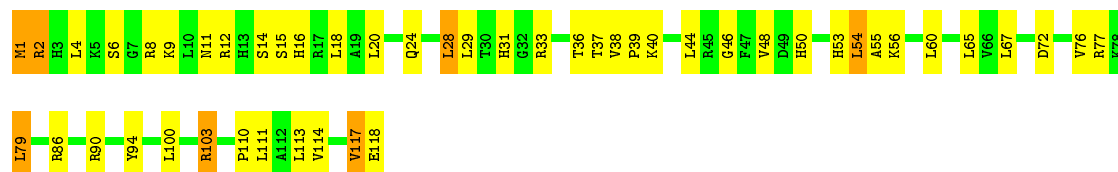
- Molecule 34: 50S Ribosomal Protein L16



- Molecule 34: 50S Ribosomal Protein L16



- Molecule 35: 50S Ribosomal Protein L17



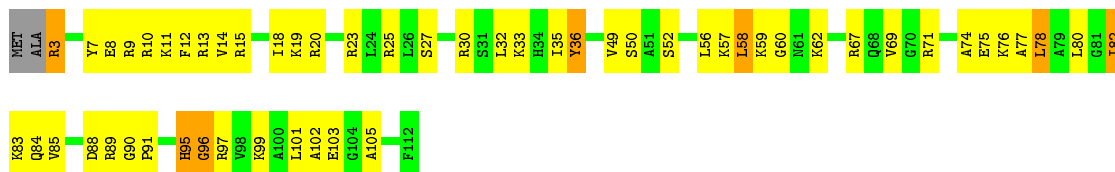
- Molecule 35: 50S Ribosomal Protein L17





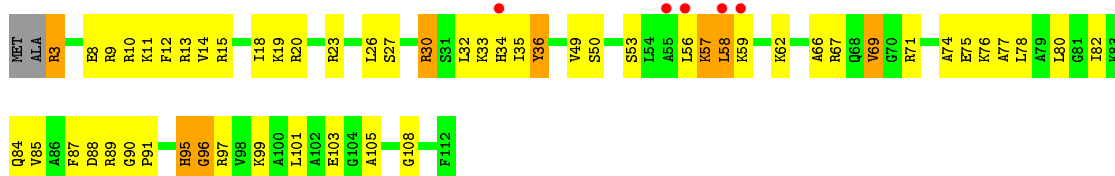
• Molecule 36: 50S Ribosomal Protein L18

Chain BS: 49% 43% 6%



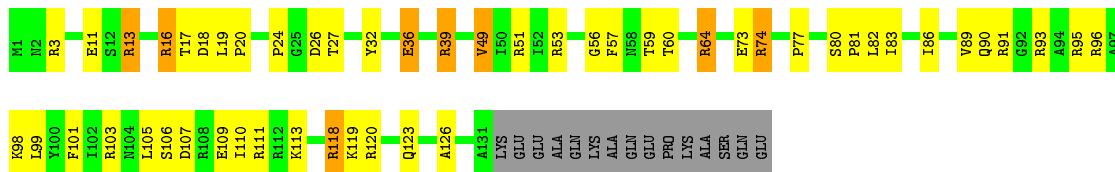
• Molecule 36: 50S Ribosomal Protein L18

Chain DS: 4% 49% 42% 7%



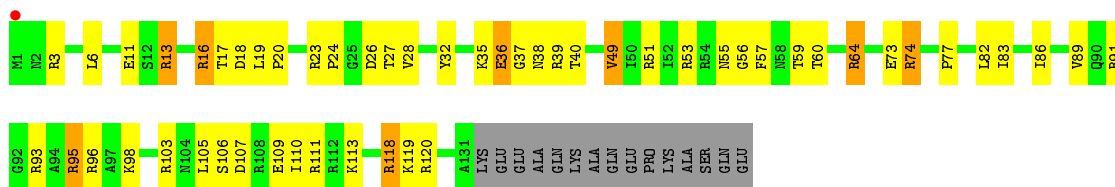
• Molecule 37: 50S Ribosomal Protein L19

Chain BT: 54% 30% 5% 10%



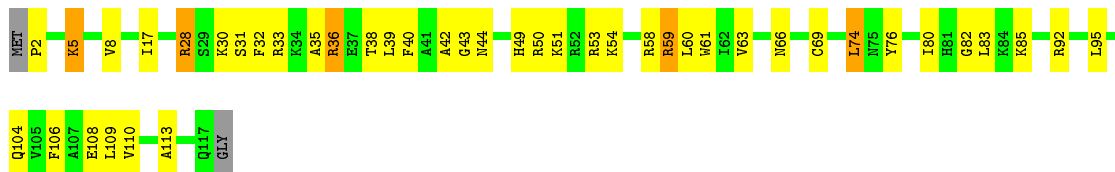
• Molecule 37: 50S Ribosomal Protein L19

Chain DT: 53% 31% 5% 10%

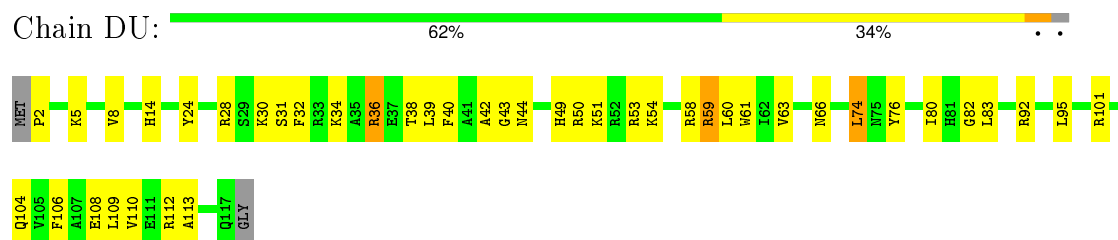


• Molecule 38: 50S Ribosomal Protein L20

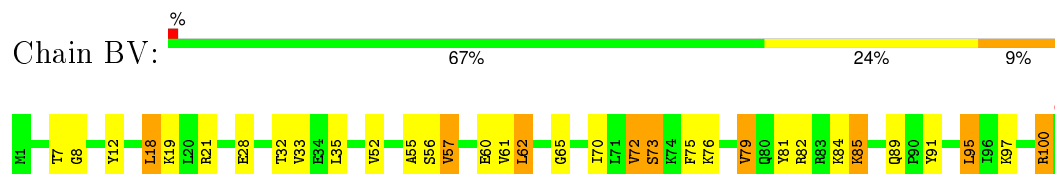
Chain BU: 62% 32% 6%



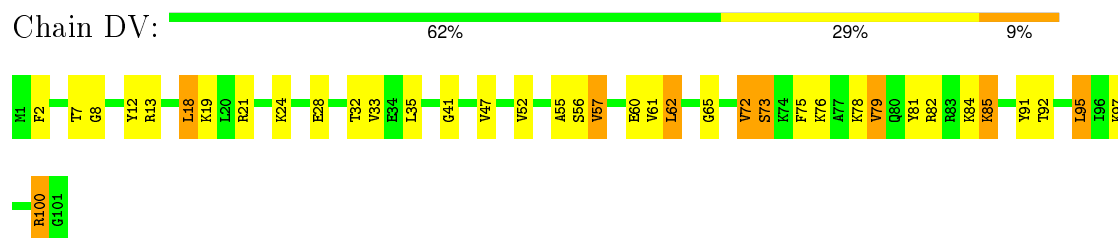
- Molecule 38: 50S Ribosomal Protein L20



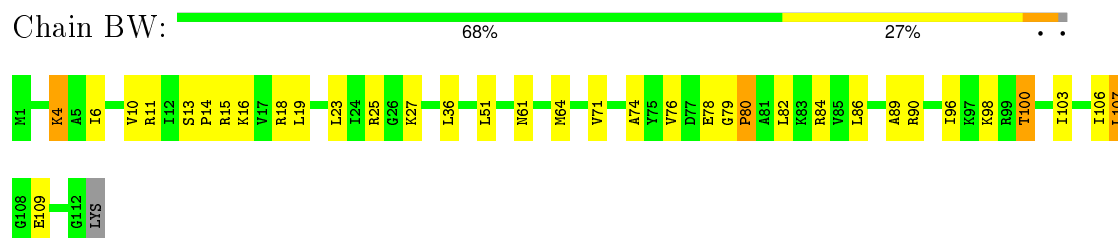
- Molecule 39: 50S Ribosomal Protein L21



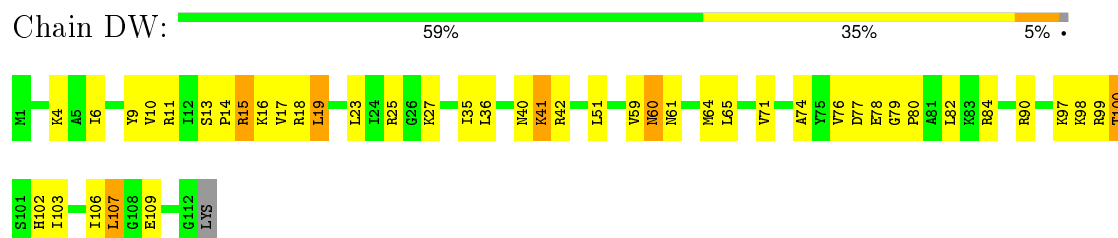
- Molecule 39: 50S Ribosomal Protein L21



- Molecule 40: 50S Ribosomal Protein L22

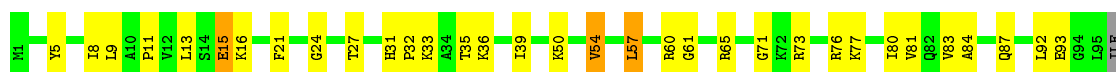


- Molecule 40: 50S Ribosomal Protein L22



- Molecule 41: 50S Ribosomal Protein L23





- Molecule 41: 50S Ribosomal Protein L23

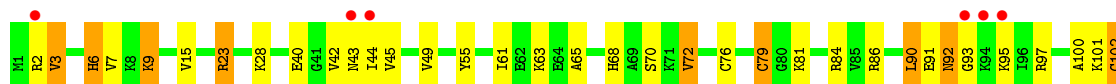


- Molecule 42: 50S Ribosomal Protein L24



THR
GLU
GLU

- Molecule 42: 50S Ribosomal Protein L24



G103
G104
D107
THR
GLU
GLU

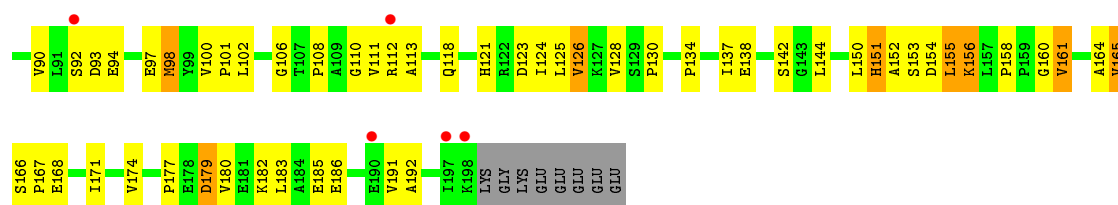
- Molecule 43: 50S Ribosomal Protein L25



E185
E186
V191
A192
K199
G200
K201
GLU
GLU
GLU
GLU

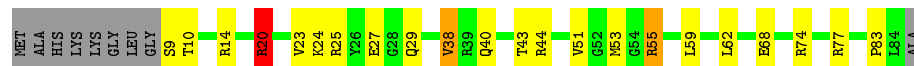
- Molecule 43: 50S Ribosomal Protein L25





• Molecule 44: 50S Ribosomal Protein L27

Chain B0: 64% 22% 11%



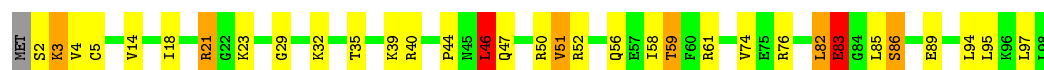
• Molecule 44: 50S Ribosomal Protein L27

Chain D0: 2% 62% 25% 11%



• Molecule 45: 50S Ribosomal Protein L28

Chain B1: 65% 26% 6%



• Molecule 45: 50S Ribosomal Protein L28

Chain D1: 2% 66% 26% 6%



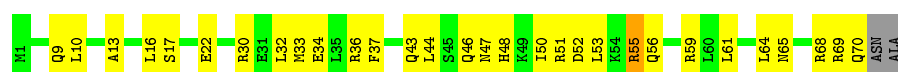
• Molecule 46: 50S Ribosomal Protein L29

Chain B2: 61% 35% 2%



• Molecule 46: 50S Ribosomal Protein L29

Chain D2: 56% 40% 2%



• Molecule 47: 50S Ribosomal Protein L30

Chain B3: 73% 17% 8%

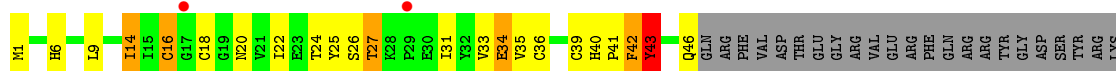
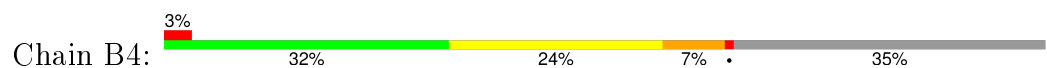




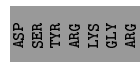
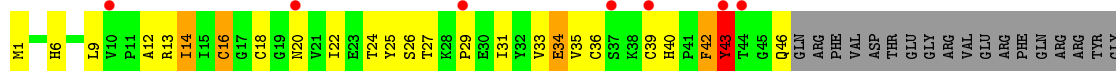
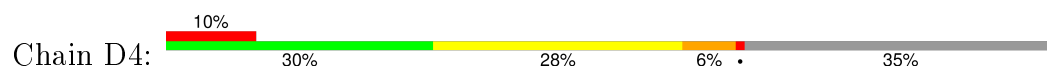
- Molecule 47: 50S Ribosomal Protein L30



- Molecule 48: 50S Ribosomal Protein L31



- Molecule 48: 50S Ribosomal Protein L31



- Molecule 49: 50S Ribosomal Protein L32



- Molecule 49: 50S Ribosomal Protein L32



- Molecule 50: 50S Ribosomal Protein L33



- Molecule 50: 50S Ribosomal Protein L33



- Molecule 51: 50S Ribosomal Protein L34



- Molecule 51: 50S Ribosomal Protein L34



- Molecule 52: 50S Ribosomal Protein L35



- Molecule 52: 50S Ribosomal Protein L35



- Molecule 53: 50S Ribosomal Protein L36



- Molecule 53: 50S Ribosomal Protein L36



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.97Å 447.24Å 617.67Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.98 – 3.10 49.98 – 3.10 | Depositor EDS |
| % Data completeness (in resolution range) | 96.0 (49.98-3.10) 96.0 (49.98-3.10) | Depositor EDS |
| R_{merge} | 0.23 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.39 (at 3.12Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.2_869) | Depositor |
| R, R_{free} | 0.216 , 0.258 0.214 , 0.257 | Depositor DCC |
| R_{free} test set | 49855 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 65.0 | Xtriage |
| Anisotropy | 0.263 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 54.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$ | Xtriage |
| Outliers | 1 of 993194 reflections (0.000%) | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 286308 | wwPDB-VP |
| Average B, all atoms (Å ²) | 74.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | AA | 1.14 | 57/36123 (0.2%) | 1.54 | 760/56379 (1.3%) |
| 1 | CA | 1.11 | 53/36028 (0.1%) | 1.55 | 750/56231 (1.3%) |
| 2 | AB | 0.69 | 0/1822 | 0.79 | 1/2468 (0.0%) |
| 2 | CB | 0.75 | 0/1809 | 0.79 | 1/2450 (0.0%) |
| 3 | AC | 0.80 | 0/1474 | 0.88 | 0/2003 |
| 3 | CC | 0.78 | 0/1474 | 0.86 | 2/2003 (0.1%) |
| 4 | AD | 0.68 | 2/1556 (0.1%) | 0.87 | 3/2113 (0.1%) |
| 4 | CD | 0.72 | 2/1556 (0.1%) | 0.87 | 3/2113 (0.1%) |
| 5 | AE | 0.61 | 0/1121 | 0.80 | 1/1517 (0.1%) |
| 5 | CE | 0.63 | 0/1121 | 0.82 | 1/1517 (0.1%) |
| 6 | AF | 0.59 | 0/790 | 0.73 | 0/1077 |
| 6 | CF | 0.62 | 0/790 | 0.73 | 0/1077 |
| 7 | AG | 1.04 | 0/1183 | 0.98 | 2/1599 (0.1%) |
| 7 | CG | 0.96 | 0/1183 | 0.90 | 0/1599 |
| 8 | AH | 0.57 | 0/1065 | 0.73 | 0/1445 |
| 8 | CH | 0.58 | 0/1065 | 0.75 | 0/1445 |
| 9 | AI | 0.92 | 0/867 | 0.92 | 0/1180 |
| 9 | CI | 1.00 | 0/867 | 0.91 | 1/1180 (0.1%) |
| 10 | AJ | 0.83 | 0/676 | 0.91 | 1/924 (0.1%) |
| 10 | CJ | 0.90 | 0/676 | 0.97 | 0/924 |
| 11 | AK | 0.62 | 0/843 | 0.75 | 1/1144 (0.1%) |
| 11 | CK | 0.61 | 0/843 | 0.75 | 1/1144 (0.1%) |
| 12 | AL | 0.63 | 0/921 | 0.78 | 0/1247 |
| 12 | CL | 0.64 | 0/921 | 0.80 | 0/1247 |
| 13 | AM | 1.02 | 0/814 | 1.00 | 0/1107 |
| 13 | CM | 1.03 | 0/814 | 1.03 | 2/1107 (0.2%) |
| 14 | AN | 0.76 | 0/487 | 0.90 | 0/649 |
| 14 | CN | 0.77 | 1/487 (0.2%) | 0.87 | 1/649 (0.2%) |
| 15 | AO | 0.62 | 0/735 | 0.84 | 0/981 |
| 15 | CO | 0.66 | 0/735 | 0.85 | 0/981 |
| 16 | AP | 0.63 | 0/667 | 0.82 | 0/905 |
| 16 | CP | 0.56 | 0/667 | 0.82 | 0/905 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.66 | 0/836 | 0.84 | 0/1117 |
| 17 | CQ | 0.69 | 1/836 (0.1%) | 0.85 | 0/1117 |
| 18 | AR | 0.59 | 0/519 | 0.76 | 1/699 (0.1%) |
| 18 | CR | 0.63 | 0/519 | 0.76 | 1/699 (0.1%) |
| 19 | AS | 0.96 | 0/574 | 0.87 | 0/781 |
| 19 | CS | 0.98 | 0/574 | 0.93 | 0/781 |
| 20 | AT | 0.63 | 0/666 | 0.79 | 0/880 |
| 20 | CT | 0.62 | 0/715 | 0.84 | 1/947 (0.1%) |
| 21 | AU | 0.82 | 0/203 | 0.92 | 0/266 |
| 21 | CU | 0.91 | 0/203 | 0.97 | 0/266 |
| 22 | AX | 0.69 | 0/637 | 0.84 | 1/864 (0.1%) |
| 22 | CX | 0.77 | 0/606 | 0.82 | 0/828 |
| 23 | BA | 1.58 | 572/68445 (0.8%) | 1.72 | 2187/106848 (2.0%) |
| 23 | DA | 1.21 | 155/67893 (0.2%) | 1.65 | 1848/105980 (1.7%) |
| 24 | BB | 1.13 | 6/2878 (0.2%) | 1.53 | 60/4490 (1.3%) |
| 24 | DB | 1.13 | 2/2878 (0.1%) | 1.52 | 49/4490 (1.1%) |
| 25 | BD | 0.90 | 1/2185 (0.0%) | 0.91 | 4/2942 (0.1%) |
| 25 | DD | 0.82 | 0/2186 | 0.91 | 2/2944 (0.1%) |
| 26 | BE | 0.90 | 0/1588 | 0.92 | 0/2145 |
| 26 | DE | 0.78 | 0/1588 | 0.92 | 3/2145 (0.1%) |
| 27 | BF | 0.91 | 0/1615 | 0.95 | 3/2188 (0.1%) |
| 27 | DF | 0.74 | 0/1615 | 0.92 | 2/2188 (0.1%) |
| 28 | BG | 0.61 | 0/1393 | 0.79 | 0/1892 |
| 28 | DG | 0.72 | 0/1393 | 0.81 | 0/1892 |
| 29 | BH | 0.72 | 0/1343 | 0.82 | 1/1820 (0.1%) |
| 29 | DH | 0.66 | 0/1343 | 0.81 | 0/1820 |
| 30 | BI | 0.64 | 0/1052 | 0.87 | 1/1441 (0.1%) |
| 30 | DI | 0.63 | 0/967 | 0.84 | 1/1334 (0.1%) |
| 31 | BN | 0.87 | 0/1139 | 0.87 | 0/1538 |
| 31 | DN | 0.71 | 0/1139 | 0.89 | 1/1538 (0.1%) |
| 32 | BO | 0.87 | 1/933 (0.1%) | 0.88 | 1/1257 (0.1%) |
| 32 | DO | 0.73 | 0/933 | 0.83 | 1/1257 (0.1%) |
| 33 | BP | 0.84 | 0/1148 | 0.91 | 1/1529 (0.1%) |
| 33 | DP | 0.73 | 0/1148 | 0.89 | 1/1529 (0.1%) |
| 34 | BQ | 0.84 | 0/1143 | 0.87 | 1/1527 (0.1%) |
| 34 | DQ | 0.74 | 0/1143 | 0.86 | 0/1527 |
| 35 | BR | 0.80 | 0/982 | 0.92 | 0/1312 |
| 35 | DR | 0.75 | 0/982 | 0.92 | 1/1312 (0.1%) |
| 36 | BS | 0.67 | 0/875 | 0.88 | 1/1168 (0.1%) |
| 36 | DS | 0.69 | 0/875 | 0.87 | 1/1168 (0.1%) |
| 37 | BT | 0.83 | 0/1077 | 0.92 | 0/1444 |
| 37 | DT | 0.73 | 0/1077 | 0.90 | 0/1444 |
| 38 | BU | 1.00 | 1/977 (0.1%) | 0.87 | 1/1301 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DU | 0.79 | 0/977 | 0.86 | 0/1301 |
| 39 | BV | 0.85 | 0/782 | 0.92 | 0/1049 |
| 39 | DV | 0.77 | 0/782 | 0.85 | 0/1049 |
| 40 | BW | 1.02 | 0/891 | 0.91 | 0/1197 |
| 40 | DW | 0.87 | 0/891 | 0.91 | 1/1197 (0.1%) |
| 41 | BX | 0.91 | 0/756 | 0.88 | 2/1016 (0.2%) |
| 41 | DX | 0.78 | 0/756 | 0.86 | 1/1016 (0.1%) |
| 42 | BY | 0.80 | 1/798 (0.1%) | 0.88 | 0/1073 |
| 42 | DY | 0.73 | 1/798 (0.1%) | 0.89 | 0/1073 |
| 43 | BZ | 0.70 | 0/1569 | 0.82 | 1/2137 (0.0%) |
| 43 | DZ | 0.72 | 0/1555 | 0.81 | 1/2118 (0.0%) |
| 44 | B0 | 0.85 | 0/602 | 0.92 | 1/804 (0.1%) |
| 44 | D0 | 0.78 | 0/602 | 0.92 | 0/804 |
| 45 | B1 | 0.85 | 0/752 | 0.90 | 2/1003 (0.2%) |
| 45 | D1 | 0.80 | 0/752 | 0.89 | 1/1003 (0.1%) |
| 46 | B2 | 0.82 | 0/590 | 0.86 | 0/781 |
| 46 | D2 | 0.79 | 0/590 | 0.86 | 0/781 |
| 47 | B3 | 0.76 | 0/463 | 0.84 | 1/623 (0.2%) |
| 47 | D3 | 0.69 | 0/463 | 0.81 | 0/623 |
| 48 | B4 | 0.68 | 0/358 | 0.84 | 1/487 (0.2%) |
| 48 | D4 | 0.85 | 0/358 | 0.83 | 1/487 (0.2%) |
| 49 | B5 | 0.93 | 1/469 (0.2%) | 1.00 | 0/634 |
| 49 | D5 | 0.86 | 1/469 (0.2%) | 0.96 | 0/634 |
| 50 | B6 | 0.93 | 2/456 (0.4%) | 0.84 | 0/609 |
| 50 | D6 | 0.75 | 0/456 | 0.87 | 2/609 (0.3%) |
| 51 | B7 | 1.03 | 1/426 (0.2%) | 1.12 | 1/561 (0.2%) |
| 51 | D7 | 0.88 | 0/426 | 1.01 | 1/561 (0.2%) |
| 52 | B8 | 0.96 | 0/516 | 0.94 | 1/679 (0.1%) |
| 52 | D8 | 0.76 | 0/516 | 0.90 | 0/679 |
| 53 | B9 | 0.79 | 0/300 | 0.95 | 0/395 |
| 53 | D9 | 0.71 | 0/300 | 0.90 | 0/395 |
| All | All | 1.18 | 861/305420 (0.3%) | 1.47 | 5724/457343 (1.3%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | AB | 0 | 3 |
| 2 | CB | 0 | 4 |
| 3 | AC | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | CC | 0 | 1 |
| 4 | AD | 0 | 1 |
| 4 | CD | 0 | 1 |
| 7 | CG | 0 | 2 |
| 9 | AI | 0 | 1 |
| 9 | CI | 0 | 1 |
| 10 | AJ | 0 | 2 |
| 10 | CJ | 0 | 2 |
| 13 | AM | 0 | 4 |
| 13 | CM | 0 | 2 |
| 14 | AN | 0 | 1 |
| 15 | AO | 0 | 1 |
| 15 | CO | 0 | 1 |
| 17 | AQ | 0 | 1 |
| 17 | CQ | 0 | 1 |
| 19 | AS | 0 | 1 |
| 19 | CS | 0 | 1 |
| 20 | AT | 0 | 1 |
| 20 | CT | 0 | 1 |
| 23 | BA | 0 | 1 |
| 23 | DA | 0 | 1 |
| 26 | BE | 0 | 1 |
| 26 | DE | 0 | 1 |
| 27 | DF | 0 | 1 |
| 30 | DI | 0 | 1 |
| 34 | BQ | 0 | 1 |
| 34 | DQ | 0 | 1 |
| 36 | BS | 0 | 1 |
| 36 | DS | 0 | 1 |
| 41 | BX | 0 | 1 |
| 41 | DX | 0 | 1 |
| 43 | BZ | 0 | 3 |
| 43 | DZ | 0 | 1 |
| 45 | B1 | 0 | 1 |
| 45 | D1 | 0 | 1 |
| 48 | B4 | 0 | 1 |
| 48 | D4 | 0 | 1 |
| All | All | 0 | 56 |

All (861) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 1 | CA | 1442(A) | G | N9-C4 | 17.19 | 1.51 | 1.38 |
| 1 | AA | 1442(A) | G | N9-C4 | 15.23 | 1.50 | 1.38 |
| 1 | AA | 1442(A) | G | C2-N3 | 15.04 | 1.44 | 1.32 |
| 1 | CA | 1442(A) | G | C2-N3 | 14.30 | 1.44 | 1.32 |
| 1 | AA | 1442(A) | G | N3-C4 | 13.24 | 1.44 | 1.35 |
| 1 | CA | 1442(A) | G | N3-C4 | 12.97 | 1.44 | 1.35 |
| 23 | BA | 1142(A) | A | N9-C4 | -12.92 | 1.30 | 1.37 |
| 23 | BA | 945 | A | N9-C4 | -12.37 | 1.30 | 1.37 |
| 23 | BA | 207 | A | N9-C4 | -12.29 | 1.30 | 1.37 |
| 23 | DA | 1142(A) | A | N9-C4 | -12.18 | 1.30 | 1.37 |
| 23 | BA | 676 | A | N9-C4 | -12.12 | 1.30 | 1.37 |
| 23 | BA | 528 | A | N9-C4 | -12.02 | 1.30 | 1.37 |
| 23 | DA | 945 | A | N9-C4 | -11.74 | 1.30 | 1.37 |
| 4 | CD | 12 | CYS | CB-SG | 11.03 | 2.00 | 1.82 |
| 23 | DA | 528 | A | N9-C4 | -9.70 | 1.32 | 1.37 |
| 23 | BA | 1204 | A | N9-C4 | -9.69 | 1.32 | 1.37 |
| 23 | BA | 2055 | C | P-OP1 | -9.53 | 1.32 | 1.49 |
| 23 | BA | 1142(A) | A | N3-C4 | -9.27 | 1.29 | 1.34 |
| 23 | BA | 330 | A | N9-C4 | -9.14 | 1.32 | 1.37 |
| 23 | BA | 2015 | A | N7-C5 | -8.94 | 1.33 | 1.39 |
| 23 | BA | 1021 | A | N9-C4 | -8.86 | 1.32 | 1.37 |
| 23 | BA | 2440 | C | N1-C6 | -8.80 | 1.31 | 1.37 |
| 23 | BA | 933 | A | N9-C4 | -8.77 | 1.32 | 1.37 |
| 23 | BA | 1762 | A | N9-C4 | 8.75 | 1.43 | 1.37 |
| 23 | BA | 2587 | A | N9-C8 | -8.67 | 1.30 | 1.37 |
| 23 | DA | 71 | A | N9-C4 | -8.63 | 1.32 | 1.37 |
| 23 | BA | 1570 | A | N9-C4 | -8.62 | 1.32 | 1.37 |
| 23 | BA | 1655 | A | N9-C4 | -8.61 | 1.32 | 1.37 |
| 23 | DA | 1308 | A | N7-C5 | -8.57 | 1.34 | 1.39 |
| 23 | BA | 1829 | A | N9-C4 | -8.52 | 1.32 | 1.37 |
| 23 | BA | 732 | C | N1-C6 | -8.51 | 1.32 | 1.37 |
| 23 | BA | 503 | A | N3-C4 | -8.48 | 1.29 | 1.34 |
| 23 | DA | 1204 | A | N9-C4 | -8.45 | 1.32 | 1.37 |
| 23 | BA | 2296 | U | C4-C5 | 8.41 | 1.51 | 1.43 |
| 23 | BA | 1785 | A | N7-C5 | -8.40 | 1.34 | 1.39 |
| 23 | DA | 1490 | A | N3-C4 | 8.38 | 1.39 | 1.34 |
| 23 | BA | 756 | C | N1-C6 | -8.38 | 1.32 | 1.37 |
| 23 | DA | 207 | A | N9-C4 | -8.37 | 1.32 | 1.37 |
| 23 | BA | 933 | A | N3-C4 | -8.32 | 1.29 | 1.34 |
| 23 | DA | 251 | A | N3-C4 | -8.31 | 1.29 | 1.34 |
| 23 | BA | 1210 | A | N3-C4 | -8.28 | 1.29 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | DA | 330 | A | N9-C4 | -8.27 | 1.32 | 1.37 |
| 23 | BA | 209 | C | N1-C6 | -8.25 | 1.32 | 1.37 |
| 23 | BA | 1570 | A | N3-C4 | -8.19 | 1.29 | 1.34 |
| 23 | BA | 1612 | C | N1-C6 | -8.15 | 1.32 | 1.37 |
| 23 | BA | 2032 | G | N7-C5 | -8.08 | 1.34 | 1.39 |
| 1 | CA | 1442(A) | G | C2-N2 | 8.08 | 1.42 | 1.34 |
| 1 | CA | 1116 | C | N1-C6 | 8.07 | 1.42 | 1.37 |
| 1 | CA | 1492 | A | N9-C4 | 8.06 | 1.42 | 1.37 |
| 23 | BA | 2030 | A | N9-C4 | -7.99 | 1.33 | 1.37 |
| 1 | AA | 1492 | A | N9-C4 | 7.99 | 1.42 | 1.37 |
| 23 | BA | 745 | G | N7-C5 | -7.95 | 1.34 | 1.39 |
| 23 | DA | 652(B) | A | N9-C4 | 7.95 | 1.42 | 1.37 |
| 23 | DA | 1788 | C | N1-C6 | -7.92 | 1.32 | 1.37 |
| 23 | BA | 209 | C | N3-C4 | -7.92 | 1.28 | 1.33 |
| 23 | DA | 2725 | A | N9-C4 | -7.90 | 1.33 | 1.37 |
| 23 | BA | 689 | A | N9-C4 | -7.89 | 1.33 | 1.37 |
| 23 | BA | 2597 | G | N7-C5 | -7.88 | 1.34 | 1.39 |
| 23 | BA | 529 | A | N9-C4 | -7.79 | 1.33 | 1.37 |
| 1 | CA | 1340 | A | N9-C4 | 7.78 | 1.42 | 1.37 |
| 50 | B6 | 13 | CYS | CB-SG | -7.75 | 1.69 | 1.82 |
| 23 | DA | 2296 | U | C4-C5 | 7.73 | 1.50 | 1.43 |
| 1 | AA | 1442(A) | G | C2-N2 | 7.68 | 1.42 | 1.34 |
| 23 | DA | 1762 | A | N9-C4 | 7.66 | 1.42 | 1.37 |
| 23 | BA | 1210 | A | N7-C5 | -7.60 | 1.34 | 1.39 |
| 23 | BA | 933 | A | C5-C6 | -7.57 | 1.34 | 1.41 |
| 23 | BA | 119 | A | N7-C5 | -7.55 | 1.34 | 1.39 |
| 23 | BA | 1791 | A | N7-C5 | -7.49 | 1.34 | 1.39 |
| 49 | D5 | 49 | CYS | CB-SG | -7.48 | 1.69 | 1.82 |
| 1 | CA | 1493 | A | N9-C4 | 7.47 | 1.42 | 1.37 |
| 23 | BA | 472 | A | N3-C4 | -7.45 | 1.30 | 1.34 |
| 23 | BA | 1755 | A | N3-C4 | -7.45 | 1.30 | 1.34 |
| 23 | BA | 191 | A | N7-C5 | -7.43 | 1.34 | 1.39 |
| 23 | BA | 1254 | A | N3-C4 | -7.43 | 1.30 | 1.34 |
| 23 | BA | 575 | A | C6-N1 | -7.33 | 1.30 | 1.35 |
| 1 | CA | 1442(B) | A | N9-C4 | 7.33 | 1.42 | 1.37 |
| 23 | BA | 197 | A | C5-C4 | -7.31 | 1.33 | 1.38 |
| 23 | DA | 676 | A | N9-C8 | 7.30 | 1.43 | 1.37 |
| 23 | BA | 2286 | A | N7-C5 | -7.30 | 1.34 | 1.39 |
| 23 | BA | 567 | A | N9-C4 | -7.30 | 1.33 | 1.37 |
| 23 | BA | 933 | A | N7-C5 | -7.29 | 1.34 | 1.39 |
| 23 | BA | 2575 | C | N1-C6 | -7.29 | 1.32 | 1.37 |
| 1 | AA | 1442(B) | A | N9-C4 | 7.26 | 1.42 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 1 | CA | 69 | G | O3'-P | -7.24 | 1.52 | 1.61 |
| 23 | BA | 983 | A | N3-C4 | -7.24 | 1.30 | 1.34 |
| 23 | BA | 2287 | A | N9-C4 | -7.22 | 1.33 | 1.37 |
| 23 | BA | 57 | C | N1-C6 | -7.21 | 1.32 | 1.37 |
| 1 | CA | 986 | A | N9-C4 | 7.21 | 1.42 | 1.37 |
| 23 | BA | 2641 | G | N7-C5 | -7.21 | 1.34 | 1.39 |
| 23 | BA | 2680 | C | N1-C6 | -7.20 | 1.32 | 1.37 |
| 23 | DA | 746 | A | N9-C4 | -7.19 | 1.33 | 1.37 |
| 23 | BA | 1308 | A | N7-C5 | -7.17 | 1.34 | 1.39 |
| 23 | BA | 804 | A | C5-C4 | -7.15 | 1.33 | 1.38 |
| 23 | BA | 679 | C | N1-C6 | -7.14 | 1.32 | 1.37 |
| 23 | DA | 204 | A | N3-C4 | -7.12 | 1.30 | 1.34 |
| 23 | BA | 1301 | A | N7-C5 | -7.11 | 1.34 | 1.39 |
| 23 | BA | 1241 | A | N9-C4 | -7.11 | 1.33 | 1.37 |
| 23 | BA | 2055 | C | P-O5' | -7.10 | 1.52 | 1.59 |
| 23 | BA | 1567 | A | N9-C4 | -7.09 | 1.33 | 1.37 |
| 23 | BA | 1789 | A | N7-C5 | -7.08 | 1.35 | 1.39 |
| 23 | BA | 1198 | U | C2-N3 | -7.07 | 1.32 | 1.37 |
| 23 | BA | 831 | G | C8-N7 | -7.06 | 1.26 | 1.30 |
| 23 | DA | 1142(A) | A | N3-C4 | -7.06 | 1.30 | 1.34 |
| 23 | DA | 1045 | A | N9-C4 | 7.04 | 1.42 | 1.37 |
| 23 | BA | 1210 | A | C5-C6 | -7.00 | 1.34 | 1.41 |
| 23 | BA | 783 | A | N7-C5 | -6.98 | 1.35 | 1.39 |
| 23 | BA | 2058 | A | N9-C4 | -6.97 | 1.33 | 1.37 |
| 1 | CA | 1333 | A | N9-C4 | 6.97 | 1.42 | 1.37 |
| 23 | BA | 577 | G | P-OP1 | -6.97 | 1.37 | 1.49 |
| 4 | CD | 9 | CYS | CB-SG | 6.96 | 1.94 | 1.82 |
| 23 | BA | 1674 | G | N7-C5 | -6.95 | 1.35 | 1.39 |
| 23 | BA | 1901 | A | C6-N1 | -6.95 | 1.30 | 1.35 |
| 23 | BA | 2335 | A | C5-C4 | -6.94 | 1.33 | 1.38 |
| 1 | AA | 1442(A) | G | C5-C6 | 6.92 | 1.49 | 1.42 |
| 23 | BA | 983 | A | N9-C4 | -6.90 | 1.33 | 1.37 |
| 23 | DA | 2252 | G | N3-C4 | -6.89 | 1.30 | 1.35 |
| 23 | BA | 850 | C | N3-C4 | -6.89 | 1.29 | 1.33 |
| 23 | BA | 2052 | G | N7-C5 | -6.89 | 1.35 | 1.39 |
| 23 | BA | 570 | G | C5-C4 | -6.88 | 1.33 | 1.38 |
| 23 | BA | 804 | A | N9-C4 | -6.87 | 1.33 | 1.37 |
| 1 | AA | 1333 | A | N9-C4 | 6.86 | 1.42 | 1.37 |
| 23 | DA | 1107 | G | N9-C4 | 6.86 | 1.43 | 1.38 |
| 23 | BA | 2248 | C | N1-C6 | -6.84 | 1.33 | 1.37 |
| 23 | BA | 676 | A | C5-C4 | 6.84 | 1.43 | 1.38 |
| 23 | DA | 2335 | A | C5-C4 | -6.82 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | DA | 2561 | A | N3-C4 | -6.82 | 1.30 | 1.34 |
| 23 | BA | 2872 | G | N3-C4 | -6.81 | 1.30 | 1.35 |
| 42 | BY | 79 | CYS | CB-SG | -6.81 | 1.70 | 1.82 |
| 23 | BA | 1225 | G | N3-C4 | -6.80 | 1.30 | 1.35 |
| 23 | DA | 2322 | A | C6-N1 | 6.80 | 1.40 | 1.35 |
| 23 | BA | 676 | A | N3-C4 | -6.77 | 1.30 | 1.34 |
| 23 | DA | 2790 | A | N9-C4 | 6.77 | 1.42 | 1.37 |
| 23 | DA | 960 | A | N9-C4 | -6.77 | 1.33 | 1.37 |
| 23 | BA | 1755 | A | N9-C4 | -6.77 | 1.33 | 1.37 |
| 23 | BA | 1571 | A | N9-C4 | -6.76 | 1.33 | 1.37 |
| 1 | CA | 946 | A | N9-C4 | 6.74 | 1.41 | 1.37 |
| 23 | BA | 587 | C | N3-C4 | -6.74 | 1.29 | 1.33 |
| 23 | BA | 1648 | C | N3-C4 | -6.73 | 1.29 | 1.33 |
| 23 | DA | 2826 | A | N3-C4 | -6.72 | 1.30 | 1.34 |
| 23 | BA | 658 | C | N3-C4 | -6.71 | 1.29 | 1.33 |
| 1 | AA | 69 | G | O3'-P | 6.70 | 1.69 | 1.61 |
| 23 | DA | 1257 | C | N1-C6 | -6.70 | 1.33 | 1.37 |
| 23 | BA | 1564 | C | N3-C4 | -6.65 | 1.29 | 1.33 |
| 23 | DA | 571 | A | N9-C4 | -6.64 | 1.33 | 1.37 |
| 23 | BA | 1571 | A | N7-C5 | -6.64 | 1.35 | 1.39 |
| 23 | BA | 1785 | A | C5-C6 | -6.64 | 1.35 | 1.41 |
| 23 | BA | 676 | A | N9-C8 | 6.63 | 1.43 | 1.37 |
| 1 | CA | 1310 | G | N7-C5 | 6.62 | 1.43 | 1.39 |
| 23 | BA | 71 | A | N9-C4 | -6.62 | 1.33 | 1.37 |
| 23 | BA | 689 | A | C5-C4 | -6.61 | 1.34 | 1.38 |
| 23 | DA | 190 | A | N9-C4 | -6.61 | 1.33 | 1.37 |
| 23 | BA | 1269 | A | N9-C4 | -6.61 | 1.33 | 1.37 |
| 23 | BA | 204 | A | N7-C5 | -6.60 | 1.35 | 1.39 |
| 23 | BA | 2015 | A | N3-C4 | -6.60 | 1.30 | 1.34 |
| 23 | BA | 804 | A | N3-C4 | -6.59 | 1.30 | 1.34 |
| 23 | BA | 2715 | C | N1-C6 | -6.59 | 1.33 | 1.37 |
| 23 | BA | 663 | G | N3-C4 | -6.57 | 1.30 | 1.35 |
| 23 | BA | 831 | G | C5-C4 | -6.57 | 1.33 | 1.38 |
| 23 | BA | 371 | A | N9-C4 | -6.56 | 1.33 | 1.37 |
| 23 | BA | 1142(A) | A | C5-C6 | -6.56 | 1.35 | 1.41 |
| 23 | BA | 1254 | A | C6-N1 | -6.56 | 1.30 | 1.35 |
| 23 | BA | 988 | A | N7-C5 | -6.55 | 1.35 | 1.39 |
| 23 | BA | 32 | C | N1-C6 | -6.55 | 1.33 | 1.37 |
| 23 | BA | 1755 | A | N7-C5 | -6.55 | 1.35 | 1.39 |
| 23 | BA | 472 | A | N9-C4 | -6.54 | 1.33 | 1.37 |
| 23 | BA | 732 | C | C4-C5 | -6.53 | 1.37 | 1.43 |
| 23 | BA | 1278 | A | N9-C8 | -6.53 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | BA | 1653 | G | N7-C5 | -6.53 | 1.35 | 1.39 |
| 23 | DA | 1960 | A | N9-C4 | -6.53 | 1.33 | 1.37 |
| 23 | BA | 819 | A | C6-N1 | -6.52 | 1.30 | 1.35 |
| 23 | BA | 1314 | C | N1-C6 | -6.52 | 1.33 | 1.37 |
| 23 | DA | 251 | A | N9-C4 | -6.52 | 1.33 | 1.37 |
| 23 | BA | 1617 | C | N1-C6 | -6.52 | 1.33 | 1.37 |
| 23 | BA | 2619 | C | N1-C6 | -6.51 | 1.33 | 1.37 |
| 23 | BA | 675 | A | C5-C6 | -6.50 | 1.35 | 1.41 |
| 23 | BA | 2790 | A | N9-C4 | 6.48 | 1.41 | 1.37 |
| 23 | BA | 32 | C | N3-C4 | -6.48 | 1.29 | 1.33 |
| 23 | BA | 577 | G | P-O5' | -6.46 | 1.53 | 1.59 |
| 23 | BA | 609 | A | N3-C4 | -6.46 | 1.30 | 1.34 |
| 23 | BA | 2765 | A | N7-C5 | -6.46 | 1.35 | 1.39 |
| 23 | BA | 2606 | C | N3-C4 | -6.45 | 1.29 | 1.33 |
| 23 | DA | 1021 | A | N9-C4 | -6.45 | 1.33 | 1.37 |
| 23 | BA | 849 | A | N9-C4 | -6.44 | 1.33 | 1.37 |
| 1 | CA | 78 | G | C6-N1 | 6.44 | 1.44 | 1.39 |
| 23 | BA | 1676 | A | N3-C4 | -6.43 | 1.30 | 1.34 |
| 23 | BA | 1278 | A | N7-C5 | -6.42 | 1.35 | 1.39 |
| 23 | BA | 1045 | A | N9-C4 | 6.42 | 1.41 | 1.37 |
| 23 | BA | 1322 | A | N9-C4 | -6.39 | 1.34 | 1.37 |
| 23 | BA | 572 | A | N3-C4 | -6.39 | 1.31 | 1.34 |
| 23 | BA | 123 | G | N3-C4 | -6.39 | 1.30 | 1.35 |
| 23 | BA | 2055 | C | P-OP2 | -6.39 | 1.38 | 1.49 |
| 23 | BA | 74 | A | N3-C4 | -6.38 | 1.31 | 1.34 |
| 23 | DA | 2593 | U | C2-N3 | -6.35 | 1.33 | 1.37 |
| 23 | DA | 676 | A | C5-C6 | -6.35 | 1.35 | 1.41 |
| 23 | BA | 561 | G | C5-C4 | -6.34 | 1.33 | 1.38 |
| 23 | BA | 69 | C | N1-C6 | -6.33 | 1.33 | 1.37 |
| 23 | BA | 1655 | A | N3-C4 | -6.33 | 1.31 | 1.34 |
| 23 | BA | 945 | A | N3-C4 | -6.30 | 1.31 | 1.34 |
| 23 | DA | 802 | A | C6-N1 | -6.30 | 1.31 | 1.35 |
| 23 | BA | 74 | A | N9-C4 | -6.29 | 1.34 | 1.37 |
| 23 | BA | 1278 | A | C5-C4 | -6.29 | 1.34 | 1.38 |
| 24 | DB | 102 | A | N7-C5 | 6.29 | 1.43 | 1.39 |
| 23 | BA | 2578 | G | N1-C2 | -6.28 | 1.32 | 1.37 |
| 23 | BA | 793 | A | N3-C4 | -6.28 | 1.31 | 1.34 |
| 23 | BA | 1046 | A | N9-C4 | 6.28 | 1.41 | 1.37 |
| 1 | AA | 1447 | A | N9-C4 | 6.27 | 1.41 | 1.37 |
| 23 | BA | 2287 | A | N3-C4 | -6.27 | 1.31 | 1.34 |
| 23 | BA | 2027 | G | N1-C2 | -6.27 | 1.32 | 1.37 |
| 23 | BA | 2621 | A | C6-N6 | -6.27 | 1.28 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | BA | 2454 | G | C5-C4 | -6.26 | 1.33 | 1.38 |
| 23 | BA | 2600 | A | N7-C5 | -6.25 | 1.35 | 1.39 |
| 23 | BA | 2587 | A | N7-C5 | -6.25 | 1.35 | 1.39 |
| 23 | BA | 750 | A | C6-N1 | -6.24 | 1.31 | 1.35 |
| 23 | BA | 1252 | G | C5-C4 | -6.23 | 1.33 | 1.38 |
| 23 | DA | 981 | A | N9-C4 | -6.23 | 1.34 | 1.37 |
| 23 | BA | 1800 | C | N1-C6 | -6.23 | 1.33 | 1.37 |
| 23 | BA | 1608 | A | N9-C4 | -6.21 | 1.34 | 1.37 |
| 23 | BA | 2199 | A | C6-N1 | -6.21 | 1.31 | 1.35 |
| 23 | BA | 1006 | C | N3-C4 | -6.21 | 1.29 | 1.33 |
| 24 | BB | 71 | C | N1-C6 | -6.21 | 1.33 | 1.37 |
| 1 | CA | 1456 | G | N3-C4 | 6.21 | 1.39 | 1.35 |
| 23 | BA | 1296 | G | N1-C2 | -6.20 | 1.32 | 1.37 |
| 23 | BA | 1843 | C | N1-C6 | -6.18 | 1.33 | 1.37 |
| 23 | BA | 204 | A | N3-C4 | -6.17 | 1.31 | 1.34 |
| 23 | BA | 2723 | C | N3-C4 | -6.16 | 1.29 | 1.33 |
| 1 | CA | 1447 | A | N9-C4 | 6.16 | 1.41 | 1.37 |
| 23 | BA | 122 | G | C5-C4 | -6.16 | 1.34 | 1.38 |
| 23 | BA | 463 | G | N3-C4 | -6.14 | 1.31 | 1.35 |
| 23 | BA | 201 | C | N1-C6 | -6.13 | 1.33 | 1.37 |
| 23 | BA | 1141 | U | C2-N3 | -6.12 | 1.33 | 1.37 |
| 23 | BA | 2515 | C | N1-C6 | -6.12 | 1.33 | 1.37 |
| 23 | BA | 959 | A | C6-N1 | -6.12 | 1.31 | 1.35 |
| 23 | BA | 2296 | U | N1-C2 | 6.12 | 1.44 | 1.38 |
| 23 | BA | 2725 | A | N9-C4 | -6.11 | 1.34 | 1.37 |
| 23 | BA | 189 | G | N9-C4 | -6.11 | 1.33 | 1.38 |
| 23 | BA | 517 | C | N1-C6 | -6.11 | 1.33 | 1.37 |
| 23 | BA | 1836 | C | N3-C4 | -6.10 | 1.29 | 1.33 |
| 23 | BA | 689 | A | N3-C4 | -6.10 | 1.31 | 1.34 |
| 23 | BA | 789 | A | N9-C4 | -6.10 | 1.34 | 1.37 |
| 23 | BA | 2382 | G | N9-C8 | -6.09 | 1.33 | 1.37 |
| 23 | BA | 2442 | C | N1-C6 | -6.08 | 1.33 | 1.37 |
| 23 | BA | 1107 | G | N9-C4 | 6.08 | 1.42 | 1.38 |
| 23 | BA | 2058 | A | N3-C4 | -6.08 | 1.31 | 1.34 |
| 23 | BA | 2505 | G | N3-C4 | -6.08 | 1.31 | 1.35 |
| 23 | BA | 531 | C | N1-C6 | -6.07 | 1.33 | 1.37 |
| 23 | BA | 652(B) | A | N9-C4 | 6.07 | 1.41 | 1.37 |
| 23 | BA | 687 | C | N3-C4 | -6.07 | 1.29 | 1.33 |
| 23 | BA | 2619 | C | N3-C4 | -6.07 | 1.29 | 1.33 |
| 23 | BA | 570 | G | C5-C6 | -6.07 | 1.36 | 1.42 |
| 23 | BA | 991 | C | N3-C4 | -6.07 | 1.29 | 1.33 |
| 23 | DA | 15 | G | N7-C5 | -6.07 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | BA | 567 | A | N3-C4 | -6.07 | 1.31 | 1.34 |
| 23 | BA | 122 | G | N7-C5 | -6.06 | 1.35 | 1.39 |
| 23 | BA | 1653 | G | N9-C8 | -6.05 | 1.33 | 1.37 |
| 1 | CA | 951 | G | N9-C4 | 6.05 | 1.42 | 1.38 |
| 23 | DA | 789 | A | N9-C4 | -6.05 | 1.34 | 1.37 |
| 1 | AA | 948 | C | N3-C4 | 6.04 | 1.38 | 1.33 |
| 1 | AA | 1377 | A | N9-C4 | 6.04 | 1.41 | 1.37 |
| 23 | BA | 2579 | C | N3-C4 | -6.04 | 1.29 | 1.33 |
| 23 | BA | 2246 | G | N1-C2 | -6.02 | 1.32 | 1.37 |
| 23 | BA | 2072 | G | C8-N7 | -6.02 | 1.27 | 1.30 |
| 23 | BA | 2017 | U | C2-N3 | -6.01 | 1.33 | 1.37 |
| 23 | DA | 278 | A | N3-C4 | 6.01 | 1.38 | 1.34 |
| 23 | BA | 90 | U | N3-C4 | 6.00 | 1.43 | 1.38 |
| 23 | BA | 745 | G | C6-N1 | -6.00 | 1.35 | 1.39 |
| 23 | DA | 2320 | A | N9-C4 | 6.00 | 1.41 | 1.37 |
| 23 | BA | 795 | C | N1-C6 | -6.00 | 1.33 | 1.37 |
| 23 | BA | 1123 | C | N1-C6 | -5.99 | 1.33 | 1.37 |
| 23 | BA | 1618 | A | C6-N1 | -5.99 | 1.31 | 1.35 |
| 23 | BA | 190 | A | N9-C4 | -5.98 | 1.34 | 1.37 |
| 23 | BA | 2046 | G | N7-C5 | -5.98 | 1.35 | 1.39 |
| 23 | BA | 468 | G | C8-N7 | -5.97 | 1.27 | 1.30 |
| 23 | BA | 1619 | G | C5-C4 | -5.97 | 1.34 | 1.38 |
| 23 | BA | 1241 | A | N3-C4 | -5.96 | 1.31 | 1.34 |
| 23 | BA | 2232 | U | C2-N3 | -5.96 | 1.33 | 1.37 |
| 23 | BA | 585 | G | C5-C4 | -5.96 | 1.34 | 1.38 |
| 24 | BB | 76 | G | N9-C4 | -5.96 | 1.33 | 1.38 |
| 23 | DA | 1569 | A | N7-C5 | -5.94 | 1.35 | 1.39 |
| 23 | DA | 2251 | G | N7-C5 | -5.94 | 1.35 | 1.39 |
| 1 | CA | 1442(A) | G | C5-C6 | 5.94 | 1.48 | 1.42 |
| 23 | BA | 2541 | A | N7-C5 | -5.93 | 1.35 | 1.39 |
| 23 | BA | 2607 | G | C8-N7 | -5.93 | 1.27 | 1.30 |
| 23 | BA | 2768 | C | N3-C4 | -5.92 | 1.29 | 1.33 |
| 1 | AA | 1350 | A | N9-C4 | 5.92 | 1.41 | 1.37 |
| 23 | BA | 381 | G | C5-C4 | -5.92 | 1.34 | 1.38 |
| 23 | BA | 1785 | A | C6-N1 | -5.91 | 1.31 | 1.35 |
| 23 | BA | 191 | A | N9-C4 | -5.91 | 1.34 | 1.37 |
| 1 | CA | 1243 | C | N1-C6 | 5.91 | 1.40 | 1.37 |
| 23 | DA | 1616 | A | C5-C6 | -5.91 | 1.35 | 1.41 |
| 23 | BA | 33 | U | N1-C2 | -5.90 | 1.33 | 1.38 |
| 23 | DA | 1981 | A | C6-N1 | -5.90 | 1.31 | 1.35 |
| 23 | BA | 940 | G | N7-C5 | -5.89 | 1.35 | 1.39 |
| 23 | BA | 2082 | A | N7-C5 | -5.89 | 1.35 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | BA | 265 | A | N7-C5 | -5.89 | 1.35 | 1.39 |
| 23 | BA | 2029 | G | N9-C8 | -5.89 | 1.33 | 1.37 |
| 1 | AA | 1014 | A | N9-C4 | 5.89 | 1.41 | 1.37 |
| 23 | BA | 1021 | A | N3-C4 | -5.88 | 1.31 | 1.34 |
| 1 | AA | 1263 | C | N1-C2 | 5.88 | 1.46 | 1.40 |
| 23 | BA | 2725 | A | N3-C4 | -5.88 | 1.31 | 1.34 |
| 23 | BA | 197 | A | N7-C5 | -5.87 | 1.35 | 1.39 |
| 23 | BA | 1819 | A | P-O5' | -5.87 | 1.53 | 1.59 |
| 23 | BA | 1603 | A | N3-C4 | -5.87 | 1.31 | 1.34 |
| 23 | BA | 1978 | A | N7-C5 | -5.87 | 1.35 | 1.39 |
| 23 | BA | 2829 | C | N1-C6 | -5.87 | 1.33 | 1.37 |
| 23 | DA | 945 | A | N3-C4 | -5.87 | 1.31 | 1.34 |
| 23 | DA | 1378 | A | N9-C4 | -5.86 | 1.34 | 1.37 |
| 23 | BA | 530 | G | C2-N3 | -5.86 | 1.28 | 1.32 |
| 23 | BA | 21 | A | N3-C4 | -5.85 | 1.31 | 1.34 |
| 23 | BA | 198 | C | N1-C6 | -5.85 | 1.33 | 1.37 |
| 23 | BA | 2321 | G | C2-N3 | -5.85 | 1.28 | 1.32 |
| 23 | BA | 1285 | G | C5-C4 | -5.84 | 1.34 | 1.38 |
| 23 | BA | 2509 | G | N7-C5 | -5.84 | 1.35 | 1.39 |
| 23 | BA | 2740 | A | N3-C4 | -5.84 | 1.31 | 1.34 |
| 23 | DA | 2031 | A | C5-C6 | -5.84 | 1.35 | 1.41 |
| 23 | BA | 184 | C | N1-C6 | -5.83 | 1.33 | 1.37 |
| 4 | AD | 12 | CYS | CB-SG | 5.83 | 1.92 | 1.82 |
| 23 | BA | 16 | G | C2-N3 | -5.83 | 1.28 | 1.32 |
| 23 | BA | 2335 | A | N9-C4 | -5.83 | 1.34 | 1.37 |
| 23 | BA | 194 | G | C2-N3 | -5.82 | 1.28 | 1.32 |
| 23 | BA | 1938 | A | N7-C5 | -5.82 | 1.35 | 1.39 |
| 23 | DA | 1998 | G | N3-C4 | -5.82 | 1.31 | 1.35 |
| 23 | DA | 2032 | G | N7-C5 | -5.82 | 1.35 | 1.39 |
| 23 | BA | 204 | A | C6-N1 | -5.82 | 1.31 | 1.35 |
| 23 | BA | 2602 | A | N9-C4 | 5.82 | 1.41 | 1.37 |
| 23 | BA | 2025 | C | N1-C6 | -5.82 | 1.33 | 1.37 |
| 1 | CA | 1030(D) | A | N9-C4 | 5.82 | 1.41 | 1.37 |
| 23 | BA | 978 | G | C5-C4 | -5.81 | 1.34 | 1.38 |
| 23 | BA | 330 | A | N3-C4 | -5.81 | 1.31 | 1.34 |
| 23 | DA | 2803 | C | N1-C6 | 5.81 | 1.40 | 1.37 |
| 1 | AA | 1210 | C | N1-C2 | 5.81 | 1.46 | 1.40 |
| 23 | BA | 1434 | A | N9-C4 | -5.81 | 1.34 | 1.37 |
| 23 | BA | 2451 | A | N3-C4 | -5.81 | 1.31 | 1.34 |
| 1 | CA | 1124 | G | N9-C4 | 5.81 | 1.42 | 1.38 |
| 23 | DA | 1252 | G | C5-C4 | -5.80 | 1.34 | 1.38 |
| 23 | BA | 1789 | A | C5-C4 | -5.80 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | BA | 2304 | G | C6-N1 | 5.80 | 1.43 | 1.39 |
| 23 | BA | 780 | G | N9-C8 | -5.79 | 1.33 | 1.37 |
| 1 | AA | 1442 | G | C8-N7 | -5.79 | 1.27 | 1.30 |
| 23 | DA | 57 | C | N3-C4 | -5.79 | 1.29 | 1.33 |
| 23 | BA | 2436 | G | N1-C2 | -5.78 | 1.33 | 1.37 |
| 23 | DA | 469 | G | C5-C4 | -5.78 | 1.34 | 1.38 |
| 23 | BA | 425 | G | C6-N1 | -5.78 | 1.35 | 1.39 |
| 23 | BA | 1669 | A | N3-C4 | -5.77 | 1.31 | 1.34 |
| 23 | DA | 1829 | A | N3-C4 | -5.77 | 1.31 | 1.34 |
| 23 | BA | 2442 | C | C2-N3 | -5.76 | 1.31 | 1.35 |
| 1 | AA | 993 | G | N9-C4 | 5.76 | 1.42 | 1.38 |
| 23 | BA | 829 | A | N9-C4 | -5.76 | 1.34 | 1.37 |
| 23 | BA | 71 | A | C5-C4 | 5.76 | 1.42 | 1.38 |
| 23 | DA | 1821 | A | C5-C4 | -5.76 | 1.34 | 1.38 |
| 23 | BA | 2740 | A | N7-C5 | -5.75 | 1.35 | 1.39 |
| 23 | DA | 2500 | U | C4-O4 | -5.75 | 1.19 | 1.23 |
| 1 | AA | 1316 | G | N7-C5 | 5.75 | 1.42 | 1.39 |
| 23 | DA | 1787 | A | N9-C4 | -5.75 | 1.34 | 1.37 |
| 23 | BA | 794 | G | C6-N1 | -5.75 | 1.35 | 1.39 |
| 23 | BA | 609 | A | C5-C4 | -5.75 | 1.34 | 1.38 |
| 23 | BA | 2382 | G | N7-C5 | -5.75 | 1.35 | 1.39 |
| 23 | DA | 2602 | A | N9-C4 | 5.75 | 1.41 | 1.37 |
| 23 | BA | 389 | G | C8-N7 | -5.75 | 1.27 | 1.30 |
| 23 | BA | 800 | A | N3-C4 | -5.74 | 1.31 | 1.34 |
| 23 | BA | 2346 | A | N7-C5 | -5.74 | 1.35 | 1.39 |
| 23 | DA | 2352 | A | N9-C4 | -5.74 | 1.34 | 1.37 |
| 23 | BA | 753 | C | N3-C4 | -5.74 | 1.29 | 1.33 |
| 1 | CA | 1004 | A | N9-C4 | 5.74 | 1.41 | 1.37 |
| 1 | AA | 1034 | G | C5-C4 | 5.73 | 1.42 | 1.38 |
| 23 | BA | 425 | G | N9-C8 | -5.73 | 1.33 | 1.37 |
| 23 | BA | 989 | G | N7-C5 | -5.72 | 1.35 | 1.39 |
| 23 | BA | 2000 | G | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | CA | 1335 | C | N1-C2 | 5.72 | 1.45 | 1.40 |
| 23 | BA | 1890 | A | N9-C4 | -5.71 | 1.34 | 1.37 |
| 23 | DA | 1649 | G | C5-C4 | -5.71 | 1.34 | 1.38 |
| 23 | BA | 181 | A | N3-C4 | -5.71 | 1.31 | 1.34 |
| 23 | BA | 571 | A | C5-C4 | -5.71 | 1.34 | 1.38 |
| 23 | BA | 47 | C | C5-C6 | -5.71 | 1.29 | 1.34 |
| 23 | BA | 344 | G | C5-C4 | -5.70 | 1.34 | 1.38 |
| 23 | BA | 2267 | A | N9-C4 | -5.70 | 1.34 | 1.37 |
| 1 | CA | 1492 | A | N3-C4 | 5.70 | 1.38 | 1.34 |
| 23 | BA | 2507 | C | C2-N3 | -5.70 | 1.31 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | BA | 1367 | A | C5-C4 | -5.70 | 1.34 | 1.38 |
| 23 | BA | 2676 | C | N1-C6 | -5.69 | 1.33 | 1.37 |
| 23 | DA | 2049 | G | N9-C4 | -5.69 | 1.33 | 1.38 |
| 23 | BA | 71 | A | N9-C8 | 5.69 | 1.42 | 1.37 |
| 23 | BA | 87 | C | N1-C6 | -5.69 | 1.33 | 1.37 |
| 23 | DA | 514 | A | N3-C4 | -5.69 | 1.31 | 1.34 |
| 1 | AA | 1447 | A | N7-C5 | 5.68 | 1.42 | 1.39 |
| 23 | BA | 1212 | G | N9-C8 | -5.67 | 1.33 | 1.37 |
| 23 | BA | 1430 | C | N1-C6 | -5.67 | 1.33 | 1.37 |
| 1 | AA | 1335 | C | N1-C2 | 5.67 | 1.45 | 1.40 |
| 23 | BA | 119 | A | N9-C8 | -5.67 | 1.33 | 1.37 |
| 23 | BA | 884 | C | N1-C6 | 5.67 | 1.40 | 1.37 |
| 1 | AA | 1355 | G | N9-C4 | 5.66 | 1.42 | 1.38 |
| 23 | DA | 1772 | G | N9-C4 | -5.66 | 1.33 | 1.38 |
| 23 | DA | 2791 | C | N1-C2 | 5.65 | 1.45 | 1.40 |
| 23 | BA | 983 | A | C5-C4 | -5.65 | 1.34 | 1.38 |
| 23 | BA | 492 | A | N7-C5 | -5.65 | 1.35 | 1.39 |
| 23 | BA | 2322 | A | C5-C6 | 5.65 | 1.46 | 1.41 |
| 23 | BA | 1535 | A | N9-C4 | 5.64 | 1.41 | 1.37 |
| 23 | BA | 197 | A | N3-C4 | -5.64 | 1.31 | 1.34 |
| 23 | BA | 788 | A | N9-C8 | -5.64 | 1.33 | 1.37 |
| 23 | BA | 1202 | C | N1-C6 | -5.64 | 1.33 | 1.37 |
| 23 | BA | 2445 | G | N9-C8 | -5.64 | 1.33 | 1.37 |
| 23 | BA | 751 | A | N3-C4 | -5.63 | 1.31 | 1.34 |
| 23 | DA | 1471 | A | N9-C4 | 5.63 | 1.41 | 1.37 |
| 23 | DA | 1698 | A | N9-C4 | -5.63 | 1.34 | 1.37 |
| 23 | BA | 1960 | A | N9-C4 | -5.63 | 1.34 | 1.37 |
| 23 | BA | 55 | G | N1-C2 | -5.63 | 1.33 | 1.37 |
| 23 | BA | 2452 | C | N1-C6 | -5.63 | 1.33 | 1.37 |
| 1 | AA | 1243 | C | N1-C6 | 5.63 | 1.40 | 1.37 |
| 23 | BA | 211 | A | C5-C4 | -5.63 | 1.34 | 1.38 |
| 23 | BA | 2322 | A | C6-N1 | 5.63 | 1.39 | 1.35 |
| 1 | AA | 1493 | A | N9-C4 | 5.62 | 1.41 | 1.37 |
| 23 | BA | 1363 | C | N3-C4 | -5.62 | 1.30 | 1.33 |
| 23 | BA | 2607 | G | N9-C8 | -5.62 | 1.33 | 1.37 |
| 23 | BA | 512 | G | P-O5' | -5.62 | 1.54 | 1.59 |
| 23 | BA | 98 | G | N9-C4 | -5.61 | 1.33 | 1.38 |
| 23 | DA | 689 | A | N9-C4 | -5.61 | 1.34 | 1.37 |
| 23 | BA | 2515 | C | C4-C5 | -5.60 | 1.38 | 1.43 |
| 23 | BA | 190 | A | C5-C6 | -5.59 | 1.36 | 1.41 |
| 1 | CA | 1330 | U | N1-C2 | 5.59 | 1.43 | 1.38 |
| 23 | BA | 682 | G | C5-C6 | -5.59 | 1.36 | 1.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | BA | 2028 | U | C2-N3 | -5.59 | 1.33 | 1.37 |
| 23 | BA | 1599 | C | N3-C4 | -5.59 | 1.30 | 1.33 |
| 23 | BA | 2541 | A | N9-C8 | -5.59 | 1.33 | 1.37 |
| 23 | BA | 425 | G | N1-C2 | -5.58 | 1.33 | 1.37 |
| 23 | BA | 815 | C | N1-C6 | -5.58 | 1.33 | 1.37 |
| 23 | BA | 1989 | G | N7-C5 | -5.58 | 1.35 | 1.39 |
| 23 | DA | 2502 | G | C5-C6 | -5.58 | 1.36 | 1.42 |
| 23 | DA | 1619 | G | C2-N3 | -5.58 | 1.28 | 1.32 |
| 23 | BA | 2695 | C | N1-C6 | -5.58 | 1.33 | 1.37 |
| 23 | DA | 2446 | G | N3-C4 | 5.58 | 1.39 | 1.35 |
| 23 | BA | 425 | G | C5-C4 | -5.58 | 1.34 | 1.38 |
| 23 | BA | 783 | A | C5-C4 | -5.57 | 1.34 | 1.38 |
| 23 | BA | 2249 | U | P-O5' | -5.57 | 1.54 | 1.59 |
| 23 | BA | 586 | A | N7-C5 | -5.57 | 1.35 | 1.39 |
| 23 | BA | 960 | A | C5-C6 | -5.56 | 1.36 | 1.41 |
| 23 | BA | 1570 | A | C5-C6 | -5.56 | 1.36 | 1.41 |
| 1 | AA | 1492 | A | N3-C4 | 5.56 | 1.38 | 1.34 |
| 23 | BA | 558 | G | C5-C4 | -5.56 | 1.34 | 1.38 |
| 23 | BA | 794 | G | N1-C2 | -5.56 | 1.33 | 1.37 |
| 23 | BA | 1297 | C | N1-C2 | -5.56 | 1.34 | 1.40 |
| 1 | CA | 1290 | G | N3-C4 | 5.56 | 1.39 | 1.35 |
| 23 | BA | 2284 | C | N3-C4 | -5.56 | 1.30 | 1.33 |
| 23 | BA | 553 | G | C5-C6 | -5.55 | 1.36 | 1.42 |
| 23 | BA | 1244 | G | C2-N3 | -5.55 | 1.28 | 1.32 |
| 23 | BA | 1653 | G | C6-N1 | -5.55 | 1.35 | 1.39 |
| 23 | DA | 1308 | A | N9-C8 | -5.55 | 1.33 | 1.37 |
| 17 | CQ | 49 | GLU | CG-CD | 5.55 | 1.60 | 1.51 |
| 23 | DA | 469 | G | N9-C8 | -5.55 | 1.33 | 1.37 |
| 23 | BA | 90 | U | C2-N3 | 5.54 | 1.41 | 1.37 |
| 23 | DA | 1037 | G | C6-N1 | 5.54 | 1.43 | 1.39 |
| 1 | CA | 1354 | C | C2-N3 | 5.54 | 1.40 | 1.35 |
| 1 | AA | 1309 | G | C6-N1 | 5.54 | 1.43 | 1.39 |
| 23 | BA | 560 | C | N1-C6 | -5.54 | 1.33 | 1.37 |
| 1 | CA | 1001 | A | N9-C4 | 5.54 | 1.41 | 1.37 |
| 23 | DA | 12 | U | N1-C2 | 5.54 | 1.43 | 1.38 |
| 23 | DA | 2607 | G | C2-N3 | 5.54 | 1.37 | 1.32 |
| 23 | BA | 830 | G | N9-C8 | -5.53 | 1.33 | 1.37 |
| 23 | BA | 2058 | A | C5-C4 | -5.53 | 1.34 | 1.38 |
| 23 | BA | 1162 | G | N7-C5 | -5.53 | 1.35 | 1.39 |
| 23 | DA | 746 | A | N3-C4 | -5.53 | 1.31 | 1.34 |
| 23 | DA | 2296 | U | N1-C2 | 5.53 | 1.43 | 1.38 |
| 23 | BA | 451 | C | N1-C6 | -5.52 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23 | BA | 1567 | A | N7-C5 | -5.52 | 1.35 | 1.39 |
| 23 | BA | 1698 | A | N7-C5 | -5.52 | 1.35 | 1.39 |
| 23 | BA | 2642 | G | N9-C8 | -5.52 | 1.33 | 1.37 |
| 23 | BA | 2052 | G | N9-C8 | -5.52 | 1.33 | 1.37 |
| 23 | DA | 1760 | A | N3-C4 | -5.52 | 1.31 | 1.34 |
| 23 | DA | 1969 | A | N9-C4 | -5.51 | 1.34 | 1.37 |
| 23 | BA | 1668 | A | C5-C4 | -5.51 | 1.34 | 1.38 |
| 23 | BA | 2015 | A | N9-C4 | -5.51 | 1.34 | 1.37 |
| 23 | BA | 113 | G | N9-C4 | -5.51 | 1.33 | 1.38 |
| 23 | DA | 1783 | A | C5-C6 | -5.50 | 1.36 | 1.41 |
| 23 | BA | 1250 | G | N7-C5 | -5.50 | 1.35 | 1.39 |
| 23 | BA | 2431 | U | N1-C2 | -5.50 | 1.33 | 1.38 |
| 23 | DA | 1213 | A | N9-C4 | -5.50 | 1.34 | 1.37 |
| 23 | DA | 2826 | A | N9-C4 | -5.50 | 1.34 | 1.37 |
| 23 | BA | 229 | A | N9-C4 | 5.50 | 1.41 | 1.37 |
| 23 | BA | 751 | A | C5-C4 | -5.50 | 1.34 | 1.38 |
| 23 | BA | 1254 | A | N7-C5 | -5.50 | 1.35 | 1.39 |
| 23 | DA | 1698 | A | N7-C5 | -5.50 | 1.35 | 1.39 |
| 23 | DA | 2606 | C | N1-C6 | -5.50 | 1.33 | 1.37 |
| 23 | BA | 480 | A | N7-C5 | -5.50 | 1.35 | 1.39 |
| 23 | BA | 745 | G | C5-C6 | -5.49 | 1.36 | 1.42 |
| 23 | BA | 2051 | A | N3-C4 | -5.49 | 1.31 | 1.34 |
| 23 | DA | 786 | C | C4-N4 | -5.49 | 1.29 | 1.33 |
| 23 | BA | 2747 | G | C6-N1 | -5.49 | 1.35 | 1.39 |
| 23 | DA | 2151 | G | C6-N1 | 5.49 | 1.43 | 1.39 |
| 23 | BA | 207 | A | N7-C5 | -5.49 | 1.35 | 1.39 |
| 23 | BA | 189 | G | N9-C8 | -5.49 | 1.34 | 1.37 |
| 23 | BA | 975 | C | N1-C6 | -5.49 | 1.33 | 1.37 |
| 23 | DA | 1267 | U | C2-N3 | -5.48 | 1.33 | 1.37 |
| 23 | BA | 2011 | U | N1-C2 | -5.48 | 1.33 | 1.38 |
| 23 | BA | 802 | A | N7-C5 | -5.48 | 1.35 | 1.39 |
| 23 | BA | 1300 | U | C3'-O3' | 5.48 | 1.49 | 1.42 |
| 23 | DA | 2149 | G | C6-N1 | 5.48 | 1.43 | 1.39 |
| 23 | BA | 1490 | A | N3-C4 | 5.48 | 1.38 | 1.34 |
| 23 | BA | 2589 | A | N9-C4 | -5.48 | 1.34 | 1.37 |
| 23 | BA | 1988 | C | N1-C6 | -5.48 | 1.33 | 1.37 |
| 23 | BA | 572 | A | N7-C5 | -5.47 | 1.35 | 1.39 |
| 23 | BA | 2017 | U | C2-O2 | -5.47 | 1.17 | 1.22 |
| 23 | BA | 804 | A | N9-C8 | -5.47 | 1.33 | 1.37 |
| 23 | BA | 1804 | C | N3-C4 | -5.47 | 1.30 | 1.33 |
| 32 | BO | 21 | CYS | CB-SG | -5.47 | 1.72 | 1.81 |
| 23 | DA | 2791 | C | N1-C6 | 5.47 | 1.40 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | DA | 1142(A) | A | C5-C6 | -5.47 | 1.36 | 1.41 |
| 23 | BA | 1698 | A | C5-C6 | -5.46 | 1.36 | 1.41 |
| 23 | DA | 1669 | A | N3-C4 | -5.46 | 1.31 | 1.34 |
| 25 | BD | 28 | GLU | CG-CD | 5.46 | 1.60 | 1.51 |
| 23 | BA | 1528 | A | N3-C4 | -5.46 | 1.31 | 1.34 |
| 23 | BA | 2426 | A | C6-N1 | -5.46 | 1.31 | 1.35 |
| 23 | BA | 1655 | A | C5-C4 | -5.45 | 1.34 | 1.38 |
| 23 | BA | 2054 | A | C5-C6 | -5.45 | 1.36 | 1.41 |
| 23 | DA | 1927 | A | N9-C4 | -5.45 | 1.34 | 1.37 |
| 23 | BA | 664 | C | N1-C6 | -5.45 | 1.33 | 1.37 |
| 23 | BA | 1330 | C | N1-C6 | -5.45 | 1.33 | 1.37 |
| 23 | DA | 2487 | G | N9-C4 | -5.45 | 1.33 | 1.38 |
| 23 | DA | 2561 | A | N9-C4 | -5.45 | 1.34 | 1.37 |
| 23 | BA | 1535 | A | N3-C4 | 5.45 | 1.38 | 1.34 |
| 23 | BA | 483 | A | C6-N1 | -5.45 | 1.31 | 1.35 |
| 23 | BA | 1252 | G | N3-C4 | -5.45 | 1.31 | 1.35 |
| 1 | AA | 1174 | G | N7-C5 | 5.44 | 1.42 | 1.39 |
| 24 | BB | 104 | U | C2-N3 | -5.44 | 1.33 | 1.37 |
| 23 | BA | 2017 | U | N1-C6 | -5.44 | 1.33 | 1.38 |
| 23 | BA | 1189 | A | C5-C6 | -5.44 | 1.36 | 1.41 |
| 23 | DA | 802 | A | C6-N6 | -5.44 | 1.29 | 1.33 |
| 1 | CA | 1149 | C | N1-C2 | 5.44 | 1.45 | 1.40 |
| 23 | BA | 756 | C | N1-C2 | -5.44 | 1.34 | 1.40 |
| 23 | BA | 1771 | C | N3-C4 | -5.43 | 1.30 | 1.33 |
| 1 | CA | 1294 | G | C6-N1 | 5.43 | 1.43 | 1.39 |
| 23 | BA | 1658 | C | P-OP1 | -5.43 | 1.39 | 1.49 |
| 23 | BA | 2058 | A | N7-C5 | -5.43 | 1.35 | 1.39 |
| 23 | BA | 2059 | A | N9-C8 | -5.43 | 1.33 | 1.37 |
| 23 | BA | 2447 | G | C5-C4 | -5.43 | 1.34 | 1.38 |
| 23 | DA | 2587 | A | N7-C5 | -5.43 | 1.35 | 1.39 |
| 23 | BA | 265 | A | C5-C6 | -5.43 | 1.36 | 1.41 |
| 23 | DA | 580 | C | N1-C6 | -5.43 | 1.33 | 1.37 |
| 23 | BA | 778 | G | N7-C5 | -5.42 | 1.35 | 1.39 |
| 23 | BA | 2053 | G | C5-C4 | -5.42 | 1.34 | 1.38 |
| 23 | BA | 2686 | G | C5-C4 | -5.42 | 1.34 | 1.38 |
| 23 | BA | 2572 | A | C5-C4 | -5.42 | 1.34 | 1.38 |
| 24 | BB | 56 | G | N7-C5 | -5.42 | 1.35 | 1.39 |
| 1 | AA | 143 | A | N3-C4 | 5.42 | 1.38 | 1.34 |
| 1 | AA | 948 | C | N1-C6 | 5.42 | 1.40 | 1.37 |
| 23 | BA | 1403 | C | N3-C4 | -5.42 | 1.30 | 1.33 |
| 24 | BB | 99 | G | C5-C4 | -5.41 | 1.34 | 1.38 |
| 4 | AD | 26 | CYS | CB-SG | 5.41 | 1.91 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|--------|-------|-------------|----------|
| 1 | CA | 1456 | G | N9-C4 | 5.41 | 1.42 | 1.38 |
| 23 | BA | 787 | U | P-OP2 | -5.41 | 1.39 | 1.49 |
| 23 | BA | 1614 | A | N9-C4 | -5.41 | 1.34 | 1.37 |
| 1 | CA | 1180 | A | N9-C4 | 5.41 | 1.41 | 1.37 |
| 23 | BA | 1638 | C | N1-C6 | -5.41 | 1.33 | 1.37 |
| 23 | BA | 1643 | G | C6-N1 | -5.41 | 1.35 | 1.39 |
| 23 | BA | 1779 | U | P-O5' | -5.41 | 1.54 | 1.59 |
| 1 | CA | 1360 | A | N9-C4 | 5.40 | 1.41 | 1.37 |
| 23 | BA | 1308 | A | C5-C4 | -5.40 | 1.34 | 1.38 |
| 1 | CA | 1149 | C | N1-C6 | 5.40 | 1.40 | 1.37 |
| 42 | DY | 79 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | AA | 1124 | G | N3-C4 | 5.40 | 1.39 | 1.35 |
| 23 | BA | 204 | A | C5-C6 | -5.40 | 1.36 | 1.41 |
| 23 | BA | 505 | A | N9-C4 | -5.40 | 1.34 | 1.37 |
| 23 | BA | 785 | G | N9-C4 | -5.40 | 1.33 | 1.38 |
| 23 | DA | 775 | G | C6-N1 | -5.40 | 1.35 | 1.39 |
| 23 | BA | 141 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 23 | DA | 676 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 23 | BA | 734 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 23 | BA | 994 | C | N1-C6 | -5.39 | 1.33 | 1.37 |
| 23 | BA | 536 | A | C5-C4 | -5.39 | 1.34 | 1.38 |
| 23 | BA | 1132 | A | C6-N1 | -5.39 | 1.31 | 1.35 |
| 23 | DA | 1567 | A | N9-C4 | -5.39 | 1.34 | 1.37 |
| 23 | BA | 971 | C | N3-C4 | -5.38 | 1.30 | 1.33 |
| 23 | DA | 2058 | A | C6-N1 | -5.38 | 1.31 | 1.35 |
| 23 | DA | 1314 | C | C4-C5 | -5.38 | 1.38 | 1.43 |
| 23 | BA | 466 | A | P-O5' | -5.38 | 1.54 | 1.59 |
| 23 | BA | 2323 | G | C5-C4 | -5.37 | 1.34 | 1.38 |
| 1 | AA | 1123 | A | N9-C4 | 5.37 | 1.41 | 1.37 |
| 23 | BA | 2251 | G | N7-C5 | -5.37 | 1.36 | 1.39 |
| 23 | BA | 57 | C | N3-C4 | -5.37 | 1.30 | 1.33 |
| 23 | BA | 1674 | G | N9-C8 | -5.37 | 1.34 | 1.37 |
| 23 | DA | 1142(A) | A | N7-C5 | -5.37 | 1.36 | 1.39 |
| 1 | AA | 1184 | G | N9-C4 | 5.36 | 1.42 | 1.38 |
| 1 | AA | 1001(A) | G | N3-C4 | 5.36 | 1.39 | 1.35 |
| 23 | BA | 2541 | A | N3-C4 | -5.36 | 1.31 | 1.34 |
| 49 | B5 | 6 | VAL | CB-CG2 | -5.36 | 1.41 | 1.52 |
| 23 | BA | 2153 | G | C6-N1 | 5.36 | 1.43 | 1.39 |
| 23 | BA | 1674 | G | C5-C4 | -5.36 | 1.34 | 1.38 |
| 23 | BA | 745 | G | C5-C4 | -5.35 | 1.34 | 1.38 |
| 23 | BA | 2614 | A | N9-C8 | -5.35 | 1.33 | 1.37 |
| 1 | AA | 994 | A | N9-C4 | 5.35 | 1.41 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 23 | DA | 1826 | G | N9-C8 | -5.35 | 1.34 | 1.37 |
| 23 | BA | 468 | G | C5-C4 | -5.34 | 1.34 | 1.38 |
| 23 | BA | 733 | G | C5-C4 | -5.34 | 1.34 | 1.38 |
| 23 | BA | 2246 | G | C2-N3 | -5.34 | 1.28 | 1.32 |
| 23 | BA | 1359 | A | C6-N6 | -5.33 | 1.29 | 1.33 |
| 23 | BA | 1606 | G | N9-C8 | -5.33 | 1.34 | 1.37 |
| 1 | CA | 1124 | G | C5-C4 | 5.33 | 1.42 | 1.38 |
| 1 | AA | 1025 | U | N3-C4 | 5.33 | 1.43 | 1.38 |
| 23 | DA | 727 | A | N7-C5 | -5.33 | 1.36 | 1.39 |
| 23 | BA | 989 | G | C8-N7 | -5.33 | 1.27 | 1.30 |
| 1 | AA | 1020 | U | N1-C2 | 5.32 | 1.43 | 1.38 |
| 1 | AA | 78 | G | C6-N1 | 5.32 | 1.43 | 1.39 |
| 23 | BA | 507 | A | N7-C5 | -5.32 | 1.36 | 1.39 |
| 23 | BA | 1157 | G | N7-C5 | -5.32 | 1.36 | 1.39 |
| 23 | BA | 981 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 23 | DA | 2436 | G | C2-N3 | -5.32 | 1.28 | 1.32 |
| 23 | BA | 271(M) | G | N9-C4 | 5.31 | 1.42 | 1.38 |
| 23 | BA | 1137 | G | C8-N7 | -5.31 | 1.27 | 1.30 |
| 23 | BA | 1031 | G | N1-C2 | -5.31 | 1.33 | 1.37 |
| 23 | DA | 1308 | A | N3-C4 | -5.31 | 1.31 | 1.34 |
| 23 | BA | 690 | G | N1-C2 | -5.31 | 1.33 | 1.37 |
| 23 | BA | 85 | G | N7-C5 | -5.30 | 1.36 | 1.39 |
| 23 | BA | 527 | C | N3-C4 | -5.30 | 1.30 | 1.33 |
| 23 | BA | 2013 | A | C5-C6 | -5.30 | 1.36 | 1.41 |
| 23 | BA | 2330 | G | N3-C4 | -5.30 | 1.31 | 1.35 |
| 23 | BA | 211 | A | N9-C4 | -5.30 | 1.34 | 1.37 |
| 23 | BA | 2162 | G | N3-C4 | 5.30 | 1.39 | 1.35 |
| 23 | BA | 1268 | A | C6-N1 | -5.30 | 1.31 | 1.35 |
| 23 | DA | 531 | C | N1-C6 | -5.29 | 1.33 | 1.37 |
| 23 | BA | 70 | G | N1-C2 | -5.29 | 1.33 | 1.37 |
| 23 | BA | 2432 | A | C5-C6 | -5.29 | 1.36 | 1.41 |
| 23 | BA | 2065 | C | N1-C6 | -5.28 | 1.33 | 1.37 |
| 23 | BA | 744 | G | N9-C8 | -5.28 | 1.34 | 1.37 |
| 23 | BA | 1132 | A | N3-C4 | -5.28 | 1.31 | 1.34 |
| 23 | DA | 255 | A | N9-C4 | -5.28 | 1.34 | 1.37 |
| 23 | BA | 1764 | G | C6-N1 | -5.27 | 1.35 | 1.39 |
| 23 | BA | 2599 | G | N9-C8 | -5.27 | 1.34 | 1.37 |
| 23 | DA | 251 | A | C5-C4 | -5.27 | 1.35 | 1.38 |
| 1 | CA | 1377 | A | N9-C4 | 5.27 | 1.41 | 1.37 |
| 23 | BA | 1616 | A | C5-C6 | -5.27 | 1.36 | 1.41 |
| 1 | AA | 1012 | U | C2-N3 | 5.26 | 1.41 | 1.37 |
| 23 | BA | 2225 | A | N9-C4 | -5.26 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | BA | 2577 | A | P-OP2 | -5.26 | 1.40 | 1.49 |
| 23 | BA | 733 | G | C8-N7 | -5.26 | 1.27 | 1.30 |
| 23 | BA | 978 | G | C5-C6 | -5.25 | 1.37 | 1.42 |
| 23 | BA | 981 | A | N7-C5 | -5.25 | 1.36 | 1.39 |
| 23 | BA | 2505 | G | C2-N3 | -5.25 | 1.28 | 1.32 |
| 23 | BA | 733 | G | N7-C5 | -5.25 | 1.36 | 1.39 |
| 23 | BA | 941 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 23 | BA | 1657 | C | N1-C6 | -5.25 | 1.33 | 1.37 |
| 23 | DA | 1026 | U | N1-C2 | 5.25 | 1.43 | 1.38 |
| 23 | BA | 13 | A | C6-N1 | -5.25 | 1.31 | 1.35 |
| 23 | BA | 994 | C | N3-C4 | -5.25 | 1.30 | 1.33 |
| 23 | DA | 38 | A | C5-C4 | -5.25 | 1.35 | 1.38 |
| 23 | BA | 2025 | C | C4-C5 | -5.25 | 1.38 | 1.43 |
| 23 | BA | 2571 | C | C2-O2 | -5.25 | 1.19 | 1.24 |
| 23 | DA | 739 | G | C5-C4 | -5.25 | 1.34 | 1.38 |
| 1 | AA | 1442(A) | G | C5-C4 | 5.25 | 1.42 | 1.38 |
| 23 | BA | 2778 | A | C6-N1 | -5.25 | 1.31 | 1.35 |
| 1 | CA | 1290 | G | N9-C4 | 5.25 | 1.42 | 1.38 |
| 1 | CA | 1279 | A | N9-C4 | 5.24 | 1.41 | 1.37 |
| 1 | CA | 1291 | G | N3-C4 | 5.24 | 1.39 | 1.35 |
| 23 | BA | 2087 | G | C5-C6 | -5.24 | 1.37 | 1.42 |
| 23 | DA | 980 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 23 | BA | 748 | G | N9-C8 | -5.24 | 1.34 | 1.37 |
| 1 | CA | 1370 | G | C6-N1 | 5.24 | 1.43 | 1.39 |
| 23 | BA | 943 | U | N1-C2 | -5.24 | 1.33 | 1.38 |
| 23 | DA | 948 | G | N3-C4 | -5.24 | 1.31 | 1.35 |
| 23 | BA | 575 | A | C6-N6 | -5.24 | 1.29 | 1.33 |
| 23 | BA | 788 | A | N7-C5 | -5.24 | 1.36 | 1.39 |
| 23 | DA | 254 | G | N9-C4 | -5.23 | 1.33 | 1.38 |
| 1 | AA | 970 | C | N1-C2 | 5.23 | 1.45 | 1.40 |
| 23 | BA | 1225 | G | C2-N3 | -5.23 | 1.28 | 1.32 |
| 23 | BA | 380 | U | N1-C6 | -5.22 | 1.33 | 1.38 |
| 23 | BA | 2778 | A | N7-C5 | -5.22 | 1.36 | 1.39 |
| 23 | BA | 2825 | C | N1-C6 | -5.22 | 1.34 | 1.37 |
| 23 | DA | 2286 | A | N7-C5 | -5.22 | 1.36 | 1.39 |
| 23 | DA | 1309 | G | C5-C4 | -5.22 | 1.34 | 1.38 |
| 23 | BA | 2506 | U | N1-C2 | 5.22 | 1.43 | 1.38 |
| 23 | DA | 1490 | A | C6-N1 | 5.22 | 1.39 | 1.35 |
| 23 | BA | 1698 | A | N3-C4 | -5.21 | 1.31 | 1.34 |
| 23 | BA | 2329 | G | N1-C2 | -5.21 | 1.33 | 1.37 |
| 23 | DA | 530 | G | C6-O6 | -5.21 | 1.19 | 1.24 |
| 23 | DA | 2028 | U | C2-N3 | -5.21 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 23 | BA | 197 | A | C5-C6 | -5.21 | 1.36 | 1.41 |
| 23 | BA | 952 | G | C5-C4 | -5.21 | 1.34 | 1.38 |
| 23 | BA | 1195 | G | C5-C4 | -5.21 | 1.34 | 1.38 |
| 23 | BA | 1262 | A | C6-N6 | -5.21 | 1.29 | 1.33 |
| 23 | BA | 2602 | A | O3'-P | 5.21 | 1.67 | 1.61 |
| 1 | CA | 1030(A) | G | N9-C4 | 5.21 | 1.42 | 1.38 |
| 23 | BA | 463 | G | C6-N1 | -5.21 | 1.35 | 1.39 |
| 51 | B7 | 30 | VAL | CA-CB | -5.21 | 1.43 | 1.54 |
| 23 | BA | 253 | C | N1-C6 | -5.20 | 1.34 | 1.37 |
| 23 | BA | 1217 | C | C4-C5 | -5.20 | 1.38 | 1.43 |
| 23 | BA | 2436 | G | C2-N3 | -5.20 | 1.28 | 1.32 |
| 23 | DA | 2424 | C | N1-C6 | -5.20 | 1.34 | 1.37 |
| 23 | BA | 71 | A | C5-C6 | -5.20 | 1.36 | 1.41 |
| 23 | BA | 1368 | G | P-O5' | -5.20 | 1.54 | 1.59 |
| 1 | AA | 1279 | A | C5-C4 | 5.20 | 1.42 | 1.38 |
| 23 | BA | 278 | A | C6-N1 | 5.20 | 1.39 | 1.35 |
| 23 | BA | 1195 | G | C2-N3 | -5.20 | 1.28 | 1.32 |
| 23 | DA | 1933 | G | C6-N1 | -5.20 | 1.35 | 1.39 |
| 23 | BA | 980 | A | C5-C6 | -5.19 | 1.36 | 1.41 |
| 23 | DA | 1257 | C | N1-C2 | -5.19 | 1.34 | 1.40 |
| 23 | BA | 936 | C | N1-C2 | -5.19 | 1.34 | 1.40 |
| 23 | BA | 1137 | G | N7-C5 | -5.19 | 1.36 | 1.39 |
| 23 | BA | 2822 | G | N9-C8 | -5.19 | 1.34 | 1.37 |
| 1 | AA | 143 | A | N9-C4 | 5.18 | 1.41 | 1.37 |
| 1 | AA | 1502 | A | C5-C6 | -5.18 | 1.36 | 1.41 |
| 23 | BA | 2764 | A | N3-C4 | -5.18 | 1.31 | 1.34 |
| 23 | BA | 2020 | A | N9-C8 | -5.18 | 1.33 | 1.37 |
| 23 | BA | 2546 | U | N1-C2 | -5.18 | 1.33 | 1.38 |
| 23 | BA | 2606 | C | N1-C6 | -5.18 | 1.34 | 1.37 |
| 23 | BA | 15 | G | N9-C8 | -5.18 | 1.34 | 1.37 |
| 23 | BA | 686 | G | C5-C6 | -5.18 | 1.37 | 1.42 |
| 23 | BA | 980 | A | N7-C5 | -5.18 | 1.36 | 1.39 |
| 23 | BA | 1256 | G | N3-C4 | -5.18 | 1.31 | 1.35 |
| 24 | BB | 96 | U | C2-N3 | -5.18 | 1.34 | 1.37 |
| 23 | BA | 2304 | G | N7-C5 | 5.17 | 1.42 | 1.39 |
| 23 | BA | 2376 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 23 | DA | 652(B) | A | N3-C4 | 5.17 | 1.38 | 1.34 |
| 23 | BA | 1204 | A | C5-C6 | -5.17 | 1.36 | 1.41 |
| 23 | BA | 1618 | A | P-O5' | -5.17 | 1.54 | 1.59 |
| 23 | BA | 733 | G | C6-N1 | -5.17 | 1.35 | 1.39 |
| 1 | AA | 1004 | A | N9-C4 | 5.17 | 1.41 | 1.37 |
| 23 | DA | 750 | A | N3-C4 | -5.17 | 1.31 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 23 | BA | 1184 | G | C2-N3 | -5.17 | 1.28 | 1.32 |
| 23 | BA | 1889 | A | N9-C4 | -5.17 | 1.34 | 1.37 |
| 23 | BA | 1933 | G | C6-N1 | -5.17 | 1.35 | 1.39 |
| 23 | BA | 975 | C | N3-C4 | -5.16 | 1.30 | 1.33 |
| 23 | BA | 2587 | A | P-O5' | -5.16 | 1.54 | 1.59 |
| 23 | BA | 819 | A | N9-C4 | -5.16 | 1.34 | 1.37 |
| 1 | AA | 1123 | A | N3-C4 | 5.16 | 1.38 | 1.34 |
| 23 | BA | 1787 | A | N3-C4 | -5.16 | 1.31 | 1.34 |
| 23 | BA | 107 | C | N1-C6 | -5.15 | 1.34 | 1.37 |
| 23 | BA | 753 | C | C2-N3 | -5.15 | 1.31 | 1.35 |
| 23 | BA | 2422 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 23 | BA | 119 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 23 | BA | 1647 | G | N9-C8 | -5.15 | 1.34 | 1.37 |
| 1 | CA | 1256 | A | N9-C4 | 5.15 | 1.41 | 1.37 |
| 23 | BA | 2517 | C | N1-C6 | -5.15 | 1.34 | 1.37 |
| 23 | DA | 2589 | A | N9-C4 | -5.15 | 1.34 | 1.37 |
| 23 | BA | 555 | U | P-O5' | -5.14 | 1.54 | 1.59 |
| 23 | BA | 20 | C | N1-C6 | -5.14 | 1.34 | 1.37 |
| 23 | BA | 1195 | G | N3-C4 | -5.14 | 1.31 | 1.35 |
| 23 | DA | 2577 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 23 | BA | 1791 | A | N3-C4 | -5.14 | 1.31 | 1.34 |
| 23 | BA | 2352 | A | N9-C4 | -5.14 | 1.34 | 1.37 |
| 23 | BA | 2149 | G | C6-N1 | 5.14 | 1.43 | 1.39 |
| 23 | BA | 2542 | A | N3-C4 | -5.14 | 1.31 | 1.34 |
| 23 | BA | 2288 | A | N9-C4 | 5.14 | 1.41 | 1.37 |
| 1 | CA | 1332 | A | C5-C4 | 5.14 | 1.42 | 1.38 |
| 23 | BA | 244 | A | C5-C6 | -5.14 | 1.36 | 1.41 |
| 23 | BA | 1285 | G | N7-C5 | -5.14 | 1.36 | 1.39 |
| 23 | BA | 2819 | G | N9-C8 | -5.14 | 1.34 | 1.37 |
| 23 | DA | 220 | G | N7-C5 | -5.14 | 1.36 | 1.39 |
| 1 | CA | 1235 | U | N1-C2 | 5.13 | 1.43 | 1.38 |
| 23 | DA | 1107 | G | N3-C4 | 5.13 | 1.39 | 1.35 |
| 23 | DA | 71 | A | C3'-O3' | 5.13 | 1.49 | 1.42 |
| 23 | BA | 2724 | C | N1-C6 | -5.13 | 1.34 | 1.37 |
| 23 | DA | 2322 | A | C5-C6 | 5.13 | 1.45 | 1.41 |
| 23 | BA | 783 | A | N3-C4 | -5.13 | 1.31 | 1.34 |
| 38 | BU | 69 | CYS | CB-SG | -5.13 | 1.73 | 1.81 |
| 23 | BA | 2072 | G | C5-C4 | -5.12 | 1.34 | 1.38 |
| 23 | BA | 2684 | U | N1-C6 | -5.12 | 1.33 | 1.38 |
| 23 | BA | 189 | G | N3-C4 | -5.12 | 1.31 | 1.35 |
| 1 | AA | 70 | G | C6-N1 | 5.12 | 1.43 | 1.39 |
| 23 | BA | 2287 | A | C6-N6 | -5.12 | 1.29 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 24 | DB | 53 | A | N9-C4 | 5.12 | 1.41 | 1.37 |
| 23 | DA | 1369 | G | N3-C4 | -5.12 | 1.31 | 1.35 |
| 1 | AA | 1447 | A | N3-C4 | 5.12 | 1.38 | 1.34 |
| 23 | BA | 204 | A | C5-C4 | -5.12 | 1.35 | 1.38 |
| 23 | BA | 2245 | U | C2-N3 | -5.12 | 1.34 | 1.37 |
| 23 | BA | 2699 | C | N1-C6 | -5.12 | 1.34 | 1.37 |
| 23 | DA | 245 | G | N7-C5 | -5.12 | 1.36 | 1.39 |
| 23 | BA | 939 | G | N3-C4 | -5.11 | 1.31 | 1.35 |
| 23 | BA | 2723 | C | C2-N3 | -5.11 | 1.31 | 1.35 |
| 23 | DA | 1301 | A | N3-C4 | -5.11 | 1.31 | 1.34 |
| 23 | BA | 2602 | A | N7-C5 | 5.11 | 1.42 | 1.39 |
| 23 | BA | 849 | A | C5-C4 | -5.11 | 1.35 | 1.38 |
| 23 | BA | 1176 | G | N3-C4 | 5.11 | 1.39 | 1.35 |
| 23 | BA | 2711 | A | N9-C4 | -5.11 | 1.34 | 1.37 |
| 23 | DA | 2437 | U | N3-C4 | -5.11 | 1.33 | 1.38 |
| 23 | BA | 1365 | A | N9-C4 | -5.10 | 1.34 | 1.37 |
| 1 | AA | 1175 | G | N3-C4 | 5.10 | 1.39 | 1.35 |
| 1 | AA | 1456 | G | N3-C4 | 5.10 | 1.39 | 1.35 |
| 23 | DA | 1989 | G | N7-C5 | -5.10 | 1.36 | 1.39 |
| 23 | BA | 1903 | G | N7-C5 | -5.10 | 1.36 | 1.39 |
| 23 | DA | 71 | A | N9-C8 | 5.10 | 1.41 | 1.37 |
| 23 | DA | 1419 | A | N9-C4 | -5.10 | 1.34 | 1.37 |
| 23 | BA | 749 | C | C4-C5 | -5.10 | 1.38 | 1.43 |
| 23 | BA | 1314 | C | N3-C4 | -5.09 | 1.30 | 1.33 |
| 23 | BA | 2741 | A | C5-C4 | -5.09 | 1.35 | 1.38 |
| 23 | BA | 1034 | G | C5-C4 | -5.09 | 1.34 | 1.38 |
| 1 | CA | 1447 | A | N3-C4 | 5.09 | 1.38 | 1.34 |
| 50 | B6 | 16 | CYS | CB-SG | -5.09 | 1.73 | 1.81 |
| 23 | DA | 2730 | C | N3-C4 | -5.09 | 1.30 | 1.33 |
| 23 | BA | 447 | A | C5-C6 | -5.09 | 1.36 | 1.41 |
| 23 | BA | 1564 | C | N1-C6 | -5.09 | 1.34 | 1.37 |
| 23 | BA | 2026 | C | N1-C6 | -5.09 | 1.34 | 1.37 |
| 23 | DA | 1022 | G | N3-C4 | -5.09 | 1.31 | 1.35 |
| 23 | DA | 2027 | G | N3-C4 | -5.09 | 1.31 | 1.35 |
| 23 | BA | 123 | G | N9-C4 | -5.09 | 1.33 | 1.38 |
| 23 | BA | 1279 | G | C6-N1 | -5.09 | 1.35 | 1.39 |
| 23 | BA | 1624 | G | C5-C4 | -5.09 | 1.34 | 1.38 |
| 23 | BA | 2063 | C | N1-C6 | -5.09 | 1.34 | 1.37 |
| 1 | AA | 947 | G | N9-C4 | 5.08 | 1.42 | 1.38 |
| 23 | DA | 805 | G | N9-C8 | -5.08 | 1.34 | 1.37 |
| 23 | BA | 1308 | A | N9-C8 | -5.08 | 1.33 | 1.37 |
| 1 | CA | 839 | U | N1-C2 | 5.08 | 1.43 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | DA | 2335 | A | N9-C4 | -5.08 | 1.34 | 1.37 |
| 1 | CA | 1124 | G | N3-C4 | 5.08 | 1.39 | 1.35 |
| 23 | BA | 745 | G | N1-C2 | -5.07 | 1.33 | 1.37 |
| 23 | BA | 188 | G | C8-N7 | -5.07 | 1.27 | 1.30 |
| 1 | CA | 1050 | G | N3-C4 | 5.07 | 1.39 | 1.35 |
| 23 | DA | 1021 | A | N3-C4 | -5.07 | 1.31 | 1.34 |
| 1 | AA | 1002 | G | C5-C4 | 5.07 | 1.41 | 1.38 |
| 23 | BA | 577 | G | P-OP2 | -5.07 | 1.40 | 1.49 |
| 23 | BA | 2445 | G | C6-N1 | -5.07 | 1.36 | 1.39 |
| 23 | BA | 109 | G | C6-N1 | -5.06 | 1.36 | 1.39 |
| 23 | BA | 1827 | C | N3-C4 | -5.06 | 1.30 | 1.33 |
| 23 | BA | 533 | G | C6-N1 | -5.06 | 1.36 | 1.39 |
| 23 | BA | 658 | C | C2-N3 | -5.06 | 1.31 | 1.35 |
| 23 | BA | 70 | G | C6-N1 | -5.06 | 1.36 | 1.39 |
| 1 | AA | 65 | U | N1-C2 | 5.05 | 1.43 | 1.38 |
| 23 | BA | 1199 | U | C2-N3 | -5.05 | 1.34 | 1.37 |
| 23 | DA | 1787 | A | N3-C4 | -5.05 | 1.31 | 1.34 |
| 23 | BA | 1199 | U | N1-C2 | -5.05 | 1.34 | 1.38 |
| 23 | BA | 1204 | A | N3-C4 | -5.05 | 1.31 | 1.34 |
| 23 | BA | 2054 | A | O3'-P | -5.05 | 1.55 | 1.61 |
| 1 | AA | 1138 | G | N9-C4 | 5.05 | 1.42 | 1.38 |
| 23 | BA | 972 | G | N1-C2 | -5.05 | 1.33 | 1.37 |
| 23 | BA | 934 | G | N9-C8 | -5.05 | 1.34 | 1.37 |
| 23 | BA | 555 | U | N1-C2 | -5.04 | 1.34 | 1.38 |
| 23 | BA | 1363 | C | C4-N4 | -5.04 | 1.29 | 1.33 |
| 1 | CA | 1033 | G | N3-C4 | 5.04 | 1.39 | 1.35 |
| 1 | CA | 1333 | A | C5-C4 | 5.04 | 1.42 | 1.38 |
| 1 | AA | 455 | C | N1-C6 | 5.04 | 1.40 | 1.37 |
| 23 | BA | 214 | G | C5-C4 | -5.04 | 1.34 | 1.38 |
| 23 | BA | 1829 | A | N3-C4 | -5.04 | 1.31 | 1.34 |
| 23 | BA | 2117 | A | N9-C4 | 5.04 | 1.40 | 1.37 |
| 23 | DA | 1981 | A | N3-C4 | -5.04 | 1.31 | 1.34 |
| 23 | BA | 1393 | A | C6-N1 | -5.04 | 1.32 | 1.35 |
| 23 | BA | 1363 | C | C2-O2 | -5.04 | 1.20 | 1.24 |
| 23 | DA | 194 | G | N9-C4 | -5.04 | 1.33 | 1.38 |
| 23 | BA | 1211 | U | P-O5' | -5.04 | 1.54 | 1.59 |
| 23 | BA | 763 | G | P-O5' | -5.03 | 1.54 | 1.59 |
| 23 | BA | 2575 | C | N3-C4 | -5.03 | 1.30 | 1.33 |
| 1 | CA | 986 | A | N3-C4 | 5.03 | 1.37 | 1.34 |
| 23 | BA | 1611 | C | N1-C6 | -5.03 | 1.34 | 1.37 |
| 14 | CN | 43 | CYS | CB-SG | -5.03 | 1.73 | 1.81 |
| 23 | DA | 585 | G | N9-C4 | -5.03 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 23 | DA | 745 | G | N7-C5 | -5.03 | 1.36 | 1.39 |
| 23 | BA | 841 | A | N3-C4 | -5.03 | 1.31 | 1.34 |
| 23 | BA | 940 | G | N3-C4 | -5.03 | 1.31 | 1.35 |
| 23 | BA | 659 | C | N1-C6 | -5.03 | 1.34 | 1.37 |
| 23 | BA | 2036 | C | N1-C2 | -5.03 | 1.35 | 1.40 |
| 23 | BA | 1970 | A | N9-C8 | -5.02 | 1.33 | 1.37 |
| 23 | DA | 1332 | G | N7-C5 | -5.02 | 1.36 | 1.39 |
| 23 | BA | 282 | A | N7-C5 | -5.02 | 1.36 | 1.39 |
| 23 | BA | 1127 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 23 | BA | 1596 | A | N9-C4 | -5.02 | 1.34 | 1.37 |
| 23 | BA | 71 | A | C6-N6 | -5.02 | 1.29 | 1.33 |
| 23 | BA | 562 | U | C2-O2 | -5.01 | 1.17 | 1.22 |
| 1 | CA | 1266 | G | N9-C4 | 5.01 | 1.42 | 1.38 |
| 23 | BA | 1251 | C | N1-C6 | -5.01 | 1.34 | 1.37 |
| 23 | BA | 2778 | A | N9-C4 | -5.01 | 1.34 | 1.37 |
| 1 | AA | 88 | A | N3-C4 | 5.01 | 1.37 | 1.34 |
| 23 | DA | 1107 | G | C2-N3 | 5.01 | 1.36 | 1.32 |
| 23 | DA | 1829 | A | N9-C4 | -5.01 | 1.34 | 1.37 |
| 23 | BA | 807 | U | N1-C6 | -5.01 | 1.33 | 1.38 |
| 1 | AA | 1272 | G | C6-N1 | 5.00 | 1.43 | 1.39 |
| 23 | BA | 693 | C | N1-C6 | -5.00 | 1.34 | 1.37 |
| 23 | BA | 2588 | G | N1-C2 | -5.00 | 1.33 | 1.37 |

All (5724) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 1 | CA | 1442(A) | G | N3-C4-C5 | -26.14 | 115.53 | 128.60 |
| 23 | DA | 2296 | U | N3-C4-O4 | -25.95 | 101.23 | 119.40 |
| 1 | AA | 1442(A) | G | N3-C4-C5 | -25.64 | 115.78 | 128.60 |
| 1 | CA | 1442(A) | G | N3-C4-N9 | 25.18 | 141.10 | 126.00 |
| 1 | AA | 1442(A) | G | N3-C4-N9 | 25.11 | 141.07 | 126.00 |
| 23 | BA | 2296 | U | N3-C4-O4 | -24.18 | 102.47 | 119.40 |
| 1 | AA | 1442(A) | G | N3-C2-N2 | 23.89 | 136.62 | 119.90 |
| 1 | CA | 1442(A) | G | N3-C2-N2 | 23.08 | 136.06 | 119.90 |
| 23 | BA | 2296 | U | C2-N3-C4 | -20.65 | 114.61 | 127.00 |
| 23 | BA | 2296 | U | C5-C6-N1 | -20.40 | 112.50 | 122.70 |
| 23 | DA | 2296 | U | C2-N3-C4 | -19.90 | 115.06 | 127.00 |
| 23 | DA | 2296 | U | C5-C6-N1 | -19.31 | 113.05 | 122.70 |
| 1 | AA | 1442(A) | G | C4-N9-C1' | 19.05 | 151.27 | 126.50 |
| 23 | DA | 2296 | U | C2-N1-C1' | -18.94 | 94.97 | 117.70 |
| 1 | CA | 1442(A) | G | C4-N9-C1' | 18.90 | 151.07 | 126.50 |
| 23 | BA | 2296 | U | C2-N1-C1' | -18.50 | 95.50 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 23 | DA | 2296 | U | C5-C4-O4 | 18.26 | 136.86 | 125.90 |
| 23 | BA | 676 | A | C2-N3-C4 | -18.16 | 101.52 | 110.60 |
| 23 | BA | 2296 | U | C5-C4-O4 | 18.02 | 136.71 | 125.90 |
| 1 | AA | 1442(A) | G | N1-C2-N2 | -17.33 | 100.61 | 116.20 |
| 23 | BA | 945 | A | C5-N7-C8 | -17.19 | 95.31 | 103.90 |
| 1 | CA | 1149 | C | N1-C2-O2 | 16.98 | 129.09 | 118.90 |
| 1 | CA | 1442(A) | G | C2-N3-C4 | 16.91 | 120.35 | 111.90 |
| 1 | AA | 1442(A) | G | C2-N3-C4 | 16.72 | 120.26 | 111.90 |
| 1 | CA | 1442(A) | G | N1-C2-N2 | -16.62 | 101.24 | 116.20 |
| 23 | BA | 330 | A | C2-N3-C4 | -16.40 | 102.40 | 110.60 |
| 1 | AA | 1442(A) | G | C8-N9-C1' | -16.11 | 106.06 | 127.00 |
| 23 | BA | 2322 | A | N9-C4-C5 | 15.93 | 112.17 | 105.80 |
| 1 | CA | 1442(A) | G | C8-N9-C1' | -15.76 | 106.52 | 127.00 |
| 23 | DA | 945 | A | C2-N3-C4 | -14.96 | 103.12 | 110.60 |
| 23 | BA | 528 | A | C2-N3-C4 | -14.74 | 103.23 | 110.60 |
| 23 | BA | 587 | C | C6-N1-C2 | -14.72 | 114.41 | 120.30 |
| 23 | BA | 1142(A) | A | C2-N3-C4 | -14.71 | 103.25 | 110.60 |
| 1 | AA | 1442(A) | G | N1-C6-O6 | -14.57 | 111.16 | 119.90 |
| 23 | DA | 1142(A) | A | C2-N3-C4 | -14.54 | 103.33 | 110.60 |
| 1 | AA | 1051 | C | N1-C2-O2 | 14.20 | 127.42 | 118.90 |
| 23 | DA | 676 | A | C5-N7-C8 | -14.08 | 96.86 | 103.90 |
| 1 | CA | 1442(A) | G | N1-C6-O6 | -13.95 | 111.53 | 119.90 |
| 1 | CA | 1442(A) | G | C5-C6-N1 | 13.88 | 118.44 | 111.50 |
| 23 | BA | 2296 | U | N1-C2-N3 | 13.85 | 123.21 | 114.90 |
| 23 | DA | 528 | A | N3-C4-N9 | -13.69 | 116.45 | 127.40 |
| 24 | DB | 115 | G | C8-N9-C4 | 13.59 | 111.84 | 106.40 |
| 1 | AA | 1442(A) | G | C5-C6-N1 | 13.40 | 118.20 | 111.50 |
| 23 | DA | 528 | A | C2-N3-C4 | -13.39 | 103.91 | 110.60 |
| 23 | BA | 1049 | C | C6-N1-C2 | -13.36 | 114.95 | 120.30 |
| 23 | DA | 2296 | U | C6-N1-C1' | 13.36 | 139.90 | 121.20 |
| 23 | DA | 945 | A | C5-N7-C8 | -13.20 | 97.30 | 103.90 |
| 23 | BA | 528 | A | N3-C4-N9 | -13.17 | 116.86 | 127.40 |
| 23 | BA | 2322 | A | C6-N1-C2 | -13.05 | 110.77 | 118.60 |
| 1 | AA | 1377 | A | C8-N9-C4 | -13.04 | 100.58 | 105.80 |
| 23 | BA | 945 | A | N7-C8-N9 | 13.03 | 120.31 | 113.80 |
| 23 | DA | 2296 | U | N1-C2-N3 | 12.91 | 122.65 | 114.90 |
| 23 | BA | 71 | A | C2-N3-C4 | -12.91 | 104.15 | 110.60 |
| 23 | DA | 330 | A | C2-N3-C4 | -12.81 | 104.19 | 110.60 |
| 23 | DA | 2335 | A | C5-C6-N1 | 12.79 | 124.10 | 117.70 |
| 23 | BA | 141 | A | C5-N7-C8 | -12.77 | 97.52 | 103.90 |
| 23 | BA | 2296 | U | C6-N1-C1' | 12.76 | 139.06 | 121.20 |
| 23 | BA | 2286 | A | N1-C6-N6 | 12.72 | 126.23 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 23 | BA | 856 | C | C6-N1-C2 | -12.70 | 115.22 | 120.30 |
| 23 | DA | 571 | A | C8-N9-C4 | 12.68 | 110.87 | 105.80 |
| 23 | BA | 528 | A | N3-C4-C5 | 12.66 | 135.66 | 126.80 |
| 23 | BA | 676 | A | N3-C4-C5 | 12.62 | 135.64 | 126.80 |
| 23 | DA | 71 | A | C5-N7-C8 | -12.58 | 97.61 | 103.90 |
| 1 | AA | 1025 | U | C5-C4-O4 | -12.52 | 118.39 | 125.90 |
| 23 | BA | 676 | A | C5-N7-C8 | -12.39 | 97.70 | 103.90 |
| 23 | DA | 1565 | C | C6-N1-C2 | 12.38 | 125.25 | 120.30 |
| 1 | CA | 1340 | A | C8-N9-C4 | -12.24 | 100.90 | 105.80 |
| 23 | BA | 975 | C | C6-N1-C2 | -12.23 | 115.41 | 120.30 |
| 23 | BA | 2296 | U | N3-C2-O2 | -12.18 | 113.67 | 122.20 |
| 23 | DA | 2296 | U | N3-C4-C5 | 12.14 | 121.88 | 114.60 |
| 23 | BA | 945 | A | C2-N3-C4 | -12.12 | 104.54 | 110.60 |
| 1 | CA | 1006 | C | C6-N1-C2 | -12.10 | 115.46 | 120.30 |
| 23 | BA | 1049 | C | C5-C6-N1 | 12.09 | 127.04 | 121.00 |
| 23 | BA | 1021 | A | C2-N3-C4 | -12.08 | 104.56 | 110.60 |
| 1 | CA | 1003 | G | C5-C6-O6 | 12.08 | 135.85 | 128.60 |
| 23 | DA | 1359 | A | N1-C6-N6 | -12.01 | 111.39 | 118.60 |
| 1 | AA | 1207 | G | C8-N9-C4 | 11.97 | 111.19 | 106.40 |
| 23 | BA | 676 | A | C5-C6-N1 | -11.91 | 111.74 | 117.70 |
| 23 | DA | 2028 | U | C6-N1-C2 | 11.88 | 128.13 | 121.00 |
| 23 | DA | 676 | A | C4-C5-N7 | 11.84 | 116.62 | 110.70 |
| 23 | DA | 2447 | G | N1-C6-O6 | 11.84 | 127.00 | 119.90 |
| 23 | BA | 2322 | A | C8-N9-C4 | -11.83 | 101.07 | 105.80 |
| 1 | CA | 1352 | C | C6-N1-C2 | -11.78 | 115.59 | 120.30 |
| 23 | DA | 2371 | G | N1-C6-O6 | 11.75 | 126.95 | 119.90 |
| 23 | DA | 928 | G | N1-C6-O6 | 11.66 | 126.89 | 119.90 |
| 23 | DA | 2572 | A | C8-N9-C4 | 11.60 | 110.44 | 105.80 |
| 1 | CA | 979 | C | C6-N1-C2 | -11.59 | 115.66 | 120.30 |
| 23 | DA | 945 | A | N7-C8-N9 | 11.58 | 119.59 | 113.80 |
| 23 | BA | 945 | A | C4-C5-N7 | 11.57 | 116.48 | 110.70 |
| 1 | AA | 1237 | C | C6-N1-C2 | -11.55 | 115.68 | 120.30 |
| 1 | CA | 1149 | C | N3-C4-N4 | -11.53 | 109.93 | 118.00 |
| 23 | DA | 676 | A | C2-N3-C4 | -11.52 | 104.84 | 110.60 |
| 23 | BA | 2286 | A | C6-C5-N7 | -11.49 | 124.25 | 132.30 |
| 23 | DA | 2322 | A | N9-C4-C5 | 11.48 | 110.39 | 105.80 |
| 23 | DA | 1437 | C | C6-N1-C2 | -11.44 | 115.72 | 120.30 |
| 1 | CA | 1379 | G | C6-C5-N7 | -11.38 | 123.57 | 130.40 |
| 23 | BA | 1762 | A | C8-N9-C4 | -11.37 | 101.25 | 105.80 |
| 23 | DA | 1021 | A | C2-N3-C4 | -11.32 | 104.94 | 110.60 |
| 23 | BA | 2335 | A | C5-C6-N1 | 11.28 | 123.34 | 117.70 |
| 23 | DA | 1204 | A | C5-N7-C8 | -11.25 | 98.27 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 23 | BA | 141 | A | N7-C8-N9 | 11.23 | 119.42 | 113.80 |
| 23 | DA | 528 | A | N3-C4-C5 | 11.19 | 134.63 | 126.80 |
| 23 | BA | 265 | A | C5-N7-C8 | -11.15 | 98.33 | 103.90 |
| 1 | AA | 359 | U | N1-C2-O2 | -11.06 | 115.06 | 122.80 |
| 23 | BA | 857 | C | C6-N1-C2 | -11.02 | 115.89 | 120.30 |
| 23 | DA | 2791 | C | C6-N1-C2 | -10.97 | 115.91 | 120.30 |
| 1 | CA | 1003 | G | C8-N9-C4 | -10.94 | 102.02 | 106.40 |
| 23 | BA | 1698 | A | C2-N3-C4 | -10.94 | 105.13 | 110.60 |
| 23 | BA | 1359 | A | N1-C6-N6 | -10.90 | 112.06 | 118.60 |
| 23 | DA | 676 | A | N7-C8-N9 | 10.90 | 119.25 | 113.80 |
| 1 | CA | 1149 | C | C5-C4-N4 | 10.89 | 127.82 | 120.20 |
| 23 | BA | 928 | G | N1-C6-O6 | 10.88 | 126.43 | 119.90 |
| 23 | BA | 933 | A | C5-N7-C8 | -10.83 | 98.48 | 103.90 |
| 1 | AA | 1335 | C | N1-C2-O2 | 10.83 | 125.40 | 118.90 |
| 1 | CA | 1379 | G | N9-C4-C5 | -10.79 | 101.08 | 105.40 |
| 23 | BA | 71 | A | C5-N7-C8 | -10.79 | 98.51 | 103.90 |
| 23 | DA | 2322 | A | C6-N1-C2 | -10.75 | 112.15 | 118.60 |
| 1 | AA | 1207 | G | N1-C6-O6 | 10.75 | 126.35 | 119.90 |
| 1 | AA | 1377 | A | N7-C8-N9 | 10.74 | 119.17 | 113.80 |
| 1 | CA | 1149 | C | N3-C2-O2 | -10.72 | 114.39 | 121.90 |
| 23 | DA | 2028 | U | N3-C4-C5 | 10.69 | 121.02 | 114.60 |
| 23 | DA | 2363 | C | C6-N1-C2 | 10.68 | 124.57 | 120.30 |
| 23 | DA | 1107 | G | N3-C4-N9 | 10.66 | 132.40 | 126.00 |
| 23 | BA | 141 | A | N1-C6-N6 | 10.66 | 125.00 | 118.60 |
| 23 | DA | 728 | G | C8-N9-C4 | 10.66 | 110.66 | 106.40 |
| 1 | CA | 1266 | G | C8-N9-C4 | -10.65 | 102.14 | 106.40 |
| 1 | CA | 1037 | C | C2-N3-C4 | 10.62 | 125.21 | 119.90 |
| 1 | AA | 358 | U | C2-N3-C4 | 10.61 | 133.37 | 127.00 |
| 1 | AA | 1003 | G | C5-C6-O6 | 10.59 | 134.96 | 128.60 |
| 1 | AA | 1502 | A | N1-C6-N6 | 10.59 | 124.95 | 118.60 |
| 1 | AA | 1277 | C | C2-N3-C4 | 10.55 | 125.17 | 119.90 |
| 1 | AA | 357 | G | N3-C2-N2 | -10.49 | 112.56 | 119.90 |
| 23 | BA | 2723 | C | N3-C4-C5 | 10.46 | 126.08 | 121.90 |
| 1 | CA | 1171 | G | C5-C6-O6 | 10.42 | 134.85 | 128.60 |
| 23 | BA | 1204 | A | C2-N3-C4 | -10.41 | 105.40 | 110.60 |
| 23 | BA | 2322 | A | C4-C5-N7 | -10.37 | 105.52 | 110.70 |
| 23 | DA | 2646 | C | C6-N1-C2 | 10.35 | 124.44 | 120.30 |
| 24 | DB | 104 | U | C5-C6-N1 | -10.32 | 117.54 | 122.70 |
| 1 | CA | 1163 | C | C6-N1-C2 | -10.31 | 116.17 | 120.30 |
| 1 | CA | 1379 | G | C4-C5-N7 | 10.31 | 114.93 | 110.80 |
| 23 | DA | 2296 | U | N3-C2-O2 | -10.31 | 114.98 | 122.20 |
| 1 | CA | 1379 | G | N3-C4-N9 | 10.31 | 132.19 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 23 | BA | 2296 | U | N3-C4-C5 | 10.29 | 120.78 | 114.60 |
| 23 | BA | 2322 | A | N1-C6-N6 | -10.28 | 112.43 | 118.60 |
| 1 | AA | 1207 | G | N9-C4-C5 | -10.27 | 101.29 | 105.40 |
| 23 | DA | 71 | A | C2-N3-C4 | -10.27 | 105.47 | 110.60 |
| 24 | BB | 30 | C | C6-N1-C2 | -10.24 | 116.20 | 120.30 |
| 23 | BA | 330 | A | N1-C2-N3 | 10.24 | 134.42 | 129.30 |
| 23 | BA | 2371 | G | N1-C6-O6 | 10.23 | 126.04 | 119.90 |
| 23 | DA | 297 | C | C6-N1-C2 | -10.22 | 116.21 | 120.30 |
| 23 | BA | 1108 | U | N3-C2-O2 | -10.22 | 115.05 | 122.20 |
| 1 | AA | 910 | C | C6-N1-C2 | 10.20 | 124.38 | 120.30 |
| 23 | DA | 1762 | A | C8-N9-C4 | -10.20 | 101.72 | 105.80 |
| 1 | AA | 1277 | C | N1-C2-O2 | 10.20 | 125.02 | 118.90 |
| 23 | DA | 154(A) | C | N1-C2-O2 | 10.19 | 125.01 | 118.90 |
| 23 | DA | 2277 | G | N1-C6-O6 | -10.15 | 113.81 | 119.90 |
| 23 | DA | 2036 | C | N1-C2-O2 | -10.15 | 112.81 | 118.90 |
| 1 | CA | 1442(A) | G | C8-N9-C4 | -10.13 | 102.35 | 106.40 |
| 23 | BA | 915 | C | C6-N1-C2 | -10.12 | 116.25 | 120.30 |
| 1 | AA | 1126 | U | N1-C2-O2 | 10.10 | 129.87 | 122.80 |
| 23 | DA | 1142(A) | A | C5-C6-N1 | -10.10 | 112.65 | 117.70 |
| 23 | DA | 2375 | G | C8-N9-C4 | 10.07 | 110.43 | 106.40 |
| 23 | BA | 90 | U | C5-C6-N1 | 10.07 | 127.73 | 122.70 |
| 23 | DA | 2619 | C | C6-N1-C2 | 10.05 | 124.32 | 120.30 |
| 23 | DA | 205 | G | N9-C4-C5 | -10.04 | 101.38 | 105.40 |
| 23 | BA | 2319 | G | C8-N9-C4 | -10.02 | 102.39 | 106.40 |
| 23 | DA | 2286 | A | C6-C5-N7 | -10.00 | 125.30 | 132.30 |
| 23 | DA | 1123 | C | C6-N1-C2 | 9.97 | 124.29 | 120.30 |
| 1 | CA | 1063 | C | C6-N1-C2 | -9.95 | 116.32 | 120.30 |
| 23 | DA | 1254 | A | N1-C2-N3 | 9.94 | 134.27 | 129.30 |
| 23 | DA | 587 | C | C6-N1-C2 | -9.94 | 116.32 | 120.30 |
| 23 | DA | 2689 | U | N3-C4-O4 | -9.94 | 112.44 | 119.40 |
| 1 | CA | 1033 | G | N3-C4-N9 | 9.94 | 131.96 | 126.00 |
| 1 | AA | 322 | C | C6-N1-C2 | 9.93 | 124.27 | 120.30 |
| 1 | CA | 458 | C | C6-N1-C2 | -9.93 | 116.33 | 120.30 |
| 23 | BA | 1243 | G | N1-C6-O6 | 9.92 | 125.85 | 119.90 |
| 23 | DA | 2286 | A | N1-C6-N6 | 9.92 | 124.55 | 118.60 |
| 23 | BA | 1227 | G | N1-C6-O6 | 9.91 | 125.85 | 119.90 |
| 23 | BA | 2040 | C | C6-N1-C2 | 9.90 | 124.26 | 120.30 |
| 1 | AA | 53 | A | C6-N1-C2 | 9.90 | 124.54 | 118.60 |
| 23 | BA | 884 | C | C5-C6-N1 | 9.89 | 125.94 | 121.00 |
| 23 | DA | 1777 | U | C5-C6-N1 | -9.87 | 117.77 | 122.70 |
| 23 | DA | 678 | C | C6-N1-C2 | 9.85 | 124.24 | 120.30 |
| 23 | DA | 1107 | G | C4-N9-C1' | 9.84 | 139.29 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 141 | A | C4-C5-N7 | 9.83 | 115.62 | 110.70 |
| 23 | BA | 1107 | G | C4-N9-C1' | 9.82 | 139.26 | 126.50 |
| 23 | DA | 676 | A | C8-N9-C4 | -9.81 | 101.88 | 105.80 |
| 23 | DA | 2619 | C | C5-C6-N1 | -9.80 | 116.10 | 121.00 |
| 23 | BA | 1210 | A | C6-C5-N7 | -9.80 | 125.44 | 132.30 |
| 23 | BA | 676 | A | N3-C4-N9 | -9.79 | 119.56 | 127.40 |
| 23 | DA | 978 | G | C8-N9-C4 | 9.79 | 110.31 | 106.40 |
| 23 | BA | 265 | A | N7-C8-N9 | 9.79 | 118.69 | 113.80 |
| 23 | BA | 2287 | A | C2-N3-C4 | -9.78 | 105.71 | 110.60 |
| 23 | BA | 2719 | G | C8-N9-C4 | 9.76 | 110.31 | 106.40 |
| 1 | CA | 1266 | G | N7-C8-N9 | 9.76 | 117.98 | 113.10 |
| 23 | BA | 1107 | G | C8-N9-C1' | -9.73 | 114.35 | 127.00 |
| 23 | DA | 1107 | G | C8-N9-C1' | -9.72 | 114.37 | 127.00 |
| 23 | DA | 1022 | G | N9-C4-C5 | 9.71 | 109.28 | 105.40 |
| 23 | DA | 201 | C | N3-C4-C5 | 9.70 | 125.78 | 121.90 |
| 23 | DA | 1049 | C | C5-C6-N1 | 9.68 | 125.84 | 121.00 |
| 23 | DA | 2626 | C | C6-N1-C2 | 9.66 | 124.17 | 120.30 |
| 1 | CA | 1054 | C | C6-N1-C2 | -9.66 | 116.44 | 120.30 |
| 23 | DA | 856 | C | C6-N1-C2 | -9.63 | 116.45 | 120.30 |
| 1 | CA | 1006 | C | C5-C6-N1 | 9.62 | 125.81 | 121.00 |
| 1 | CA | 1124 | G | N3-C2-N2 | 9.62 | 126.63 | 119.90 |
| 23 | DA | 1565 | C | N3-C4-C5 | 9.60 | 125.74 | 121.90 |
| 1 | AA | 1074 | G | N1-C6-O6 | 9.60 | 125.66 | 119.90 |
| 23 | DA | 1800 | C | C6-N1-C2 | 9.60 | 124.14 | 120.30 |
| 1 | AA | 1279 | A | N7-C8-N9 | 9.58 | 118.59 | 113.80 |
| 23 | BA | 209 | C | C5-C6-N1 | -9.57 | 116.22 | 121.00 |
| 23 | DA | 62 | C | C5-C6-N1 | -9.56 | 116.22 | 121.00 |
| 23 | DA | 915 | C | C6-N1-C2 | -9.55 | 116.48 | 120.30 |
| 23 | DA | 2624 | G | N1-C6-O6 | 9.55 | 125.63 | 119.90 |
| 1 | AA | 1169 | A | C8-N9-C4 | -9.54 | 101.98 | 105.80 |
| 23 | BA | 570 | G | C8-N9-C4 | 9.54 | 110.22 | 106.40 |
| 1 | CA | 1335 | C | N1-C2-O2 | 9.54 | 124.62 | 118.90 |
| 23 | BA | 409 | C | C6-N1-C2 | 9.54 | 124.11 | 120.30 |
| 1 | CA | 1124 | G | C5-C6-O6 | 9.53 | 134.32 | 128.60 |
| 23 | DA | 2107 | C | C2-N3-C4 | 9.52 | 124.66 | 119.90 |
| 23 | DA | 2593 | U | N3-C4-O4 | -9.52 | 112.74 | 119.40 |
| 1 | AA | 1051 | C | N3-C4-C5 | 9.50 | 125.70 | 121.90 |
| 23 | DA | 560 | C | C6-N1-C2 | 9.48 | 124.09 | 120.30 |
| 23 | BA | 154(A) | C | N1-C2-O2 | 9.47 | 124.58 | 118.90 |
| 23 | BA | 754 | C | C5-C4-N4 | -9.46 | 113.58 | 120.20 |
| 1 | AA | 1025 | U | N3-C4-O4 | 9.46 | 126.02 | 119.40 |
| 23 | BA | 1248 | G | C5-C6-O6 | -9.46 | 122.92 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|----------|-------|-------------|----------|
| 23 | BA | 1626 | G | C5-C6-O6 | 9.46 | 134.27 | 128.60 |
| 24 | BB | 104 | U | C5-C6-N1 | -9.45 | 117.97 | 122.70 |
| 1 | CA | 1379 | G | C5-C6-O6 | -9.45 | 122.93 | 128.60 |
| 23 | BA | 2107 | C | C2-N3-C4 | 9.44 | 124.62 | 119.90 |
| 23 | BA | 2581 | G | C5-C6-O6 | 9.44 | 134.26 | 128.60 |
| 23 | DA | 735 | A | C8-N9-C4 | 9.43 | 109.57 | 105.80 |
| 23 | DA | 122 | G | C5-C6-O6 | -9.43 | 122.94 | 128.60 |
| 1 | AA | 1442(A) | G | C8-N9-C4 | -9.42 | 102.63 | 106.40 |
| 23 | BA | 265 | A | C6-C5-N7 | -9.41 | 125.71 | 132.30 |
| 23 | BA | 2017 | U | N1-C2-N3 | 9.41 | 120.55 | 114.90 |
| 23 | BA | 47 | C | C6-N1-C2 | 9.40 | 124.06 | 120.30 |
| 1 | CA | 972 | C | C6-N1-C2 | -9.39 | 116.54 | 120.30 |
| 23 | DA | 2591 | C | N1-C2-O2 | -9.39 | 113.27 | 118.90 |
| 1 | CA | 1044 | A | C5-C6-N6 | 9.39 | 131.21 | 123.70 |
| 23 | BA | 2251 | G | C8-N9-C4 | -9.38 | 102.65 | 106.40 |
| 23 | DA | 123 | G | C8-N9-C4 | 9.38 | 110.15 | 106.40 |
| 1 | AA | 1292 | U | C5-C6-N1 | 9.36 | 127.38 | 122.70 |
| 1 | CA | 1335 | C | N3-C2-O2 | -9.36 | 115.35 | 121.90 |
| 23 | DA | 2322 | A | N1-C6-N6 | -9.36 | 112.98 | 118.60 |
| 23 | BA | 463 | G | C5-C6-O6 | 9.34 | 134.21 | 128.60 |
| 1 | CA | 1044 | A | N1-C6-N6 | -9.34 | 112.99 | 118.60 |
| 23 | BA | 835 | A | C2-N3-C4 | 9.34 | 115.27 | 110.60 |
| 23 | BA | 202 | U | N3-C4-O4 | -9.33 | 112.87 | 119.40 |
| 23 | BA | 194 | G | N3-C2-N2 | -9.33 | 113.37 | 119.90 |
| 23 | BA | 265 | A | N1-C6-N6 | 9.30 | 124.18 | 118.60 |
| 23 | DA | 645 | C | N1-C2-O2 | 9.30 | 124.48 | 118.90 |
| 23 | DA | 2447 | G | C5-C6-O6 | -9.30 | 123.02 | 128.60 |
| 23 | BA | 265 | A | C4-C5-N7 | 9.30 | 115.35 | 110.70 |
| 1 | AA | 896 | C | C6-N1-C2 | 9.29 | 124.02 | 120.30 |
| 23 | DA | 2286 | A | C2-N3-C4 | -9.29 | 105.95 | 110.60 |
| 23 | DA | 179 | G | N1-C6-O6 | 9.29 | 125.47 | 119.90 |
| 1 | CA | 1502 | A | C5-N7-C8 | -9.29 | 99.26 | 103.90 |
| 23 | BA | 2375 | G | C8-N9-C4 | 9.29 | 110.11 | 106.40 |
| 23 | DA | 1108 | U | N3-C2-O2 | -9.29 | 115.70 | 122.20 |
| 23 | DA | 1616 | A | N1-C6-N6 | 9.28 | 124.17 | 118.60 |
| 23 | DA | 62 | C | C6-N1-C2 | 9.27 | 124.01 | 120.30 |
| 23 | BA | 1142(A) | A | N3-C4-C5 | 9.27 | 133.29 | 126.80 |
| 23 | DA | 928 | G | C6-C5-N7 | -9.27 | 124.84 | 130.40 |
| 1 | AA | 1381 | U | N1-C2-O2 | 9.27 | 129.28 | 122.80 |
| 23 | BA | 1437 | C | C6-N1-C2 | -9.26 | 116.59 | 120.30 |
| 23 | BA | 1612 | C | C6-N1-C2 | 9.26 | 124.01 | 120.30 |
| 23 | BA | 391 | G | N1-C6-O6 | 9.24 | 125.45 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 1565 | C | C5-C6-N1 | -9.23 | 116.38 | 121.00 |
| 23 | DA | 2828 | C | C6-N1-C2 | 9.23 | 123.99 | 120.30 |
| 23 | DA | 2322 | A | C8-N9-C4 | -9.22 | 102.11 | 105.80 |
| 1 | CA | 1116 | C | C2-N3-C4 | 9.21 | 124.51 | 119.90 |
| 23 | BA | 508 | G | N1-C6-O6 | 9.20 | 125.42 | 119.90 |
| 23 | BA | 2015 | A | C8-N9-C4 | -9.19 | 102.12 | 105.80 |
| 23 | BA | 933 | A | C4-C5-N7 | 9.19 | 115.30 | 110.70 |
| 23 | BA | 465 | G | C8-N9-C4 | -9.19 | 102.72 | 106.40 |
| 23 | DA | 1107 | G | N3-C4-C5 | -9.18 | 124.01 | 128.60 |
| 23 | BA | 2572 | A | C8-N9-C4 | 9.16 | 109.47 | 105.80 |
| 23 | BA | 1142(A) | A | N1-C6-N6 | 9.15 | 124.09 | 118.60 |
| 1 | CA | 1033 | G | C4-C5-N7 | 9.15 | 114.46 | 110.80 |
| 23 | BA | 945 | A | C8-N9-C4 | -9.13 | 102.15 | 105.80 |
| 23 | DA | 2676 | C | C2-N3-C4 | -9.13 | 115.33 | 119.90 |
| 23 | DA | 2570 | G | N1-C6-O6 | 9.13 | 125.38 | 119.90 |
| 23 | BA | 1490 | A | C8-N9-C4 | 9.13 | 109.45 | 105.80 |
| 23 | DA | 2329 | G | C8-N9-C4 | 9.12 | 110.05 | 106.40 |
| 23 | DA | 2277 | G | C5-C6-O6 | 9.11 | 134.07 | 128.60 |
| 1 | AA | 934 | C | C6-N1-C2 | -9.11 | 116.66 | 120.30 |
| 1 | AA | 1158 | C | C2-N1-C1' | 9.11 | 128.82 | 118.80 |
| 23 | DA | 1490 | A | C8-N9-C4 | 9.11 | 109.44 | 105.80 |
| 23 | BA | 928 | G | C6-C5-N7 | -9.10 | 124.94 | 130.40 |
| 23 | BA | 1210 | A | C5-N7-C8 | -9.08 | 99.36 | 103.90 |
| 23 | BA | 1142(A) | A | C5-N7-C8 | -9.06 | 99.37 | 103.90 |
| 1 | CA | 818 | G | C4-C5-N7 | -9.06 | 107.18 | 110.80 |
| 23 | DA | 141 | A | N7-C8-N9 | 9.06 | 118.33 | 113.80 |
| 23 | BA | 2036 | C | C6-N1-C2 | -9.05 | 116.68 | 120.30 |
| 23 | BA | 570 | G | N9-C4-C5 | -9.05 | 101.78 | 105.40 |
| 1 | AA | 357 | G | N1-C2-N2 | 9.05 | 124.34 | 116.20 |
| 23 | BA | 2502 | G | C5-C6-N1 | 9.04 | 116.02 | 111.50 |
| 1 | CA | 1293 | G | C5-C6-N1 | 9.04 | 116.02 | 111.50 |
| 23 | BA | 1618 | A | N1-C6-N6 | -9.04 | 113.18 | 118.60 |
| 1 | AA | 998 | G | N3-C4-N9 | -9.03 | 120.58 | 126.00 |
| 23 | DA | 2755 | C | C5-C6-N1 | 9.03 | 125.51 | 121.00 |
| 23 | BA | 94 | C | C6-N1-C2 | -9.03 | 116.69 | 120.30 |
| 23 | BA | 759 | G | N1-C6-O6 | 9.02 | 125.31 | 119.90 |
| 23 | BA | 1391 | U | N1-C2-O2 | 9.02 | 129.11 | 122.80 |
| 23 | BA | 2581 | G | N1-C6-O6 | -9.01 | 114.49 | 119.90 |
| 23 | DA | 71 | A | N7-C8-N9 | 9.01 | 118.31 | 113.80 |
| 1 | AA | 1149 | C | N1-C2-O2 | 9.01 | 124.31 | 118.90 |
| 1 | AA | 1442(A) | G | N7-C8-N9 | 9.01 | 117.60 | 113.10 |
| 23 | DA | 1049 | C | C6-N1-C2 | -9.00 | 116.70 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|----------|-------|-------------|----------|
| 23 | BA | 2322 | A | N1-C2-N3 | 9.00 | 133.80 | 129.30 |
| 23 | BA | 1210 | A | N7-C8-N9 | 8.99 | 118.30 | 113.80 |
| 23 | BA | 179 | G | N1-C6-O6 | 8.99 | 125.29 | 119.90 |
| 23 | BA | 2572 | A | N7-C8-N9 | -8.99 | 109.31 | 113.80 |
| 23 | BA | 2273 | A | C8-N9-C4 | -8.98 | 102.21 | 105.80 |
| 23 | BA | 982 | C | N3-C2-O2 | -8.97 | 115.62 | 121.90 |
| 23 | BA | 71 | A | N7-C8-N9 | 8.96 | 118.28 | 113.80 |
| 23 | BA | 391 | G | C4-C5-N7 | 8.96 | 114.39 | 110.80 |
| 23 | BA | 1142(A) | A | C5-C6-N1 | -8.96 | 113.22 | 117.70 |
| 23 | BA | 1210 | A | N1-C6-N6 | 8.97 | 123.98 | 118.60 |
| 23 | BA | 1243 | G | C2-N3-C4 | -8.96 | 107.42 | 111.90 |
| 1 | CA | 1030(B) | C | C6-N1-C2 | -8.96 | 116.72 | 120.30 |
| 23 | BA | 452 | G | C5-C6-O6 | 8.96 | 133.97 | 128.60 |
| 23 | DA | 988 | A | N1-C6-N6 | 8.96 | 123.97 | 118.60 |
| 23 | BA | 572 | A | C8-N9-C4 | -8.95 | 102.22 | 105.80 |
| 23 | DA | 764 | A | N1-C2-N3 | -8.95 | 124.82 | 129.30 |
| 1 | AA | 1153 | C | N1-C2-O2 | 8.95 | 124.27 | 118.90 |
| 23 | BA | 2729 | G | N1-C6-O6 | 8.95 | 125.27 | 119.90 |
| 23 | DA | 2723 | C | C5-C6-N1 | -8.94 | 116.53 | 121.00 |
| 23 | DA | 2393 | A | C8-N9-C4 | -8.94 | 102.22 | 105.80 |
| 1 | AA | 1169 | A | N7-C8-N9 | 8.93 | 118.27 | 113.80 |
| 23 | BA | 141 | A | C6-C5-N7 | -8.93 | 126.05 | 132.30 |
| 23 | DA | 141 | A | C5-N7-C8 | -8.92 | 99.44 | 103.90 |
| 23 | BA | 574 | C | C6-N1-C2 | -8.91 | 116.74 | 120.30 |
| 23 | BA | 1992 | G | C4-C5-N7 | -8.91 | 107.24 | 110.80 |
| 23 | DA | 945 | A | N1-C2-N3 | 8.90 | 133.75 | 129.30 |
| 23 | DA | 2615 | U | N3-C4-O4 | -8.90 | 113.17 | 119.40 |
| 1 | AA | 52 | G | C6-N1-C2 | 8.89 | 130.44 | 125.10 |
| 23 | BA | 945 | A | N3-C4-C5 | 8.89 | 133.03 | 126.80 |
| 23 | DA | 122 | G | N1-C6-O6 | 8.89 | 125.23 | 119.90 |
| 1 | CA | 1343 | G | C5-C6-O6 | -8.89 | 123.27 | 128.60 |
| 1 | CA | 634 | C | C6-N1-C2 | -8.88 | 116.75 | 120.30 |
| 1 | CA | 1456 | G | C2-N3-C4 | 8.87 | 116.33 | 111.90 |
| 23 | DA | 2624 | G | C5-C6-O6 | -8.87 | 123.28 | 128.60 |
| 23 | BA | 2250 | G | C8-N9-C4 | -8.86 | 102.86 | 106.40 |
| 23 | DA | 1230 | C | C6-N1-C2 | 8.86 | 123.84 | 120.30 |
| 1 | CA | 1003 | G | N1-C6-O6 | -8.86 | 114.58 | 119.90 |
| 23 | BA | 2371 | G | C5-C6-O6 | -8.85 | 123.29 | 128.60 |
| 23 | DA | 1490 | A | N9-C4-C5 | -8.85 | 102.26 | 105.80 |
| 23 | DA | 71 | A | C4-C5-N7 | 8.84 | 115.12 | 110.70 |
| 1 | AA | 1018 | C | C5-C6-N1 | 8.83 | 125.42 | 121.00 |
| 23 | DA | 571 | A | N9-C4-C5 | -8.83 | 102.27 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | CA | 435 | C | N1-C2-O2 | 8.83 | 124.20 | 118.90 |
| 23 | DA | 1248 | G | C8-N9-C4 | 8.83 | 109.93 | 106.40 |
| 23 | BA | 689 | A | C8-N9-C4 | 8.82 | 109.33 | 105.80 |
| 23 | BA | 676 | A | N7-C8-N9 | 8.82 | 118.21 | 113.80 |
| 23 | BA | 794 | G | N1-C6-O6 | -8.82 | 114.61 | 119.90 |
| 1 | CA | 1033 | G | N9-C4-C5 | -8.81 | 101.88 | 105.40 |
| 1 | AA | 1258 | G | N3-C2-N2 | 8.81 | 126.06 | 119.90 |
| 23 | BA | 1779 | U | C6-N1-C2 | 8.81 | 126.28 | 121.00 |
| 23 | BA | 2538 | C | C6-N1-C2 | 8.80 | 123.82 | 120.30 |
| 23 | BA | 2522 | U | N3-C4-O4 | 8.79 | 125.55 | 119.40 |
| 1 | AA | 839 | U | N1-C2-O2 | 8.79 | 128.95 | 122.80 |
| 23 | DA | 1328 | G | C8-N9-C4 | 8.77 | 109.91 | 106.40 |
| 23 | BA | 675 | A | N1-C6-N6 | 8.77 | 123.86 | 118.60 |
| 23 | BA | 759 | G | C5-C6-O6 | -8.76 | 123.34 | 128.60 |
| 23 | BA | 2791 | C | C6-N1-C2 | -8.76 | 116.80 | 120.30 |
| 23 | DA | 128 | C | C6-N1-C2 | 8.76 | 123.80 | 120.30 |
| 23 | BA | 777 | A | C5-N7-C8 | 8.75 | 108.28 | 103.90 |
| 23 | BA | 2041 | U | N3-C2-O2 | -8.75 | 116.08 | 122.20 |
| 23 | DA | 1325 | G | C6-C5-N7 | -8.74 | 125.15 | 130.40 |
| 23 | DA | 2449 | U | N3-C2-O2 | 8.74 | 128.32 | 122.20 |
| 23 | BA | 2646 | C | C6-N1-C2 | 8.74 | 123.80 | 120.30 |
| 23 | BA | 391 | G | N9-C4-C5 | -8.73 | 101.91 | 105.40 |
| 1 | CA | 910 | C | C6-N1-C2 | 8.73 | 123.79 | 120.30 |
| 23 | DA | 1142(A) | A | N3-C4-C5 | 8.73 | 132.91 | 126.80 |
| 24 | DB | 79 | C | C6-N1-C2 | -8.73 | 116.81 | 120.30 |
| 1 | AA | 1059 | C | N3-C2-O2 | -8.73 | 115.79 | 121.90 |
| 1 | AA | 1043 | C | N3-C4-C5 | -8.71 | 118.42 | 121.90 |
| 23 | BA | 1845 | G | N1-C6-O6 | -8.71 | 114.67 | 119.90 |
| 23 | BA | 389 | G | N9-C4-C5 | -8.71 | 101.92 | 105.40 |
| 1 | AA | 943 | U | C5-C6-N1 | 8.70 | 127.05 | 122.70 |
| 23 | DA | 528 | A | C5-C6-N1 | -8.70 | 113.35 | 117.70 |
| 1 | AA | 1333 | A | C8-N9-C4 | -8.70 | 102.32 | 105.80 |
| 23 | DA | 945 | A | C8-N9-C4 | -8.70 | 102.32 | 105.80 |
| 23 | DA | 760 | G | C5-C6-O6 | -8.70 | 123.38 | 128.60 |
| 23 | BA | 2440 | C | C4-C5-C6 | 8.69 | 121.75 | 117.40 |
| 23 | BA | 1022 | G | C4-C5-N7 | -8.69 | 107.32 | 110.80 |
| 23 | BA | 2286 | A | C4-C5-C6 | 8.69 | 121.34 | 117.00 |
| 23 | BA | 124 | G | C4-C5-N7 | 8.68 | 114.27 | 110.80 |
| 23 | BA | 1107 | G | N3-C4-N9 | 8.68 | 131.21 | 126.00 |
| 23 | BA | 698 | C | N1-C2-O2 | -8.67 | 113.70 | 118.90 |
| 23 | BA | 1779 | U | C6-N1-C1' | -8.67 | 109.06 | 121.20 |
| 23 | BA | 2607 | G | N1-C2-N2 | -8.67 | 108.40 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 23 | DA | 179 | G | C5-C6-N1 | -8.66 | 107.17 | 111.50 |
| 23 | DA | 945 | A | N3-C4-C5 | 8.66 | 132.86 | 126.80 |
| 23 | DA | 665 | C | C6-N1-C2 | 8.65 | 123.76 | 120.30 |
| 23 | DA | 676 | A | N3-C4-C5 | 8.65 | 132.86 | 126.80 |
| 1 | AA | 1279 | A | C8-N9-C4 | -8.64 | 102.34 | 105.80 |
| 1 | CA | 1077 | G | C8-N9-C4 | 8.64 | 109.86 | 106.40 |
| 1 | CA | 1379 | G | N1-C6-O6 | 8.64 | 125.09 | 119.90 |
| 23 | BA | 885 | C | N1-C2-O2 | 8.64 | 124.08 | 118.90 |
| 1 | AA | 112 | G | N1-C6-O6 | 8.64 | 125.08 | 119.90 |
| 1 | AA | 1003 | G | N1-C6-O6 | -8.63 | 114.72 | 119.90 |
| 1 | CA | 818 | G | C5-C6-O6 | 8.62 | 133.78 | 128.60 |
| 23 | BA | 528 | A | C5-C6-N1 | -8.62 | 113.39 | 117.70 |
| 23 | BA | 154(A) | C | N3-C4-N4 | -8.61 | 111.97 | 118.00 |
| 23 | DA | 1437 | C | C5-C6-N1 | 8.61 | 125.31 | 121.00 |
| 23 | BA | 735 | A | C8-N9-C4 | 8.61 | 109.24 | 105.80 |
| 23 | BA | 884 | C | C2-N3-C4 | 8.61 | 124.20 | 119.90 |
| 23 | DA | 915 | C | N3-C2-O2 | -8.60 | 115.88 | 121.90 |
| 23 | DA | 1698 | A | C5-N7-C8 | -8.59 | 99.60 | 103.90 |
| 23 | DA | 792 | G | C8-N9-C4 | 8.59 | 109.83 | 106.40 |
| 23 | DA | 1992 | G | C4-C5-N7 | -8.57 | 107.37 | 110.80 |
| 23 | BA | 1001 | A | C8-N9-C4 | 8.56 | 109.22 | 105.80 |
| 24 | DB | 89 | G | N1-C6-O6 | 8.56 | 125.04 | 119.90 |
| 23 | BA | 1698 | A | C6-C5-N7 | -8.56 | 126.31 | 132.30 |
| 23 | BA | 2429 | G | C8-N9-C4 | -8.56 | 102.98 | 106.40 |
| 23 | BA | 2440 | C | N3-C4-C5 | -8.56 | 118.48 | 121.90 |
| 1 | CA | 117 | G | N9-C4-C5 | -8.55 | 101.98 | 105.40 |
| 23 | BA | 386 | G | C8-N9-C4 | -8.54 | 102.98 | 106.40 |
| 23 | BA | 1021 | A | C5-N7-C8 | -8.54 | 99.63 | 103.90 |
| 23 | DA | 2371 | G | C5-C6-O6 | -8.54 | 123.48 | 128.60 |
| 23 | BA | 1222 | C | N3-C4-C5 | 8.54 | 125.31 | 121.90 |
| 1 | CA | 1243 | C | C6-N1-C2 | -8.53 | 116.89 | 120.30 |
| 23 | DA | 330 | A | C5-N7-C8 | -8.53 | 99.64 | 103.90 |
| 23 | DA | 2821 | A | C8-N9-C4 | 8.53 | 109.21 | 105.80 |
| 1 | CA | 1340 | A | N9-C4-C5 | 8.53 | 109.21 | 105.80 |
| 23 | DA | 1207 | C | C6-N1-C2 | 8.52 | 123.71 | 120.30 |
| 23 | BA | 205 | G | N9-C4-C5 | -8.51 | 102.00 | 105.40 |
| 23 | BA | 1565 | C | C6-N1-C2 | 8.51 | 123.70 | 120.30 |
| 23 | DA | 2087 | G | C8-N9-C4 | 8.51 | 109.80 | 106.40 |
| 23 | BA | 330 | A | N3-C4-C5 | 8.51 | 132.75 | 126.80 |
| 23 | DA | 2521 | C | C6-N1-C2 | 8.50 | 123.70 | 120.30 |
| 23 | DA | 1204 | A | C4-C5-N7 | 8.50 | 114.95 | 110.70 |
| 23 | BA | 1313 | U | C6-N1-C2 | -8.50 | 115.90 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 1977 | A | C8-N9-C4 | 8.49 | 109.20 | 105.80 |
| 23 | BA | 1645 | G | C8-N9-C4 | -8.48 | 103.01 | 106.40 |
| 1 | AA | 1371 | G | C5-C6-O6 | -8.48 | 123.51 | 128.60 |
| 23 | DA | 12 | U | N1-C2-O2 | 8.48 | 128.73 | 122.80 |
| 1 | AA | 1018 | C | C6-N1-C2 | -8.47 | 116.91 | 120.30 |
| 1 | AA | 1002 | G | C8-N9-C4 | -8.47 | 103.01 | 106.40 |
| 23 | BA | 510 | C | N3-C4-C5 | -8.46 | 118.51 | 121.90 |
| 1 | CA | 1108 | G | C4-C5-N7 | -8.46 | 107.41 | 110.80 |
| 23 | BA | 1604 | C | N1-C2-O2 | -8.46 | 113.82 | 118.90 |
| 24 | DB | 104 | U | C6-N1-C2 | 8.46 | 126.08 | 121.00 |
| 23 | BA | 1248 | G | N1-C6-O6 | 8.46 | 124.97 | 119.90 |
| 23 | BA | 2286 | A | C2-N3-C4 | -8.45 | 106.37 | 110.60 |
| 23 | BA | 1695 | G | C4-C5-N7 | 8.44 | 114.17 | 110.80 |
| 24 | DB | 115 | G | N7-C8-N9 | -8.43 | 108.89 | 113.10 |
| 1 | CA | 1442(A) | G | N7-C8-N9 | 8.43 | 117.31 | 113.10 |
| 23 | DA | 1022 | G | C4-C5-N7 | -8.42 | 107.43 | 110.80 |
| 23 | BA | 455 | C | N1-C2-O2 | 8.42 | 123.95 | 118.90 |
| 23 | BA | 2725 | A | C2-N3-C4 | -8.42 | 106.39 | 110.60 |
| 23 | BA | 676 | A | C4-C5-N7 | 8.42 | 114.91 | 110.70 |
| 1 | CA | 1442(A) | G | C6-N1-C2 | -8.41 | 120.05 | 125.10 |
| 23 | DA | 2881 | C | N1-C2-O2 | -8.41 | 113.86 | 118.90 |
| 51 | B7 | 47 | ARG | NE-CZ-NH1 | 8.41 | 124.50 | 120.30 |
| 23 | DA | 446 | G | C8-N9-C4 | 8.40 | 109.76 | 106.40 |
| 1 | AA | 77 | G | C4-C5-N7 | 8.40 | 114.16 | 110.80 |
| 23 | DA | 2791 | C | N1-C2-O2 | 8.40 | 123.94 | 118.90 |
| 23 | BA | 154(A) | C | N3-C2-O2 | -8.40 | 116.02 | 121.90 |
| 1 | CA | 1343 | G | N1-C6-O6 | 8.38 | 124.93 | 119.90 |
| 23 | BA | 684 | G | N3-C2-N2 | -8.38 | 114.04 | 119.90 |
| 1 | AA | 1034 | G | C5-C6-O6 | 8.37 | 133.62 | 128.60 |
| 23 | BA | 1216 | G | C6-C5-N7 | -8.37 | 125.38 | 130.40 |
| 23 | BA | 1315 | C | N3-C2-O2 | -8.37 | 116.04 | 121.90 |
| 23 | DA | 154(A) | C | N3-C2-O2 | -8.37 | 116.04 | 121.90 |
| 23 | BA | 975 | C | N3-C2-O2 | -8.36 | 116.05 | 121.90 |
| 1 | CA | 1158 | C | N1-C2-O2 | 8.36 | 123.91 | 118.90 |
| 4 | CD | 12 | CYS | CA-CB-SG | 8.36 | 129.04 | 114.00 |
| 1 | CA | 1033 | G | C5-C6-O6 | -8.35 | 123.59 | 128.60 |
| 23 | DA | 2286 | A | C4-C5-C6 | 8.35 | 121.18 | 117.00 |
| 23 | DA | 2287 | A | N1-C6-N6 | 8.35 | 123.61 | 118.60 |
| 1 | AA | 1443 | G | C5-C6-O6 | -8.35 | 123.59 | 128.60 |
| 23 | BA | 1049 | C | C2-N1-C1' | 8.35 | 127.98 | 118.80 |
| 23 | BA | 2723 | C | N3-C4-N4 | -8.35 | 112.16 | 118.00 |
| 1 | AA | 283 | C | N1-C2-O2 | 8.34 | 123.91 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 24 | BB | 4 | C | C6-N1-C2 | 8.34 | 123.64 | 120.30 |
| 23 | BA | 2318 | G | C8-N9-C4 | -8.34 | 103.06 | 106.40 |
| 1 | AA | 1051 | C | N3-C2-O2 | -8.34 | 116.06 | 121.90 |
| 1 | AA | 1051 | C | C6-N1-C1' | -8.33 | 110.80 | 120.80 |
| 23 | BA | 2375 | G | N7-C8-N9 | -8.33 | 108.94 | 113.10 |
| 1 | CA | 1052 | U | N1-C2-O2 | 8.33 | 128.63 | 122.80 |
| 1 | CA | 357 | G | N1-C6-O6 | -8.32 | 114.91 | 119.90 |
| 23 | BA | 910 | A | C8-N9-C4 | 8.32 | 109.13 | 105.80 |
| 23 | BA | 1762 | A | N7-C8-N9 | 8.32 | 117.96 | 113.80 |
| 23 | BA | 804 | A | C8-N9-C4 | 8.31 | 109.12 | 105.80 |
| 1 | CA | 1171 | G | N1-C6-O6 | -8.31 | 114.91 | 119.90 |
| 24 | DB | 83 | G | N1-C6-O6 | 8.31 | 124.89 | 119.90 |
| 23 | DA | 566 | U | C6-N1-C2 | 8.31 | 125.98 | 121.00 |
| 1 | CA | 1192 | C | C6-N1-C2 | -8.30 | 116.98 | 120.30 |
| 23 | BA | 988 | A | N1-C6-N6 | 8.30 | 123.58 | 118.60 |
| 1 | CA | 1230 | C | C6-N1-C2 | -8.30 | 116.98 | 120.30 |
| 23 | BA | 2286 | A | N7-C8-N9 | 8.30 | 117.95 | 113.80 |
| 1 | CA | 1283 | G | C8-N9-C4 | -8.29 | 103.09 | 106.40 |
| 23 | DA | 1565 | C | C2-N3-C4 | -8.29 | 115.76 | 119.90 |
| 23 | BA | 508 | G | C5-C6-O6 | -8.28 | 123.63 | 128.60 |
| 23 | BA | 2321 | G | N3-C2-N2 | -8.28 | 114.10 | 119.90 |
| 23 | BA | 145 | G | C8-N9-C4 | 8.28 | 109.71 | 106.40 |
| 23 | BA | 2619 | C | C5-C6-N1 | -8.27 | 116.86 | 121.00 |
| 23 | BA | 959 | A | C5-C6-N6 | 8.27 | 130.32 | 123.70 |
| 23 | BA | 1695 | G | N1-C6-O6 | 8.27 | 124.86 | 119.90 |
| 24 | BB | 76 | G | C8-N9-C4 | 8.26 | 109.70 | 106.40 |
| 23 | BA | 188 | G | C2-N3-C4 | -8.26 | 107.77 | 111.90 |
| 23 | BA | 1210 | A | C8-N9-C4 | -8.26 | 102.50 | 105.80 |
| 1 | CA | 1216 | G | N3-C4-C5 | 8.26 | 132.73 | 128.60 |
| 23 | DA | 2498 | C | C6-N1-C2 | 8.26 | 123.60 | 120.30 |
| 23 | BA | 645 | C | N1-C2-O2 | 8.25 | 123.85 | 118.90 |
| 23 | BA | 959 | A | N1-C6-N6 | -8.25 | 113.65 | 118.60 |
| 23 | BA | 2206 | G | C4-N9-C1' | -8.25 | 115.78 | 126.50 |
| 1 | CA | 943 | U | C5-C4-O4 | 8.25 | 130.85 | 125.90 |
| 23 | BA | 2100 | G | N3-C4-N9 | 8.24 | 130.95 | 126.00 |
| 23 | BA | 971 | C | C6-N1-C2 | -8.24 | 117.00 | 120.30 |
| 23 | DA | 2572 | A | N7-C8-N9 | -8.24 | 109.68 | 113.80 |
| 23 | BA | 678 | C | C6-N1-C2 | 8.24 | 123.60 | 120.30 |
| 23 | DA | 568 | U | C5-C4-O4 | -8.24 | 120.96 | 125.90 |
| 23 | BA | 844 | C | C6-N1-C2 | 8.23 | 123.59 | 120.30 |
| 23 | BA | 1022 | G | N9-C4-C5 | 8.23 | 108.69 | 105.40 |
| 23 | DA | 2827 | C | C6-N1-C2 | 8.23 | 123.59 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 1022 | G | N3-C2-N2 | -8.23 | 114.14 | 119.90 |
| 1 | CA | 839 | U | N1-C2-O2 | 8.23 | 128.56 | 122.80 |
| 23 | BA | 849 | A | C8-N9-C4 | 8.23 | 109.09 | 105.80 |
| 23 | DA | 440 | G | N1-C6-O6 | -8.23 | 114.96 | 119.90 |
| 23 | BA | 1655 | A | C8-N9-C4 | 8.22 | 109.09 | 105.80 |
| 23 | DA | 2040 | C | C6-N1-C2 | 8.22 | 123.59 | 120.30 |
| 23 | DA | 201 | C | C6-N1-C2 | 8.22 | 123.59 | 120.30 |
| 23 | DA | 945 | A | C5-C6-N1 | -8.22 | 113.59 | 117.70 |
| 23 | DA | 2589 | A | C2-N3-C4 | -8.22 | 106.49 | 110.60 |
| 23 | DA | 2606 | C | N3-C4-C5 | 8.22 | 125.19 | 121.90 |
| 23 | DA | 528 | A | C5-C6-N6 | 8.22 | 130.27 | 123.70 |
| 23 | DA | 2690 | C | N3-C4-C5 | -8.22 | 118.61 | 121.90 |
| 23 | DA | 448 | U | N1-C2-N3 | 8.21 | 119.83 | 114.90 |
| 27 | BF | 74 | ARG | NE-CZ-NH2 | -8.21 | 116.20 | 120.30 |
| 23 | DA | 271(S) | G | N1-C6-O6 | 8.21 | 124.82 | 119.90 |
| 23 | DA | 1698 | A | N7-C8-N9 | 8.20 | 117.90 | 113.80 |
| 1 | AA | 458 | C | C6-N1-C2 | -8.20 | 117.02 | 120.30 |
| 1 | CA | 1050 | G | N3-C2-N2 | 8.20 | 125.64 | 119.90 |
| 23 | DA | 945 | A | N3-C4-N9 | -8.20 | 120.84 | 127.40 |
| 1 | AA | 1174 | G | C8-N9-C4 | 8.20 | 109.68 | 106.40 |
| 23 | BA | 1021 | A | C5-C6-N1 | -8.20 | 113.60 | 117.70 |
| 23 | BA | 2206 | G | N3-C4-C5 | 8.19 | 132.69 | 128.60 |
| 38 | BU | 28 | ARG | NE-CZ-NH1 | -8.19 | 116.21 | 120.30 |
| 1 | CA | 52 | G | C5-C6-O6 | 8.19 | 133.51 | 128.60 |
| 23 | BA | 782 | A | C6-N1-C2 | -8.18 | 113.69 | 118.60 |
| 23 | DA | 789 | A | C8-N9-C4 | 8.18 | 109.07 | 105.80 |
| 23 | BA | 130 | C | C6-N1-C2 | 8.18 | 123.57 | 120.30 |
| 1 | CA | 1351 | U | C5-C6-N1 | -8.18 | 118.61 | 122.70 |
| 23 | BA | 2700 | C | C6-N1-C2 | 8.17 | 123.57 | 120.30 |
| 23 | BA | 745 | G | N3-C4-C5 | -8.16 | 124.52 | 128.60 |
| 23 | BA | 1328 | G | C8-N9-C4 | 8.16 | 109.66 | 106.40 |
| 1 | AA | 1223 | C | C6-N1-C2 | -8.15 | 117.04 | 120.30 |
| 23 | BA | 2689 | U | C5-C4-O4 | 8.15 | 130.79 | 125.90 |
| 23 | DA | 2371 | G | N9-C4-C5 | -8.14 | 102.14 | 105.40 |
| 1 | CA | 28 | G | N1-C6-O6 | 8.13 | 124.78 | 119.90 |
| 23 | BA | 2105 | C | C6-N1-C2 | -8.13 | 117.05 | 120.30 |
| 23 | DA | 413 | C | N1-C2-O2 | -8.13 | 114.02 | 118.90 |
| 23 | BA | 1977 | A | C8-N9-C4 | 8.13 | 109.05 | 105.80 |
| 1 | AA | 1158 | C | N1-C2-O2 | 8.13 | 123.78 | 118.90 |
| 1 | AA | 1502 | A | C6-C5-N7 | -8.12 | 126.62 | 132.30 |
| 1 | AA | 1443 | G | N9-C4-C5 | -8.12 | 102.15 | 105.40 |
| 1 | AA | 1502 | A | C5-N7-C8 | -8.12 | 99.84 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 23 | DA | 1108 | U | N1-C2-O2 | 8.12 | 128.48 | 122.80 |
| 1 | AA | 1210 | C | C2-N1-C1' | 8.12 | 127.73 | 118.80 |
| 1 | AA | 1006 | C | C5-C6-N1 | 8.11 | 125.06 | 121.00 |
| 23 | BA | 2349 | G | C8-N9-C4 | -8.11 | 103.16 | 106.40 |
| 23 | DA | 1760 | A | N1-C6-N6 | -8.11 | 113.74 | 118.60 |
| 24 | DB | 30 | C | C6-N1-C2 | -8.11 | 117.06 | 120.30 |
| 23 | DA | 453 | C | C6-N1-C2 | 8.10 | 123.54 | 120.30 |
| 23 | DA | 2296 | U | O4'-C1'-N1 | 8.10 | 114.68 | 108.20 |
| 1 | AA | 557 | G | N3-C4-C5 | -8.10 | 124.55 | 128.60 |
| 1 | AA | 1051 | C | C2-N1-C1' | 8.09 | 127.70 | 118.80 |
| 23 | DA | 1350 | C | C6-N1-C2 | 8.09 | 123.54 | 120.30 |
| 23 | BA | 272(D) | G | C8-N9-C4 | 8.09 | 109.64 | 106.40 |
| 23 | BA | 2261 | C | C4-C5-C6 | 8.09 | 121.44 | 117.40 |
| 1 | AA | 1456 | G | N3-C4-N9 | 8.09 | 130.85 | 126.00 |
| 23 | BA | 1452 | A | C8-N9-C4 | 8.08 | 109.03 | 105.80 |
| 23 | BA | 1695 | G | C5-N7-C8 | -8.08 | 100.26 | 104.30 |
| 1 | CA | 1442(B) | A | N3-C4-C5 | -8.08 | 121.14 | 126.80 |
| 23 | DA | 933 | A | C5-N7-C8 | -8.08 | 99.86 | 103.90 |
| 23 | BA | 552 | G | C8-N9-C4 | 8.08 | 109.63 | 106.40 |
| 23 | BA | 2084 | C | C5-C6-N1 | -8.08 | 116.96 | 121.00 |
| 23 | BA | 1314 | C | C2-N1-C1' | 8.07 | 127.68 | 118.80 |
| 23 | BA | 207 | A | C2-N3-C4 | -8.07 | 106.56 | 110.60 |
| 23 | BA | 612 | C | C6-N1-C2 | 8.07 | 123.53 | 120.30 |
| 23 | BA | 527 | C | N3-C2-O2 | -8.06 | 116.25 | 121.90 |
| 1 | AA | 1442 | G | C5-N7-C8 | 8.06 | 108.33 | 104.30 |
| 23 | BA | 2596 | U | N1-C2-O2 | -8.05 | 117.16 | 122.80 |
| 24 | BB | 85 | G | C5-C6-O6 | -8.05 | 123.77 | 128.60 |
| 1 | CA | 936 | C | C2-N1-C1' | 8.05 | 127.66 | 118.80 |
| 23 | BA | 1695 | G | C6-C5-N7 | -8.05 | 125.57 | 130.40 |
| 23 | BA | 205 | G | N3-C2-N2 | 8.04 | 125.53 | 119.90 |
| 23 | BA | 2242 | G | N3-C2-N2 | -8.04 | 114.27 | 119.90 |
| 23 | DA | 1992 | G | N9-C4-C5 | 8.04 | 108.62 | 105.40 |
| 1 | AA | 1243 | C | C5-C6-N1 | 8.04 | 125.02 | 121.00 |
| 23 | BA | 1617 | C | N3-C4-C5 | -8.04 | 118.68 | 121.90 |
| 23 | DA | 1779 | U | C6-N1-C1' | -8.04 | 109.95 | 121.20 |
| 1 | CA | 1282 | C | C6-N1-C2 | -8.03 | 117.09 | 120.30 |
| 23 | BA | 2306 | C | C2-N1-C1' | 8.03 | 127.63 | 118.80 |
| 1 | CA | 1305 | G | N1-C6-O6 | 8.03 | 124.72 | 119.90 |
| 23 | BA | 745 | G | N3-C4-N9 | 8.03 | 130.82 | 126.00 |
| 23 | BA | 2497 | A | C6-N1-C2 | -8.03 | 113.78 | 118.60 |
| 1 | CA | 986 | A | C2-N3-C4 | 8.03 | 114.61 | 110.60 |
| 23 | DA | 39 | C | C5-C6-N1 | -8.02 | 116.99 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|----------|-------|-------------|----------|
| 23 | BA | 2044 | C | N1-C2-O2 | -8.02 | 114.09 | 118.90 |
| 23 | BA | 2010 | G | N1-C6-O6 | 8.02 | 124.71 | 119.90 |
| 23 | BA | 13 | A | N1-C6-N6 | -8.01 | 113.79 | 118.60 |
| 23 | DA | 2676 | C | C5-C6-N1 | -8.01 | 116.99 | 121.00 |
| 1 | CA | 1502 | A | C6-C5-N7 | -8.01 | 126.69 | 132.30 |
| 23 | BA | 587 | C | N3-C4-C5 | -8.01 | 118.70 | 121.90 |
| 1 | AA | 818 | G | C5-C6-O6 | 8.00 | 133.40 | 128.60 |
| 23 | DA | 1608 | A | C2-N3-C4 | -8.00 | 106.60 | 110.60 |
| 23 | BA | 928 | G | C5-C6-O6 | -8.00 | 123.80 | 128.60 |
| 1 | AA | 927 | G | C8-N9-C4 | 8.00 | 109.60 | 106.40 |
| 23 | BA | 1647 | G | N1-C6-O6 | 8.00 | 124.70 | 119.90 |
| 23 | DA | 2292 | C | C5-C6-N1 | -8.00 | 117.00 | 121.00 |
| 1 | AA | 1442(A) | G | C6-N1-C2 | -7.99 | 120.31 | 125.10 |
| 23 | BA | 1217 | C | C6-N1-C2 | 7.99 | 123.50 | 120.30 |
| 23 | DA | 1377 | G | N3-C4-C5 | -7.99 | 124.61 | 128.60 |
| 23 | BA | 271(J) | C | C6-N1-C2 | 7.99 | 123.49 | 120.30 |
| 1 | AA | 1292 | U | N1-C2-O2 | 7.98 | 128.39 | 122.80 |
| 23 | DA | 826 | U | N1-C2-N3 | 7.98 | 119.69 | 114.90 |
| 1 | AA | 1014 | A | C8-N9-C4 | -7.98 | 102.61 | 105.80 |
| 23 | BA | 185 | U | C5-C6-N1 | -7.98 | 118.71 | 122.70 |
| 23 | DA | 2306 | C | C5-C6-N1 | 7.98 | 124.99 | 121.00 |
| 1 | AA | 333 | G | N1-C6-O6 | 7.98 | 124.69 | 119.90 |
| 23 | DA | 729 | G | C5-C6-O6 | -7.98 | 123.81 | 128.60 |
| 23 | BA | 71 | A | C8-N9-C4 | -7.97 | 102.61 | 105.80 |
| 1 | CA | 1456 | G | N3-C4-N9 | 7.97 | 130.78 | 126.00 |
| 1 | AA | 1312 | G | N3-C4-C5 | -7.97 | 124.62 | 128.60 |
| 23 | DA | 208 | C | N3-C4-C5 | 7.96 | 125.08 | 121.90 |
| 23 | DA | 736 | C | N1-C2-O2 | -7.96 | 114.12 | 118.90 |
| 1 | CA | 1039 | C | N1-C2-O2 | 7.95 | 123.67 | 118.90 |
| 1 | AA | 1402 | C | C6-N1-C2 | -7.95 | 117.12 | 120.30 |
| 23 | BA | 2087 | G | N1-C6-O6 | 7.95 | 124.67 | 119.90 |
| 23 | DA | 468 | G | C8-N9-C4 | 7.95 | 109.58 | 106.40 |
| 23 | BA | 2286 | A | C5-N7-C8 | -7.95 | 99.93 | 103.90 |
| 23 | BA | 2080 | G | C8-N9-C4 | 7.94 | 109.58 | 106.40 |
| 23 | BA | 2689 | U | N3-C4-O4 | -7.94 | 113.84 | 119.40 |
| 24 | BB | 61 | G | N3-C2-N2 | -7.94 | 114.34 | 119.90 |
| 23 | BA | 2307 | G | N7-C8-N9 | 7.94 | 117.07 | 113.10 |
| 23 | DA | 12 | U | N3-C2-O2 | -7.93 | 116.64 | 122.20 |
| 23 | DA | 2100 | G | N3-C4-N9 | 7.93 | 130.76 | 126.00 |
| 1 | CA | 242 | C | N1-C2-O2 | -7.93 | 114.14 | 118.90 |
| 23 | BA | 2404 | C | C6-N1-C2 | 7.93 | 123.47 | 120.30 |
| 23 | DA | 1967 | C | C6-N1-C2 | 7.93 | 123.47 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 844 | C | C5-C6-N1 | -7.92 | 117.04 | 121.00 |
| 23 | DA | 2250 | G | C4-C5-N7 | -7.92 | 107.63 | 110.80 |
| 23 | BA | 1372 | U | N3-C2-O2 | -7.92 | 116.66 | 122.20 |
| 1 | CA | 1081 | G | N9-C4-C5 | -7.92 | 102.23 | 105.40 |
| 1 | AA | 1274 | G | N1-C6-O6 | 7.92 | 124.65 | 119.90 |
| 23 | DA | 1937 | A | N1-C6-N6 | 7.92 | 123.35 | 118.60 |
| 23 | BA | 1992 | G | N9-C4-C5 | 7.91 | 108.56 | 105.40 |
| 1 | AA | 1050 | G | N1-C6-O6 | 7.91 | 124.64 | 119.90 |
| 23 | DA | 1142(A) | A | N1-C6-N6 | 7.91 | 123.34 | 118.60 |
| 1 | AA | 634 | C | C6-N1-C2 | -7.90 | 117.14 | 120.30 |
| 1 | AA | 1210 | C | N1-C2-O2 | 7.90 | 123.64 | 118.90 |
| 23 | DA | 389 | G | N9-C4-C5 | -7.90 | 102.24 | 105.40 |
| 1 | AA | 1417 | G | N3-C4-N9 | 7.90 | 130.74 | 126.00 |
| 23 | DA | 1993 | U | N1-C2-O2 | -7.90 | 117.27 | 122.80 |
| 23 | DA | 2319 | G | N3-C2-N2 | -7.89 | 114.38 | 119.90 |
| 23 | DA | 1021 | A | C5-N7-C8 | -7.89 | 99.95 | 103.90 |
| 1 | CA | 117 | G | N1-C6-O6 | 7.89 | 124.63 | 119.90 |
| 23 | BA | 546 | C | C5-C6-N1 | 7.88 | 124.94 | 121.00 |
| 23 | DA | 652(E) | G | C6-N1-C2 | 7.88 | 129.83 | 125.10 |
| 1 | CA | 77 | G | C4-C5-N7 | 7.88 | 113.95 | 110.80 |
| 23 | BA | 475 | U | C6-N1-C2 | -7.88 | 116.28 | 121.00 |
| 23 | BA | 1570 | A | C2-N3-C4 | -7.87 | 106.67 | 110.60 |
| 1 | CA | 1116 | C | C5-C4-N4 | 7.87 | 125.71 | 120.20 |
| 1 | AA | 1174 | G | C6-C5-N7 | 7.86 | 135.12 | 130.40 |
| 1 | CA | 1409 | C | C6-N1-C2 | 7.86 | 123.44 | 120.30 |
| 1 | AA | 1292 | U | C2-N1-C1' | 7.86 | 127.13 | 117.70 |
| 23 | DA | 1983 | C | N1-C2-O2 | -7.86 | 114.19 | 118.90 |
| 23 | BA | 1283 | G | C5-C6-O6 | 7.85 | 133.31 | 128.60 |
| 1 | CA | 529 | G | N1-C6-O6 | 7.85 | 124.61 | 119.90 |
| 23 | BA | 1047 | G | N3-C4-N9 | 7.85 | 130.71 | 126.00 |
| 23 | BA | 2623 | G | N3-C4-C5 | -7.85 | 124.68 | 128.60 |
| 1 | CA | 1442(A) | G | C6-C5-N7 | -7.84 | 125.69 | 130.40 |
| 23 | BA | 1128 | A | C6-N1-C2 | -7.84 | 113.90 | 118.60 |
| 1 | AA | 1243 | C | C2-N3-C4 | 7.84 | 123.82 | 119.90 |
| 23 | BA | 1698 | A | C5-N7-C8 | -7.84 | 99.98 | 103.90 |
| 23 | DA | 1006 | C | N3-C4-N4 | -7.83 | 112.52 | 118.00 |
| 23 | DA | 1284 | A | N1-C6-N6 | 7.83 | 123.30 | 118.60 |
| 23 | DA | 201 | C | C2-N3-C4 | -7.83 | 115.99 | 119.90 |
| 23 | BA | 124 | G | N9-C4-C5 | -7.83 | 102.27 | 105.40 |
| 23 | DA | 2335 | A | C5-C6-N6 | -7.83 | 117.44 | 123.70 |
| 23 | BA | 982 | C | N1-C2-O2 | 7.83 | 123.60 | 118.90 |
| 1 | AA | 1263 | C | N3-C2-O2 | -7.82 | 116.42 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 928 | G | C5-C6-O6 | -7.82 | 123.91 | 128.60 |
| 1 | AA | 1502 | A | C4-C5-N7 | 7.82 | 114.61 | 110.70 |
| 23 | BA | 2496 | C | N1-C2-O2 | -7.82 | 114.21 | 118.90 |
| 23 | BA | 972 | G | C5-C6-O6 | 7.81 | 133.29 | 128.60 |
| 1 | AA | 1335 | C | C2-N1-C1' | 7.81 | 127.39 | 118.80 |
| 23 | BA | 572 | A | N9-C4-C5 | 7.81 | 108.92 | 105.80 |
| 23 | DA | 1124 | C | C6-N1-C2 | 7.81 | 123.42 | 120.30 |
| 1 | AA | 1442(A) | G | C6-C5-N7 | -7.81 | 125.72 | 130.40 |
| 23 | BA | 737 | C | C6-N1-C2 | 7.81 | 123.42 | 120.30 |
| 23 | BA | 2488 | A | C8-N9-C4 | 7.80 | 108.92 | 105.80 |
| 23 | DA | 1001 | A | C8-N9-C4 | 7.80 | 108.92 | 105.80 |
| 23 | DA | 2449 | U | N1-C2-O2 | -7.80 | 117.34 | 122.80 |
| 1 | CA | 925 | G | C8-N9-C4 | 7.79 | 109.52 | 106.40 |
| 1 | AA | 1012 | U | N1-C2-O2 | -7.79 | 117.34 | 122.80 |
| 23 | BA | 202 | U | N3-C4-C5 | 7.79 | 119.27 | 114.60 |
| 23 | DA | 528 | A | N9-C4-C5 | 7.79 | 108.92 | 105.80 |
| 23 | DA | 1348 | G | N1-C6-O6 | 7.79 | 124.57 | 119.90 |
| 23 | DA | 1333 | C | N3-C4-C5 | 7.79 | 125.01 | 121.90 |
| 1 | AA | 1126 | U | N3-C2-O2 | -7.78 | 116.75 | 122.20 |
| 23 | DA | 205 | G | C8-N9-C4 | 7.78 | 109.51 | 106.40 |
| 23 | DA | 792 | G | N9-C4-C5 | -7.78 | 102.29 | 105.40 |
| 1 | CA | 1050 | G | N3-C4-N9 | 7.78 | 130.67 | 126.00 |
| 1 | AA | 1237 | C | C5-C6-N1 | 7.78 | 124.89 | 121.00 |
| 23 | BA | 2505 | G | C5-C6-N1 | -7.78 | 107.61 | 111.50 |
| 23 | DA | 627 | A | C8-N9-C4 | 7.78 | 108.91 | 105.80 |
| 23 | DA | 1204 | A | N7-C8-N9 | 7.78 | 117.69 | 113.80 |
| 23 | DA | 2340 | G | C8-N9-C4 | 7.78 | 109.51 | 106.40 |
| 23 | BA | 2306 | C | N1-C2-O2 | 7.77 | 123.56 | 118.90 |
| 23 | DA | 121 | G | C8-N9-C4 | 7.77 | 109.51 | 106.40 |
| 24 | DB | 61 | G | N3-C2-N2 | -7.77 | 114.46 | 119.90 |
| 1 | AA | 980 | C | N1-C2-O2 | 7.77 | 123.56 | 118.90 |
| 23 | DA | 728 | G | N7-C8-N9 | -7.76 | 109.22 | 113.10 |
| 1 | AA | 1153 | C | C6-N1-C1' | -7.76 | 111.49 | 120.80 |
| 23 | BA | 729 | G | C5-N7-C8 | -7.75 | 100.42 | 104.30 |
| 23 | DA | 2607 | G | N1-C2-N2 | -7.75 | 109.22 | 116.20 |
| 23 | BA | 2538 | C | C5-C6-N1 | -7.75 | 117.12 | 121.00 |
| 23 | DA | 2371 | G | C4-C5-N7 | 7.75 | 113.90 | 110.80 |
| 23 | DA | 2502 | G | C4-C5-N7 | 7.75 | 113.90 | 110.80 |
| 23 | BA | 2863 | C | C6-N1-C2 | 7.75 | 123.40 | 120.30 |
| 23 | DA | 2515 | C | N3-C4-C5 | 7.75 | 125.00 | 121.90 |
| 23 | BA | 2791 | C | N1-C2-O2 | 7.74 | 123.55 | 118.90 |
| 23 | BA | 1657 | C | N1-C2-O2 | -7.74 | 114.26 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1054 | C | N3-C2-O2 | -7.74 | 116.48 | 121.90 |
| 23 | DA | 1979 | C | C6-N1-C2 | -7.73 | 117.21 | 120.30 |
| 1 | CA | 1033 | G | C6-C5-N7 | -7.73 | 125.76 | 130.40 |
| 23 | DA | 1659 | U | C5-C6-N1 | -7.73 | 118.83 | 122.70 |
| 1 | AA | 989 | C | C2-N3-C4 | 7.73 | 123.77 | 119.90 |
| 23 | BA | 689 | A | N7-C8-N9 | -7.73 | 109.94 | 113.80 |
| 23 | DA | 1792 | G | C8-N9-C4 | 7.73 | 109.49 | 106.40 |
| 23 | DA | 1807 | G | N1-C6-O6 | 7.73 | 124.54 | 119.90 |
| 23 | DA | 1022 | G | N3-C4-N9 | -7.73 | 121.36 | 126.00 |
| 23 | BA | 287 | C | C6-N1-C2 | 7.72 | 123.39 | 120.30 |
| 23 | DA | 2594 | C | N1-C2-O2 | -7.72 | 114.27 | 118.90 |
| 23 | BA | 676 | A | N1-C6-N6 | 7.72 | 123.23 | 118.60 |
| 23 | DA | 934 | G | C8-N9-C4 | 7.72 | 109.49 | 106.40 |
| 23 | BA | 455 | C | N3-C2-O2 | -7.72 | 116.50 | 121.90 |
| 50 | D6 | 40 | CYS | CA-CB-SG | -7.72 | 100.11 | 114.00 |
| 23 | BA | 2200 | C | N3-C2-O2 | -7.72 | 116.50 | 121.90 |
| 23 | DA | 1762 | A | N7-C8-N9 | 7.72 | 117.66 | 113.80 |
| 23 | BA | 1343 | G | N7-C8-N9 | 7.71 | 116.96 | 113.10 |
| 23 | BA | 2296 | U | O4'-C1'-N1 | 7.71 | 114.37 | 108.20 |
| 23 | BA | 729 | G | C4-C5-N7 | 7.71 | 113.89 | 110.80 |
| 1 | CA | 44 | G | N1-C6-O6 | 7.71 | 124.53 | 119.90 |
| 23 | DA | 1776 | G | C8-N9-C4 | 7.71 | 109.48 | 106.40 |
| 23 | DA | 759 | G | N1-C6-O6 | 7.71 | 124.53 | 119.90 |
| 23 | DA | 47 | C | C6-N1-C2 | 7.71 | 123.38 | 120.30 |
| 23 | BA | 102 | G | C8-N9-C4 | -7.70 | 103.32 | 106.40 |
| 1 | CA | 896 | C | C6-N1-C2 | 7.70 | 123.38 | 120.30 |
| 23 | BA | 2182 | G | C6-N1-C2 | 7.70 | 129.72 | 125.10 |
| 1 | AA | 1261 | A | N1-C6-N6 | 7.70 | 123.22 | 118.60 |
| 1 | CA | 1216 | G | N3-C4-N9 | -7.70 | 121.38 | 126.00 |
| 1 | CA | 27 | G | C5-C6-O6 | -7.69 | 123.98 | 128.60 |
| 23 | DA | 572 | A | N1-C2-N3 | 7.69 | 133.15 | 129.30 |
| 1 | CA | 1353 | G | C2-N3-C4 | 7.69 | 115.74 | 111.90 |
| 23 | BA | 655 | A | C8-N9-C4 | -7.69 | 102.72 | 105.80 |
| 23 | DA | 2856 | C | C5-C6-N1 | 7.68 | 124.84 | 121.00 |
| 23 | BA | 2364 | C | C6-N1-C2 | 7.68 | 123.37 | 120.30 |
| 23 | BA | 2579 | C | C5-C6-N1 | -7.68 | 117.16 | 121.00 |
| 1 | CA | 572 | A | C8-N9-C4 | 7.68 | 108.87 | 105.80 |
| 24 | DB | 83 | G | C5-C6-O6 | -7.68 | 123.99 | 128.60 |
| 23 | BA | 528 | A | C5-N7-C8 | -7.68 | 100.06 | 103.90 |
| 1 | AA | 998 | G | C6-C5-N7 | 7.68 | 135.01 | 130.40 |
| 24 | BB | 117 | G | C8-N9-C4 | 7.67 | 109.47 | 106.40 |
| 23 | BA | 745 | G | C5-C6-N1 | 7.67 | 115.33 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1602 | U | N3-C4-C5 | -7.67 | 110.00 | 114.60 |
| 23 | DA | 2324 | C | N3-C4-C5 | 7.67 | 124.97 | 121.90 |
| 23 | BA | 2144 | U | C5-C6-N1 | 7.67 | 126.53 | 122.70 |
| 1 | CA | 1357 | A | C8-N9-C4 | -7.67 | 102.73 | 105.80 |
| 1 | CA | 691 | G | N9-C4-C5 | -7.66 | 102.34 | 105.40 |
| 1 | CA | 1223 | C | C6-N1-C2 | -7.65 | 117.24 | 120.30 |
| 1 | CA | 1165 | C | C2-N3-C4 | 7.65 | 123.72 | 119.90 |
| 1 | AA | 1174 | G | C4-N9-C1' | -7.64 | 116.56 | 126.50 |
| 23 | BA | 2694 | G | N3-C4-C5 | -7.64 | 124.78 | 128.60 |
| 23 | DA | 197 | A | C6-N1-C2 | -7.64 | 114.02 | 118.60 |
| 3 | CC | 52 | LEU | CA-CB-CG | 7.64 | 132.87 | 115.30 |
| 23 | BA | 1490 | A | N9-C4-C5 | -7.64 | 102.75 | 105.80 |
| 23 | BA | 655 | A | N7-C8-N9 | 7.63 | 117.62 | 113.80 |
| 23 | DA | 1603 | A | C8-N9-C4 | -7.63 | 102.75 | 105.80 |
| 23 | BA | 2041 | U | N1-C2-N3 | 7.63 | 119.48 | 114.90 |
| 23 | BA | 2286 | A | C5-C6-N1 | -7.63 | 113.89 | 117.70 |
| 1 | AA | 1006 | C | C2-N3-C4 | 7.62 | 123.71 | 119.90 |
| 23 | BA | 1254 | A | C8-N9-C4 | -7.62 | 102.75 | 105.80 |
| 24 | BB | 76 | G | N3-C4-C5 | 7.62 | 132.41 | 128.60 |
| 4 | AD | 12 | CYS | CA-CB-SG | 7.62 | 127.72 | 114.00 |
| 23 | BA | 465 | G | N3-C4-C5 | -7.62 | 124.79 | 128.60 |
| 24 | BB | 7 | G | N1-C6-O6 | 7.62 | 124.47 | 119.90 |
| 1 | CA | 359 | U | C2-N3-C4 | -7.62 | 122.43 | 127.00 |
| 1 | CA | 1502 | A | C4-C5-N7 | 7.62 | 114.51 | 110.70 |
| 23 | DA | 13 | A | N1-C6-N6 | -7.62 | 114.03 | 118.60 |
| 23 | BA | 945 | A | N3-C4-N9 | -7.61 | 121.31 | 127.40 |
| 1 | AA | 1274 | G | N7-C8-N9 | 7.61 | 116.91 | 113.10 |
| 23 | BA | 756 | C | N3-C4-C5 | -7.61 | 118.86 | 121.90 |
| 23 | DA | 1302 | A | N1-C6-N6 | -7.61 | 114.03 | 118.60 |
| 23 | DA | 560 | C | N3-C4-C5 | 7.61 | 124.94 | 121.90 |
| 23 | DA | 202 | U | C6-N1-C2 | 7.61 | 125.56 | 121.00 |
| 23 | DA | 772 | C | N1-C2-O2 | -7.61 | 114.34 | 118.90 |
| 23 | DA | 2704 | C | C6-N1-C2 | 7.61 | 123.34 | 120.30 |
| 1 | AA | 1120 | G | C5-C6-O6 | -7.60 | 124.04 | 128.60 |
| 23 | DA | 1314 | C | C2-N1-C1' | 7.60 | 127.16 | 118.80 |
| 1 | AA | 1059 | C | N1-C2-O2 | 7.60 | 123.46 | 118.90 |
| 23 | BA | 2619 | C | C6-N1-C2 | 7.60 | 123.34 | 120.30 |
| 23 | DA | 452 | G | C8-N9-C4 | -7.60 | 103.36 | 106.40 |
| 1 | AA | 1000 | U | C5-C6-N1 | 7.59 | 126.50 | 122.70 |
| 23 | BA | 1314 | C | C6-N1-C1' | -7.59 | 111.69 | 120.80 |
| 23 | DA | 729 | G | N1-C6-O6 | 7.59 | 124.45 | 119.90 |
| 23 | BA | 655 | A | C5-N7-C8 | -7.59 | 100.11 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | BA | 2200 | C | N1-C2-O2 | 7.59 | 123.45 | 118.90 |
| 23 | BA | 530 | G | N3-C4-C5 | 7.58 | 132.39 | 128.60 |
| 1 | CA | 1206 | G | C5-C6-O6 | -7.58 | 124.05 | 128.60 |
| 1 | AA | 1307 | U | C5-C6-N1 | 7.58 | 126.49 | 122.70 |
| 23 | DA | 940 | G | N1-C6-O6 | 7.58 | 124.45 | 119.90 |
| 23 | BA | 530 | G | C4-C5-N7 | 7.58 | 113.83 | 110.80 |
| 23 | BA | 1779 | U | N1-C2-N3 | -7.58 | 110.35 | 114.90 |
| 23 | BA | 2641 | G | C6-C5-N7 | -7.58 | 125.85 | 130.40 |
| 23 | BA | 789 | A | C8-N9-C4 | 7.57 | 108.83 | 105.80 |
| 1 | AA | 1350 | A | C6-N1-C2 | -7.57 | 114.06 | 118.60 |
| 23 | DA | 818 | G | C8-N9-C4 | 7.57 | 109.43 | 106.40 |
| 23 | DA | 1821 | A | C6-N1-C2 | -7.57 | 114.06 | 118.60 |
| 1 | AA | 756 | C | C6-N1-C2 | 7.57 | 123.33 | 120.30 |
| 23 | BA | 2028 | U | N3-C4-C5 | 7.56 | 119.14 | 114.60 |
| 1 | CA | 1081 | G | N1-C6-O6 | 7.56 | 124.44 | 119.90 |
| 23 | DA | 1325 | G | N1-C6-O6 | 7.56 | 124.44 | 119.90 |
| 1 | CA | 1032 | G | N3-C4-N9 | -7.55 | 121.47 | 126.00 |
| 1 | AA | 1133 | G | C4-C5-N7 | -7.55 | 107.78 | 110.80 |
| 23 | BA | 2791 | C | C5-C6-N1 | 7.55 | 124.77 | 121.00 |
| 23 | BA | 2768 | C | C5-C6-N1 | -7.54 | 117.23 | 121.00 |
| 23 | BA | 1464 | C | C6-N1-C2 | -7.54 | 117.28 | 120.30 |
| 23 | DA | 2501 | C | C5-C4-N4 | -7.54 | 114.92 | 120.20 |
| 23 | BA | 556 | G | C8-N9-C4 | 7.54 | 109.42 | 106.40 |
| 23 | BA | 693 | C | C6-N1-C2 | -7.54 | 117.28 | 120.30 |
| 23 | DA | 2789 | C | C6-N1-C2 | 7.54 | 123.31 | 120.30 |
| 23 | BA | 735 | A | N7-C8-N9 | -7.54 | 110.03 | 113.80 |
| 1 | AA | 352 | C | N1-C2-O2 | 7.53 | 123.42 | 118.90 |
| 1 | AA | 1042 | G | N9-C4-C5 | 7.53 | 108.41 | 105.40 |
| 1 | CA | 357 | G | N9-C4-C5 | 7.53 | 108.41 | 105.40 |
| 23 | BA | 2597 | G | C8-N9-C4 | -7.53 | 103.39 | 106.40 |
| 1 | CA | 1108 | G | N1-C6-O6 | -7.53 | 115.38 | 119.90 |
| 23 | DA | 684 | G | N3-C2-N2 | -7.53 | 114.63 | 119.90 |
| 23 | BA | 202 | U | C5-C6-N1 | -7.53 | 118.94 | 122.70 |
| 23 | BA | 468 | G | C8-N9-C4 | 7.53 | 109.41 | 106.40 |
| 36 | BS | 96 | GLY | N-CA-C | -7.53 | 94.28 | 113.10 |
| 1 | CA | 21 | G | C5-C6-O6 | 7.52 | 133.12 | 128.60 |
| 1 | AA | 418 | C | N3-C2-O2 | -7.52 | 116.63 | 121.90 |
| 23 | BA | 793 | A | N1-C6-N6 | 7.52 | 123.11 | 118.60 |
| 23 | BA | 2567 | G | C8-N9-C4 | 7.52 | 109.41 | 106.40 |
| 1 | AA | 1420 | C | C6-N1-C2 | -7.52 | 117.29 | 120.30 |
| 23 | BA | 297 | C | N3-C4-C5 | -7.52 | 118.89 | 121.90 |
| 1 | CA | 1446 | U | N1-C2-N3 | -7.52 | 110.39 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 24 | DB | 89 | G | C5-C6-O6 | -7.52 | 124.09 | 128.60 |
| 23 | BA | 2764 | A | N1-C6-N6 | -7.51 | 114.09 | 118.60 |
| 23 | DA | 330 | A | N3-C4-C5 | 7.51 | 132.06 | 126.80 |
| 23 | BA | 936 | C | C6-N1-C2 | 7.51 | 123.31 | 120.30 |
| 23 | DA | 2791 | C | N3-C2-O2 | -7.51 | 116.64 | 121.90 |
| 1 | AA | 77 | G | N3-C2-N2 | 7.51 | 125.16 | 119.90 |
| 23 | BA | 265 | A | C8-N9-C4 | -7.51 | 102.80 | 105.80 |
| 23 | BA | 188 | G | N9-C4-C5 | -7.51 | 102.40 | 105.40 |
| 23 | BA | 452 | G | N1-C6-O6 | -7.51 | 115.40 | 119.90 |
| 23 | BA | 1108 | U | N1-C2-O2 | 7.50 | 128.05 | 122.80 |
| 23 | DA | 2241 | A | C2-N3-C4 | -7.50 | 106.85 | 110.60 |
| 23 | DA | 2306 | C | C2-N1-C1' | 7.50 | 127.05 | 118.80 |
| 23 | BA | 1616 | A | C5-C6-N6 | -7.50 | 117.70 | 123.70 |
| 23 | DA | 1950 | G | C4-C5-N7 | -7.50 | 107.80 | 110.80 |
| 23 | BA | 533 | G | N3-C2-N2 | -7.50 | 114.65 | 119.90 |
| 23 | BA | 664 | C | C6-N1-C2 | 7.50 | 123.30 | 120.30 |
| 23 | BA | 577 | G | C2-N3-C4 | -7.50 | 108.15 | 111.90 |
| 23 | BA | 1047 | G | N3-C2-N2 | 7.50 | 125.15 | 119.90 |
| 23 | BA | 62 | C | C6-N1-C2 | 7.49 | 123.30 | 120.30 |
| 23 | BA | 1616 | A | N1-C6-N6 | 7.49 | 123.10 | 118.60 |
| 23 | DA | 1800 | C | C5-C6-N1 | -7.49 | 117.25 | 121.00 |
| 1 | CA | 691 | G | C8-N9-C4 | 7.49 | 109.40 | 106.40 |
| 23 | BA | 893 | C | N1-C2-O2 | 7.49 | 123.39 | 118.90 |
| 1 | CA | 1030 | C | N1-C2-O2 | 7.49 | 123.39 | 118.90 |
| 23 | DA | 51 | G | N1-C6-O6 | -7.49 | 115.41 | 119.90 |
| 1 | CA | 1343 | G | C6-C5-N7 | -7.49 | 125.91 | 130.40 |
| 1 | CA | 1003 | G | N9-C4-C5 | 7.48 | 108.39 | 105.40 |
| 1 | CA | 1165 | C | C5-C4-N4 | 7.48 | 125.44 | 120.20 |
| 23 | DA | 2206 | G | C4-N9-C1' | -7.48 | 116.78 | 126.50 |
| 1 | AA | 1241 | G | C8-N9-C4 | -7.48 | 103.41 | 106.40 |
| 23 | DA | 945 | A | C4-C5-N7 | 7.47 | 114.44 | 110.70 |
| 23 | DA | 2182 | G | N3-C4-N9 | -7.47 | 121.52 | 126.00 |
| 1 | AA | 1158 | C | C6-N1-C2 | -7.47 | 117.31 | 120.30 |
| 23 | BA | 1162 | G | C8-N9-C4 | -7.47 | 103.41 | 106.40 |
| 24 | BB | 37 | C | C6-N1-C2 | -7.47 | 117.31 | 120.30 |
| 23 | DA | 1415 | U | C5-C6-N1 | -7.47 | 118.96 | 122.70 |
| 1 | CA | 1184 | G | C5-C6-O6 | 7.47 | 133.08 | 128.60 |
| 1 | AA | 1442 | G | C8-N9-C4 | 7.47 | 109.39 | 106.40 |
| 23 | BA | 675 | A | C4-C5-N7 | 7.47 | 114.43 | 110.70 |
| 23 | DA | 71 | A | N1-C6-N6 | 7.46 | 123.08 | 118.60 |
| 23 | DA | 1021 | A | C5-C6-N1 | -7.46 | 113.97 | 117.70 |
| 23 | BA | 2449 | U | N3-C4-O4 | 7.46 | 124.62 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 141 | A | C8-N9-C4 | -7.45 | 102.82 | 105.80 |
| 1 | CA | 1263 | C | C5-C4-N4 | -7.45 | 114.98 | 120.20 |
| 23 | BA | 386 | G | C4-C5-N7 | 7.45 | 113.78 | 110.80 |
| 23 | BA | 562 | U | N1-C2-N3 | 7.45 | 119.37 | 114.90 |
| 1 | AA | 372 | C | C6-N1-C2 | 7.45 | 123.28 | 120.30 |
| 23 | BA | 2711 | A | C8-N9-C4 | 7.45 | 108.78 | 105.80 |
| 23 | DA | 2346 | A | C6-N1-C2 | -7.45 | 114.13 | 118.60 |
| 1 | AA | 1310 | G | N3-C4-C5 | 7.45 | 132.32 | 128.60 |
| 1 | CA | 1336 | C | C6-N1-C2 | -7.45 | 117.32 | 120.30 |
| 23 | DA | 751 | A | C8-N9-C4 | 7.44 | 108.78 | 105.80 |
| 23 | DA | 1005 | C | C6-N1-C2 | 7.44 | 123.28 | 120.30 |
| 1 | AA | 1502 | A | C2-N3-C4 | -7.44 | 106.88 | 110.60 |
| 1 | AA | 948 | C | C5-C6-N1 | 7.44 | 124.72 | 121.00 |
| 23 | BA | 652(T) | C | C2-N3-C4 | 7.44 | 123.62 | 119.90 |
| 23 | BA | 1582 | C | N3-C2-O2 | -7.43 | 116.70 | 121.90 |
| 1 | CA | 1108 | G | C5-C6-O6 | 7.43 | 133.06 | 128.60 |
| 23 | BA | 574 | C | C5-C6-N1 | 7.43 | 124.72 | 121.00 |
| 23 | BA | 2893 | G | C2-N3-C4 | 7.43 | 115.61 | 111.90 |
| 23 | BA | 1901 | A | N1-C6-N6 | -7.43 | 114.14 | 118.60 |
| 23 | BA | 810 | U | N1-C2-O2 | -7.42 | 117.60 | 122.80 |
| 23 | BA | 933 | A | C8-N9-C4 | -7.42 | 102.83 | 105.80 |
| 23 | DA | 2307 | G | N7-C8-N9 | 7.42 | 116.81 | 113.10 |
| 1 | AA | 971 | G | C8-N9-C4 | -7.42 | 103.43 | 106.40 |
| 1 | AA | 1012 | U | N3-C2-O2 | 7.42 | 127.39 | 122.20 |
| 23 | BA | 2464 | C | C6-N1-C1' | -7.42 | 111.90 | 120.80 |
| 1 | AA | 1120 | G | N3-C4-N9 | 7.42 | 130.45 | 126.00 |
| 23 | DA | 727 | A | N1-C6-N6 | 7.42 | 123.05 | 118.60 |
| 1 | AA | 1124 | G | N3-C4-N9 | 7.41 | 130.45 | 126.00 |
| 23 | DA | 1026 | U | N1-C2-O2 | 7.41 | 127.99 | 122.80 |
| 23 | DA | 1779 | U | C6-N1-C2 | 7.41 | 125.44 | 121.00 |
| 1 | CA | 998 | G | C4-C5-N7 | -7.41 | 107.84 | 110.80 |
| 23 | BA | 209 | C | C6-N1-C2 | 7.41 | 123.26 | 120.30 |
| 1 | CA | 577 | G | C8-N9-C4 | 7.41 | 109.36 | 106.40 |
| 23 | DA | 2013 | A | C8-N9-C4 | 7.41 | 108.76 | 105.80 |
| 23 | DA | 2322 | A | C4-C5-N7 | -7.41 | 107.00 | 110.70 |
| 1 | AA | 1207 | G | C5-C6-O6 | -7.40 | 124.16 | 128.60 |
| 23 | BA | 1994 | C | N3-C4-N4 | -7.40 | 112.82 | 118.00 |
| 23 | BA | 2286 | A | C4-C5-N7 | 7.40 | 114.40 | 110.70 |
| 23 | DA | 1698 | A | C8-N9-C4 | -7.40 | 102.84 | 105.80 |
| 23 | DA | 528 | A | C6-N1-C2 | 7.40 | 123.04 | 118.60 |
| 23 | DA | 2700 | C | C6-N1-C2 | 7.40 | 123.26 | 120.30 |
| 1 | AA | 53 | A | N1-C2-N3 | -7.40 | 125.60 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 769 | G | C8-N9-C4 | 7.40 | 109.36 | 106.40 |
| 4 | AD | 26 | CYS | CA-CB-SG | 7.40 | 127.31 | 114.00 |
| 23 | DA | 932 | G | N3-C4-N9 | -7.39 | 121.56 | 126.00 |
| 23 | BA | 463 | G | N9-C4-C5 | 7.39 | 108.36 | 105.40 |
| 1 | CA | 972 | C | C5-C6-N1 | 7.39 | 124.70 | 121.00 |
| 23 | BA | 1653 | G | N3-C4-C5 | -7.39 | 124.91 | 128.60 |
| 23 | DA | 516 | C | C6-N1-C2 | -7.39 | 117.34 | 120.30 |
| 23 | DA | 1325 | G | C4-C5-N7 | 7.39 | 113.76 | 110.80 |
| 23 | BA | 760 | G | N1-C6-O6 | 7.39 | 124.33 | 119.90 |
| 23 | DA | 1251 | C | N3-C4-C5 | -7.38 | 118.95 | 121.90 |
| 23 | DA | 2307 | G | C8-N9-C4 | -7.38 | 103.45 | 106.40 |
| 23 | BA | 1258 | C | N3-C4-C5 | 7.38 | 124.85 | 121.90 |
| 23 | BA | 2335 | A | C8-N9-C4 | 7.38 | 108.75 | 105.80 |
| 23 | DA | 847 | U | N3-C2-O2 | -7.38 | 117.04 | 122.20 |
| 1 | CA | 1063 | C | C5-C6-N1 | 7.37 | 124.69 | 121.00 |
| 23 | BA | 2018 | G | C8-N9-C4 | -7.37 | 103.45 | 106.40 |
| 23 | DA | 1663 | C | C2-N3-C4 | -7.37 | 116.21 | 119.90 |
| 1 | CA | 946 | A | C6-N1-C2 | -7.37 | 114.18 | 118.60 |
| 23 | DA | 1776 | G | N9-C4-C5 | -7.37 | 102.45 | 105.40 |
| 23 | BA | 2785 | C | C6-N1-C2 | -7.36 | 117.36 | 120.30 |
| 1 | CA | 47 | C | N3-C2-O2 | 7.36 | 127.05 | 121.90 |
| 23 | BA | 1301 | A | C8-N9-C4 | -7.36 | 102.86 | 105.80 |
| 23 | BA | 1558 | A | C8-N9-C4 | 7.36 | 108.74 | 105.80 |
| 1 | CA | 1163 | C | C5-C6-N1 | 7.35 | 124.68 | 121.00 |
| 23 | DA | 2077 | A | C5-C6-N1 | 7.35 | 121.38 | 117.70 |
| 23 | DA | 665 | C | N3-C4-C5 | 7.35 | 124.84 | 121.90 |
| 1 | CA | 1120 | G | N3-C4-N9 | -7.35 | 121.59 | 126.00 |
| 23 | BA | 2312 | U | N3-C2-O2 | -7.35 | 117.06 | 122.20 |
| 23 | DA | 787 | U | C5-C4-O4 | 7.35 | 130.31 | 125.90 |
| 23 | DA | 936 | C | C6-N1-C2 | 7.35 | 123.24 | 120.30 |
| 23 | BA | 1990 | C | N1-C2-O2 | -7.35 | 114.49 | 118.90 |
| 1 | AA | 970 | C | N1-C2-O2 | 7.34 | 123.31 | 118.90 |
| 23 | BA | 1937 | A | N1-C2-N3 | 7.34 | 132.97 | 129.30 |
| 23 | DA | 569 | U | C5-C4-O4 | -7.34 | 121.49 | 125.90 |
| 23 | DA | 2247 | A | C2-N3-C4 | -7.34 | 106.93 | 110.60 |
| 23 | BA | 362 | U | C5-C4-O4 | -7.34 | 121.50 | 125.90 |
| 23 | BA | 2041 | U | C4-C5-C6 | 7.34 | 124.10 | 119.70 |
| 23 | DA | 2593 | U | C5-C4-O4 | 7.33 | 130.30 | 125.90 |
| 1 | CA | 1446 | U | C5-C4-O4 | -7.33 | 121.50 | 125.90 |
| 23 | DA | 263 | C | N1-C2-O2 | 7.33 | 123.30 | 118.90 |
| 23 | DA | 764 | A | C6-N1-C2 | 7.33 | 123.00 | 118.60 |
| 23 | DA | 1974 | C | C6-N1-C2 | 7.33 | 123.23 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2375 | G | N7-C8-N9 | -7.33 | 109.44 | 113.10 |
| 1 | AA | 991 | U | C5-C6-N1 | 7.33 | 126.36 | 122.70 |
| 23 | BA | 2689 | U | C5-C6-N1 | -7.33 | 119.04 | 122.70 |
| 23 | BA | 1815 | A | N1-C6-N6 | -7.33 | 114.20 | 118.60 |
| 1 | CA | 1124 | G | C5-C6-N1 | -7.33 | 107.84 | 111.50 |
| 1 | CA | 1231 | G | N3-C4-C5 | -7.33 | 124.94 | 128.60 |
| 23 | BA | 265 | A | C2-N3-C4 | -7.32 | 106.94 | 110.60 |
| 1 | AA | 1258 | G | C5-C6-O6 | 7.32 | 132.99 | 128.60 |
| 23 | BA | 1123 | C | C6-N1-C2 | 7.32 | 123.23 | 120.30 |
| 23 | DA | 570 | G | C8-N9-C4 | 7.32 | 109.33 | 106.40 |
| 23 | BA | 736 | C | C5-C4-N4 | -7.32 | 115.08 | 120.20 |
| 1 | CA | 460 | G | N7-C8-N9 | 7.32 | 116.76 | 113.10 |
| 1 | CA | 1352 | C | N3-C2-O2 | -7.32 | 116.78 | 121.90 |
| 23 | BA | 211 | A | C8-N9-C4 | 7.31 | 108.72 | 105.80 |
| 23 | BA | 673 | C | C6-N1-C2 | 7.31 | 123.22 | 120.30 |
| 23 | DA | 1655 | A | C8-N9-C4 | 7.31 | 108.72 | 105.80 |
| 1 | CA | 1442 | G | C5-N7-C8 | 7.31 | 107.95 | 104.30 |
| 23 | BA | 124 | G | C2-N3-C4 | -7.31 | 108.25 | 111.90 |
| 23 | BA | 674 | G | N1-C6-O6 | 7.30 | 124.28 | 119.90 |
| 23 | BA | 271(M) | G | N3-C4-C5 | -7.30 | 124.95 | 128.60 |
| 23 | DA | 1405 | U | C5-C6-N1 | -7.30 | 119.05 | 122.70 |
| 1 | AA | 346 | G | N1-C2-N2 | -7.30 | 109.63 | 116.20 |
| 23 | BA | 777 | A | C2-N3-C4 | 7.30 | 114.25 | 110.60 |
| 23 | DA | 2338 | G | N1-C6-O6 | 7.29 | 124.28 | 119.90 |
| 23 | BA | 1819 | A | N1-C6-N6 | -7.29 | 114.23 | 118.60 |
| 23 | BA | 117 | G | N1-C2-N2 | -7.29 | 109.64 | 116.20 |
| 23 | BA | 2321 | G | N9-C4-C5 | 7.28 | 108.31 | 105.40 |
| 23 | BA | 975 | C | N3-C4-C5 | -7.27 | 118.99 | 121.90 |
| 23 | BA | 1471 | A | C8-N9-C4 | -7.27 | 102.89 | 105.80 |
| 23 | BA | 1963 | U | C2-N1-C1' | 7.27 | 126.43 | 117.70 |
| 23 | DA | 2015 | A | N1-C6-N6 | -7.27 | 114.24 | 118.60 |
| 23 | DA | 679 | C | C2-N3-C4 | -7.27 | 116.27 | 119.90 |
| 23 | BA | 47 | C | N3-C4-C5 | 7.26 | 124.81 | 121.90 |
| 23 | BA | 933 | A | N7-C8-N9 | 7.26 | 117.43 | 113.80 |
| 23 | DA | 2070 | G | C5-C6-N1 | 7.26 | 115.13 | 111.50 |
| 23 | DA | 2293 | C | C6-N1-C2 | 7.26 | 123.20 | 120.30 |
| 23 | BA | 2840 | C | N3-C4-C5 | 7.26 | 124.80 | 121.90 |
| 23 | DA | 2501 | C | N3-C4-C5 | 7.26 | 124.80 | 121.90 |
| 23 | DA | 2571 | C | N1-C2-O2 | -7.26 | 114.54 | 118.90 |
| 23 | BA | 135 | G | C8-N9-C4 | 7.26 | 109.30 | 106.40 |
| 23 | BA | 1204 | A | C5-N7-C8 | -7.26 | 100.27 | 103.90 |
| 23 | BA | 2296 | U | C4-C5-C6 | 7.26 | 124.05 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | AA | 79 | G | C5-C6-O6 | -7.25 | 124.25 | 128.60 |
| 1 | AA | 435 | C | N1-C2-O2 | 7.25 | 123.25 | 118.90 |
| 23 | DA | 71 | A | C8-N9-C4 | -7.25 | 102.90 | 105.80 |
| 1 | AA | 930 | C | C5-C6-N1 | -7.25 | 117.38 | 121.00 |
| 1 | AA | 955 | U | C5-C6-N1 | 7.25 | 126.33 | 122.70 |
| 1 | AA | 1258 | G | C6-N1-C2 | 7.25 | 129.45 | 125.10 |
| 1 | CA | 1124 | G | N1-C2-N2 | -7.25 | 109.67 | 116.20 |
| 23 | DA | 308 | G | C8-N9-C4 | -7.25 | 103.50 | 106.40 |
| 23 | BA | 102 | G | C4-N9-C1' | 7.25 | 135.92 | 126.50 |
| 23 | BA | 745 | G | C6-N1-C2 | -7.25 | 120.75 | 125.10 |
| 23 | DA | 141 | A | C4-C5-N7 | 7.24 | 114.32 | 110.70 |
| 23 | BA | 1367 | A | C8-N9-C4 | 7.24 | 108.70 | 105.80 |
| 1 | AA | 1059 | C | C6-N1-C2 | -7.24 | 117.41 | 120.30 |
| 23 | BA | 1359 | A | N9-C4-C5 | 7.24 | 108.69 | 105.80 |
| 1 | CA | 299 | G | N3-C4-C5 | 7.24 | 132.22 | 128.60 |
| 24 | BB | 104 | U | C2-N3-C4 | -7.24 | 122.66 | 127.00 |
| 23 | DA | 1815 | A | N1-C6-N6 | -7.24 | 114.26 | 118.60 |
| 23 | BA | 765 | G | N1-C6-O6 | 7.24 | 124.24 | 119.90 |
| 23 | BA | 1334 | G | C8-N9-C4 | -7.24 | 103.51 | 106.40 |
| 1 | CA | 1126 | U | N1-C2-O2 | 7.24 | 127.86 | 122.80 |
| 1 | CA | 1502 | A | N1-C6-N6 | 7.24 | 122.94 | 118.60 |
| 23 | DA | 271(J) | C | C6-N1-C2 | 7.24 | 123.19 | 120.30 |
| 1 | AA | 1033 | G | N3-C4-N9 | 7.23 | 130.34 | 126.00 |
| 23 | BA | 2206 | G | C8-N9-C1' | 7.23 | 136.40 | 127.00 |
| 23 | DA | 1391 | U | N1-C2-O2 | 7.23 | 127.86 | 122.80 |
| 23 | DA | 2144 | U | C5-C6-N1 | 7.23 | 126.32 | 122.70 |
| 23 | DA | 265 | A | N7-C8-N9 | 7.23 | 117.42 | 113.80 |
| 23 | BA | 570 | G | C4-C5-N7 | 7.23 | 113.69 | 110.80 |
| 23 | DA | 1654 | A | N1-C6-N6 | -7.23 | 114.26 | 118.60 |
| 23 | DA | 657 | U | C5-C6-N1 | -7.23 | 119.09 | 122.70 |
| 23 | DA | 1779 | U | N3-C4-C5 | 7.23 | 118.94 | 114.60 |
| 23 | DA | 2277 | G | C4-C5-N7 | -7.23 | 107.91 | 110.80 |
| 23 | BA | 1555 | G | N1-C6-O6 | 7.22 | 124.23 | 119.90 |
| 1 | CA | 1502 | A | C2-N3-C4 | -7.22 | 106.99 | 110.60 |
| 23 | DA | 760 | G | C4-C5-N7 | 7.22 | 113.69 | 110.80 |
| 23 | BA | 2361 | A | N1-C6-N6 | 7.22 | 122.93 | 118.60 |
| 23 | DA | 265 | A | C8-N9-C4 | -7.22 | 102.91 | 105.80 |
| 1 | AA | 28 | G | N1-C6-O6 | 7.21 | 124.23 | 119.90 |
| 1 | AA | 345 | C | C6-N1-C2 | 7.21 | 123.19 | 120.30 |
| 23 | BA | 2015 | A | N9-C4-C5 | 7.21 | 108.69 | 105.80 |
| 1 | CA | 936 | C | C5-C4-N4 | -7.21 | 115.15 | 120.20 |
| 1 | AA | 1174 | G | N7-C8-N9 | -7.21 | 109.50 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 446 | G | N1-C6-O6 | 7.21 | 124.22 | 119.90 |
| 23 | DA | 2821 | A | N9-C4-C5 | -7.21 | 102.92 | 105.80 |
| 23 | BA | 1189 | A | N1-C6-N6 | 7.20 | 122.92 | 118.60 |
| 23 | DA | 1698 | A | C2-N3-C4 | -7.20 | 107.00 | 110.60 |
| 23 | BA | 207 | A | N3-C4-C5 | 7.20 | 131.84 | 126.80 |
| 23 | BA | 733 | G | C5-N7-C8 | 7.20 | 107.90 | 104.30 |
| 23 | BA | 747 | U | C5-C4-O4 | -7.20 | 121.58 | 125.90 |
| 23 | DA | 2878 | U | N1-C2-O2 | 7.19 | 127.83 | 122.80 |
| 23 | BA | 2017 | U | N3-C2-O2 | -7.19 | 117.17 | 122.20 |
| 23 | DA | 1142(A) | A | N3-C4-N9 | -7.19 | 121.65 | 127.40 |
| 23 | DA | 912 | C | C6-N1-C2 | -7.19 | 117.43 | 120.30 |
| 23 | DA | 2598 | A | N1-C6-N6 | 7.19 | 122.91 | 118.60 |
| 23 | DA | 1790 | C | N1-C2-O2 | -7.18 | 114.59 | 118.90 |
| 23 | BA | 1992 | G | N1-C6-O6 | -7.18 | 115.59 | 119.90 |
| 23 | DA | 1049 | C | C2-N1-C1' | 7.18 | 126.70 | 118.80 |
| 23 | DA | 2318 | G | C8-N9-C4 | -7.18 | 103.53 | 106.40 |
| 23 | BA | 777 | A | C4-C5-N7 | -7.18 | 107.11 | 110.70 |
| 23 | BA | 2028 | U | C6-N1-C2 | 7.18 | 125.31 | 121.00 |
| 1 | CA | 1124 | G | C6-N1-C2 | 7.18 | 129.41 | 125.10 |
| 23 | DA | 583 | G | N1-C6-O6 | 7.18 | 124.21 | 119.90 |
| 23 | DA | 1698 | A | C6-C5-N7 | -7.17 | 127.28 | 132.30 |
| 1 | AA | 1059 | C | C5-C4-N4 | 7.17 | 125.22 | 120.20 |
| 23 | DA | 735 | A | N7-C8-N9 | -7.17 | 110.22 | 113.80 |
| 23 | DA | 2803 | C | C5-C6-N1 | 7.17 | 124.58 | 121.00 |
| 23 | BA | 2251 | G | N3-C4-C5 | -7.17 | 125.02 | 128.60 |
| 23 | DA | 2162 | G | C2-N3-C4 | 7.16 | 115.48 | 111.90 |
| 23 | BA | 2312 | U | N1-C2-O2 | 7.16 | 127.81 | 122.80 |
| 23 | BA | 2316 | C | C6-N1-C2 | -7.16 | 117.44 | 120.30 |
| 1 | CA | 21 | G | N1-C6-O6 | -7.16 | 115.61 | 119.90 |
| 23 | BA | 2041 | U | C5-C6-N1 | -7.15 | 119.12 | 122.70 |
| 44 | B0 | 20 | ARG | NE-CZ-NH1 | -7.15 | 116.72 | 120.30 |
| 1 | AA | 1100 | C | C6-N1-C2 | 7.15 | 123.16 | 120.30 |
| 23 | BA | 330 | A | C5-N7-C8 | -7.15 | 100.33 | 103.90 |
| 23 | BA | 570 | G | C5-C6-O6 | -7.15 | 124.31 | 128.60 |
| 23 | BA | 2182 | G | N3-C4-N9 | -7.15 | 121.71 | 126.00 |
| 1 | CA | 1149 | C | C2-N3-C4 | 7.15 | 123.47 | 119.90 |
| 23 | BA | 652(E) | G | C6-N1-C2 | 7.14 | 129.39 | 125.10 |
| 1 | AA | 1297 | C | C5-C6-N1 | 7.14 | 124.57 | 121.00 |
| 23 | BA | 575 | A | N1-C2-N3 | 7.14 | 132.87 | 129.30 |
| 23 | DA | 280 | C | C6-N1-C2 | -7.14 | 117.44 | 120.30 |
| 23 | BA | 500 | G | C4-C5-N7 | -7.14 | 107.94 | 110.80 |
| 23 | BA | 2335 | A | C6-N1-C2 | -7.14 | 114.32 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | CA | 91 | C | C5-C6-N1 | 7.14 | 124.57 | 121.00 |
| 1 | CA | 1029 | C | C5-C4-N4 | 7.14 | 125.20 | 120.20 |
| 23 | DA | 679 | C | N1-C2-O2 | -7.14 | 114.62 | 118.90 |
| 1 | CA | 1284 | C | C6-N1-C2 | -7.14 | 117.45 | 120.30 |
| 23 | BA | 675 | A | N9-C4-C5 | -7.13 | 102.95 | 105.80 |
| 23 | BA | 1189 | A | C5-N7-C8 | -7.13 | 100.33 | 103.90 |
| 1 | CA | 1502 | A | N1-C2-N3 | 7.13 | 132.87 | 129.30 |
| 23 | BA | 2020 | A | C8-N9-C4 | 7.13 | 108.65 | 105.80 |
| 23 | DA | 751 | A | N7-C8-N9 | -7.12 | 110.24 | 113.80 |
| 23 | BA | 1610 | A | N1-C6-N6 | 7.12 | 122.87 | 118.60 |
| 23 | DA | 123 | G | N7-C8-N9 | -7.12 | 109.54 | 113.10 |
| 23 | BA | 676 | A | C6-N1-C2 | 7.12 | 122.87 | 118.60 |
| 23 | BA | 386 | G | N7-C8-N9 | 7.12 | 116.66 | 113.10 |
| 23 | BA | 1107 | G | N3-C4-C5 | -7.12 | 125.04 | 128.60 |
| 23 | DA | 1807 | G | C5-C6-O6 | -7.12 | 124.33 | 128.60 |
| 1 | AA | 1029 | C | C2-N1-C1' | -7.11 | 110.97 | 118.80 |
| 1 | AA | 1198 | G | N1-C6-O6 | -7.11 | 115.63 | 119.90 |
| 23 | BA | 910 | A | N9-C4-C5 | -7.11 | 102.95 | 105.80 |
| 1 | CA | 27 | G | N1-C6-O6 | 7.11 | 124.17 | 119.90 |
| 1 | CA | 839 | U | C2-N1-C1' | 7.11 | 126.24 | 117.70 |
| 1 | CA | 991 | U | N1-C2-O2 | 7.11 | 127.78 | 122.80 |
| 1 | CA | 1024 | G | C4-C5-N7 | 7.11 | 113.64 | 110.80 |
| 1 | CA | 909 | A | N1-C6-N6 | 7.11 | 122.87 | 118.60 |
| 23 | DA | 1558 | A | C2-N3-C4 | -7.11 | 107.04 | 110.60 |
| 23 | DA | 2315 | G | C8-N9-C4 | 7.11 | 109.24 | 106.40 |
| 23 | BA | 1992 | G | N3-C4-C5 | -7.11 | 125.05 | 128.60 |
| 1 | AA | 1442(B) | A | C8-N9-C4 | -7.11 | 102.96 | 105.80 |
| 23 | DA | 530 | G | C5-C6-N1 | 7.11 | 115.05 | 111.50 |
| 23 | BA | 1790 | C | N1-C2-O2 | -7.11 | 114.64 | 118.90 |
| 23 | BA | 2761 | G | C8-N9-C4 | -7.10 | 103.56 | 106.40 |
| 1 | CA | 529 | G | C6-C5-N7 | -7.10 | 126.14 | 130.40 |
| 23 | BA | 691 | C | N3-C4-C5 | 7.10 | 124.74 | 121.90 |
| 36 | DS | 96 | GLY | N-CA-C | -7.10 | 95.35 | 113.10 |
| 23 | BA | 1604 | C | N3-C2-O2 | 7.10 | 126.87 | 121.90 |
| 1 | CA | 936 | C | C6-N1-C1' | -7.10 | 112.28 | 120.80 |
| 23 | BA | 1180 | C | C6-N1-C2 | 7.10 | 123.14 | 120.30 |
| 1 | AA | 444 | C | C6-N1-C2 | 7.10 | 123.14 | 120.30 |
| 23 | BA | 702 | G | C2-N3-C4 | -7.10 | 108.35 | 111.90 |
| 23 | BA | 1045 | A | C2-N3-C4 | 7.09 | 114.15 | 110.60 |
| 23 | BA | 2755 | C | C5-C6-N1 | 7.09 | 124.55 | 121.00 |
| 23 | BA | 536 | A | C8-N9-C4 | 7.09 | 108.64 | 105.80 |
| 1 | CA | 940 | C | C5-C6-N1 | 7.09 | 124.54 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 681 | C | C6-N1-C2 | 7.09 | 123.13 | 120.30 |
| 23 | BA | 1951 | U | N3-C4-C5 | -7.08 | 110.35 | 114.60 |
| 23 | DA | 94 | C | C2-N1-C1' | 7.08 | 126.59 | 118.80 |
| 23 | BA | 595 | C | N3-C4-N4 | 7.08 | 122.96 | 118.00 |
| 23 | DA | 2312 | U | C6-N1-C2 | -7.08 | 116.75 | 121.00 |
| 23 | BA | 2251 | G | N9-C4-C5 | 7.08 | 108.23 | 105.40 |
| 23 | DA | 676 | A | N3-C4-N9 | -7.08 | 121.74 | 127.40 |
| 23 | DA | 2791 | C | C2-N1-C1' | 7.08 | 126.58 | 118.80 |
| 23 | BA | 1681 | G | C4-C5-N7 | 7.07 | 113.63 | 110.80 |
| 23 | DA | 535 | C | N1-C2-O2 | -7.07 | 114.66 | 118.90 |
| 24 | BB | 89 | G | C5-C6-O6 | -7.07 | 124.36 | 128.60 |
| 23 | DA | 729 | G | N3-C2-N2 | -7.07 | 114.95 | 119.90 |
| 23 | DA | 2251 | G | C8-N9-C4 | -7.07 | 103.57 | 106.40 |
| 23 | DA | 2361 | A | N1-C6-N6 | 7.07 | 122.84 | 118.60 |
| 23 | BA | 2319 | G | N7-C8-N9 | 7.06 | 116.63 | 113.10 |
| 23 | DA | 330 | A | C4-C5-N7 | 7.06 | 114.23 | 110.70 |
| 23 | DA | 1325 | G | C5-C6-O6 | -7.06 | 124.36 | 128.60 |
| 1 | CA | 460 | G | C8-N9-C4 | -7.06 | 103.58 | 106.40 |
| 1 | CA | 942 | G | C5-C6-O6 | 7.06 | 132.84 | 128.60 |
| 23 | BA | 1698 | A | N1-C2-N3 | 7.06 | 132.83 | 129.30 |
| 23 | DA | 2437 | U | C5-C4-O4 | 7.06 | 130.13 | 125.90 |
| 23 | BA | 90 | U | N3-C4-O4 | 7.06 | 124.34 | 119.40 |
| 24 | DB | 6 | C | C6-N1-C2 | 7.05 | 123.12 | 120.30 |
| 23 | DA | 774 | A | C8-N9-C4 | -7.05 | 102.98 | 105.80 |
| 1 | CA | 163 | C | N3-C4-C5 | -7.05 | 119.08 | 121.90 |
| 23 | BA | 2503 | A | N1-C2-N3 | -7.05 | 125.78 | 129.30 |
| 23 | DA | 728 | G | N9-C4-C5 | -7.05 | 102.58 | 105.40 |
| 23 | DA | 791 | C | C5-C6-N1 | -7.04 | 117.48 | 121.00 |
| 23 | BA | 1745 | C | N1-C2-O2 | -7.04 | 114.67 | 118.90 |
| 1 | CA | 442 | C | C6-N1-C2 | -7.04 | 117.48 | 120.30 |
| 23 | BA | 1989 | G | N1-C6-O6 | 7.04 | 124.12 | 119.90 |
| 23 | DA | 893 | C | N1-C2-O2 | 7.04 | 123.12 | 118.90 |
| 23 | BA | 821 | A | C8-N9-C4 | -7.03 | 102.99 | 105.80 |
| 23 | BA | 1243 | G | C4-C5-N7 | 7.03 | 113.61 | 110.80 |
| 23 | BA | 2609 | U | N1-C2-O2 | -7.03 | 117.88 | 122.80 |
| 1 | AA | 266 | G | C8-N9-C4 | 7.03 | 109.21 | 106.40 |
| 23 | BA | 148 | C | C2-N3-C4 | -7.03 | 116.39 | 119.90 |
| 23 | BA | 1229 | G | N1-C6-O6 | 7.03 | 124.12 | 119.90 |
| 1 | CA | 1230 | C | C5-C6-N1 | 7.03 | 124.51 | 121.00 |
| 23 | DA | 1566 | A | N1-C6-N6 | 7.03 | 122.82 | 118.60 |
| 23 | BA | 1776 | G | C8-N9-C4 | 7.03 | 109.21 | 106.40 |
| 23 | BA | 884 | C | C6-N1-C2 | -7.02 | 117.49 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1940 | U | N3-C4-O4 | 7.02 | 124.32 | 119.40 |
| 1 | CA | 1330 | U | N1-C2-O2 | 7.02 | 127.72 | 122.80 |
| 23 | BA | 1835 | G | C8-N9-C4 | -7.02 | 103.59 | 106.40 |
| 23 | BA | 1249 | U | N1-C2-O2 | -7.02 | 117.89 | 122.80 |
| 1 | CA | 1045 | C | C2-N3-C4 | 7.02 | 123.41 | 119.90 |
| 23 | BA | 141 | A | C2-N3-C4 | -7.02 | 107.09 | 110.60 |
| 23 | BA | 271(A) | A | C8-N9-C4 | 7.02 | 108.61 | 105.80 |
| 1 | CA | 936 | C | N1-C2-O2 | 7.02 | 123.11 | 118.90 |
| 23 | DA | 1372 | U | N3-C2-O2 | -7.02 | 117.29 | 122.20 |
| 23 | BA | 1358 | G | N1-C6-O6 | -7.02 | 115.69 | 119.90 |
| 23 | DA | 587 | C | N3-C4-C5 | -7.02 | 119.09 | 121.90 |
| 23 | BA | 1784 | A | C8-N9-C4 | 7.02 | 108.61 | 105.80 |
| 23 | BA | 2073 | C | C5-C6-N1 | -7.01 | 117.49 | 121.00 |
| 23 | BA | 673 | C | N3-C4-C5 | 7.01 | 124.70 | 121.90 |
| 1 | AA | 1162 | C | C6-N1-C2 | 7.01 | 123.10 | 120.30 |
| 23 | BA | 2351 | G | C8-N9-C1' | -7.01 | 117.89 | 127.00 |
| 23 | BA | 2100 | G | N3-C4-C5 | -7.01 | 125.10 | 128.60 |
| 23 | BA | 2307 | G | C8-N9-C4 | -7.01 | 103.60 | 106.40 |
| 1 | CA | 1321 | C | N3-C4-C5 | -7.01 | 119.10 | 121.90 |
| 23 | DA | 1762 | A | C2-N3-C4 | 7.00 | 114.10 | 110.60 |
| 23 | DA | 2324 | C | C6-N1-C2 | 7.00 | 123.10 | 120.30 |
| 1 | AA | 1165 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 1 | CA | 1177 | G | N7-C8-N9 | 7.00 | 116.60 | 113.10 |
| 23 | DA | 41 | C | C5-C6-N1 | -7.00 | 117.50 | 121.00 |
| 23 | DA | 154(A) | C | N3-C4-N4 | -7.00 | 113.10 | 118.00 |
| 23 | DA | 2182 | G | C8-N9-C1' | 7.00 | 136.10 | 127.00 |
| 23 | BA | 729 | G | C8-N9-C4 | -7.00 | 103.60 | 106.40 |
| 23 | BA | 1343 | G | C5-N7-C8 | -7.00 | 100.80 | 104.30 |
| 1 | CA | 52 | G | N1-C6-O6 | -7.00 | 115.70 | 119.90 |
| 23 | DA | 1653 | G | N3-C4-C5 | -7.00 | 125.10 | 128.60 |
| 23 | BA | 102 | G | N7-C8-N9 | 7.00 | 116.60 | 113.10 |
| 23 | BA | 729 | G | N7-C8-N9 | 7.00 | 116.60 | 113.10 |
| 23 | DA | 2353 | G | C8-N9-C4 | 6.99 | 109.20 | 106.40 |
| 1 | AA | 1074 | G | C5-C6-O6 | -6.99 | 124.41 | 128.60 |
| 23 | BA | 362 | U | C2-N3-C4 | -6.99 | 122.81 | 127.00 |
| 23 | BA | 1558 | A | C2-N3-C4 | -6.99 | 107.11 | 110.60 |
| 1 | CA | 117 | G | C6-C5-N7 | -6.99 | 126.21 | 130.40 |
| 1 | CA | 997 | U | C2-N3-C4 | 6.99 | 131.19 | 127.00 |
| 23 | DA | 1612 | C | C6-N1-C2 | 6.99 | 123.10 | 120.30 |
| 1 | AA | 21 | G | N1-C6-O6 | -6.99 | 115.71 | 119.90 |
| 23 | BA | 1250 | G | N1-C6-O6 | 6.99 | 124.09 | 119.90 |
| 23 | BA | 804 | A | N7-C8-N9 | -6.99 | 110.31 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 391 | G | C6-C5-N7 | -6.99 | 126.21 | 130.40 |
| 1 | AA | 1442 | G | C8-N9-C1' | -6.98 | 117.92 | 127.00 |
| 23 | DA | 1142(A) | A | C5-N7-C8 | -6.98 | 100.41 | 103.90 |
| 1 | AA | 77 | G | N9-C4-C5 | -6.98 | 102.61 | 105.40 |
| 23 | BA | 425 | G | N3-C4-C5 | -6.98 | 125.11 | 128.60 |
| 23 | BA | 1776 | G | N9-C4-C5 | -6.98 | 102.61 | 105.40 |
| 1 | CA | 1350 | A | C8-N9-C4 | -6.98 | 103.01 | 105.80 |
| 23 | DA | 2250 | G | C5-C6-O6 | 6.98 | 132.79 | 128.60 |
| 23 | BA | 1698 | A | N7-C8-N9 | 6.98 | 117.29 | 113.80 |
| 23 | BA | 1628 | G | C8-N9-C4 | -6.98 | 103.61 | 106.40 |
| 23 | BA | 1625 | C | N3-C4-C5 | 6.98 | 124.69 | 121.90 |
| 23 | BA | 1315 | C | C6-N1-C2 | -6.98 | 117.51 | 120.30 |
| 23 | BA | 1643 | G | N1-C6-O6 | -6.97 | 115.72 | 119.90 |
| 23 | DA | 2360 | A | C8-N9-C4 | 6.97 | 108.59 | 105.80 |
| 23 | BA | 767 | U | N3-C2-O2 | -6.97 | 117.32 | 122.20 |
| 23 | DA | 2087 | G | N9-C4-C5 | -6.97 | 102.61 | 105.40 |
| 1 | CA | 1502 | A | N7-C8-N9 | 6.97 | 117.28 | 113.80 |
| 23 | BA | 2191 | G | C5-C6-O6 | -6.96 | 124.42 | 128.60 |
| 23 | BA | 2579 | C | C4-C5-C6 | 6.96 | 120.88 | 117.40 |
| 23 | DA | 2525 | G | N9-C4-C5 | -6.96 | 102.61 | 105.40 |
| 23 | BA | 1184 | G | N3-C2-N2 | -6.96 | 115.03 | 119.90 |
| 23 | BA | 1145 | C | C6-N1-C2 | -6.96 | 117.52 | 120.30 |
| 23 | DA | 102 | G | C4-N9-C1' | 6.96 | 135.55 | 126.50 |
| 23 | BA | 940 | G | N1-C6-O6 | 6.96 | 124.07 | 119.90 |
| 1 | CA | 357 | G | C6-N1-C2 | -6.96 | 120.93 | 125.10 |
| 23 | DA | 2182 | G | C6-C5-N7 | 6.96 | 134.57 | 130.40 |
| 23 | DA | 2420 | C | C5-C4-N4 | -6.96 | 115.33 | 120.20 |
| 1 | AA | 839 | U | C2-N1-C1' | 6.95 | 126.04 | 117.70 |
| 23 | BA | 71 | A | N3-C4-N9 | -6.95 | 121.84 | 127.40 |
| 23 | DA | 1989 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 23 | BA | 33 | U | C2-N1-C1' | -6.95 | 109.36 | 117.70 |
| 23 | DA | 2087 | G | N1-C6-O6 | 6.95 | 124.07 | 119.90 |
| 23 | BA | 690 | G | C5-C6-N1 | 6.95 | 114.97 | 111.50 |
| 23 | BA | 1757 | U | C5-C4-O4 | -6.95 | 121.73 | 125.90 |
| 1 | CA | 1153 | C | C2-N1-C1' | -6.95 | 111.15 | 118.80 |
| 23 | BA | 793 | A | C5-N7-C8 | -6.95 | 100.43 | 103.90 |
| 23 | BA | 975 | C | C5-C4-N4 | 6.95 | 125.06 | 120.20 |
| 1 | AA | 372 | C | N1-C2-O2 | 6.95 | 123.07 | 118.90 |
| 1 | AA | 1120 | G | N9-C4-C5 | -6.94 | 102.62 | 105.40 |
| 1 | AA | 1198 | G | C8-N9-C4 | -6.94 | 103.62 | 106.40 |
| 1 | AA | 998 | G | C5-C6-O6 | 6.94 | 132.76 | 128.60 |
| 23 | BA | 1313 | U | C2-N1-C1' | 6.94 | 126.03 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 2346 | A | C6-N1-C2 | -6.94 | 114.43 | 118.60 |
| 23 | BA | 1340 | U | C5-C6-N1 | -6.94 | 119.23 | 122.70 |
| 23 | BA | 2837 | G | C5-C6-O6 | -6.94 | 124.44 | 128.60 |
| 23 | DA | 750 | A | N1-C2-N3 | 6.94 | 132.77 | 129.30 |
| 1 | AA | 171 | A | C8-N9-C4 | -6.94 | 103.03 | 105.80 |
| 1 | AA | 1150 | U | C5-C4-O4 | 6.94 | 130.06 | 125.90 |
| 23 | BA | 1006 | C | C5-C4-N4 | 6.93 | 125.05 | 120.20 |
| 23 | BA | 575 | A | C2-N3-C4 | -6.93 | 107.13 | 110.60 |
| 23 | DA | 2146 | C | N1-C2-O2 | 6.93 | 123.06 | 118.90 |
| 1 | CA | 1241 | G | N7-C8-N9 | 6.93 | 116.56 | 113.10 |
| 23 | DA | 731 | C | C6-N1-C2 | 6.92 | 123.07 | 120.30 |
| 23 | DA | 2476 | A | C8-N9-C4 | -6.92 | 103.03 | 105.80 |
| 1 | CA | 1457 | G | C5-C6-N1 | 6.92 | 114.96 | 111.50 |
| 23 | DA | 1755 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 1 | AA | 317 | G | N1-C6-O6 | 6.92 | 124.05 | 119.90 |
| 24 | BB | 102 | A | N1-C6-N6 | -6.92 | 114.45 | 118.60 |
| 23 | DA | 2277 | G | C6-C5-N7 | 6.92 | 134.55 | 130.40 |
| 1 | AA | 1263 | C | N1-C2-O2 | 6.92 | 123.05 | 118.90 |
| 23 | BA | 751 | A | C8-N9-C4 | 6.92 | 108.57 | 105.80 |
| 23 | BA | 1210 | A | C4-C5-C6 | 6.92 | 120.46 | 117.00 |
| 23 | BA | 2803 | C | C6-N1-C2 | -6.92 | 117.53 | 120.30 |
| 1 | CA | 713 | G | N1-C6-O6 | -6.92 | 115.75 | 119.90 |
| 23 | DA | 2221 | G | N1-C6-O6 | 6.92 | 124.05 | 119.90 |
| 23 | BA | 1939 | U | N3-C4-C5 | 6.92 | 118.75 | 114.60 |
| 1 | AA | 355 | C | N1-C2-O2 | -6.91 | 114.75 | 118.90 |
| 23 | BA | 2689 | U | N1-C2-N3 | 6.91 | 119.05 | 114.90 |
| 23 | BA | 2728 | U | C5-C6-N1 | -6.91 | 119.25 | 122.70 |
| 1 | CA | 721 | G | N1-C6-O6 | 6.91 | 124.05 | 119.90 |
| 23 | BA | 934 | G | C8-N9-C4 | 6.91 | 109.16 | 106.40 |
| 23 | BA | 2182 | G | C5-C6-O6 | 6.91 | 132.74 | 128.60 |
| 23 | DA | 652(T) | C | C2-N3-C4 | 6.91 | 123.35 | 119.90 |
| 23 | DA | 1372 | U | N1-C2-O2 | 6.91 | 127.63 | 122.80 |
| 23 | DA | 2680 | C | C5-C6-N1 | -6.91 | 117.55 | 121.00 |
| 23 | DA | 122 | G | C6-C5-N7 | -6.90 | 126.26 | 130.40 |
| 23 | DA | 1490 | A | N1-C2-N3 | -6.90 | 125.85 | 129.30 |
| 23 | BA | 188 | G | C6-C5-N7 | -6.90 | 126.26 | 130.40 |
| 1 | AA | 1217 | C | C6-N1-C2 | 6.90 | 123.06 | 120.30 |
| 23 | BA | 645 | C | C2-N1-C1' | 6.90 | 126.39 | 118.80 |
| 23 | DA | 679 | C | C6-N1-C2 | 6.90 | 123.06 | 120.30 |
| 1 | AA | 731 | G | C8-N9-C4 | -6.90 | 103.64 | 106.40 |
| 23 | DA | 198 | C | C2-N3-C4 | -6.90 | 116.45 | 119.90 |
| 1 | CA | 1237 | C | C6-N1-C2 | -6.89 | 117.54 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|----------|-------|-------------|----------|
| 1 | AA | 1263 | C | C6-N1-C2 | -6.89 | 117.55 | 120.30 |
| 23 | BA | 2036 | C | C5-C6-N1 | 6.89 | 124.44 | 121.00 |
| 24 | DB | 61 | G | N1-C6-O6 | 6.88 | 124.03 | 119.90 |
| 23 | DA | 679 | C | N3-C4-C5 | 6.88 | 124.65 | 121.90 |
| 23 | DA | 1800 | C | C2-N3-C4 | -6.88 | 116.46 | 119.90 |
| 23 | DA | 2323 | G | C8-N9-C4 | 6.88 | 109.15 | 106.40 |
| 23 | DA | 2724 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 1 | AA | 1312 | G | N3-C4-N9 | 6.88 | 130.13 | 126.00 |
| 23 | DA | 2782 | G | N1-C6-O6 | 6.88 | 124.03 | 119.90 |
| 23 | DA | 409 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 23 | DA | 1252 | G | N7-C8-N9 | -6.88 | 109.66 | 113.10 |
| 1 | AA | 1198 | G | C5-C6-O6 | 6.88 | 132.72 | 128.60 |
| 23 | BA | 803 | U | C5-C6-N1 | -6.88 | 119.26 | 122.70 |
| 23 | DA | 1123 | C | C5-C6-N1 | -6.88 | 117.56 | 121.00 |
| 23 | BA | 530 | G | N3-C2-N2 | -6.87 | 115.09 | 119.90 |
| 23 | DA | 1645 | G | C4-C5-N7 | -6.87 | 108.05 | 110.80 |
| 1 | AA | 925 | G | C5-C6-O6 | -6.87 | 124.48 | 128.60 |
| 1 | AA | 1244 | C | C6-N1-C2 | -6.87 | 117.55 | 120.30 |
| 23 | BA | 2471 | C | N1-C2-O2 | 6.87 | 123.02 | 118.90 |
| 23 | BA | 2723 | C | C2-N3-C4 | -6.87 | 116.46 | 119.90 |
| 23 | DA | 1698 | A | N1-C2-N3 | 6.87 | 132.74 | 129.30 |
| 23 | DA | 1795 | C | N3-C4-C5 | 6.87 | 124.65 | 121.90 |
| 23 | BA | 196 | A | C4-C5-N7 | 6.87 | 114.13 | 110.70 |
| 23 | BA | 475 | U | N3-C4-C5 | -6.87 | 110.48 | 114.60 |
| 1 | CA | 1442(A) | G | C4-C5-C6 | 6.87 | 122.92 | 118.80 |
| 23 | DA | 736 | C | N3-C2-O2 | 6.87 | 126.71 | 121.90 |
| 23 | DA | 769 | G | N7-C8-N9 | -6.87 | 109.67 | 113.10 |
| 23 | DA | 2689 | U | C5-C6-N1 | -6.87 | 119.27 | 122.70 |
| 23 | BA | 1269 | A | N9-C4-C5 | -6.87 | 103.05 | 105.80 |
| 1 | CA | 1044 | A | C6-N1-C2 | 6.87 | 122.72 | 118.60 |
| 23 | DA | 988 | A | C5-C6-N6 | -6.87 | 118.21 | 123.70 |
| 23 | BA | 807 | U | C5-C4-O4 | -6.87 | 121.78 | 125.90 |
| 23 | BA | 1207 | C | C6-N1-C2 | 6.87 | 123.05 | 120.30 |
| 23 | BA | 2011 | U | N3-C2-O2 | 6.87 | 127.00 | 122.20 |
| 1 | CA | 1160 | G | N9-C4-C5 | -6.87 | 102.65 | 105.40 |
| 23 | DA | 928 | G | N7-C8-N9 | 6.86 | 116.53 | 113.10 |
| 23 | BA | 910 | A | N1-C6-N6 | 6.86 | 122.72 | 118.60 |
| 1 | CA | 1017 | G | N1-C6-O6 | -6.86 | 115.78 | 119.90 |
| 23 | BA | 2371 | G | C4-C5-N7 | 6.86 | 113.54 | 110.80 |
| 1 | AA | 226 | G | C8-N9-C4 | 6.86 | 109.14 | 106.40 |
| 23 | DA | 2322 | A | N1-C2-N3 | 6.86 | 132.73 | 129.30 |
| 1 | AA | 1225 | A | N1-C2-N3 | -6.85 | 125.87 | 129.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1710 | C | C6-N1-C2 | 6.85 | 123.04 | 120.30 |
| 1 | AA | 1263 | C | C2-N1-C1' | 6.85 | 126.34 | 118.80 |
| 23 | DA | 2835 | A | N1-C6-N6 | -6.85 | 114.49 | 118.60 |
| 30 | DI | 106 | GLY | N-CA-C | 6.84 | 130.21 | 113.10 |
| 1 | AA | 946 | A | N1-C6-N6 | 6.84 | 122.71 | 118.60 |
| 23 | DA | 271(J) | C | N3-C4-C5 | 6.84 | 124.64 | 121.90 |
| 23 | BA | 988 | A | N9-C4-C5 | -6.84 | 103.06 | 105.80 |
| 23 | BA | 1041 | C | C6-N1-C2 | -6.84 | 117.56 | 120.30 |
| 23 | BA | 1210 | A | C2-N3-C4 | -6.84 | 107.18 | 110.60 |
| 23 | DA | 1403 | C | C2-N1-C1' | -6.84 | 111.28 | 118.80 |
| 24 | BB | 37 | C | N3-C4-C5 | -6.83 | 119.17 | 121.90 |
| 23 | DA | 2375 | G | N3-C4-C5 | 6.83 | 132.02 | 128.60 |
| 23 | DA | 2791 | C | C5-C6-N1 | 6.83 | 124.42 | 121.00 |
| 23 | BA | 547 | A | C2-N3-C4 | 6.83 | 114.02 | 110.60 |
| 23 | BA | 2059 | A | N7-C8-N9 | -6.83 | 110.38 | 113.80 |
| 23 | DA | 1791 | A | N1-C6-N6 | 6.83 | 122.70 | 118.60 |
| 23 | DA | 2107 | C | N3-C4-C5 | -6.83 | 119.17 | 121.90 |
| 23 | DA | 2497 | A | N1-C6-N6 | 6.83 | 122.70 | 118.60 |
| 1 | CA | 691 | G | N1-C6-O6 | 6.83 | 124.00 | 119.90 |
| 1 | CA | 1266 | G | N3-C4-C5 | -6.83 | 125.19 | 128.60 |
| 1 | CA | 921 | U | C2-N3-C4 | 6.83 | 131.10 | 127.00 |
| 23 | DA | 147 | U | C5-C6-N1 | -6.83 | 119.29 | 122.70 |
| 23 | BA | 207 | A | C5-N7-C8 | -6.83 | 100.49 | 103.90 |
| 23 | BA | 1243 | G | C6-C5-N7 | -6.83 | 126.30 | 130.40 |
| 1 | CA | 1081 | G | C8-N9-C4 | 6.83 | 109.13 | 106.40 |
| 23 | DA | 2744 | G | N1-C6-O6 | 6.83 | 124.00 | 119.90 |
| 23 | DA | 2286 | A | N1-C2-N3 | 6.82 | 132.71 | 129.30 |
| 1 | AA | 359 | U | N3-C2-O2 | 6.82 | 126.97 | 122.20 |
| 23 | BA | 512 | G | N1-C6-O6 | -6.82 | 115.81 | 119.90 |
| 1 | AA | 52 | G | C5-C6-N1 | -6.82 | 108.09 | 111.50 |
| 23 | BA | 2705 | A | C8-N9-C4 | 6.81 | 108.53 | 105.80 |
| 1 | CA | 365 | U | C5-C6-N1 | -6.81 | 119.29 | 122.70 |
| 23 | BA | 2442 | C | C2-N3-C4 | -6.81 | 116.49 | 119.90 |
| 1 | CA | 1443 | G | N9-C4-C5 | -6.81 | 102.67 | 105.40 |
| 23 | DA | 1829 | A | C8-N9-C4 | 6.81 | 108.53 | 105.80 |
| 23 | BA | 2397 | G | C8-N9-C4 | -6.81 | 103.67 | 106.40 |
| 1 | AA | 93 | G | C8-N9-C4 | 6.81 | 109.12 | 106.40 |
| 1 | CA | 1114 | C | N1-C2-O2 | 6.81 | 122.99 | 118.90 |
| 1 | CA | 1357 | A | N7-C8-N9 | 6.81 | 117.20 | 113.80 |
| 23 | BA | 1021 | A | N3-C4-C5 | 6.81 | 131.56 | 126.80 |
| 23 | BA | 2582 | G | N1-C6-O6 | -6.81 | 115.81 | 119.90 |
| 24 | BB | 27 | C | C6-N1-C2 | -6.81 | 117.58 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | CA | 940 | C | N1-C2-O2 | 6.81 | 122.98 | 118.90 |
| 23 | DA | 1949 | G | C8-N9-C4 | 6.81 | 109.12 | 106.40 |
| 23 | DA | 2321 | G | C8-N9-C4 | -6.81 | 103.68 | 106.40 |
| 23 | DA | 2323 | G | N3-C4-C5 | 6.80 | 132.00 | 128.60 |
| 1 | AA | 1229 | A | C8-N9-C4 | -6.80 | 103.08 | 105.80 |
| 23 | BA | 213 | A | N1-C6-N6 | 6.80 | 122.68 | 118.60 |
| 23 | BA | 678 | C | N3-C4-C5 | 6.80 | 124.62 | 121.90 |
| 23 | BA | 1758 | G | N1-C6-O6 | 6.80 | 123.98 | 119.90 |
| 23 | DA | 2189 | U | N1-C2-O2 | 6.80 | 127.56 | 122.80 |
| 23 | BA | 578 | A | N9-C4-C5 | 6.80 | 108.52 | 105.80 |
| 23 | BA | 1210 | A | C4-C5-N7 | 6.80 | 114.10 | 110.70 |
| 23 | BA | 1605 | C | N3-C2-O2 | -6.80 | 117.14 | 121.90 |
| 1 | CA | 1108 | G | N3-C4-C5 | -6.80 | 125.20 | 128.60 |
| 23 | DA | 645 | C | C2-N1-C1' | 6.80 | 126.28 | 118.80 |
| 23 | BA | 2363 | C | C6-N1-C2 | 6.80 | 123.02 | 120.30 |
| 1 | CA | 1030(B) | C | C5-C6-N1 | 6.80 | 124.40 | 121.00 |
| 1 | CA | 1231 | G | C5-C6-N1 | 6.80 | 114.90 | 111.50 |
| 23 | DA | 1827 | C | N3-C4-N4 | -6.79 | 113.24 | 118.00 |
| 23 | DA | 2782 | G | C4-C5-N7 | 6.79 | 113.52 | 110.80 |
| 23 | DA | 253 | C | N3-C4-C5 | -6.79 | 119.18 | 121.90 |
| 23 | BA | 446 | G | N3-C4-N9 | 6.79 | 130.07 | 126.00 |
| 23 | BA | 2571 | C | N1-C2-O2 | -6.79 | 114.83 | 118.90 |
| 23 | DA | 2074 | U | C5-C6-N1 | 6.79 | 126.09 | 122.70 |
| 23 | DA | 2312 | U | N3-C2-O2 | -6.79 | 117.45 | 122.20 |
| 23 | BA | 744 | G | C5-C6-N1 | -6.79 | 108.11 | 111.50 |
| 1 | CA | 1024 | G | N1-C6-O6 | 6.79 | 123.97 | 119.90 |
| 23 | DA | 647 | G | C8-N9-C4 | -6.79 | 103.69 | 106.40 |
| 23 | BA | 1405 | U | N3-C4-O4 | -6.79 | 114.65 | 119.40 |
| 23 | BA | 2821 | A | N1-C6-N6 | 6.79 | 122.67 | 118.60 |
| 23 | DA | 1304 | C | C6-N1-C2 | 6.79 | 123.01 | 120.30 |
| 23 | DA | 840 | C | C6-N1-C2 | 6.78 | 123.01 | 120.30 |
| 23 | BA | 786 | C | C5-C6-N1 | -6.78 | 117.61 | 121.00 |
| 23 | BA | 2897 | U | C2-N1-C1' | 6.78 | 125.84 | 117.70 |
| 23 | BA | 1047 | G | N3-C4-C5 | -6.78 | 125.21 | 128.60 |
| 23 | BA | 885 | C | C2-N1-C1' | 6.78 | 126.25 | 118.80 |
| 1 | CA | 776 | G | C5-C6-N1 | -6.78 | 108.11 | 111.50 |
| 1 | CA | 1370 | G | N3-C2-N2 | -6.78 | 115.16 | 119.90 |
| 1 | AA | 913 | A | N1-C6-N6 | -6.77 | 114.54 | 118.60 |
| 1 | AA | 972 | C | C6-N1-C2 | -6.77 | 117.59 | 120.30 |
| 23 | DA | 389 | G | C8-N9-C1' | -6.77 | 118.19 | 127.00 |
| 23 | DA | 1567 | A | C2-N3-C4 | -6.77 | 107.21 | 110.60 |
| 23 | BA | 458 | G | N9-C4-C5 | 6.77 | 108.11 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2351 | G | C4-N9-C1' | 6.77 | 135.30 | 126.50 |
| 23 | DA | 1992 | G | N1-C6-O6 | -6.77 | 115.84 | 119.90 |
| 23 | DA | 2179 | C | N1-C2-O2 | 6.77 | 122.96 | 118.90 |
| 23 | DA | 2289 | G | C8-N9-C4 | 6.77 | 109.11 | 106.40 |
| 23 | DA | 2699 | C | C6-N1-C2 | 6.77 | 123.01 | 120.30 |
| 23 | DA | 195 | A | N1-C6-N6 | 6.77 | 122.66 | 118.60 |
| 1 | AA | 945 | G | N9-C4-C5 | -6.76 | 102.69 | 105.40 |
| 23 | BA | 1204 | A | N3-C4-C5 | 6.76 | 131.53 | 126.80 |
| 1 | CA | 150 | C | C5-C6-N1 | 6.76 | 124.38 | 121.00 |
| 23 | BA | 1021 | A | N1-C6-N6 | 6.76 | 122.66 | 118.60 |
| 23 | DA | 2618 | G | C4-C5-N7 | -6.76 | 108.09 | 110.80 |
| 23 | BA | 530 | G | N3-C4-N9 | -6.76 | 121.94 | 126.00 |
| 1 | CA | 1235 | U | C5-C4-O4 | -6.76 | 121.84 | 125.90 |
| 23 | BA | 188 | G | C5-C6-N1 | -6.76 | 108.12 | 111.50 |
| 1 | CA | 34 | C | C6-N1-C2 | 6.76 | 123.00 | 120.30 |
| 23 | DA | 141 | A | N1-C6-N6 | 6.76 | 122.65 | 118.60 |
| 23 | DA | 205 | G | C4-C5-N7 | 6.76 | 113.50 | 110.80 |
| 23 | DA | 2031 | A | N1-C6-N6 | 6.76 | 122.65 | 118.60 |
| 23 | DA | 2238 | G | N3-C4-C5 | -6.76 | 125.22 | 128.60 |
| 1 | AA | 1377 | A | N1-C2-N3 | 6.75 | 132.68 | 129.30 |
| 23 | DA | 132 | G | N1-C6-O6 | 6.75 | 123.95 | 119.90 |
| 23 | DA | 2725 | A | C2-N3-C4 | -6.75 | 107.22 | 110.60 |
| 23 | BA | 2321 | G | C8-N9-C4 | -6.75 | 103.70 | 106.40 |
| 1 | AA | 1184 | G | N3-C4-C5 | -6.75 | 125.22 | 128.60 |
| 23 | BA | 2041 | U | C2-N3-C4 | -6.75 | 122.95 | 127.00 |
| 23 | BA | 2571 | C | N1-C2-N3 | 6.75 | 123.92 | 119.20 |
| 1 | CA | 818 | G | N9-C4-C5 | 6.75 | 108.10 | 105.40 |
| 23 | DA | 2335 | A | C8-N9-C4 | 6.75 | 108.50 | 105.80 |
| 1 | AA | 939 | G | C8-N9-C4 | 6.74 | 109.10 | 106.40 |
| 23 | BA | 1674 | G | C5-C6-O6 | -6.74 | 124.55 | 128.60 |
| 23 | BA | 1698 | A | C4-C5-N7 | 6.74 | 114.07 | 110.70 |
| 23 | BA | 785 | G | N3-C2-N2 | -6.74 | 115.18 | 119.90 |
| 1 | CA | 1325 | C | C2-N3-C4 | 6.74 | 123.27 | 119.90 |
| 23 | DA | 1277 | G | C2-N3-C4 | -6.74 | 108.53 | 111.90 |
| 1 | AA | 1309 | G | N1-C2-N2 | 6.74 | 122.27 | 116.20 |
| 23 | BA | 1790 | C | C2-N3-C4 | -6.73 | 116.53 | 119.90 |
| 23 | BA | 1983 | C | N1-C2-O2 | -6.73 | 114.86 | 118.90 |
| 23 | DA | 417 | C | C6-N1-C2 | 6.73 | 122.99 | 120.30 |
| 23 | DA | 2226 | C | C6-N1-C2 | 6.73 | 122.99 | 120.30 |
| 23 | DA | 197 | A | C5-C6-N1 | 6.73 | 121.06 | 117.70 |
| 23 | BA | 1283 | G | N1-C6-O6 | -6.73 | 115.86 | 119.90 |
| 23 | DA | 2411 | A | C8-N9-C4 | 6.73 | 108.49 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 924 | C | N3-C4-C5 | 6.73 | 124.59 | 121.90 |
| 1 | AA | 1371 | G | N3-C4-N9 | 6.72 | 130.03 | 126.00 |
| 1 | AA | 934 | C | C5-C6-N1 | 6.72 | 124.36 | 121.00 |
| 23 | DA | 426 | C | C6-N1-C2 | 6.72 | 122.99 | 120.30 |
| 1 | AA | 1015 | A | N1-C6-N6 | 6.72 | 122.63 | 118.60 |
| 23 | BA | 258 | G | N1-C2-N2 | -6.72 | 110.15 | 116.20 |
| 23 | DA | 2515 | C | C2-N3-C4 | -6.72 | 116.54 | 119.90 |
| 1 | AA | 54 | C | N1-C2-O2 | -6.72 | 114.87 | 118.90 |
| 23 | DA | 680 | G | C2-N3-C4 | -6.72 | 108.54 | 111.90 |
| 23 | DA | 2304 | G | C8-N9-C1' | 6.72 | 135.74 | 127.00 |
| 23 | BA | 2321 | G | N1-C2-N2 | 6.72 | 122.25 | 116.20 |
| 1 | AA | 1273 | G | C8-N9-C4 | -6.72 | 103.71 | 106.40 |
| 23 | BA | 525 | U | C6-N1-C2 | -6.72 | 116.97 | 121.00 |
| 23 | BA | 2020 | A | N7-C8-N9 | -6.72 | 110.44 | 113.80 |
| 23 | DA | 1612 | C | C5-C4-N4 | -6.71 | 115.50 | 120.20 |
| 23 | DA | 1611 | C | C6-N1-C2 | 6.71 | 122.98 | 120.30 |
| 23 | DA | 2464 | C | C6-N1-C1' | -6.71 | 112.74 | 120.80 |
| 1 | AA | 806 | C | N3-C4-C5 | 6.71 | 124.58 | 121.90 |
| 1 | AA | 836 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 23 | DA | 2028 | U | C4-C5-C6 | -6.71 | 115.67 | 119.70 |
| 1 | AA | 1023 | G | C6-N1-C2 | 6.71 | 129.12 | 125.10 |
| 23 | DA | 1256 | G | N3-C2-N2 | -6.71 | 115.20 | 119.90 |
| 1 | CA | 1158 | C | C2-N1-C1' | 6.71 | 126.18 | 118.80 |
| 23 | BA | 945 | A | C6-C5-N7 | -6.71 | 127.61 | 132.30 |
| 23 | DA | 588 | U | C5-C4-O4 | 6.71 | 129.92 | 125.90 |
| 23 | BA | 94 | C | C5-C6-N1 | 6.70 | 124.35 | 121.00 |
| 23 | BA | 1026 | U | N1-C2-O2 | 6.70 | 127.49 | 122.80 |
| 23 | DA | 39 | C | N3-C2-O2 | -6.70 | 117.21 | 121.90 |
| 23 | BA | 204 | A | C8-N9-C4 | -6.70 | 103.12 | 105.80 |
| 23 | BA | 1142(A) | A | N3-C4-N9 | -6.70 | 122.04 | 127.40 |
| 23 | DA | 1021 | A | N1-C2-N3 | 6.70 | 132.65 | 129.30 |
| 23 | DA | 1531 | C | C5-C6-N1 | 6.70 | 124.35 | 121.00 |
| 1 | AA | 1274 | G | C6-C5-N7 | -6.70 | 126.38 | 130.40 |
| 23 | BA | 940 | G | C6-C5-N7 | -6.70 | 126.38 | 130.40 |
| 23 | BA | 2575 | C | N3-C4-C5 | -6.70 | 119.22 | 121.90 |
| 23 | DA | 1112 | G | N3-C4-C5 | 6.70 | 131.95 | 128.60 |
| 1 | CA | 77 | G | C5-C6-O6 | -6.70 | 124.58 | 128.60 |
| 23 | DA | 2856 | C | C6-N1-C2 | -6.70 | 117.62 | 120.30 |
| 23 | BA | 465 | G | C4-C5-C6 | 6.70 | 122.82 | 118.80 |
| 23 | BA | 2593 | U | N3-C4-O4 | -6.70 | 114.71 | 119.40 |
| 23 | BA | 2609 | U | C2-N3-C4 | -6.70 | 122.98 | 127.00 |
| 23 | DA | 446 | G | N3-C4-N9 | 6.70 | 130.02 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 1471 | A | C8-N9-C4 | -6.70 | 103.12 | 105.80 |
| 23 | DA | 1616 | A | C4-C5-N7 | 6.70 | 114.05 | 110.70 |
| 23 | BA | 682 | G | C4-C5-N7 | 6.69 | 113.48 | 110.80 |
| 23 | BA | 839 | U | C5-C4-O4 | 6.69 | 129.92 | 125.90 |
| 23 | BA | 972 | G | N1-C6-O6 | -6.69 | 115.88 | 119.90 |
| 23 | DA | 570 | G | N9-C4-C5 | -6.69 | 102.72 | 105.40 |
| 23 | DA | 2321 | G | N9-C4-C5 | 6.69 | 108.08 | 105.40 |
| 23 | BA | 1038 | C | N3-C2-O2 | -6.69 | 117.22 | 121.90 |
| 23 | DA | 1304 | C | C5-C6-N1 | -6.69 | 117.66 | 121.00 |
| 1 | AA | 1442(B) | A | N3-C4-C5 | -6.68 | 122.12 | 126.80 |
| 23 | BA | 1254 | A | N1-C2-N3 | 6.68 | 132.64 | 129.30 |
| 23 | BA | 754 | C | N3-C4-C5 | 6.68 | 124.57 | 121.90 |
| 23 | BA | 1653 | G | C4-N9-C1' | 6.68 | 135.19 | 126.50 |
| 23 | DA | 12 | U | C2-N1-C1' | 6.68 | 125.72 | 117.70 |
| 23 | DA | 994 | C | C6-N1-C2 | 6.68 | 122.97 | 120.30 |
| 23 | BA | 2107 | C | N3-C4-C5 | -6.68 | 119.23 | 121.90 |
| 23 | DA | 2371 | G | C6-C5-N7 | -6.68 | 126.39 | 130.40 |
| 23 | DA | 71 | A | N3-C4-C5 | 6.68 | 131.47 | 126.80 |
| 23 | DA | 936 | C | N3-C2-O2 | 6.68 | 126.57 | 121.90 |
| 23 | DA | 2182 | G | C5-C6-O6 | 6.68 | 132.61 | 128.60 |
| 23 | BA | 1758 | G | N3-C2-N2 | -6.67 | 115.23 | 119.90 |
| 1 | CA | 1288 | A | C8-N9-C4 | 6.67 | 108.47 | 105.80 |
| 23 | DA | 465 | G | N1-C6-O6 | 6.67 | 123.90 | 119.90 |
| 24 | BB | 81 | G | N1-C6-O6 | 6.67 | 123.90 | 119.90 |
| 23 | DA | 272(H) | C | C5-C4-N4 | -6.67 | 115.53 | 120.20 |
| 23 | DA | 669 | G | C8-N9-C4 | 6.67 | 109.07 | 106.40 |
| 23 | DA | 2070 | G | N3-C4-N9 | 6.67 | 130.00 | 126.00 |
| 1 | CA | 972 | C | N1-C2-O2 | 6.67 | 122.90 | 118.90 |
| 23 | DA | 94 | C | C6-N1-C2 | -6.67 | 117.63 | 120.30 |
| 23 | DA | 271(M) | G | N3-C4-C5 | -6.67 | 125.27 | 128.60 |
| 23 | BA | 2519 | U | N1-C2-O2 | -6.67 | 118.13 | 122.80 |
| 23 | DA | 2491 | U | N3-C4-C5 | 6.67 | 118.60 | 114.60 |
| 23 | DA | 2609 | U | N1-C2-O2 | -6.67 | 118.13 | 122.80 |
| 1 | CA | 1029 | C | C2-N3-C4 | 6.67 | 123.23 | 119.90 |
| 23 | BA | 1934 | C | C6-N1-C2 | 6.66 | 122.97 | 120.30 |
| 1 | AA | 1377 | A | C4-C5-C6 | 6.66 | 120.33 | 117.00 |
| 23 | BA | 1327 | C | C6-N1-C2 | -6.66 | 117.64 | 120.30 |
| 1 | CA | 361 | G | N1-C6-O6 | 6.66 | 123.90 | 119.90 |
| 23 | DA | 113 | G | C5-C6-O6 | -6.66 | 124.60 | 128.60 |
| 23 | DA | 2632 | A | C8-N9-C4 | 6.66 | 108.46 | 105.80 |
| 23 | BA | 17 | G | N1-C6-O6 | -6.66 | 115.90 | 119.90 |
| 23 | DA | 389 | G | C8-N9-C4 | 6.66 | 109.06 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 60 | G | N1-C6-O6 | 6.66 | 123.89 | 119.90 |
| 23 | DA | 895 | U | C5-C6-N1 | 6.66 | 126.03 | 122.70 |
| 1 | AA | 1329 | A | C6-N1-C2 | 6.66 | 122.59 | 118.60 |
| 23 | BA | 1999 | C | C2-N3-C4 | -6.66 | 116.57 | 119.90 |
| 23 | BA | 12 | U | N3-C2-O2 | -6.65 | 117.54 | 122.20 |
| 1 | CA | 1030(A) | G | C2-N3-C4 | 6.65 | 115.23 | 111.90 |
| 23 | DA | 265 | A | C6-C5-N7 | -6.65 | 127.64 | 132.30 |
| 23 | DA | 444 | C | N3-C4-C5 | 6.65 | 124.56 | 121.90 |
| 1 | CA | 1378 | C | C6-N1-C2 | -6.65 | 117.64 | 120.30 |
| 23 | BA | 1217 | C | N3-C2-O2 | 6.65 | 126.55 | 121.90 |
| 23 | DA | 607 | U | C6-N1-C2 | 6.64 | 124.99 | 121.00 |
| 23 | DA | 1925 | C | N1-C2-O2 | -6.64 | 114.91 | 118.90 |
| 23 | BA | 2100 | G | C4-N9-C1' | 6.64 | 135.14 | 126.50 |
| 23 | DA | 682 | G | C5-C6-O6 | -6.64 | 124.61 | 128.60 |
| 23 | DA | 1785 | A | N1-C6-N6 | 6.64 | 122.59 | 118.60 |
| 23 | DA | 2286 | A | C5-C6-N1 | -6.64 | 114.38 | 117.70 |
| 1 | AA | 139 | G | N1-C6-O6 | 6.64 | 123.88 | 119.90 |
| 1 | CA | 953 | G | C8-N9-C4 | 6.64 | 109.06 | 106.40 |
| 23 | DA | 663 | G | N3-C2-N2 | -6.64 | 115.25 | 119.90 |
| 23 | BA | 675 | A | C5-C6-N6 | -6.64 | 118.39 | 123.70 |
| 23 | BA | 2676 | C | C6-N1-C2 | 6.64 | 122.96 | 120.30 |
| 23 | BA | 1022 | G | C6-C5-N7 | 6.64 | 134.38 | 130.40 |
| 23 | DA | 2464 | C | N3-C4-C5 | 6.64 | 124.56 | 121.90 |
| 23 | BA | 213 | A | C8-N9-C4 | 6.64 | 108.45 | 105.80 |
| 23 | BA | 330 | A | N3-C4-N9 | -6.63 | 122.09 | 127.40 |
| 1 | CA | 1166 | G | C4-C5-N7 | -6.63 | 108.15 | 110.80 |
| 1 | CA | 1231 | G | C2-N3-C4 | 6.63 | 115.22 | 111.90 |
| 23 | DA | 772 | C | N3-C2-O2 | 6.63 | 126.54 | 121.90 |
| 23 | BA | 698 | C | N3-C2-O2 | 6.63 | 126.54 | 121.90 |
| 1 | CA | 979 | C | C5-C6-N1 | 6.63 | 124.31 | 121.00 |
| 23 | DA | 1264 | G | N1-C6-O6 | 6.63 | 123.88 | 119.90 |
| 1 | AA | 1119 | C | C5-C6-N1 | 6.63 | 124.31 | 121.00 |
| 23 | BA | 577 | G | N1-C6-O6 | 6.63 | 123.88 | 119.90 |
| 23 | BA | 2371 | G | N9-C4-C5 | -6.63 | 102.75 | 105.40 |
| 24 | DB | 64 | C | C5-C6-N1 | -6.63 | 117.69 | 121.00 |
| 23 | BA | 669 | G | C8-N9-C4 | 6.62 | 109.05 | 106.40 |
| 23 | BA | 1345 | C | C6-N1-C2 | -6.62 | 117.65 | 120.30 |
| 23 | BA | 2020 | A | C5-N7-C8 | 6.62 | 107.21 | 103.90 |
| 1 | CA | 484 | G | N1-C6-O6 | -6.62 | 115.93 | 119.90 |
| 23 | BA | 592 | G | C8-N9-C4 | -6.62 | 103.75 | 106.40 |
| 23 | BA | 2609 | U | C5-C6-N1 | -6.62 | 119.39 | 122.70 |
| 23 | DA | 335 | C | N3-C4-C5 | -6.62 | 119.25 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2329 | G | N7-C8-N9 | -6.62 | 109.79 | 113.10 |
| 1 | CA | 357 | G | C5-C6-N1 | 6.62 | 114.81 | 111.50 |
| 23 | BA | 2464 | C | C5-C4-N4 | -6.62 | 115.57 | 120.20 |
| 1 | CA | 831 | U | C6-N1-C2 | -6.62 | 117.03 | 121.00 |
| 23 | DA | 1374 | G | C8-N9-C4 | -6.62 | 103.75 | 106.40 |
| 23 | DA | 2396 | G | C8-N9-C4 | -6.62 | 103.75 | 106.40 |
| 23 | BA | 885 | C | C6-N1-C1' | -6.61 | 112.86 | 120.80 |
| 1 | CA | 1443 | G | C5-C6-O6 | -6.61 | 124.63 | 128.60 |
| 23 | DA | 1107 | G | N3-C2-N2 | 6.61 | 124.53 | 119.90 |
| 1 | AA | 418 | C | N1-C2-O2 | 6.61 | 122.87 | 118.90 |
| 23 | BA | 1132 | A | C2-N3-C4 | -6.61 | 107.29 | 110.60 |
| 23 | BA | 47 | C | C5-C4-N4 | -6.61 | 115.57 | 120.20 |
| 23 | BA | 2582 | G | N7-C8-N9 | 6.61 | 116.41 | 113.10 |
| 23 | BA | 793 | A | N7-C8-N9 | 6.61 | 117.10 | 113.80 |
| 23 | BA | 1613 | G | N3-C2-N2 | 6.61 | 124.53 | 119.90 |
| 1 | CA | 1206 | G | N3-C4-N9 | 6.61 | 129.96 | 126.00 |
| 1 | AA | 1371 | G | N9-C4-C5 | -6.61 | 102.76 | 105.40 |
| 23 | BA | 2832 | U | C2-N1-C1' | 6.61 | 125.63 | 117.70 |
| 23 | DA | 2591 | C | C6-N1-C2 | -6.61 | 117.66 | 120.30 |
| 1 | AA | 615 | C | C6-N1-C2 | -6.60 | 117.66 | 120.30 |
| 23 | BA | 1359 | A | C5-C6-N1 | 6.60 | 121.00 | 117.70 |
| 23 | BA | 1217 | C | C5-C4-N4 | -6.60 | 115.58 | 120.20 |
| 23 | BA | 2250 | G | N9-C4-C5 | 6.60 | 108.04 | 105.40 |
| 1 | AA | 1261 | A | C5-C6-N6 | -6.60 | 118.42 | 123.70 |
| 23 | BA | 458 | G | C8-N9-C4 | -6.60 | 103.76 | 106.40 |
| 23 | BA | 750 | A | C8-N9-C4 | -6.60 | 103.16 | 105.80 |
| 23 | DA | 188 | G | N1-C2-N2 | -6.60 | 110.26 | 116.20 |
| 23 | BA | 1013 | C | N1-C2-O2 | -6.60 | 114.94 | 118.90 |
| 23 | BA | 2182 | G | C6-C5-N7 | 6.60 | 134.36 | 130.40 |
| 1 | CA | 1210 | C | N1-C2-O2 | 6.60 | 122.86 | 118.90 |
| 1 | AA | 1477 | C | N1-C2-O2 | -6.59 | 114.94 | 118.90 |
| 1 | CA | 932 | C | C2-N1-C1' | 6.59 | 126.06 | 118.80 |
| 23 | DA | 465 | G | C6-C5-N7 | -6.59 | 126.44 | 130.40 |
| 23 | DA | 1604 | C | N1-C2-O2 | -6.59 | 114.94 | 118.90 |
| 23 | DA | 2335 | A | C4-C5-C6 | -6.59 | 113.70 | 117.00 |
| 23 | DA | 2487 | G | N1-C6-O6 | 6.59 | 123.86 | 119.90 |
| 23 | BA | 2000 | G | N7-C8-N9 | -6.59 | 109.80 | 113.10 |
| 23 | BA | 2725 | A | N1-C2-N3 | 6.59 | 132.60 | 129.30 |
| 1 | AA | 190 | U | C5-C6-N1 | 6.59 | 125.99 | 122.70 |
| 23 | BA | 71 | A | N3-C4-C5 | 6.58 | 131.41 | 126.80 |
| 1 | AA | 1301 | U | C2-N1-C1' | 6.58 | 125.60 | 117.70 |
| 23 | BA | 148 | C | N3-C4-C5 | 6.58 | 124.53 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 1275 | A | N1-C6-N6 | 6.58 | 122.55 | 118.60 |
| 23 | BA | 1778 | U | C5-C6-N1 | -6.58 | 119.41 | 122.70 |
| 1 | CA | 1192 | C | C5-C6-N1 | 6.58 | 124.29 | 121.00 |
| 23 | DA | 286 | C | N1-C2-O2 | 6.58 | 122.85 | 118.90 |
| 23 | DA | 2206 | G | C8-N9-C1' | 6.58 | 135.56 | 127.00 |
| 23 | DA | 2552 | U | C2-N3-C4 | -6.58 | 123.05 | 127.00 |
| 1 | AA | 1335 | C | N3-C2-O2 | -6.58 | 117.29 | 121.90 |
| 1 | CA | 1003 | G | N7-C8-N9 | 6.58 | 116.39 | 113.10 |
| 23 | BA | 90 | U | C2-N3-C4 | 6.58 | 130.95 | 127.00 |
| 1 | CA | 951 | G | N3-C4-C5 | -6.58 | 125.31 | 128.60 |
| 23 | DA | 2487 | G | C6-C5-N7 | -6.58 | 126.45 | 130.40 |
| 23 | DA | 2689 | U | C5-C4-O4 | 6.58 | 129.85 | 125.90 |
| 23 | DA | 802 | A | C5-C6-N1 | 6.58 | 120.99 | 117.70 |
| 1 | AA | 1050 | G | C5-C6-N1 | -6.58 | 108.21 | 111.50 |
| 23 | BA | 1142(A) | A | C4-C5-N7 | 6.57 | 113.99 | 110.70 |
| 23 | BA | 552 | G | N7-C8-N9 | -6.57 | 109.81 | 113.10 |
| 23 | DA | 1963 | U | C2-N1-C1' | 6.57 | 125.59 | 117.70 |
| 1 | CA | 1050 | G | N9-C4-C5 | -6.57 | 102.77 | 105.40 |
| 23 | BA | 2572 | A | C5-N7-C8 | 6.57 | 107.19 | 103.90 |
| 23 | DA | 449 | A | C5-N7-C8 | -6.57 | 100.62 | 103.90 |
| 1 | AA | 442 | C | C6-N1-C2 | -6.57 | 117.67 | 120.30 |
| 23 | BA | 2304 | G | C6-C5-N7 | 6.56 | 134.34 | 130.40 |
| 1 | AA | 112 | G | C5-C6-O6 | -6.56 | 124.66 | 128.60 |
| 23 | BA | 124 | G | C5-C6-O6 | -6.56 | 124.66 | 128.60 |
| 23 | DA | 746 | A | C6-N1-C2 | -6.56 | 114.66 | 118.60 |
| 1 | AA | 998 | G | C4-C5-N7 | -6.56 | 108.18 | 110.80 |
| 23 | BA | 391 | G | C5-C6-O6 | -6.56 | 124.66 | 128.60 |
| 23 | BA | 1536 | C | C6-N1-C2 | -6.56 | 117.68 | 120.30 |
| 23 | DA | 327 | G | N1-C6-O6 | 6.56 | 123.83 | 119.90 |
| 1 | AA | 286 | G | N9-C4-C5 | 6.56 | 108.02 | 105.40 |
| 1 | AA | 1443 | G | N3-C4-N9 | 6.56 | 129.93 | 126.00 |
| 23 | BA | 13 | A | C8-N9-C4 | -6.56 | 103.18 | 105.80 |
| 23 | DA | 1200 | C | C6-N1-C2 | 6.56 | 122.92 | 120.30 |
| 23 | BA | 1342 | A | C5-C6-N1 | 6.56 | 120.98 | 117.70 |
| 23 | BA | 2306 | C | C5-C6-N1 | 6.56 | 124.28 | 121.00 |
| 23 | BA | 1229 | G | C5-C6-O6 | -6.55 | 124.67 | 128.60 |
| 1 | AA | 1153 | C | C2-N1-C1' | 6.55 | 126.01 | 118.80 |
| 23 | DA | 2264 | C | C5-C6-N1 | -6.55 | 117.72 | 121.00 |
| 23 | BA | 796 | C | N3-C4-C5 | 6.55 | 124.52 | 121.90 |
| 24 | BB | 7 | G | C4-C5-N7 | 6.55 | 113.42 | 110.80 |
| 23 | DA | 1459 | G | C8-N9-C4 | -6.55 | 103.78 | 106.40 |
| 23 | DA | 2609 | U | N3-C2-O2 | 6.55 | 126.78 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 24 | DB | 81 | G | C4-C5-N7 | 6.55 | 113.42 | 110.80 |
| 1 | AA | 79 | G | N1-C6-O6 | 6.55 | 123.83 | 119.90 |
| 1 | AA | 1344 | C | N1-C2-O2 | 6.55 | 122.83 | 118.90 |
| 23 | BA | 1391 | U | N3-C2-O2 | -6.55 | 117.62 | 122.20 |
| 1 | CA | 1392 | G | N1-C2-N2 | -6.55 | 110.31 | 116.20 |
| 1 | AA | 993 | G | N3-C4-C5 | -6.55 | 125.33 | 128.60 |
| 23 | BA | 769 | G | C8-N9-C4 | 6.55 | 109.02 | 106.40 |
| 23 | DA | 2849 | U | C5-C6-N1 | -6.55 | 119.43 | 122.70 |
| 23 | BA | 527 | C | N3-C4-N4 | -6.55 | 113.42 | 118.00 |
| 23 | BA | 530 | G | C5-N7-C8 | -6.55 | 101.03 | 104.30 |
| 23 | DA | 978 | G | N7-C8-N9 | -6.55 | 109.83 | 113.10 |
| 23 | DA | 1269 | A | C8-N9-C4 | 6.55 | 108.42 | 105.80 |
| 23 | DA | 1204 | A | C2-N3-C4 | -6.54 | 107.33 | 110.60 |
| 23 | DA | 207 | A | C2-N3-C4 | -6.54 | 107.33 | 110.60 |
| 23 | DA | 2329 | G | N9-C4-C5 | -6.54 | 102.78 | 105.40 |
| 1 | CA | 979 | C | C2-N1-C1' | 6.54 | 126.00 | 118.80 |
| 23 | DA | 2283 | C | N1-C2-O2 | -6.54 | 114.97 | 118.90 |
| 23 | DA | 2525 | G | C5-C6-O6 | -6.54 | 124.67 | 128.60 |
| 23 | DA | 2596 | U | N1-C2-N3 | 6.54 | 118.83 | 114.90 |
| 23 | DA | 2615 | U | C5-C4-O4 | 6.54 | 129.82 | 125.90 |
| 23 | BA | 2607 | G | N1-C2-N3 | 6.54 | 127.82 | 123.90 |
| 23 | DA | 114 | U | C2-N1-C1' | 6.54 | 125.55 | 117.70 |
| 23 | BA | 1207 | C | C5-C6-N1 | -6.54 | 117.73 | 121.00 |
| 23 | BA | 1698 | A | N1-C6-N6 | 6.54 | 122.52 | 118.60 |
| 23 | BA | 2623 | G | C5-C6-O6 | 6.54 | 132.52 | 128.60 |
| 23 | DA | 185 | U | C5-C6-N1 | -6.54 | 119.43 | 122.70 |
| 23 | BA | 1125 | G | C8-N9-C1' | -6.53 | 118.51 | 127.00 |
| 23 | BA | 1328 | G | N9-C4-C5 | -6.53 | 102.79 | 105.40 |
| 24 | BB | 89 | G | N1-C6-O6 | 6.53 | 123.82 | 119.90 |
| 1 | CA | 102 | G | C8-N9-C4 | -6.53 | 103.79 | 106.40 |
| 23 | DA | 154 | G | N1-C6-O6 | 6.53 | 123.82 | 119.90 |
| 1 | AA | 610 | G | C8-N9-C1' | -6.53 | 118.51 | 127.00 |
| 23 | BA | 2107 | C | C5-C4-N4 | 6.53 | 124.77 | 120.20 |
| 23 | DA | 535 | C | C2-N1-C1' | -6.53 | 111.61 | 118.80 |
| 23 | BA | 2087 | G | C4-C5-N7 | 6.53 | 113.41 | 110.80 |
| 1 | AA | 880 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 23 | BA | 2206 | G | N3-C4-N9 | -6.53 | 122.08 | 126.00 |
| 23 | DA | 96 | G | C2-N3-C4 | -6.53 | 108.64 | 111.90 |
| 23 | DA | 1763 | G | N3-C4-N9 | -6.53 | 122.08 | 126.00 |
| 23 | DA | 727 | A | C6-C5-N7 | -6.53 | 127.73 | 132.30 |
| 23 | BA | 1334 | G | N9-C4-C5 | 6.52 | 108.01 | 105.40 |
| 1 | CA | 1284 | C | N3-C4-C5 | -6.52 | 119.29 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 23 | BA | 1822 | G | C8-N9-C4 | 6.52 | 109.01 | 106.40 |
| 1 | CA | 117 | G | N3-C4-N9 | 6.51 | 129.91 | 126.00 |
| 23 | BA | 145 | G | N7-C8-N9 | -6.51 | 109.84 | 113.10 |
| 23 | BA | 2224 | G | N1-C6-O6 | 6.51 | 123.81 | 119.90 |
| 23 | DA | 1613 | G | N3-C2-N2 | 6.51 | 124.46 | 119.90 |
| 23 | BA | 210 | C | C6-N1-C2 | 6.51 | 122.90 | 120.30 |
| 23 | BA | 2767 | C | C6-N1-C2 | 6.51 | 122.90 | 120.30 |
| 23 | DA | 535 | C | C6-N1-C2 | 6.51 | 122.90 | 120.30 |
| 23 | BA | 1222 | C | C5-C4-N4 | -6.51 | 115.64 | 120.20 |
| 1 | CA | 1270 | C | C5-C6-N1 | 6.51 | 124.25 | 121.00 |
| 1 | CA | 1382 | C | N1-C2-O2 | 6.51 | 122.80 | 118.90 |
| 23 | DA | 2689 | U | C2-N3-C4 | -6.51 | 123.10 | 127.00 |
| 23 | BA | 1189 | A | C6-C5-N7 | -6.50 | 127.75 | 132.30 |
| 23 | BA | 2391 | G | C4-C5-N7 | -6.50 | 108.20 | 110.80 |
| 23 | DA | 652(B) | A | C2-N3-C4 | 6.50 | 113.85 | 110.60 |
| 23 | BA | 324 | A | C8-N9-C4 | 6.50 | 108.40 | 105.80 |
| 23 | DA | 1365 | A | C8-N9-C4 | -6.50 | 103.20 | 105.80 |
| 23 | BA | 1279 | G | N1-C6-O6 | -6.50 | 116.00 | 119.90 |
| 23 | BA | 271(O) | C | C5-C6-N1 | -6.50 | 117.75 | 121.00 |
| 23 | BA | 1625 | C | C6-N1-C2 | 6.50 | 122.90 | 120.30 |
| 23 | BA | 2334 | G | C8-N9-C4 | 6.50 | 109.00 | 106.40 |
| 24 | BB | 30 | C | C5-C6-N1 | 6.50 | 124.25 | 121.00 |
| 23 | BA | 2037 | G | N1-C6-O6 | -6.50 | 116.00 | 119.90 |
| 23 | BA | 2039 | C | C5-C6-N1 | 6.50 | 124.25 | 121.00 |
| 23 | BA | 2068 | U | N3-C4-C5 | 6.50 | 118.50 | 114.60 |
| 23 | DA | 1045 | A | C2-N3-C4 | 6.50 | 113.85 | 110.60 |
| 23 | DA | 1677 | A | C2-N3-C4 | -6.50 | 107.35 | 110.60 |
| 23 | DA | 1539 | G | C6-C5-N7 | -6.50 | 126.50 | 130.40 |
| 23 | BA | 674 | G | C5-C6-O6 | -6.49 | 124.70 | 128.60 |
| 23 | DA | 463 | G | C5-C6-O6 | 6.49 | 132.50 | 128.60 |
| 23 | BA | 1325 | G | N3-C4-N9 | 6.49 | 129.90 | 126.00 |
| 23 | BA | 2306 | C | C2-N3-C4 | 6.49 | 123.15 | 119.90 |
| 23 | BA | 2498 | C | C6-N1-C2 | 6.49 | 122.89 | 120.30 |
| 1 | AA | 38 | G | C5-C6-O6 | -6.49 | 124.71 | 128.60 |
| 1 | AA | 1042 | G | C8-N9-C4 | -6.49 | 103.81 | 106.40 |
| 23 | BA | 1141 | U | N1-C2-N3 | 6.49 | 118.79 | 114.90 |
| 23 | BA | 1674 | G | N1-C6-O6 | 6.49 | 123.79 | 119.90 |
| 23 | BA | 205 | G | N1-C2-N2 | -6.49 | 110.36 | 116.20 |
| 23 | BA | 1141 | U | N3-C2-O2 | -6.49 | 117.66 | 122.20 |
| 23 | BA | 1343 | G | C8-N9-C4 | -6.49 | 103.81 | 106.40 |
| 24 | BB | 87 | G | C8-N9-C4 | 6.49 | 108.99 | 106.40 |
| 1 | AA | 970 | C | C6-N1-C2 | -6.48 | 117.71 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 2849 | U | C5-C6-N1 | -6.48 | 119.46 | 122.70 |
| 23 | BA | 71 | A | N1-C2-N3 | 6.48 | 132.54 | 129.30 |
| 1 | CA | 54 | C | C2-N3-C4 | -6.48 | 116.66 | 119.90 |
| 23 | DA | 1192 | G | C8-N9-C4 | 6.48 | 108.99 | 106.40 |
| 1 | AA | 939 | G | N9-C4-C5 | -6.48 | 102.81 | 105.40 |
| 23 | BA | 205 | G | C8-N9-C4 | 6.48 | 108.99 | 106.40 |
| 23 | BA | 624 | C | C6-N1-C2 | 6.48 | 122.89 | 120.30 |
| 23 | BA | 830 | G | C4-C5-N7 | -6.48 | 108.21 | 110.80 |
| 23 | BA | 1137 | G | C5-C6-N1 | -6.48 | 108.26 | 111.50 |
| 23 | DA | 746 | A | C5-N7-C8 | -6.48 | 100.66 | 103.90 |
| 23 | BA | 2107 | C | C6-N1-C2 | -6.48 | 117.71 | 120.30 |
| 1 | CA | 1178 | G | N7-C8-N9 | 6.48 | 116.34 | 113.10 |
| 23 | DA | 2420 | C | N3-C4-C5 | 6.48 | 124.49 | 121.90 |
| 23 | DA | 2618 | G | C6-N1-C2 | -6.48 | 121.21 | 125.10 |
| 1 | CA | 1325 | C | N1-C2-O2 | 6.48 | 122.79 | 118.90 |
| 23 | DA | 1258 | C | C6-N1-C2 | 6.48 | 122.89 | 120.30 |
| 23 | DA | 1788 | C | N3-C4-C5 | -6.48 | 119.31 | 121.90 |
| 23 | DA | 2461 | C | C5-C6-N1 | -6.48 | 117.76 | 121.00 |
| 23 | BA | 2659 | G | C8-N9-C4 | -6.47 | 103.81 | 106.40 |
| 1 | CA | 1056 | U | N3-C4-C5 | -6.47 | 110.72 | 114.60 |
| 23 | DA | 584 | C | N1-C2-O2 | -6.47 | 115.02 | 118.90 |
| 1 | AA | 1442(A) | G | C4-C5-C6 | 6.47 | 122.68 | 118.80 |
| 23 | BA | 33 | U | C5-C4-O4 | 6.47 | 129.78 | 125.90 |
| 1 | CA | 839 | U | N3-C2-O2 | -6.47 | 117.67 | 122.20 |
| 1 | CA | 1120 | G | N9-C4-C5 | 6.47 | 107.99 | 105.40 |
| 24 | DB | 63 | G | C8-N9-C4 | 6.47 | 108.99 | 106.40 |
| 23 | DA | 2047 | U | C5-C6-N1 | -6.47 | 119.47 | 122.70 |
| 1 | AA | 32 | A | N1-C6-N6 | -6.47 | 114.72 | 118.60 |
| 1 | AA | 955 | U | C6-N1-C2 | -6.47 | 117.12 | 121.00 |
| 23 | BA | 1001 | A | N7-C8-N9 | -6.47 | 110.56 | 113.80 |
| 1 | CA | 1185 | G | C4-C5-N7 | -6.47 | 108.21 | 110.80 |
| 23 | DA | 2182 | G | C6-N1-C2 | 6.47 | 128.98 | 125.10 |
| 23 | BA | 968 | G | C8-N9-C4 | 6.47 | 108.99 | 106.40 |
| 23 | BA | 2129 | C | C6-N1-C2 | -6.47 | 117.71 | 120.30 |
| 23 | BA | 2336 | A | C2-N3-C4 | 6.47 | 113.83 | 110.60 |
| 23 | BA | 2501 | C | C6-N1-C2 | 6.47 | 122.89 | 120.30 |
| 1 | CA | 1166 | G | C4-N9-C1' | -6.47 | 118.09 | 126.50 |
| 23 | BA | 62 | C | C5-C6-N1 | -6.46 | 117.77 | 121.00 |
| 23 | BA | 2318 | G | N7-C8-N9 | 6.46 | 116.33 | 113.10 |
| 23 | DA | 102 | G | C8-N9-C1' | -6.46 | 118.60 | 127.00 |
| 23 | DA | 2028 | U | N1-C2-N3 | -6.46 | 111.02 | 114.90 |
| 23 | DA | 2312 | U | C5-C6-N1 | 6.46 | 125.93 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 23 | BA | 663 | G | N9-C4-C5 | 6.46 | 107.98 | 105.40 |
| 23 | BA | 1304 | C | C6-N1-C2 | 6.46 | 122.89 | 120.30 |
| 1 | CA | 1305 | G | C5-C6-N1 | -6.46 | 108.27 | 111.50 |
| 23 | BA | 2198 | A | C8-N9-C4 | 6.46 | 108.38 | 105.80 |
| 23 | DA | 39 | C | C2-N3-C4 | -6.46 | 116.67 | 119.90 |
| 1 | CA | 1442(B) | A | C4-N9-C1' | 6.46 | 137.92 | 126.30 |
| 23 | DA | 62 | C | C2-N3-C4 | -6.46 | 116.67 | 119.90 |
| 23 | DA | 453 | C | C5-C6-N1 | -6.46 | 117.77 | 121.00 |
| 1 | AA | 1502 | A | N7-C8-N9 | 6.46 | 117.03 | 113.80 |
| 23 | BA | 966 | G | N1-C2-N2 | -6.46 | 110.39 | 116.20 |
| 23 | DA | 1368 | G | N3-C2-N2 | -6.46 | 115.38 | 119.90 |
| 23 | DA | 1979 | C | C5-C6-N1 | 6.46 | 124.23 | 121.00 |
| 1 | AA | 299 | G | N3-C4-C5 | 6.45 | 131.83 | 128.60 |
| 1 | AA | 1034 | G | N1-C6-O6 | -6.45 | 116.03 | 119.90 |
| 23 | BA | 195 | A | N1-C6-N6 | 6.45 | 122.47 | 118.60 |
| 1 | CA | 352 | C | N1-C2-O2 | 6.45 | 122.77 | 118.90 |
| 1 | AA | 228 | A | N1-C6-N6 | 6.45 | 122.47 | 118.60 |
| 23 | BA | 389 | G | N3-C2-N2 | 6.45 | 124.42 | 119.90 |
| 23 | BA | 1970 | A | C8-N9-C4 | 6.45 | 108.38 | 105.80 |
| 23 | BA | 2503 | A | C2-N3-C4 | 6.45 | 113.83 | 110.60 |
| 23 | BA | 2259 | G | N1-C6-O6 | 6.45 | 123.77 | 119.90 |
| 23 | DA | 287 | C | C6-N1-C2 | 6.45 | 122.88 | 120.30 |
| 1 | AA | 1125 | U | N3-C2-O2 | 6.45 | 126.71 | 122.20 |
| 23 | BA | 1610 | A | N9-C4-C5 | -6.45 | 103.22 | 105.80 |
| 23 | BA | 333 | G | C4-N9-C1' | 6.45 | 134.88 | 126.50 |
| 23 | BA | 2840 | C | N3-C4-N4 | -6.45 | 113.49 | 118.00 |
| 23 | DA | 1021 | A | N7-C8-N9 | 6.45 | 117.02 | 113.80 |
| 23 | DA | 1141 | U | N3-C4-O4 | -6.45 | 114.89 | 119.40 |
| 1 | AA | 598 | U | N3-C4-C5 | -6.44 | 110.73 | 114.60 |
| 23 | DA | 1299 | G | C8-N9-C4 | -6.44 | 103.82 | 106.40 |
| 23 | DA | 2680 | C | C6-N1-C2 | 6.44 | 122.88 | 120.30 |
| 1 | AA | 925 | G | N1-C6-O6 | 6.44 | 123.76 | 119.90 |
| 23 | BA | 2385 | C | C2-N3-C4 | -6.44 | 116.68 | 119.90 |
| 23 | BA | 2441 | C | N3-C2-O2 | -6.44 | 117.39 | 121.90 |
| 23 | DA | 2335 | A | O4'-C1'-N9 | 6.44 | 113.35 | 108.20 |
| 1 | AA | 987 | G | N7-C8-N9 | 6.43 | 116.32 | 113.10 |
| 23 | DA | 2048 | G | C8-N9-C4 | -6.43 | 103.83 | 106.40 |
| 1 | AA | 1316 | G | N1-C6-O6 | -6.43 | 116.04 | 119.90 |
| 23 | BA | 213 | A | N9-C4-C5 | -6.43 | 103.23 | 105.80 |
| 23 | BA | 560 | C | N1-C2-O2 | -6.43 | 115.04 | 118.90 |
| 1 | CA | 1024 | G | C6-C5-N7 | -6.43 | 126.54 | 130.40 |
| 23 | DA | 1191 | G | C8-N9-C4 | 6.43 | 108.97 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 196 | A | N1-C6-N6 | 6.43 | 122.46 | 118.60 |
| 23 | BA | 974 | G | N3-C4-C5 | -6.43 | 125.39 | 128.60 |
| 23 | DA | 2321 | G | N3-C2-N2 | -6.43 | 115.40 | 119.90 |
| 23 | DA | 2393 | A | N9-C4-C5 | 6.43 | 108.37 | 105.80 |
| 23 | BA | 2312 | U | C2-N1-C1' | 6.43 | 125.41 | 117.70 |
| 1 | AA | 1381 | U | C2-N1-C1' | 6.43 | 125.41 | 117.70 |
| 23 | BA | 781 | A | C8-N9-C4 | 6.43 | 108.37 | 105.80 |
| 23 | BA | 984 | A | N9-C4-C5 | -6.43 | 103.23 | 105.80 |
| 23 | BA | 1041 | C | C5-C6-N1 | 6.43 | 124.21 | 121.00 |
| 23 | BA | 1342 | A | C6-N1-C2 | -6.43 | 114.74 | 118.60 |
| 23 | DA | 1239 | G | N3-C2-N2 | -6.43 | 115.40 | 119.90 |
| 1 | AA | 967 | C | C5-C6-N1 | 6.42 | 124.21 | 121.00 |
| 23 | BA | 1464 | C | N3-C4-C5 | -6.42 | 119.33 | 121.90 |
| 23 | BA | 1576 | U | N3-C2-O2 | -6.42 | 117.70 | 122.20 |
| 23 | BA | 2065 | C | N3-C2-O2 | -6.42 | 117.40 | 121.90 |
| 1 | CA | 322 | C | C6-N1-C2 | 6.42 | 122.87 | 120.30 |
| 1 | AA | 1346 | A | N1-C6-N6 | 6.42 | 122.45 | 118.60 |
| 23 | BA | 1802 | A | C2-N3-C4 | -6.42 | 107.39 | 110.60 |
| 23 | BA | 2587 | A | N1-C6-N6 | 6.42 | 122.45 | 118.60 |
| 23 | DA | 265 | A | C4-C5-C6 | 6.42 | 120.21 | 117.00 |
| 23 | DA | 1315 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 23 | BA | 776 | G | C6-N1-C2 | -6.42 | 121.25 | 125.10 |
| 1 | CA | 1367 | C | C6-N1-C2 | -6.42 | 117.73 | 120.30 |
| 23 | DA | 2681 | C | C2-N3-C4 | -6.42 | 116.69 | 119.90 |
| 23 | BA | 1616 | A | C4-C5-N7 | 6.42 | 113.91 | 110.70 |
| 23 | BA | 2819 | G | C8-N9-C4 | 6.42 | 108.97 | 106.40 |
| 1 | AA | 955 | U | C2-N3-C4 | 6.42 | 130.85 | 127.00 |
| 23 | BA | 251 | A | N1-C6-N6 | -6.42 | 114.75 | 118.60 |
| 23 | BA | 229 | A | C8-N9-C4 | -6.41 | 103.23 | 105.80 |
| 23 | BA | 553 | G | C4-C5-N7 | 6.41 | 113.37 | 110.80 |
| 1 | CA | 117 | G | C4-C5-N7 | 6.41 | 113.36 | 110.80 |
| 23 | DA | 1955 | U | C5-C6-N1 | -6.41 | 119.49 | 122.70 |
| 24 | DB | 76 | G | N3-C4-C5 | 6.41 | 131.81 | 128.60 |
| 23 | BA | 1648 | C | N3-C2-O2 | -6.41 | 117.41 | 121.90 |
| 23 | BA | 1273 | U | N1-C2-N3 | 6.41 | 118.75 | 114.90 |
| 23 | DA | 113 | G | N1-C6-O6 | 6.41 | 123.75 | 119.90 |
| 23 | BA | 1658 | C | C5-C4-N4 | -6.41 | 115.71 | 120.20 |
| 23 | BA | 2277 | G | C5-C6-O6 | 6.41 | 132.44 | 128.60 |
| 23 | DA | 1207 | C | C5-C6-N1 | -6.41 | 117.80 | 121.00 |
| 23 | BA | 2067 | G | N3-C4-C5 | -6.41 | 125.40 | 128.60 |
| 1 | CA | 1241 | G | N3-C4-N9 | 6.41 | 129.84 | 126.00 |
| 23 | BA | 2751 | G | C5-C6-O6 | 6.41 | 132.44 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 297 | C | N3-C4-C5 | -6.41 | 119.34 | 121.90 |
| 23 | DA | 2676 | C | C6-N1-C2 | 6.41 | 122.86 | 120.30 |
| 23 | BA | 696 | G | N9-C4-C5 | -6.40 | 102.84 | 105.40 |
| 23 | BA | 870 | A | N7-C8-N9 | -6.40 | 110.60 | 113.80 |
| 23 | BA | 1231 | G | C2-N3-C4 | -6.40 | 108.70 | 111.90 |
| 23 | BA | 2539 | C | C6-N1-C2 | 6.40 | 122.86 | 120.30 |
| 23 | DA | 664 | C | C2-N3-C4 | -6.40 | 116.70 | 119.90 |
| 23 | DA | 673 | C | N1-C2-O2 | -6.40 | 115.06 | 118.90 |
| 23 | DA | 1651 | G | C5-C6-N1 | 6.40 | 114.70 | 111.50 |
| 23 | DA | 2250 | G | N9-C4-C5 | 6.40 | 107.96 | 105.40 |
| 23 | DA | 2623 | G | N3-C4-C5 | -6.40 | 125.40 | 128.60 |
| 23 | BA | 47 | C | C2-N3-C4 | -6.40 | 116.70 | 119.90 |
| 1 | AA | 1034 | G | C8-N9-C4 | -6.40 | 103.84 | 106.40 |
| 1 | CA | 330 | C | C6-N1-C2 | -6.40 | 117.74 | 120.30 |
| 23 | DA | 862 | G | N9-C4-C5 | 6.40 | 107.96 | 105.40 |
| 23 | DA | 1254 | A | C6-N1-C2 | -6.40 | 114.76 | 118.60 |
| 23 | DA | 2421 | G | N9-C4-C5 | -6.40 | 102.84 | 105.40 |
| 23 | BA | 1216 | G | C4-C5-N7 | 6.40 | 113.36 | 110.80 |
| 23 | BA | 1813 | G | N1-C6-O6 | 6.40 | 123.74 | 119.90 |
| 23 | DA | 2675 | A | N1-C6-N6 | 6.40 | 122.44 | 118.60 |
| 23 | DA | 2680 | C | C2-N3-C4 | -6.40 | 116.70 | 119.90 |
| 1 | AA | 945 | G | N3-C4-N9 | 6.39 | 129.84 | 126.00 |
| 1 | AA | 998 | G | N9-C4-C5 | 6.39 | 107.96 | 105.40 |
| 23 | BA | 2897 | U | C5-C6-N1 | 6.39 | 125.90 | 122.70 |
| 23 | DA | 1308 | A | C4-C5-C6 | 6.39 | 120.20 | 117.00 |
| 23 | DA | 1950 | G | C5-N7-C8 | 6.39 | 107.50 | 104.30 |
| 23 | DA | 129 | C | C2-N3-C4 | -6.39 | 116.70 | 119.90 |
| 23 | BA | 760 | G | C5-C6-O6 | -6.39 | 124.77 | 128.60 |
| 23 | DA | 1942 | C | N3-C4-N4 | -6.39 | 113.53 | 118.00 |
| 23 | DA | 2485 | G | N9-C4-C5 | -6.39 | 102.84 | 105.40 |
| 23 | BA | 1639 | U | N3-C2-O2 | -6.39 | 117.73 | 122.20 |
| 23 | DA | 845 | G | C6-C5-N7 | -6.39 | 126.57 | 130.40 |
| 23 | DA | 2356 | C | N1-C2-O2 | -6.39 | 115.07 | 118.90 |
| 1 | AA | 557 | G | N3-C4-N9 | 6.38 | 129.83 | 126.00 |
| 23 | BA | 296 | C | N3-C4-C5 | 6.38 | 124.45 | 121.90 |
| 23 | BA | 2429 | G | N9-C4-C5 | 6.38 | 107.95 | 105.40 |
| 23 | DA | 389 | G | N3-C2-N2 | 6.38 | 124.37 | 119.90 |
| 23 | BA | 1695 | G | N7-C8-N9 | 6.38 | 116.29 | 113.10 |
| 1 | CA | 1024 | G | N7-C8-N9 | 6.38 | 116.29 | 113.10 |
| 23 | DA | 2030 | A | C4-N9-C1' | -6.38 | 114.81 | 126.30 |
| 26 | DE | 118 | LYS | N-CA-C | -6.38 | 93.77 | 111.00 |
| 1 | AA | 967 | C | C6-N1-C2 | -6.38 | 117.75 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1050 | G | C6-C5-N7 | -6.38 | 126.57 | 130.40 |
| 1 | AA | 1513 | A | C8-N9-C4 | 6.38 | 108.35 | 105.80 |
| 23 | BA | 179 | G | C8-N9-C4 | 6.38 | 108.95 | 106.40 |
| 23 | BA | 2043 | C | N1-C2-O2 | -6.38 | 115.07 | 118.90 |
| 23 | BA | 2633 | G | N1-C6-O6 | -6.38 | 116.07 | 119.90 |
| 1 | CA | 295 | C | C6-N1-C2 | 6.38 | 122.85 | 120.30 |
| 23 | BA | 1261 | C | N3-C2-O2 | 6.38 | 126.36 | 121.90 |
| 23 | DA | 664 | C | C6-N1-C2 | 6.38 | 122.85 | 120.30 |
| 1 | AA | 433 | C | N3-C2-O2 | -6.37 | 117.44 | 121.90 |
| 1 | AA | 1261 | A | N9-C4-C5 | -6.37 | 103.25 | 105.80 |
| 23 | BA | 464 | U | C5-C4-O4 | 6.37 | 129.72 | 125.90 |
| 23 | BA | 1204 | A | C5-C6-N1 | -6.37 | 114.51 | 117.70 |
| 23 | BA | 1325 | G | C5-C6-O6 | -6.37 | 124.78 | 128.60 |
| 23 | BA | 2182 | G | C4-N9-C1' | -6.37 | 118.22 | 126.50 |
| 1 | CA | 163 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 23 | DA | 1864 | U | C5-C6-N1 | -6.37 | 119.51 | 122.70 |
| 23 | BA | 1790 | C | C5-C4-N4 | -6.37 | 115.74 | 120.20 |
| 23 | BA | 2607 | G | C4-C5-C6 | 6.37 | 122.62 | 118.80 |
| 23 | BA | 453 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 23 | BA | 731 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 23 | BA | 886 | C | C5-C6-N1 | 6.37 | 124.19 | 121.00 |
| 1 | AA | 328 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 23 | BA | 302 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 23 | DA | 1359 | A | C4-C5-C6 | -6.37 | 113.82 | 117.00 |
| 23 | DA | 1616 | A | N9-C4-C5 | -6.37 | 103.25 | 105.80 |
| 23 | DA | 1930 | G | C4-N9-C1' | -6.37 | 118.22 | 126.50 |
| 1 | AA | 1445 | C | C6-N1-C2 | -6.37 | 117.75 | 120.30 |
| 23 | BA | 1269 | A | C4-C5-N7 | 6.37 | 113.88 | 110.70 |
| 23 | BA | 2837 | G | N1-C6-O6 | 6.37 | 123.72 | 119.90 |
| 1 | CA | 1232 | U | C6-N1-C2 | -6.37 | 117.18 | 121.00 |
| 23 | BA | 206 | U | N1-C2-O2 | -6.36 | 118.34 | 122.80 |
| 23 | BA | 2080 | G | N9-C4-C5 | -6.36 | 102.86 | 105.40 |
| 23 | BA | 2571 | C | C2-N3-C4 | -6.36 | 116.72 | 119.90 |
| 1 | CA | 1178 | G | C8-N9-C4 | -6.36 | 103.85 | 106.40 |
| 23 | DA | 1216 | G | N9-C4-C5 | -6.36 | 102.85 | 105.40 |
| 23 | DA | 2070 | G | C6-N1-C2 | -6.36 | 121.28 | 125.10 |
| 1 | AA | 433 | C | N3-C4-N4 | -6.36 | 113.55 | 118.00 |
| 23 | BA | 278 | A | C6-N1-C2 | -6.36 | 114.78 | 118.60 |
| 23 | DA | 2285 | C | C5-C4-N4 | 6.36 | 124.65 | 120.20 |
| 23 | BA | 893 | C | C2-N1-C1' | 6.36 | 125.80 | 118.80 |
| 23 | BA | 1982 | C | C5-C6-N1 | 6.36 | 124.18 | 121.00 |
| 23 | BA | 2430 | A | C6-N1-C2 | -6.36 | 114.78 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | AA | 1059 | C | N3-C4-C5 | -6.36 | 119.36 | 121.90 |
| 1 | AA | 1184 | G | N3-C4-N9 | 6.36 | 129.81 | 126.00 |
| 23 | BA | 1555 | G | C6-C5-N7 | -6.36 | 126.58 | 130.40 |
| 23 | BA | 2761 | G | N7-C8-N9 | 6.36 | 116.28 | 113.10 |
| 24 | BB | 85 | G | C4-C5-N7 | 6.36 | 113.34 | 110.80 |
| 23 | DA | 1942 | C | C2-N1-C1' | -6.36 | 111.81 | 118.80 |
| 23 | BA | 272(D) | G | N7-C8-N9 | -6.36 | 109.92 | 113.10 |
| 23 | BA | 576 | U | N3-C2-O2 | -6.36 | 117.75 | 122.20 |
| 23 | DA | 1284 | A | C5-C6-N6 | -6.36 | 118.61 | 123.70 |
| 24 | DB | 76 | G | C4-C5-N7 | 6.36 | 113.34 | 110.80 |
| 23 | BA | 679 | C | C6-N1-C2 | 6.35 | 122.84 | 120.30 |
| 23 | BA | 2369 | A | C5-C6-N1 | 6.35 | 120.88 | 117.70 |
| 23 | DA | 2755 | C | C4-C5-C6 | -6.35 | 114.22 | 117.40 |
| 1 | AA | 1000 | U | C2-N3-C4 | 6.35 | 130.81 | 127.00 |
| 23 | BA | 760 | G | C4-C5-N7 | 6.35 | 113.34 | 110.80 |
| 23 | BA | 2791 | C | C2-N1-C1' | 6.35 | 125.78 | 118.80 |
| 1 | CA | 1330 | U | C2-N1-C1' | 6.35 | 125.32 | 117.70 |
| 23 | BA | 48 | G | C5-C6-N1 | -6.35 | 108.33 | 111.50 |
| 23 | DA | 179 | G | C2-N3-C4 | -6.35 | 108.73 | 111.90 |
| 23 | DA | 1267 | U | C4-C5-C6 | -6.35 | 115.89 | 119.70 |
| 23 | DA | 2030 | A | C4-C5-C6 | -6.35 | 113.83 | 117.00 |
| 23 | DA | 2238 | G | C2-N3-C4 | 6.35 | 115.07 | 111.90 |
| 23 | BA | 1791 | A | C6-C5-N7 | -6.35 | 127.86 | 132.30 |
| 23 | BA | 840 | C | C6-N1-C2 | 6.34 | 122.84 | 120.30 |
| 23 | BA | 1125 | G | C4-N9-C1' | 6.34 | 134.75 | 126.50 |
| 23 | BA | 2259 | G | C2-N3-C4 | -6.34 | 108.73 | 111.90 |
| 23 | DA | 745 | G | C6-C5-N7 | -6.34 | 126.59 | 130.40 |
| 23 | BA | 61 | G | C8-N9-C4 | 6.34 | 108.94 | 106.40 |
| 23 | BA | 2803 | C | C5-C6-N1 | 6.34 | 124.17 | 121.00 |
| 1 | AA | 1225 | A | C2-N3-C4 | 6.34 | 113.77 | 110.60 |
| 23 | BA | 512 | G | C5-C6-O6 | 6.34 | 132.40 | 128.60 |
| 24 | BB | 7 | G | C5-C6-O6 | -6.34 | 124.80 | 128.60 |
| 1 | CA | 971 | G | C8-N9-C4 | -6.34 | 103.86 | 106.40 |
| 1 | CA | 976 | G | C4-N9-C1' | -6.34 | 118.26 | 126.50 |
| 23 | BA | 2628 | C | C6-N1-C2 | 6.34 | 122.83 | 120.30 |
| 23 | BA | 2719 | G | N7-C8-N9 | -6.34 | 109.93 | 113.10 |
| 23 | BA | 1243 | G | C5-C6-N1 | -6.34 | 108.33 | 111.50 |
| 23 | BA | 1938 | A | C4-C5-C6 | 6.34 | 120.17 | 117.00 |
| 23 | BA | 2778 | A | C2-N3-C4 | -6.34 | 107.43 | 110.60 |
| 23 | DA | 80 | G | C8-N9-C4 | -6.34 | 103.87 | 106.40 |
| 23 | DA | 1647 | G | N1-C6-O6 | 6.34 | 123.70 | 119.90 |
| 23 | BA | 570 | G | N7-C8-N9 | -6.33 | 109.93 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | BA | 1478 | G | N3-C4-N9 | 6.33 | 129.80 | 126.00 |
| 23 | BA | 200 | U | C2-N3-C4 | -6.33 | 123.20 | 127.00 |
| 23 | BA | 2181 | G | N3-C4-N9 | -6.33 | 122.20 | 126.00 |
| 23 | DA | 2030 | A | C8-N9-C4 | 6.33 | 108.33 | 105.80 |
| 1 | AA | 1239 | A | C8-N9-C4 | -6.33 | 103.27 | 105.80 |
| 23 | BA | 1437 | C | N3-C4-C5 | -6.33 | 119.37 | 121.90 |
| 23 | DA | 1248 | G | N9-C4-C5 | -6.33 | 102.87 | 105.40 |
| 23 | BA | 829 | A | C8-N9-C4 | 6.33 | 108.33 | 105.80 |
| 1 | AA | 1329 | A | C5-C6-N6 | 6.33 | 128.76 | 123.70 |
| 23 | BA | 558 | G | C8-N9-C4 | 6.33 | 108.93 | 106.40 |
| 23 | DA | 122 | G | N9-C4-C5 | -6.33 | 102.87 | 105.40 |
| 23 | DA | 458 | G | C8-N9-C4 | -6.33 | 103.87 | 106.40 |
| 23 | DA | 2803 | C | C2-N3-C4 | 6.33 | 123.06 | 119.90 |
| 23 | BA | 745 | G | C6-C5-N7 | -6.33 | 126.61 | 130.40 |
| 23 | BA | 2306 | C | C6-N1-C1' | -6.33 | 113.21 | 120.80 |
| 23 | DA | 1767 | C | C2-N3-C4 | -6.33 | 116.74 | 119.90 |
| 23 | DA | 2396 | G | N7-C8-N9 | 6.33 | 116.26 | 113.10 |
| 23 | DA | 2607 | G | C8-N9-C1' | -6.33 | 118.78 | 127.00 |
| 1 | AA | 1020 | U | N1-C2-O2 | 6.32 | 127.23 | 122.80 |
| 23 | BA | 2721 | A | C6-N1-C2 | -6.32 | 114.81 | 118.60 |
| 23 | DA | 58 | G | C8-N9-C4 | -6.32 | 103.87 | 106.40 |
| 23 | DA | 933 | A | C4-C5-N7 | 6.32 | 113.86 | 110.70 |
| 23 | DA | 2572 | A | N9-C4-C5 | -6.32 | 103.27 | 105.80 |
| 23 | DA | 2332 | U | N1-C2-O2 | 6.32 | 127.23 | 122.80 |
| 23 | BA | 778 | G | N1-C6-O6 | -6.32 | 116.11 | 119.90 |
| 23 | DA | 2499 | C | C5-C6-N1 | 6.32 | 124.16 | 121.00 |
| 23 | BA | 1404 | C | N3-C2-O2 | -6.32 | 117.48 | 121.90 |
| 23 | BA | 2296 | U | C1'-O4'-C4' | -6.32 | 104.84 | 109.90 |
| 23 | DA | 760 | G | N1-C6-O6 | 6.32 | 123.69 | 119.90 |
| 1 | AA | 1456 | G | C8-N9-C4 | 6.32 | 108.93 | 106.40 |
| 23 | BA | 794 | G | C5-C6-O6 | 6.32 | 132.39 | 128.60 |
| 23 | BA | 1696 | G | C8-N9-C4 | 6.32 | 108.93 | 106.40 |
| 23 | BA | 1782 | C | C5-C4-N4 | -6.32 | 115.78 | 120.20 |
| 23 | BA | 2680 | C | N3-C4-N4 | 6.32 | 122.42 | 118.00 |
| 23 | DA | 2496 | C | N3-C4-C5 | 6.32 | 124.43 | 121.90 |
| 1 | AA | 506 | G | C8-N9-C4 | -6.32 | 103.87 | 106.40 |
| 23 | BA | 777 | A | N1-C6-N6 | -6.32 | 114.81 | 118.60 |
| 23 | BA | 2612 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 23 | BA | 2617 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 23 | BA | 2719 | G | N9-C4-C5 | -6.32 | 102.87 | 105.40 |
| 23 | DA | 188 | G | C2-N3-C4 | -6.32 | 108.74 | 111.90 |
| 23 | DA | 664 | C | C5-C6-N1 | -6.32 | 117.84 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23 | BA | 756 | C | C4-C5-C6 | 6.31 | 120.56 | 117.40 |
| 23 | DA | 1781 | C | N1-C2-O2 | 6.31 | 122.69 | 118.90 |
| 23 | BA | 1202 | C | N1-C2-O2 | -6.31 | 115.11 | 118.90 |
| 23 | BA | 2182 | G | C8-N9-C1' | 6.31 | 135.21 | 127.00 |
| 23 | BA | 2577 | A | N1-C2-N3 | -6.31 | 126.14 | 129.30 |
| 23 | BA | 1189 | A | N7-C8-N9 | 6.31 | 116.95 | 113.80 |
| 23 | BA | 1189 | A | C8-N9-C4 | -6.31 | 103.28 | 105.80 |
| 23 | BA | 614(B) | G | C6-C5-N7 | 6.31 | 134.19 | 130.40 |
| 1 | CA | 1194 | U | C6-N1-C2 | -6.31 | 117.21 | 121.00 |
| 1 | CA | 1267 | C | C6-N1-C2 | -6.31 | 117.78 | 120.30 |
| 23 | DA | 444 | C | N3-C4-N4 | -6.31 | 113.58 | 118.00 |
| 23 | DA | 1950 | G | N9-C4-C5 | 6.31 | 107.92 | 105.40 |
| 23 | DA | 2394 | C | C5-C6-N1 | -6.31 | 117.85 | 121.00 |
| 1 | AA | 1342 | C | C6-N1-C2 | 6.31 | 122.82 | 120.30 |
| 23 | BA | 147 | U | C5-C6-N1 | -6.31 | 119.55 | 122.70 |
| 23 | BA | 189 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 23 | BA | 2789 | C | C6-N1-C2 | 6.31 | 122.82 | 120.30 |
| 23 | DA | 2224 | G | N1-C6-O6 | 6.31 | 123.69 | 119.90 |
| 23 | DA | 98 | G | C8-N9-C4 | 6.31 | 108.92 | 106.40 |
| 23 | DA | 1781 | C | N3-C2-O2 | -6.31 | 117.49 | 121.90 |
| 51 | D7 | 47 | ARG | NE-CZ-NH1 | 6.31 | 123.45 | 120.30 |
| 1 | AA | 28 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 23 | BA | 657 | U | C5-C6-N1 | -6.30 | 119.55 | 122.70 |
| 23 | BA | 2087 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 23 | BA | 60 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 23 | BA | 1044 | G | N3-C4-C5 | -6.30 | 125.45 | 128.60 |
| 23 | BA | 129 | C | C2-N3-C4 | -6.30 | 116.75 | 119.90 |
| 23 | BA | 753 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 23 | BA | 1593 | G | C5-C6-N1 | 6.30 | 114.65 | 111.50 |
| 23 | DA | 449 | A | C5-C6-N6 | -6.30 | 118.66 | 123.70 |
| 23 | DA | 1614 | A | C8-N9-C4 | 6.30 | 108.32 | 105.80 |
| 23 | DA | 2182 | G | C4-N9-C1' | -6.30 | 118.31 | 126.50 |
| 24 | DB | 113 | G | N9-C4-C5 | -6.30 | 102.88 | 105.40 |
| 1 | AA | 1210 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 1 | AA | 1368 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 23 | BA | 1881 | C | C6-N1-C2 | -6.30 | 117.78 | 120.30 |
| 1 | CA | 73 | G | C5-C6-O6 | -6.30 | 124.82 | 128.60 |
| 1 | CA | 721 | G | C5-C6-N1 | -6.30 | 108.35 | 111.50 |
| 1 | AA | 577 | G | C8-N9-C4 | 6.29 | 108.92 | 106.40 |
| 23 | DA | 2296 | U | C1'-O4'-C4' | -6.29 | 104.86 | 109.90 |
| 23 | BA | 202 | U | C6-N1-C2 | 6.29 | 124.78 | 121.00 |
| 23 | BA | 723 | G | C8-N9-C4 | 6.29 | 108.92 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 23 | BA | 1896 | G | N1-C6-O6 | 6.29 | 123.68 | 119.90 |
| 1 | CA | 1166 | G | C5-C6-O6 | 6.29 | 132.38 | 128.60 |
| 23 | BA | 389 | G | C4-C5-N7 | 6.29 | 113.32 | 110.80 |
| 23 | BA | 659 | C | C5-C6-N1 | -6.29 | 117.85 | 121.00 |
| 23 | BA | 1785 | A | C2-N3-C4 | -6.29 | 107.45 | 110.60 |
| 1 | AA | 73 | G | C5-C6-O6 | -6.29 | 124.83 | 128.60 |
| 1 | AA | 839 | U | N3-C2-O2 | -6.29 | 117.80 | 122.20 |
| 1 | CA | 888 | G | C5-C6-O6 | 6.29 | 132.37 | 128.60 |
| 1 | AA | 818 | G | N1-C6-O6 | -6.29 | 116.13 | 119.90 |
| 1 | AA | 970 | C | N3-C2-O2 | -6.29 | 117.50 | 121.90 |
| 1 | AA | 1058 | G | C8-N9-C4 | 6.29 | 108.91 | 106.40 |
| 23 | BA | 528 | A | C8-N9-C1' | 6.29 | 139.01 | 127.70 |
| 1 | CA | 1148 | U | C5-C6-N1 | 6.29 | 125.84 | 122.70 |
| 23 | BA | 262 | A | C6-N1-C2 | -6.28 | 114.83 | 118.60 |
| 23 | BA | 1791 | A | N1-C6-N6 | 6.28 | 122.37 | 118.60 |
| 23 | BA | 2487 | G | N1-C6-O6 | 6.28 | 123.67 | 119.90 |
| 23 | DA | 1309 | G | N7-C8-N9 | -6.28 | 109.96 | 113.10 |
| 23 | DA | 1314 | C | C6-N1-C1' | -6.28 | 113.26 | 120.80 |
| 1 | AA | 698 | G | N1-C6-O6 | 6.28 | 123.67 | 119.90 |
| 1 | AA | 1175 | G | C2-N3-C4 | 6.28 | 115.04 | 111.90 |
| 1 | AA | 1312 | G | C4-N9-C1' | 6.28 | 134.67 | 126.50 |
| 23 | BA | 386 | G | C5-N7-C8 | -6.28 | 101.16 | 104.30 |
| 23 | BA | 2335 | A | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 23 | DA | 645 | C | C5-C6-N1 | 6.28 | 124.14 | 121.00 |
| 23 | BA | 2371 | G | C6-C5-N7 | -6.28 | 126.63 | 130.40 |
| 1 | AA | 989 | C | C5-C6-N1 | 6.28 | 124.14 | 121.00 |
| 23 | DA | 2525 | G | N1-C6-O6 | 6.28 | 123.67 | 119.90 |
| 23 | DA | 82 | G | C8-N9-C4 | 6.28 | 108.91 | 106.40 |
| 23 | BA | 148 | C | C6-N1-C2 | 6.27 | 122.81 | 120.30 |
| 23 | BA | 1616 | A | N9-C4-C5 | -6.27 | 103.29 | 105.80 |
| 1 | CA | 117 | G | C5-C6-O6 | -6.27 | 124.83 | 128.60 |
| 1 | AA | 1308 | U | C5-C4-O4 | 6.27 | 129.66 | 125.90 |
| 1 | AA | 1316 | G | C6-C5-N7 | 6.27 | 134.16 | 130.40 |
| 23 | DA | 2100 | G | N3-C4-C5 | -6.27 | 125.46 | 128.60 |
| 23 | BA | 271(J) | C | N3-C4-C5 | 6.27 | 124.41 | 121.90 |
| 23 | BA | 1227 | G | C5-C6-O6 | -6.27 | 124.84 | 128.60 |
| 1 | AA | 240 | C | C5-C6-N1 | -6.27 | 117.87 | 121.00 |
| 1 | CA | 435 | C | N3-C2-O2 | -6.27 | 117.51 | 121.90 |
| 1 | CA | 976 | G | N3-C4-N9 | -6.27 | 122.24 | 126.00 |
| 1 | AA | 1217 | C | C2-N1-C1' | -6.27 | 111.91 | 118.80 |
| 23 | BA | 1661 | G | N1-C2-N3 | 6.27 | 127.66 | 123.90 |
| 23 | DA | 2435 | A | C5-N7-C8 | -6.27 | 100.77 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 750 | A | C4-C5-C6 | 6.27 | 120.13 | 117.00 |
| 23 | BA | 1021 | A | N7-C8-N9 | 6.26 | 116.93 | 113.80 |
| 23 | BA | 2623 | G | C4-C5-N7 | -6.26 | 108.29 | 110.80 |
| 24 | BB | 8 | U | C6-N1-C2 | -6.26 | 117.24 | 121.00 |
| 1 | CA | 1017 | G | C6-C5-N7 | 6.26 | 134.16 | 130.40 |
| 23 | DA | 2306 | C | C2-N3-C4 | 6.26 | 123.03 | 119.90 |
| 23 | BA | 661 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 1 | CA | 1379 | G | C8-N9-C1' | -6.26 | 118.86 | 127.00 |
| 23 | BA | 71 | A | C4-C5-N7 | 6.26 | 113.83 | 110.70 |
| 23 | BA | 988 | A | C6-C5-N7 | -6.26 | 127.92 | 132.30 |
| 23 | DA | 2084 | C | C6-N1-C2 | 6.26 | 122.80 | 120.30 |
| 1 | AA | 964 | A | C8-N9-C4 | 6.26 | 108.30 | 105.80 |
| 1 | AA | 1043 | C | C6-N1-C2 | -6.26 | 117.80 | 120.30 |
| 1 | CA | 495 | A | N1-C6-N6 | -6.26 | 114.85 | 118.60 |
| 1 | CA | 1443 | G | C4-C5-N7 | 6.26 | 113.30 | 110.80 |
| 23 | DA | 2353 | G | N9-C4-C5 | -6.26 | 102.90 | 105.40 |
| 23 | BA | 1005 | C | N3-C4-C5 | 6.25 | 124.40 | 121.90 |
| 1 | CA | 1060 | C | C6-N1-C2 | -6.25 | 117.80 | 120.30 |
| 23 | DA | 928 | G | C4-C5-N7 | 6.25 | 113.30 | 110.80 |
| 1 | AA | 930 | C | C2-N1-C1' | -6.25 | 111.92 | 118.80 |
| 1 | AA | 1175 | G | N1-C2-N3 | -6.25 | 120.15 | 123.90 |
| 23 | BA | 1256 | G | N1-C2-N3 | 6.25 | 127.65 | 123.90 |
| 23 | BA | 2036 | C | C6-N1-C1' | 6.25 | 128.31 | 120.80 |
| 1 | CA | 1076 | C | C6-N1-C2 | 6.25 | 122.80 | 120.30 |
| 1 | CA | 765 | G | C8-N9-C4 | -6.25 | 103.90 | 106.40 |
| 23 | DA | 2322 | A | C5-C6-N1 | 6.25 | 120.83 | 117.70 |
| 23 | BA | 2510 | C | N3-C2-O2 | -6.25 | 117.53 | 121.90 |
| 23 | BA | 859 | G | N1-C6-O6 | 6.25 | 123.65 | 119.90 |
| 23 | BA | 109 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 23 | BA | 536 | A | N7-C8-N9 | -6.25 | 110.68 | 113.80 |
| 23 | BA | 2059 | A | C5-N7-C8 | 6.25 | 107.02 | 103.90 |
| 23 | BA | 2700 | C | N3-C4-C5 | 6.25 | 124.40 | 121.90 |
| 23 | DA | 776 | G | C8-N9-C4 | -6.25 | 103.90 | 106.40 |
| 23 | DA | 1603 | A | N7-C8-N9 | 6.25 | 116.92 | 113.80 |
| 23 | DA | 2023 | G | C5-C6-O6 | -6.25 | 124.85 | 128.60 |
| 23 | BA | 526 | A | C8-N9-C4 | -6.24 | 103.30 | 105.80 |
| 23 | BA | 1431 | U | C5-C6-N1 | 6.24 | 125.82 | 122.70 |
| 23 | BA | 2179 | C | N1-C2-O2 | 6.24 | 122.65 | 118.90 |
| 23 | BA | 2683 | C | C6-N1-C2 | -6.24 | 117.80 | 120.30 |
| 23 | BA | 2712(A) | A | C2-N3-C4 | -6.24 | 107.48 | 110.60 |
| 23 | DA | 530 | G | C5-C6-O6 | -6.24 | 124.85 | 128.60 |
| 23 | DA | 2260 | C | C4-C5-C6 | 6.24 | 120.52 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 982 | C | N3-C4-N4 | -6.24 | 113.63 | 118.00 |
| 23 | DA | 1839 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 23 | DA | 2570 | G | C5-C6-N1 | -6.24 | 108.38 | 111.50 |
| 23 | BA | 194 | G | N3-C4-C5 | 6.24 | 131.72 | 128.60 |
| 23 | BA | 640 | C | N3-C4-C5 | -6.24 | 119.40 | 121.90 |
| 23 | BA | 793 | A | C8-N9-C4 | -6.24 | 103.30 | 105.80 |
| 23 | BA | 988 | A | C5-C6-N6 | -6.24 | 118.71 | 123.70 |
| 23 | DA | 1022 | G | C8-N9-C1' | 6.24 | 135.11 | 127.00 |
| 1 | AA | 598 | U | N3-C4-O4 | 6.24 | 123.77 | 119.40 |
| 23 | BA | 2338 | G | N1-C6-O6 | 6.24 | 123.64 | 119.90 |
| 23 | BA | 2729 | G | C5-C6-N1 | -6.24 | 108.38 | 111.50 |
| 23 | DA | 1792 | G | N7-C8-N9 | -6.24 | 109.98 | 113.10 |
| 23 | BA | 416 | C | N3-C4-C5 | 6.24 | 124.39 | 121.90 |
| 23 | BA | 2439 | A | C2-N3-C4 | -6.24 | 107.48 | 110.60 |
| 23 | BA | 2621 | A | C5-C6-N1 | 6.24 | 120.82 | 117.70 |
| 23 | BA | 446 | G | N9-C4-C5 | -6.24 | 102.91 | 105.40 |
| 23 | BA | 2502 | G | C6-N1-C2 | -6.24 | 121.36 | 125.10 |
| 1 | CA | 1047 | G | C6-N1-C2 | 6.24 | 128.84 | 125.10 |
| 1 | CA | 1235 | U | C2-N3-C4 | -6.24 | 123.26 | 127.00 |
| 23 | DA | 2827 | C | N3-C2-O2 | 6.24 | 126.27 | 121.90 |
| 23 | BA | 2015 | A | C2-N3-C4 | -6.23 | 107.48 | 110.60 |
| 1 | AA | 1443 | G | C4-C5-N7 | 6.23 | 113.29 | 110.80 |
| 1 | AA | 1158 | C | C5-C6-N1 | 6.23 | 124.11 | 121.00 |
| 1 | CA | 63 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 23 | BA | 2011 | U | N1-C2-O2 | -6.23 | 118.44 | 122.80 |
| 23 | DA | 2596 | U | C2-N3-C4 | -6.23 | 123.26 | 127.00 |
| 23 | BA | 2587 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 24 | DB | 115 | G | N9-C4-C5 | -6.22 | 102.91 | 105.40 |
| 1 | AA | 665 | A | C8-N9-C4 | 6.22 | 108.29 | 105.80 |
| 23 | DA | 404 | C | C6-N1-C2 | 6.22 | 122.79 | 120.30 |
| 23 | BA | 652(F) | G | N1-C6-O6 | 6.22 | 123.63 | 119.90 |
| 23 | BA | 2164 | C | N3-C4-C5 | -6.22 | 119.41 | 121.90 |
| 23 | BA | 2100 | G | C6-C5-N7 | -6.22 | 126.67 | 130.40 |
| 1 | AA | 1346 | A | N9-C4-C5 | -6.22 | 103.31 | 105.80 |
| 23 | BA | 745 | G | C5-C6-O6 | -6.22 | 124.87 | 128.60 |
| 23 | BA | 799 | G | C6-N1-C2 | -6.22 | 121.37 | 125.10 |
| 23 | DA | 2723 | C | C4-C5-C6 | 6.22 | 120.51 | 117.40 |
| 1 | AA | 818 | G | C4-C5-N7 | -6.21 | 108.31 | 110.80 |
| 1 | CA | 866 | C | N3-C4-C5 | -6.21 | 119.42 | 121.90 |
| 1 | CA | 1246 | C | C5-C6-N1 | 6.21 | 124.11 | 121.00 |
| 1 | CA | 1301 | U | C6-N1-C2 | -6.21 | 117.27 | 121.00 |
| 23 | DA | 271(G) | C | N1-C2-O2 | 6.21 | 122.63 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | DA | 1616 | A | C6-C5-N7 | -6.21 | 127.95 | 132.30 |
| 23 | BA | 196 | A | C5-N7-C8 | -6.21 | 100.79 | 103.90 |
| 23 | BA | 1698 | A | C8-N9-C4 | -6.21 | 103.31 | 105.80 |
| 23 | BA | 2292 | C | N3-C4-C5 | 6.21 | 124.39 | 121.90 |
| 23 | BA | 960 | A | N1-C6-N6 | 6.21 | 122.33 | 118.60 |
| 23 | BA | 2692 | C | N3-C4-C5 | 6.21 | 124.39 | 121.90 |
| 23 | DA | 675 | A | C2-N3-C4 | -6.21 | 107.49 | 110.60 |
| 23 | DA | 2728 | U | C2-N3-C4 | -6.21 | 123.27 | 127.00 |
| 23 | BA | 2769 | C | N3-C4-C5 | 6.21 | 124.38 | 121.90 |
| 1 | CA | 1184 | G | C6-N1-C2 | 6.21 | 128.83 | 125.10 |
| 1 | AA | 529 | G | C5-C6-O6 | -6.21 | 124.88 | 128.60 |
| 1 | AA | 1274 | G | C5-C6-N1 | -6.21 | 108.39 | 111.50 |
| 1 | CA | 963 | G | N3-C4-N9 | 6.21 | 129.72 | 126.00 |
| 1 | CA | 998 | G | N9-C4-C5 | 6.21 | 107.88 | 105.40 |
| 1 | CA | 1343 | G | C4-C5-N7 | 6.21 | 113.28 | 110.80 |
| 24 | DB | 75 | G | C8-N9-C4 | 6.21 | 108.88 | 106.40 |
| 23 | BA | 586 | A | C8-N9-C4 | -6.21 | 103.32 | 105.80 |
| 23 | BA | 763 | G | C6-N1-C2 | -6.21 | 121.38 | 125.10 |
| 23 | BA | 1243 | G | N3-C4-C5 | 6.21 | 131.70 | 128.60 |
| 23 | BA | 2353 | G | N9-C4-C5 | -6.21 | 102.92 | 105.40 |
| 1 | CA | 1119 | C | C6-N1-C2 | -6.21 | 117.82 | 120.30 |
| 23 | DA | 2379 | G | N7-C8-N9 | 6.21 | 116.20 | 113.10 |
| 23 | BA | 1803 | A | C2-N3-C4 | 6.21 | 113.70 | 110.60 |
| 23 | BA | 2555 | U | N1-C2-O2 | -6.21 | 118.46 | 122.80 |
| 1 | CA | 976 | G | N3-C4-C5 | 6.21 | 131.70 | 128.60 |
| 1 | CA | 1340 | A | N7-C8-N9 | 6.21 | 116.90 | 113.80 |
| 23 | DA | 2028 | U | C5-C6-N1 | -6.21 | 119.60 | 122.70 |
| 1 | AA | 988 | G | N9-C4-C5 | 6.20 | 107.88 | 105.40 |
| 23 | BA | 529 | A | C5-N7-C8 | -6.20 | 100.80 | 103.90 |
| 1 | CA | 529 | G | C5-C6-O6 | -6.20 | 124.88 | 128.60 |
| 23 | DA | 977 | G | C5-C6-N1 | 6.20 | 114.60 | 111.50 |
| 23 | DA | 196 | A | N1-C6-N6 | 6.20 | 122.32 | 118.60 |
| 23 | BA | 1864 | U | N3-C2-O2 | 6.20 | 126.54 | 122.20 |
| 23 | DA | 2782 | G | C6-C5-N7 | -6.20 | 126.68 | 130.40 |
| 1 | AA | 366 | C | C5-C6-N1 | -6.20 | 117.90 | 121.00 |
| 1 | AA | 767 | A | N1-C6-N6 | -6.20 | 114.88 | 118.60 |
| 1 | AA | 855 | G | N9-C4-C5 | 6.20 | 107.88 | 105.40 |
| 23 | BA | 124 | G | C8-N9-C4 | 6.20 | 108.88 | 106.40 |
| 23 | BA | 1602 | U | C4-C5-C6 | 6.20 | 123.42 | 119.70 |
| 1 | CA | 770 | C | C5-C6-N1 | -6.20 | 117.90 | 121.00 |
| 23 | DA | 1755 | A | C5-C6-N6 | 6.20 | 128.66 | 123.70 |
| 1 | AA | 1297 | C | C6-N1-C2 | -6.20 | 117.82 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|----------|-------|-------------|----------|
| 23 | BA | 2353 | G | C8-N9-C4 | 6.20 | 108.88 | 106.40 |
| 23 | BA | 2425 | A | C8-N9-C4 | -6.20 | 103.32 | 105.80 |
| 23 | BA | 2768 | C | C2-N3-C4 | -6.20 | 116.80 | 119.90 |
| 24 | BB | 118 | G | C8-N9-C4 | 6.20 | 108.88 | 106.40 |
| 23 | DA | 389 | G | C4-C5-N7 | 6.20 | 113.28 | 110.80 |
| 23 | DA | 673 | C | N3-C4-C5 | 6.20 | 124.38 | 121.90 |
| 23 | DA | 1314 | C | C5-C4-N4 | -6.20 | 115.86 | 120.20 |
| 23 | DA | 1987 | G | N1-C6-O6 | 6.20 | 123.62 | 119.90 |
| 1 | CA | 1042 | G | C6-C5-N7 | 6.19 | 134.12 | 130.40 |
| 1 | AA | 1108 | G | C5-C6-O6 | 6.19 | 132.32 | 128.60 |
| 23 | BA | 1304 | C | N3-C4-C5 | 6.19 | 124.38 | 121.90 |
| 1 | CA | 1343 | G | N3-C4-N9 | 6.19 | 129.72 | 126.00 |
| 23 | DA | 910 | A | N1-C6-N6 | 6.19 | 122.31 | 118.60 |
| 23 | BA | 2296 | U | C6-N1-C2 | 6.19 | 124.71 | 121.00 |
| 23 | DA | 2031 | A | C4-C5-C6 | 6.19 | 120.10 | 117.00 |
| 23 | BA | 2059 | A | C8-N9-C4 | 6.19 | 108.28 | 105.80 |
| 23 | BA | 2454 | G | N7-C8-N9 | -6.19 | 110.01 | 113.10 |
| 23 | BA | 989 | G | N9-C4-C5 | -6.19 | 102.92 | 105.40 |
| 23 | BA | 1021 | A | N1-C2-N3 | 6.19 | 132.39 | 129.30 |
| 23 | BA | 1992 | G | C5-C6-O6 | 6.19 | 132.31 | 128.60 |
| 23 | DA | 2038 | G | C4-C5-N7 | 6.19 | 113.27 | 110.80 |
| 1 | AA | 1158 | C | N3-C2-O2 | -6.18 | 117.57 | 121.90 |
| 23 | BA | 1979 | C | C5-C6-N1 | 6.18 | 124.09 | 121.00 |
| 23 | DA | 1298 | C | N3-C2-O2 | -6.18 | 117.57 | 121.90 |
| 1 | AA | 1093 | A | N1-C6-N6 | 6.18 | 122.31 | 118.60 |
| 23 | BA | 729 | G | N1-C6-O6 | 6.18 | 123.61 | 119.90 |
| 23 | DA | 766 | C | C6-N1-C2 | -6.18 | 117.83 | 120.30 |
| 23 | BA | 984 | A | C8-N9-C4 | 6.18 | 108.27 | 105.80 |
| 23 | BA | 1128 | A | C8-N9-C4 | -6.18 | 103.33 | 105.80 |
| 23 | BA | 1578 | U | C5-C4-O4 | 6.18 | 129.61 | 125.90 |
| 23 | DA | 1938 | A | C4-C5-C6 | 6.18 | 120.09 | 117.00 |
| 23 | DA | 330 | A | N1-C2-N3 | 6.18 | 132.39 | 129.30 |
| 23 | DA | 1977 | A | N7-C8-N9 | -6.18 | 110.71 | 113.80 |
| 1 | AA | 1239 | A | N1-C6-N6 | -6.18 | 114.89 | 118.60 |
| 23 | BA | 2018 | G | N7-C8-N9 | 6.18 | 116.19 | 113.10 |
| 25 | DD | 229 | VAL | CB-CA-C | -6.18 | 99.67 | 111.40 |
| 23 | BA | 558 | G | N7-C8-N9 | -6.17 | 110.01 | 113.10 |
| 23 | BA | 2487 | G | C5-C6-O6 | -6.17 | 124.89 | 128.60 |
| 23 | BA | 2808 | U | N3-C4-O4 | 6.17 | 123.72 | 119.40 |
| 1 | CA | 1442(B) | A | C4-C5-C6 | 6.17 | 120.09 | 117.00 |
| 23 | DA | 459 | U | N3-C4-O4 | -6.17 | 115.08 | 119.40 |
| 23 | BA | 272(H) | C | C5-C6-N1 | 6.17 | 124.09 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1262 | A | C8-N9-C4 | -6.17 | 103.33 | 105.80 |
| 23 | BA | 2782 | G | N1-C6-O6 | 6.17 | 123.60 | 119.90 |
| 23 | BA | 2768 | C | N3-C2-O2 | -6.17 | 117.58 | 121.90 |
| 1 | CA | 954 | G | C8-N9-C4 | 6.17 | 108.87 | 106.40 |
| 1 | CA | 1527 | C | C6-N1-C2 | 6.17 | 122.77 | 120.30 |
| 1 | AA | 60 | A | N1-C6-N6 | -6.17 | 114.90 | 118.60 |
| 1 | AA | 956 | U | C5-C6-N1 | 6.17 | 125.78 | 122.70 |
| 23 | BA | 623 | G | C8-N9-C4 | 6.17 | 108.87 | 106.40 |
| 1 | CA | 358 | U | N1-C2-N3 | 6.17 | 118.60 | 114.90 |
| 23 | DA | 1391 | U | C2-N1-C1' | 6.17 | 125.10 | 117.70 |
| 23 | BA | 1655 | A | N7-C8-N9 | -6.17 | 110.72 | 113.80 |
| 23 | BA | 1858 | G | C8-N9-C4 | -6.17 | 103.93 | 106.40 |
| 23 | DA | 535 | C | N3-C2-O2 | 6.17 | 126.22 | 121.90 |
| 23 | DA | 995 | C | N1-C2-O2 | -6.17 | 115.20 | 118.90 |
| 23 | DA | 1802 | A | N1-C2-N3 | 6.17 | 132.38 | 129.30 |
| 23 | DA | 2364 | C | C5-C6-N1 | -6.17 | 117.92 | 121.00 |
| 1 | AA | 938 | A | N7-C8-N9 | 6.17 | 116.88 | 113.80 |
| 23 | BA | 1200 | C | C5-C6-N1 | -6.16 | 117.92 | 121.00 |
| 1 | CA | 818 | G | N1-C6-O6 | -6.16 | 116.20 | 119.90 |
| 23 | DA | 1478 | G | N3-C2-N2 | 6.16 | 124.22 | 119.90 |
| 23 | DA | 1963 | U | C5-C6-N1 | 6.16 | 125.78 | 122.70 |
| 23 | DA | 2055 | C | C2-N1-C1' | -6.16 | 112.02 | 118.80 |
| 23 | BA | 1304 | C | C2-N3-C4 | -6.16 | 116.82 | 119.90 |
| 23 | BA | 1350 | C | C6-N1-C2 | 6.16 | 122.77 | 120.30 |
| 23 | BA | 1667 | G | C5-C6-O6 | -6.16 | 124.90 | 128.60 |
| 1 | AA | 357 | G | N9-C4-C5 | 6.16 | 107.86 | 105.40 |
| 23 | DA | 2371 | G | C8-N9-C4 | 6.16 | 108.86 | 106.40 |
| 23 | BA | 688 | U | N1-C2-O2 | -6.16 | 118.49 | 122.80 |
| 1 | CA | 39 | G | C4-C5-N7 | -6.16 | 108.34 | 110.80 |
| 23 | DA | 775 | G | N1-C2-N2 | -6.16 | 110.66 | 116.20 |
| 23 | DA | 1327 | C | N1-C2-O2 | -6.16 | 115.20 | 118.90 |
| 23 | DA | 1653 | G | C4-N9-C1' | 6.16 | 134.50 | 126.50 |
| 23 | BA | 12 | U | N1-C2-O2 | 6.16 | 127.11 | 122.80 |
| 23 | BA | 1755 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 23 | BA | 2764 | A | N9-C4-C5 | 6.16 | 108.26 | 105.80 |
| 23 | BA | 1950 | G | C5-C6-O6 | 6.15 | 132.29 | 128.60 |
| 1 | CA | 1009 | G | N1-C6-O6 | 6.15 | 123.59 | 119.90 |
| 23 | DA | 397 | G | N3-C4-C5 | 6.15 | 131.68 | 128.60 |
| 23 | DA | 2103 | C | C2-N3-C4 | 6.15 | 122.98 | 119.90 |
| 23 | DA | 361 | G | N1-C6-O6 | 6.15 | 123.59 | 119.90 |
| 23 | DA | 1204 | A | N3-C4-C5 | 6.15 | 131.11 | 126.80 |
| 23 | DA | 2182 | G | N9-C4-C5 | 6.15 | 107.86 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 1 | AA | 1443 | G | C8-N9-C4 | 6.15 | 108.86 | 106.40 |
| 23 | BA | 678 | C | C2-N3-C4 | -6.15 | 116.83 | 119.90 |
| 23 | BA | 764 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 23 | BA | 2621 | A | C4-C5-C6 | -6.15 | 113.92 | 117.00 |
| 1 | CA | 1246 | C | N1-C2-O2 | 6.15 | 122.59 | 118.90 |
| 1 | AA | 1333 | A | N7-C8-N9 | 6.15 | 116.87 | 113.80 |
| 23 | BA | 278 | A | C5-C6-N6 | -6.15 | 118.78 | 123.70 |
| 23 | BA | 688 | U | N1-C2-N3 | 6.15 | 118.59 | 114.90 |
| 23 | BA | 2286 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 23 | DA | 2581 | G | C5-C6-O6 | 6.15 | 132.29 | 128.60 |
| 1 | CA | 1392 | G | N3-C2-N2 | 6.15 | 124.20 | 119.90 |
| 23 | DA | 2335 | A | N9-C4-C5 | -6.15 | 103.34 | 105.80 |
| 23 | BA | 1178 | C | C5-C6-N1 | 6.14 | 124.07 | 121.00 |
| 23 | DA | 1264 | G | C5-C6-O6 | -6.14 | 124.91 | 128.60 |
| 1 | AA | 1047 | G | C5-C6-O6 | -6.14 | 124.91 | 128.60 |
| 23 | BA | 1448 | G | N1-C6-O6 | 6.14 | 123.59 | 119.90 |
| 23 | DA | 71 | A | N3-C4-N9 | -6.14 | 122.49 | 127.40 |
| 23 | BA | 2582 | G | C5-C6-O6 | 6.14 | 132.28 | 128.60 |
| 1 | CA | 1214 | C | N3-C4-C5 | -6.14 | 119.44 | 121.90 |
| 1 | CA | 1231 | G | C6-N1-C2 | -6.14 | 121.42 | 125.10 |
| 23 | DA | 1371 | G | N1-C6-O6 | 6.14 | 123.58 | 119.90 |
| 1 | AA | 1067 | A | C8-N9-C4 | -6.14 | 103.34 | 105.80 |
| 23 | BA | 1819 | A | C4-C5-N7 | -6.14 | 107.63 | 110.70 |
| 23 | BA | 2220 | G | C8-N9-C4 | -6.14 | 103.94 | 106.40 |
| 23 | DA | 201 | C | C5-C6-N1 | -6.14 | 117.93 | 121.00 |
| 23 | DA | 1934 | C | C6-N1-C2 | 6.14 | 122.75 | 120.30 |
| 23 | BA | 2592 | G | C8-N9-C4 | -6.13 | 103.95 | 106.40 |
| 1 | CA | 804 | U | C5-C6-N1 | -6.13 | 119.63 | 122.70 |
| 23 | DA | 1047 | G | N3-C4-N9 | 6.13 | 129.68 | 126.00 |
| 23 | BA | 272(H) | C | C5-C4-N4 | -6.13 | 115.91 | 120.20 |
| 23 | BA | 452 | G | N3-C4-C5 | -6.13 | 125.53 | 128.60 |
| 1 | CA | 458 | C | N3-C2-O2 | -6.13 | 117.61 | 121.90 |
| 23 | DA | 1992 | G | C8-N9-C4 | -6.13 | 103.95 | 106.40 |
| 1 | AA | 1442 | G | N3-C4-N9 | 6.13 | 129.68 | 126.00 |
| 1 | AA | 670 | G | C4-C5-N7 | -6.13 | 108.35 | 110.80 |
| 23 | BA | 380 | U | C5-C6-N1 | -6.13 | 119.64 | 122.70 |
| 23 | BA | 2300 | G | N3-C4-N9 | 6.13 | 129.68 | 126.00 |
| 23 | BA | 2596 | U | N1-C2-N3 | 6.13 | 118.58 | 114.90 |
| 1 | CA | 1286 | A | N1-C2-N3 | 6.13 | 132.36 | 129.30 |
| 23 | DA | 2323 | G | N9-C4-C5 | -6.13 | 102.95 | 105.40 |
| 23 | DA | 1991 | U | C5-C6-N1 | -6.12 | 119.64 | 122.70 |
| 1 | AA | 1343 | G | N3-C4-N9 | 6.12 | 129.67 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 2446 | G | C5-C6-O6 | -6.12 | 124.93 | 128.60 |
| 23 | DA | 2751 | G | C8-N9-C4 | -6.12 | 103.95 | 106.40 |
| 23 | BA | 475 | U | N3-C2-O2 | -6.12 | 117.92 | 122.20 |
| 23 | BA | 2257 | U | N3-C2-O2 | 6.12 | 126.48 | 122.20 |
| 23 | DA | 154 | G | C5-C6-O6 | -6.12 | 124.93 | 128.60 |
| 1 | AA | 1442 | G | N9-C4-C5 | -6.12 | 102.95 | 105.40 |
| 23 | BA | 363(B) | G | N3-C4-N9 | 6.12 | 129.67 | 126.00 |
| 23 | BA | 1200 | C | C2-N3-C4 | -6.12 | 116.84 | 119.90 |
| 23 | BA | 1531 | C | C6-N1-C2 | -6.12 | 117.85 | 120.30 |
| 23 | DA | 2107 | C | C5-C4-N4 | 6.12 | 124.48 | 120.20 |
| 23 | DA | 1419 | A | C8-N9-C4 | 6.12 | 108.25 | 105.80 |
| 23 | DA | 2607 | G | N3-C2-N2 | 6.12 | 124.18 | 119.90 |
| 23 | BA | 667 | U | N1-C2-O2 | -6.12 | 118.52 | 122.80 |
| 23 | BA | 2445 | G | C5-C6-O6 | 6.12 | 132.27 | 128.60 |
| 1 | CA | 1333 | A | C8-N9-C4 | -6.12 | 103.35 | 105.80 |
| 23 | DA | 691 | C | C6-N1-C2 | 6.12 | 122.75 | 120.30 |
| 23 | DA | 865 | C | C6-N1-C2 | 6.12 | 122.75 | 120.30 |
| 23 | DA | 2689 | U | C2-N1-C1' | -6.12 | 110.36 | 117.70 |
| 23 | DA | 2340 | G | N9-C4-C5 | -6.11 | 102.95 | 105.40 |
| 23 | DA | 530 | G | C4-C5-N7 | 6.11 | 113.25 | 110.80 |
| 23 | BA | 201 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |
| 23 | BA | 1936 | A | C8-N9-C4 | -6.11 | 103.36 | 105.80 |
| 23 | DA | 205 | G | N3-C2-N2 | 6.11 | 124.18 | 119.90 |
| 23 | DA | 446 | G | N9-C4-C5 | -6.11 | 102.96 | 105.40 |
| 1 | AA | 1312 | G | C8-N9-C4 | -6.11 | 103.96 | 106.40 |
| 23 | DA | 279 | C | C5-C6-N1 | 6.11 | 124.05 | 121.00 |
| 1 | AA | 1166 | G | C4-N9-C1' | -6.11 | 118.56 | 126.50 |
| 23 | BA | 1536 | C | C2-N1-C1' | 6.11 | 125.52 | 118.80 |
| 23 | BA | 2100 | G | C8-N9-C1' | -6.11 | 119.06 | 127.00 |
| 1 | CA | 444 | C | C6-N1-C2 | 6.11 | 122.74 | 120.30 |
| 23 | BA | 2103 | C | C2-N3-C4 | 6.10 | 122.95 | 119.90 |
| 1 | CA | 1008 | C | N3-C4-N4 | 6.10 | 122.27 | 118.00 |
| 23 | BA | 196 | A | N9-C4-C5 | -6.10 | 103.36 | 105.80 |
| 1 | CA | 1165 | C | N3-C4-C5 | -6.10 | 119.46 | 121.90 |
| 1 | CA | 1283 | G | N1-C6-O6 | -6.10 | 116.24 | 119.90 |
| 23 | DA | 1006 | C | C2-N1-C1' | -6.10 | 112.09 | 118.80 |
| 1 | CA | 1131 | G | C8-N9-C4 | 6.10 | 108.84 | 106.40 |
| 1 | CA | 1277 | C | C5-C4-N4 | 6.10 | 124.47 | 120.20 |
| 23 | DA | 1531 | C | C6-N1-C2 | -6.10 | 117.86 | 120.30 |
| 23 | BA | 592 | G | N9-C4-C5 | 6.10 | 107.84 | 105.40 |
| 23 | BA | 1681 | G | C6-C5-N7 | -6.10 | 126.74 | 130.40 |
| 23 | DA | 1617 | C | C5-C6-N1 | -6.10 | 117.95 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2421 | G | C5-C6-O6 | -6.10 | 124.94 | 128.60 |
| 23 | BA | 1268 | A | C2-N3-C4 | -6.10 | 107.55 | 110.60 |
| 1 | CA | 1004 | A | C8-N9-C4 | -6.10 | 103.36 | 105.80 |
| 23 | DA | 278 | A | N9-C4-C5 | -6.10 | 103.36 | 105.80 |
| 23 | DA | 2031 | A | C6-C5-N7 | -6.10 | 128.03 | 132.30 |
| 23 | DA | 2731 | G | C6-N1-C2 | -6.10 | 121.44 | 125.10 |
| 1 | CA | 557 | G | N3-C4-C5 | -6.09 | 125.55 | 128.60 |
| 23 | DA | 847 | U | N1-C2-O2 | 6.09 | 127.07 | 122.80 |
| 23 | DA | 1755 | A | N1-C2-N3 | 6.09 | 132.35 | 129.30 |
| 23 | DA | 2335 | A | C6-N1-C2 | -6.09 | 114.94 | 118.60 |
| 1 | AA | 1216 | G | C6-N1-C2 | 6.09 | 128.76 | 125.10 |
| 23 | BA | 2013 | A | C5-N7-C8 | -6.09 | 100.85 | 103.90 |
| 23 | BA | 682 | G | C6-C5-N7 | -6.09 | 126.75 | 130.40 |
| 1 | CA | 1166 | G | C6-C5-N7 | 6.09 | 134.06 | 130.40 |
| 23 | DA | 2623 | G | C2-N3-C4 | 6.09 | 114.95 | 111.90 |
| 23 | BA | 2049 | G | C2-N3-C4 | -6.09 | 108.86 | 111.90 |
| 23 | BA | 2286 | A | N1-C2-N3 | 6.09 | 132.34 | 129.30 |
| 23 | BA | 2875 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 1 | CA | 1171 | G | C6-N1-C2 | 6.09 | 128.75 | 125.10 |
| 1 | CA | 1456 | G | N3-C4-C5 | -6.09 | 125.56 | 128.60 |
| 23 | DA | 893 | C | C2-N1-C1' | 6.09 | 125.50 | 118.80 |
| 24 | BB | 92 | C | C5-C6-N1 | 6.09 | 124.04 | 121.00 |
| 23 | BA | 1137 | G | N1-C6-O6 | 6.09 | 123.55 | 119.90 |
| 23 | BA | 1816 | G | N9-C4-C5 | -6.09 | 102.97 | 105.40 |
| 25 | BD | 131 | LEU | CB-CG-CD2 | -6.09 | 100.65 | 111.00 |
| 23 | DA | 2510 | C | C5-C4-N4 | 6.09 | 124.46 | 120.20 |
| 23 | DA | 747 | U | N1-C2-O2 | -6.08 | 118.54 | 122.80 |
| 23 | DA | 2881 | C | N3-C2-O2 | 6.08 | 126.16 | 121.90 |
| 23 | BA | 742 | G | C8-N9-C4 | 6.08 | 108.83 | 106.40 |
| 23 | BA | 1391 | U | C2-N1-C1' | 6.08 | 125.00 | 117.70 |
| 23 | DA | 1830 | C | C6-N1-C2 | 6.08 | 122.73 | 120.30 |
| 23 | BA | 143 | G | C4-N9-C1' | -6.08 | 118.59 | 126.50 |
| 23 | BA | 759 | G | C8-N9-C4 | 6.08 | 108.83 | 106.40 |
| 23 | BA | 2273 | A | C5-N7-C8 | -6.08 | 100.86 | 103.90 |
| 23 | BA | 2856 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 23 | DA | 2129 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 23 | DA | 2300 | G | N3-C4-N9 | 6.08 | 129.65 | 126.00 |
| 23 | DA | 693 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 23 | DA | 2768 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 23 | BA | 546 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 23 | BA | 2225 | A | C4-C5-C6 | -6.08 | 113.96 | 117.00 |
| 23 | DA | 271(W) | G | C8-N9-C4 | -6.08 | 103.97 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 2397 | G | N7-C8-N9 | 6.08 | 116.14 | 113.10 |
| 1 | AA | 1279 | A | C4-N9-C1' | 6.08 | 137.24 | 126.30 |
| 23 | BA | 122 | G | N1-C6-O6 | 6.08 | 123.55 | 119.90 |
| 23 | BA | 468 | G | N9-C4-C5 | -6.08 | 102.97 | 105.40 |
| 23 | BA | 679 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 23 | BA | 2015 | A | C4-C5-C6 | 6.08 | 120.04 | 117.00 |
| 1 | CA | 1314 | C | N1-C2-O2 | 6.08 | 122.55 | 118.90 |
| 23 | DA | 739 | G | N7-C8-N9 | -6.08 | 110.06 | 113.10 |
| 23 | DA | 2264 | C | C2-N3-C4 | -6.08 | 116.86 | 119.90 |
| 23 | BA | 533 | G | N1-C2-N3 | 6.07 | 127.54 | 123.90 |
| 23 | BA | 1315 | C | N1-C2-N3 | 6.07 | 123.45 | 119.20 |
| 23 | DA | 695 | G | C5-C6-O6 | 6.07 | 132.24 | 128.60 |
| 23 | BA | 2003 | G | C5-C6-N1 | 6.07 | 114.54 | 111.50 |
| 23 | BA | 886 | C | N1-C2-O2 | 6.07 | 122.54 | 118.90 |
| 23 | BA | 2287 | A | C5-N7-C8 | -6.07 | 100.86 | 103.90 |
| 23 | BA | 2464 | C | C2-N1-C1' | 6.07 | 125.48 | 118.80 |
| 23 | BA | 2672 | G | N1-C6-O6 | 6.07 | 123.54 | 119.90 |
| 23 | DA | 1989 | G | C5-C6-O6 | -6.07 | 124.96 | 128.60 |
| 1 | AA | 1442(B) | A | C4-N9-C1' | 6.07 | 137.22 | 126.30 |
| 23 | BA | 239 | U | C5-C6-N1 | -6.07 | 119.67 | 122.70 |
| 23 | BA | 763 | G | C4-C5-N7 | -6.07 | 108.37 | 110.80 |
| 1 | CA | 1330 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 23 | DA | 1121 | C | C5-C6-N1 | -6.07 | 117.97 | 121.00 |
| 23 | DA | 2099 | U | C6-N1-C2 | -6.07 | 117.36 | 121.00 |
| 23 | BA | 527 | C | C5-C4-N4 | 6.07 | 124.45 | 120.20 |
| 23 | BA | 2004 | G | C5-N7-C8 | -6.07 | 101.27 | 104.30 |
| 23 | BA | 2707 | G | C4-C5-N7 | 6.07 | 113.23 | 110.80 |
| 1 | CA | 1030 | C | N3-C2-O2 | -6.07 | 117.65 | 121.90 |
| 23 | DA | 62 | C | N3-C4-N4 | -6.07 | 113.75 | 118.00 |
| 23 | DA | 791 | C | N3-C2-O2 | -6.07 | 117.65 | 121.90 |
| 23 | DA | 1316 | U | N3-C2-O2 | -6.07 | 117.95 | 122.20 |
| 23 | DA | 1845 | G | N1-C6-O6 | -6.07 | 116.26 | 119.90 |
| 23 | DA | 2100 | G | C4-N9-C1' | 6.07 | 134.38 | 126.50 |
| 1 | AA | 822 | C | C6-N1-C2 | 6.06 | 122.72 | 120.30 |
| 23 | BA | 1478 | G | N3-C2-N2 | 6.06 | 124.14 | 119.90 |
| 23 | BA | 2279 | G | N1-C2-N2 | -6.06 | 110.74 | 116.20 |
| 23 | BA | 2587 | A | N1-C2-N3 | 6.06 | 132.33 | 129.30 |
| 23 | DA | 391 | G | N9-C4-C5 | -6.06 | 102.97 | 105.40 |
| 1 | AA | 1365 | G | C5-C6-O6 | -6.06 | 124.96 | 128.60 |
| 1 | AA | 1456 | G | N9-C4-C5 | -6.06 | 102.98 | 105.40 |
| 23 | BA | 1530 | C | C6-N1-C1' | -6.06 | 113.53 | 120.80 |
| 1 | AA | 993 | G | C4-N9-C1' | 6.06 | 134.38 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 1108 | G | C8-N9-C4 | -6.06 | 103.98 | 106.40 |
| 23 | BA | 1142(A) | A | N1-C2-N3 | 6.06 | 132.33 | 129.30 |
| 23 | DA | 2500 | U | N3-C4-C5 | 6.06 | 118.23 | 114.60 |
| 23 | BA | 1471 | A | N7-C8-N9 | 6.06 | 116.83 | 113.80 |
| 23 | BA | 1900 | A | C2-N3-C4 | 6.06 | 113.63 | 110.60 |
| 23 | BA | 2065 | C | N3-C4-C5 | -6.06 | 119.48 | 121.90 |
| 23 | BA | 2607 | G | C8-N9-C1' | -6.06 | 119.12 | 127.00 |
| 1 | CA | 741 | G | C8-N9-C4 | 6.06 | 108.82 | 106.40 |
| 1 | CA | 1266 | G | C2-N3-C4 | 6.06 | 114.93 | 111.90 |
| 23 | DA | 1313 | U | C6-N1-C2 | -6.06 | 117.37 | 121.00 |
| 23 | BA | 1358 | G | N3-C4-C5 | -6.05 | 125.57 | 128.60 |
| 23 | BA | 2312 | U | C5-C6-N1 | 6.05 | 125.73 | 122.70 |
| 1 | CA | 1322 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 23 | DA | 1784 | A | N1-C6-N6 | -6.05 | 114.97 | 118.60 |
| 23 | BA | 535 | C | C2-N1-C1' | -6.05 | 112.14 | 118.80 |
| 23 | BA | 1276 | A | C2-N3-C4 | -6.05 | 107.57 | 110.60 |
| 23 | BA | 1368 | G | N9-C4-C5 | 6.05 | 107.82 | 105.40 |
| 23 | BA | 1970 | A | C8-N9-C1' | -6.05 | 116.81 | 127.70 |
| 1 | CA | 1267 | C | C5-C6-N1 | 6.05 | 124.03 | 121.00 |
| 1 | AA | 818 | G | N9-C4-C5 | 6.05 | 107.82 | 105.40 |
| 1 | AA | 1066 | C | C4-C5-C6 | 6.05 | 120.43 | 117.40 |
| 23 | DA | 300 | A | C8-N9-C4 | 6.05 | 108.22 | 105.80 |
| 23 | DA | 975 | C | C6-N1-C2 | -6.05 | 117.88 | 120.30 |
| 1 | AA | 1268 | A | C2-N3-C4 | 6.05 | 113.62 | 110.60 |
| 23 | BA | 2072 | G | C6-C5-N7 | -6.05 | 126.77 | 130.40 |
| 23 | BA | 2279 | G | N3-C2-N2 | 6.05 | 124.13 | 119.90 |
| 23 | BA | 2575 | C | C4-C5-C6 | 6.05 | 120.42 | 117.40 |
| 23 | DA | 1216 | G | N1-C6-O6 | 6.05 | 123.53 | 119.90 |
| 23 | BA | 1698 | A | C5-C6-N1 | -6.05 | 114.68 | 117.70 |
| 23 | BA | 2026 | C | N3-C4-C5 | -6.04 | 119.48 | 121.90 |
| 23 | DA | 1653 | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |
| 1 | AA | 1277 | C | C5-C4-N4 | 6.04 | 124.43 | 120.20 |
| 23 | BA | 12 | U | C2-N1-C1' | 6.04 | 124.95 | 117.70 |
| 23 | BA | 20 | C | C2-N3-C4 | -6.04 | 116.88 | 119.90 |
| 23 | BA | 94 | C | C2-N1-C1' | 6.04 | 125.45 | 118.80 |
| 23 | BA | 1245 | G | N1-C6-O6 | -6.04 | 116.27 | 119.90 |
| 23 | DA | 845 | G | C8-N9-C1' | -6.04 | 119.14 | 127.00 |
| 23 | DA | 1575 | C | C6-N1-C2 | 6.04 | 122.72 | 120.30 |
| 23 | DA | 468 | G | N9-C4-C5 | -6.04 | 102.98 | 105.40 |
| 23 | BA | 1130 | U | C4-C5-C6 | 6.04 | 123.32 | 119.70 |
| 23 | DA | 2354 | G | C8-N9-C4 | -6.04 | 103.98 | 106.40 |
| 23 | DA | 2782 | G | C5-C6-O6 | -6.04 | 124.98 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1864 | U | N1-C2-O2 | -6.04 | 118.57 | 122.80 |
| 1 | CA | 836 | G | C5-C6-O6 | -6.04 | 124.98 | 128.60 |
| 23 | DA | 465 | G | C4-C5-C6 | 6.04 | 122.42 | 118.80 |
| 23 | DA | 1530 | C | C6-N1-C1' | -6.04 | 113.55 | 120.80 |
| 23 | BA | 1608 | A | C2-N3-C4 | -6.04 | 107.58 | 110.60 |
| 23 | DA | 1313 | U | C2-N1-C1' | 6.04 | 124.94 | 117.70 |
| 23 | BA | 1242 | A | C8-N9-C4 | 6.04 | 108.22 | 105.80 |
| 1 | CA | 1442 | G | C8-N9-C1' | -6.04 | 119.15 | 127.00 |
| 23 | DA | 1351 | C | C6-N1-C2 | 6.04 | 122.71 | 120.30 |
| 1 | AA | 529 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 23 | BA | 2304 | G | C4-N9-C1' | -6.03 | 118.66 | 126.50 |
| 24 | BB | 61 | G | N1-C2-N2 | 6.03 | 121.63 | 116.20 |
| 23 | DA | 90 | U | C5-C6-N1 | 6.03 | 125.72 | 122.70 |
| 23 | DA | 403 | U | N3-C2-O2 | -6.03 | 117.98 | 122.20 |
| 1 | AA | 593 | G | C8-N9-C4 | -6.03 | 103.99 | 106.40 |
| 1 | CA | 1033 | G | N3-C2-N2 | 6.03 | 124.12 | 119.90 |
| 1 | CA | 940 | C | C2-N1-C1' | 6.03 | 125.43 | 118.80 |
| 23 | DA | 2111 | C | C6-N1-C2 | -6.03 | 117.89 | 120.30 |
| 1 | CA | 1008 | C | C5-C4-N4 | -6.03 | 115.98 | 120.20 |
| 23 | DA | 2521 | C | C5-C6-N1 | -6.03 | 117.98 | 121.00 |
| 23 | BA | 2200 | C | C2-N1-C1' | 6.03 | 125.43 | 118.80 |
| 23 | BA | 2238 | G | C2-N3-C4 | 6.03 | 114.91 | 111.90 |
| 23 | BA | 2578 | G | N1-C2-N3 | 6.03 | 127.52 | 123.90 |
| 1 | CA | 1379 | G | C4-N9-C1' | 6.03 | 134.34 | 126.50 |
| 23 | DA | 529 | A | C2-N3-C4 | -6.03 | 107.59 | 110.60 |
| 23 | BA | 751 | A | C6-N1-C2 | -6.03 | 114.98 | 118.60 |
| 23 | DA | 103 | A | N1-C6-N6 | 6.03 | 122.22 | 118.60 |
| 23 | DA | 122 | G | C8-N9-C4 | 6.03 | 108.81 | 106.40 |
| 23 | DA | 528 | A | C8-N9-C1' | 6.03 | 138.55 | 127.70 |
| 23 | DA | 2719 | G | C8-N9-C4 | 6.03 | 108.81 | 106.40 |
| 23 | BA | 131 | G | C4-C5-N7 | 6.02 | 113.21 | 110.80 |
| 23 | BA | 752 | A | N1-C2-N3 | 6.02 | 132.31 | 129.30 |
| 23 | BA | 2319 | G | N3-C4-N9 | -6.02 | 122.39 | 126.00 |
| 23 | DA | 783 | A | C2-N3-C4 | 6.02 | 113.61 | 110.60 |
| 23 | DA | 988 | A | N9-C4-C5 | -6.02 | 103.39 | 105.80 |
| 23 | DA | 2387 | U | C5-C6-N1 | -6.02 | 119.69 | 122.70 |
| 1 | CA | 901 | A | C2-N3-C4 | -6.02 | 107.59 | 110.60 |
| 23 | DA | 2805 | G | N1-C6-O6 | -6.02 | 116.29 | 119.90 |
| 1 | AA | 1028 | C | C5-C6-N1 | 6.02 | 124.01 | 121.00 |
| 23 | BA | 975 | C | C4-C5-C6 | 6.02 | 120.41 | 117.40 |
| 23 | BA | 1632 | A | N1-C6-N6 | 6.02 | 122.21 | 118.60 |
| 23 | DA | 926 | A | N1-C6-N6 | 6.02 | 122.21 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1290 | G | C4-N9-C1' | 6.02 | 134.32 | 126.50 |
| 1 | CA | 365 | U | C2-N1-C1' | -6.02 | 110.48 | 117.70 |
| 23 | DA | 445 | C | C2-N3-C4 | -6.02 | 116.89 | 119.90 |
| 23 | DA | 825 | C | N3-C4-N4 | 6.02 | 122.21 | 118.00 |
| 1 | AA | 1014 | A | N3-C4-C5 | -6.01 | 122.59 | 126.80 |
| 23 | BA | 385 | C | N3-C4-C5 | -6.01 | 119.50 | 121.90 |
| 1 | CA | 946 | A | N1-C6-N6 | -6.01 | 114.99 | 118.60 |
| 23 | DA | 2790 | A | C2-N3-C4 | 6.01 | 113.61 | 110.60 |
| 1 | CA | 1096 | C | N3-C4-C5 | 6.01 | 124.31 | 121.90 |
| 1 | AA | 158 | G | C8-N9-C4 | -6.01 | 104.00 | 106.40 |
| 1 | AA | 1223 | C | N1-C2-O2 | 6.01 | 122.51 | 118.90 |
| 23 | BA | 624 | C | N3-C4-C5 | 6.01 | 124.30 | 121.90 |
| 23 | BA | 941 | A | C2-N3-C4 | 6.01 | 113.61 | 110.60 |
| 23 | DA | 1210 | A | C5-N7-C8 | -6.01 | 100.89 | 103.90 |
| 23 | DA | 2312 | U | C2-N1-C1' | 6.01 | 124.91 | 117.70 |
| 1 | AA | 1205 | U | C6-N1-C2 | -6.01 | 117.39 | 121.00 |
| 23 | BA | 940 | G | C8-N9-C4 | -6.01 | 104.00 | 106.40 |
| 1 | CA | 1158 | C | N3-C2-O2 | -6.01 | 117.69 | 121.90 |
| 1 | CA | 1293 | G | N3-C4-N9 | 6.01 | 129.61 | 126.00 |
| 23 | DA | 141 | A | C6-C5-N7 | -6.01 | 128.09 | 132.30 |
| 1 | AA | 38 | G | N1-C6-O6 | 6.01 | 123.50 | 119.90 |
| 1 | AA | 1355 | G | N3-C4-C5 | -6.01 | 125.60 | 128.60 |
| 23 | DA | 205 | G | C5-C6-O6 | -6.01 | 125.00 | 128.60 |
| 1 | AA | 93 | G | N9-C4-C5 | -6.01 | 103.00 | 105.40 |
| 1 | AA | 359 | U | C5-C6-N1 | -6.01 | 119.70 | 122.70 |
| 1 | AA | 940 | C | C5-C6-N1 | 6.01 | 124.00 | 121.00 |
| 1 | CA | 1320 | C | N3-C2-O2 | -6.01 | 117.69 | 121.90 |
| 23 | DA | 2708 | G | N1-C6-O6 | -6.01 | 116.30 | 119.90 |
| 1 | AA | 47 | C | C2-N3-C4 | -6.00 | 116.90 | 119.90 |
| 1 | AA | 1036 | G | C5-C6-O6 | 6.00 | 132.20 | 128.60 |
| 23 | BA | 595 | C | C5-C4-N4 | -6.00 | 116.00 | 120.20 |
| 23 | BA | 737 | C | N3-C2-O2 | 6.00 | 126.10 | 121.90 |
| 23 | BA | 1159 | U | N1-C2-N3 | 6.00 | 118.50 | 114.90 |
| 1 | CA | 986 | A | C5-C6-N1 | 6.00 | 120.70 | 117.70 |
| 23 | DA | 132 | G | C5-C6-N1 | -6.00 | 108.50 | 111.50 |
| 23 | DA | 1808 | U | C2-N3-C4 | 6.00 | 130.60 | 127.00 |
| 23 | DA | 2759 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 23 | DA | 1337 | G | N1-C6-O6 | -6.00 | 116.30 | 119.90 |
| 1 | AA | 365 | U | C5-C6-N1 | -6.00 | 119.70 | 122.70 |
| 1 | AA | 998 | G | C8-N9-C1' | 6.00 | 134.80 | 127.00 |
| 23 | BA | 2361 | A | C5-C6-N6 | -6.00 | 118.90 | 123.70 |
| 1 | AA | 485 | G | C4-N9-C1' | -6.00 | 118.70 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 392 | C | N3-C4-C5 | 6.00 | 124.30 | 121.90 |
| 23 | BA | 723 | G | N9-C4-C5 | -6.00 | 103.00 | 105.40 |
| 23 | BA | 2319 | G | N9-C4-C5 | 6.00 | 107.80 | 105.40 |
| 23 | DA | 465 | G | C8-N9-C4 | -6.00 | 104.00 | 106.40 |
| 23 | DA | 1762 | A | N3-C4-C5 | -6.00 | 122.60 | 126.80 |
| 1 | AA | 92 | C | C2-N3-C4 | 6.00 | 122.90 | 119.90 |
| 23 | BA | 1243 | G | N9-C4-C5 | -6.00 | 103.00 | 105.40 |
| 1 | CA | 1081 | G | C4-C5-N7 | 6.00 | 113.20 | 110.80 |
| 1 | AA | 698 | G | C5-C6-O6 | -6.00 | 125.00 | 128.60 |
| 23 | BA | 706 | A | C8-N9-C4 | 6.00 | 108.20 | 105.80 |
| 1 | CA | 1028 | C | C2-N3-C4 | 6.00 | 122.90 | 119.90 |
| 23 | BA | 920 | G | N1-C2-N2 | -5.99 | 110.81 | 116.20 |
| 23 | BA | 2727 | G | N1-C6-O6 | 5.99 | 123.50 | 119.90 |
| 1 | CA | 1417 | G | N3-C4-N9 | 5.99 | 129.60 | 126.00 |
| 1 | CA | 1442(B) | A | C8-N9-C4 | -5.99 | 103.40 | 105.80 |
| 23 | DA | 1760 | A | C6-N1-C2 | -5.99 | 115.00 | 118.60 |
| 43 | DZ | 151 | HIS | N-CA-C | 5.99 | 127.18 | 111.00 |
| 23 | BA | 684 | G | N1-C2-N2 | 5.99 | 121.59 | 116.20 |
| 23 | DA | 1325 | G | N9-C4-C5 | -5.99 | 103.00 | 105.40 |
| 1 | AA | 936 | C | C2-N3-C4 | -5.99 | 116.91 | 119.90 |
| 23 | BA | 893 | C | C6-N1-C1' | -5.99 | 113.61 | 120.80 |
| 23 | BA | 1273 | U | N3-C4-O4 | -5.99 | 115.21 | 119.40 |
| 23 | BA | 1721 | G | C4-C5-N7 | 5.99 | 113.20 | 110.80 |
| 23 | BA | 1819 | A | N9-C4-C5 | 5.99 | 108.20 | 105.80 |
| 1 | CA | 1133 | G | C4-C5-N7 | -5.99 | 108.40 | 110.80 |
| 23 | DA | 1577 | C | C6-N1-C2 | 5.99 | 122.70 | 120.30 |
| 23 | DA | 2523 | G | C8-N9-C4 | 5.99 | 108.80 | 106.40 |
| 23 | DA | 2844 | G | N1-C6-O6 | 5.99 | 123.49 | 119.90 |
| 1 | AA | 930 | C | C2-N3-C4 | -5.99 | 116.91 | 119.90 |
| 23 | BA | 782 | A | C5-C6-N6 | -5.99 | 118.91 | 123.70 |
| 23 | BA | 1531 | C | C5-C6-N1 | 5.99 | 123.99 | 121.00 |
| 23 | BA | 1952 | A | C8-N9-C4 | -5.99 | 103.40 | 105.80 |
| 1 | CA | 122 | G | N1-C6-O6 | 5.99 | 123.49 | 119.90 |
| 1 | CA | 1121 | U | C5-C6-N1 | 5.99 | 125.69 | 122.70 |
| 1 | CA | 1045 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |
| 23 | DA | 627 | A | N7-C8-N9 | -5.99 | 110.81 | 113.80 |
| 23 | BA | 912 | C | C6-N1-C2 | -5.99 | 117.91 | 120.30 |
| 1 | CA | 204 | U | C5-C6-N1 | 5.99 | 125.69 | 122.70 |
| 23 | DA | 2787 | C | N1-C2-O2 | 5.99 | 122.49 | 118.90 |
| 1 | AA | 1023 | G | N7-C8-N9 | 5.98 | 116.09 | 113.10 |
| 23 | BA | 2497 | A | C5-C6-N1 | 5.98 | 120.69 | 117.70 |
| 1 | CA | 1487 | G | C2-N3-C4 | -5.98 | 108.91 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1643 | G | C5-C6-O6 | 5.98 | 132.19 | 128.60 |
| 30 | BI | 123 | LEU | CA-CB-CG | 5.98 | 129.06 | 115.30 |
| 23 | BA | 1779 | U | N1-C2-O2 | 5.98 | 126.99 | 122.80 |
| 23 | DA | 1992 | G | C5-C6-O6 | 5.98 | 132.19 | 128.60 |
| 24 | DB | 7 | G | C8-N9-C4 | 5.98 | 108.79 | 106.40 |
| 23 | DA | 1316 | U | N1-C2-O2 | 5.98 | 126.98 | 122.80 |
| 23 | DA | 1350 | C | N3-C4-C5 | 5.98 | 124.29 | 121.90 |
| 1 | AA | 594 | G | N3-C4-C5 | -5.98 | 125.61 | 128.60 |
| 23 | BA | 448 | U | C6-N1-C2 | -5.98 | 117.41 | 121.00 |
| 23 | DA | 2364 | C | C6-N1-C2 | 5.98 | 122.69 | 120.30 |
| 23 | BA | 180 | G | C5-C6-O6 | -5.98 | 125.01 | 128.60 |
| 1 | AA | 999 | C | N3-C4-N4 | -5.97 | 113.82 | 118.00 |
| 23 | BA | 794 | G | N1-C2-N2 | -5.97 | 110.82 | 116.20 |
| 23 | DA | 179 | G | C8-N9-C4 | 5.97 | 108.79 | 106.40 |
| 1 | AA | 779 | C | N3-C4-C5 | 5.97 | 124.29 | 121.90 |
| 23 | BA | 500 | G | C5-C6-O6 | 5.97 | 132.18 | 128.60 |
| 1 | AA | 1038 | C | C2-N3-C4 | 5.97 | 122.89 | 119.90 |
| 1 | AA | 1424 | C | C5-C6-N1 | -5.97 | 118.02 | 121.00 |
| 23 | BA | 2028 | U | N3-C4-O4 | -5.97 | 115.22 | 119.40 |
| 1 | CA | 1277 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 23 | DA | 583 | G | C5-C6-O6 | -5.97 | 125.02 | 128.60 |
| 23 | DA | 2452 | C | N3-C4-C5 | -5.97 | 119.51 | 121.90 |
| 1 | AA | 346 | G | C4-N9-C1' | 5.97 | 134.26 | 126.50 |
| 23 | BA | 1811 | G | N3-C2-N2 | -5.97 | 115.72 | 119.90 |
| 23 | BA | 2791 | C | N3-C2-O2 | -5.97 | 117.72 | 121.90 |
| 1 | CA | 376 | G | N1-C6-O6 | 5.97 | 123.48 | 119.90 |
| 23 | DA | 1777 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 23 | DA | 2315 | G | N7-C8-N9 | -5.97 | 110.11 | 113.10 |
| 23 | DA | 2580 | U | C5-C6-N1 | -5.97 | 119.72 | 122.70 |
| 23 | DA | 2599 | G | N1-C2-N3 | 5.97 | 127.48 | 123.90 |
| 1 | AA | 1266 | G | C2-N3-C4 | 5.97 | 114.88 | 111.90 |
| 23 | BA | 1760 | A | N1-C6-N6 | -5.97 | 115.02 | 118.60 |
| 1 | CA | 1154 | G | C4-C5-N7 | -5.97 | 108.41 | 110.80 |
| 23 | DA | 1698 | A | C4-C5-N7 | 5.97 | 113.68 | 110.70 |
| 23 | BA | 652(T) | C | N1-C2-O2 | 5.97 | 122.48 | 118.90 |
| 23 | BA | 990 | A | C2-N3-C4 | -5.97 | 107.62 | 110.60 |
| 23 | BA | 2621 | A | N1-C6-N6 | -5.97 | 115.02 | 118.60 |
| 23 | DA | 389 | G | N3-C4-N9 | 5.97 | 129.58 | 126.00 |
| 23 | DA | 446 | G | C8-N9-C1' | -5.97 | 119.24 | 127.00 |
| 1 | AA | 1456 | G | N3-C2-N2 | 5.96 | 124.08 | 119.90 |
| 24 | BB | 117 | G | N7-C8-N9 | -5.96 | 110.12 | 113.10 |
| 23 | DA | 70 | G | C4-C5-N7 | 5.96 | 113.19 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 23 | DA | 327 | G | C5-C6-N1 | -5.96 | 108.52 | 111.50 |
| 23 | DA | 915 | C | N1-C2-O2 | 5.96 | 122.48 | 118.90 |
| 23 | DA | 1282 | U | C5-C6-N1 | -5.96 | 119.72 | 122.70 |
| 23 | DA | 1377 | G | N3-C4-N9 | 5.96 | 129.58 | 126.00 |
| 23 | DA | 2351 | G | N3-C4-C5 | -5.96 | 125.62 | 128.60 |
| 1 | AA | 1249 | C | C5-C6-N1 | 5.96 | 123.98 | 121.00 |
| 23 | DA | 566 | U | C5-C6-N1 | -5.96 | 119.72 | 122.70 |
| 23 | BA | 1546 | C | C2-N1-C1' | 5.96 | 125.36 | 118.80 |
| 23 | BA | 2522 | U | N3-C4-C5 | -5.96 | 111.02 | 114.60 |
| 23 | DA | 208 | C | C5-C4-N4 | -5.96 | 116.03 | 120.20 |
| 23 | BA | 1773 | A | C2-N3-C4 | 5.96 | 113.58 | 110.60 |
| 23 | BA | 194 | G | C5-C6-N1 | -5.96 | 108.52 | 111.50 |
| 23 | BA | 2292 | C | C2-N3-C4 | -5.96 | 116.92 | 119.90 |
| 23 | DA | 587 | C | N3-C2-O2 | -5.96 | 117.73 | 121.90 |
| 23 | DA | 924 | C | N3-C4-N4 | -5.96 | 113.83 | 118.00 |
| 23 | DA | 1270 | C | C5-C6-N1 | -5.96 | 118.02 | 121.00 |
| 23 | BA | 892 | G | C6-N1-C2 | 5.96 | 128.67 | 125.10 |
| 1 | CA | 831 | U | N1-C2-N3 | 5.96 | 118.47 | 114.90 |
| 23 | DA | 1980 | G | N3-C2-N2 | -5.96 | 115.73 | 119.90 |
| 23 | DA | 2622 | C | C6-N1-C2 | 5.96 | 122.68 | 120.30 |
| 23 | BA | 215 | G | N1-C2-N3 | 5.96 | 127.47 | 123.90 |
| 23 | BA | 945 | A | C1'-O4'-C4' | -5.96 | 105.14 | 109.90 |
| 23 | DA | 781 | A | C8-N9-C4 | 5.96 | 108.18 | 105.80 |
| 1 | AA | 1001(A) | G | N3-C4-N9 | 5.95 | 129.57 | 126.00 |
| 23 | BA | 746 | A | N1-C6-N6 | 5.95 | 122.17 | 118.60 |
| 23 | BA | 988 | A | C4-C5-N7 | 5.95 | 113.68 | 110.70 |
| 23 | DA | 676 | A | C6-C5-N7 | -5.95 | 128.13 | 132.30 |
| 23 | DA | 392 | C | N3-C2-O2 | 5.95 | 126.06 | 121.90 |
| 23 | DA | 862 | G | N1-C6-O6 | -5.95 | 116.33 | 119.90 |
| 23 | DA | 1129 | A | N9-C4-C5 | 5.95 | 108.18 | 105.80 |
| 23 | DA | 2240 | C | C4-C5-C6 | -5.95 | 114.42 | 117.40 |
| 1 | AA | 1002 | G | N7-C8-N9 | 5.95 | 116.07 | 113.10 |
| 23 | DA | 512 | G | N1-C6-O6 | -5.95 | 116.33 | 119.90 |
| 23 | DA | 756 | C | C5-C6-N1 | -5.95 | 118.03 | 121.00 |
| 23 | DA | 629 | G | N3-C4-N9 | -5.95 | 122.43 | 126.00 |
| 1 | AA | 1036 | G | C4-C5-N7 | -5.95 | 108.42 | 110.80 |
| 1 | AA | 1264 | C | C2-N3-C4 | 5.95 | 122.87 | 119.90 |
| 1 | CA | 972 | C | N3-C2-O2 | -5.95 | 117.74 | 121.90 |
| 23 | DA | 34 | C | N1-C2-O2 | 5.95 | 122.47 | 118.90 |
| 23 | DA | 1896 | G | N1-C6-O6 | 5.95 | 123.47 | 119.90 |
| 23 | DA | 196 | A | N9-C4-C5 | -5.94 | 103.42 | 105.80 |
| 23 | BA | 114 | U | C2-N1-C1' | 5.94 | 124.83 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 508 | G | N9-C4-C5 | -5.94 | 103.02 | 105.40 |
| 23 | BA | 516 | C | N1-C2-O2 | -5.94 | 115.33 | 118.90 |
| 23 | BA | 2680 | C | C6-N1-C2 | 5.94 | 122.68 | 120.30 |
| 1 | CA | 420 | U | C6-N1-C2 | -5.94 | 117.44 | 121.00 |
| 23 | DA | 572 | A | C2-N3-C4 | -5.94 | 107.63 | 110.60 |
| 23 | DA | 1618 | A | C5-C6-N6 | 5.94 | 128.45 | 123.70 |
| 1 | AA | 139 | G | C5-C6-O6 | -5.94 | 125.04 | 128.60 |
| 1 | CA | 1234 | C | N1-C2-O2 | 5.94 | 122.46 | 118.90 |
| 23 | DA | 508 | G | C8-N9-C4 | 5.94 | 108.78 | 106.40 |
| 23 | DA | 762 | U | N1-C2-N3 | -5.94 | 111.34 | 114.90 |
| 23 | DA | 1944 | U | C5-C6-N1 | -5.94 | 119.73 | 122.70 |
| 23 | DA | 1992 | G | P-O3'-C3' | 5.94 | 126.82 | 119.70 |
| 23 | DA | 2107 | C | C6-N1-C2 | -5.94 | 117.92 | 120.30 |
| 23 | BA | 2894 | G | C4-C5-N7 | 5.94 | 113.17 | 110.80 |
| 1 | CA | 1081 | G | C2-N3-C4 | -5.94 | 108.93 | 111.90 |
| 1 | CA | 1108 | G | N9-C4-C5 | 5.94 | 107.77 | 105.40 |
| 1 | CA | 1456 | G | N3-C2-N2 | 5.94 | 124.06 | 119.90 |
| 23 | DA | 659 | C | C6-N1-C2 | 5.94 | 122.67 | 120.30 |
| 1 | AA | 1417 | G | N3-C4-C5 | -5.93 | 125.63 | 128.60 |
| 7 | AG | 104 | LEU | CA-CB-CG | 5.93 | 128.95 | 115.30 |
| 1 | CA | 1148 | U | C6-N1-C2 | -5.93 | 117.44 | 121.00 |
| 23 | DA | 1301 | A | N1-C2-N3 | 5.93 | 132.27 | 129.30 |
| 23 | BA | 268 | C | N3-C4-N4 | 5.93 | 122.15 | 118.00 |
| 23 | BA | 2518 | A | C8-N9-C4 | -5.93 | 103.43 | 105.80 |
| 23 | DA | 1296 | G | N1-C2-N2 | -5.93 | 110.86 | 116.20 |
| 23 | BA | 2335 | A | C5-C6-N6 | -5.93 | 118.95 | 123.70 |
| 23 | DA | 2612 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 23 | BA | 1298 | C | N3-C4-C5 | 5.93 | 124.27 | 121.90 |
| 24 | BB | 97 | G | N7-C8-N9 | -5.93 | 110.14 | 113.10 |
| 1 | CA | 944 | G | N3-C4-N9 | 5.93 | 129.56 | 126.00 |
| 23 | DA | 2200 | C | C2-N1-C1' | 5.93 | 125.32 | 118.80 |
| 23 | DA | 2746 | U | C5-C6-N1 | -5.93 | 119.73 | 122.70 |
| 23 | DA | 652(T) | C | N1-C2-O2 | 5.93 | 122.46 | 118.90 |
| 23 | BA | 386 | G | C6-C5-N7 | -5.93 | 126.84 | 130.40 |
| 23 | BA | 951 | C | C6-N1-C2 | 5.93 | 122.67 | 120.30 |
| 23 | BA | 1208 | C | C5-C4-N4 | -5.93 | 116.05 | 120.20 |
| 23 | BA | 1300 | U | P-O3'-C3' | 5.93 | 126.81 | 119.70 |
| 23 | BA | 2641 | G | C4-N9-C1' | 5.93 | 134.21 | 126.50 |
| 1 | CA | 1320 | C | C6-N1-C2 | -5.93 | 117.93 | 120.30 |
| 23 | DA | 776 | G | N7-C8-N9 | 5.93 | 116.06 | 113.10 |
| 23 | DA | 1213 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |
| 23 | DA | 1583 | A | C8-N9-C4 | 5.93 | 108.17 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 645 | C | C2-N3-C4 | 5.92 | 122.86 | 119.90 |
| 23 | BA | 213 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 23 | BA | 1565 | C | N3-C4-C5 | 5.92 | 124.27 | 121.90 |
| 23 | DA | 2105 | C | C5-C6-N1 | 5.92 | 123.96 | 121.00 |
| 1 | AA | 1166 | G | C6-C5-N7 | 5.92 | 133.95 | 130.40 |
| 23 | BA | 777 | A | N3-C4-C5 | -5.92 | 122.65 | 126.80 |
| 23 | DA | 1427 | A | C6-N1-C2 | -5.92 | 115.05 | 118.60 |
| 23 | DA | 2641 | G | C4-N9-C1' | 5.92 | 134.19 | 126.50 |
| 23 | BA | 989 | G | C4-C5-N7 | 5.92 | 113.17 | 110.80 |
| 1 | CA | 1274 | G | N1-C6-O6 | 5.92 | 123.45 | 119.90 |
| 23 | DA | 51 | G | C5-C6-O6 | 5.92 | 132.15 | 128.60 |
| 23 | BA | 1681 | G | N1-C6-O6 | 5.92 | 123.45 | 119.90 |
| 1 | CA | 1297 | C | N3-C4-C5 | -5.92 | 119.53 | 121.90 |
| 23 | BA | 1132 | A | N1-C2-N3 | 5.91 | 132.26 | 129.30 |
| 23 | BA | 1208 | C | N1-C2-O2 | -5.91 | 115.35 | 118.90 |
| 23 | BA | 1858 | G | N7-C8-N9 | 5.91 | 116.06 | 113.10 |
| 23 | DA | 777 | A | N9-C4-C5 | 5.91 | 108.17 | 105.80 |
| 23 | DA | 2304 | G | C4-N9-C1' | -5.91 | 118.81 | 126.50 |
| 23 | BA | 271(M) | G | N3-C4-N9 | 5.91 | 129.55 | 126.00 |
| 1 | AA | 1188 | A | C8-N9-C4 | 5.91 | 108.16 | 105.80 |
| 23 | BA | 2609 | U | C4-C5-C6 | 5.91 | 123.25 | 119.70 |
| 23 | DA | 2304 | G | N9-C4-C5 | 5.91 | 107.76 | 105.40 |
| 1 | CA | 433 | C | C5-C6-N1 | -5.91 | 118.05 | 121.00 |
| 23 | DA | 363(B) | G | N3-C4-N9 | 5.91 | 129.54 | 126.00 |
| 23 | DA | 679 | C | C5-C6-N1 | -5.91 | 118.05 | 121.00 |
| 23 | BA | 886 | C | C2-N1-C1' | 5.91 | 125.30 | 118.80 |
| 1 | AA | 962 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 23 | BA | 271(G) | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 23 | BA | 578 | A | C8-N9-C4 | -5.91 | 103.44 | 105.80 |
| 23 | BA | 2391 | G | N9-C4-C5 | 5.91 | 107.76 | 105.40 |
| 1 | CA | 1071 | C | C6-N1-C2 | -5.91 | 117.94 | 120.30 |
| 23 | DA | 765 | G | N1-C6-O6 | 5.91 | 123.44 | 119.90 |
| 23 | DA | 1777 | U | N1-C2-O2 | 5.91 | 126.93 | 122.80 |
| 23 | DA | 2525 | G | C8-N9-C4 | 5.91 | 108.76 | 106.40 |
| 23 | BA | 2581 | G | N3-C2-N2 | 5.90 | 124.03 | 119.90 |
| 23 | BA | 431 | U | C5-C6-N1 | 5.90 | 125.65 | 122.70 |
| 23 | BA | 826 | U | N3-C4-C5 | -5.90 | 111.06 | 114.60 |
| 23 | BA | 2277 | G | N1-C6-O6 | -5.90 | 116.36 | 119.90 |
| 23 | DA | 673 | C | C2-N3-C4 | -5.90 | 116.95 | 119.90 |
| 1 | AA | 1032 | G | N1-C2-N3 | -5.90 | 120.36 | 123.90 |
| 1 | AA | 1457 | G | C5-C6-O6 | -5.90 | 125.06 | 128.60 |
| 23 | BA | 1290 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 792 | G | C8-N9-C1' | -5.90 | 119.33 | 127.00 |
| 23 | DA | 645 | C | C6-N1-C2 | -5.90 | 117.94 | 120.30 |
| 23 | DA | 652(E) | G | N3-C2-N2 | 5.90 | 124.03 | 119.90 |
| 23 | DA | 1695 | G | N7-C8-N9 | 5.90 | 116.05 | 113.10 |
| 1 | AA | 1299 | A | N1-C6-N6 | -5.90 | 115.06 | 118.60 |
| 1 | CA | 1342 | C | N1-C2-O2 | 5.90 | 122.44 | 118.90 |
| 23 | DA | 1539 | G | N1-C6-O6 | 5.90 | 123.44 | 119.90 |
| 23 | BA | 179 | G | C5-C6-O6 | -5.89 | 125.06 | 128.60 |
| 23 | BA | 424 | G | C5-C6-O6 | -5.89 | 125.06 | 128.60 |
| 23 | DA | 2162 | G | N3-C4-N9 | 5.89 | 129.54 | 126.00 |
| 1 | AA | 121 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 1 | AA | 1335 | C | C6-N1-C1' | -5.89 | 113.73 | 120.80 |
| 23 | BA | 844 | C | N3-C4-C5 | 5.89 | 124.26 | 121.90 |
| 23 | DA | 1271 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |
| 23 | DA | 984 | A | C8-N9-C4 | 5.89 | 108.16 | 105.80 |
| 23 | BA | 297 | C | N3-C4-N4 | 5.89 | 122.12 | 118.00 |
| 23 | BA | 1422 | G | C2-N3-C4 | 5.89 | 114.84 | 111.90 |
| 23 | BA | 2381 | C | N1-C2-N3 | 5.89 | 123.32 | 119.20 |
| 1 | CA | 1024 | G | C5-C6-O6 | -5.89 | 125.07 | 128.60 |
| 4 | AD | 26 | CYS | N-CA-C | -5.89 | 95.10 | 111.00 |
| 1 | CA | 1153 | C | C6-N1-C1' | 5.89 | 127.87 | 120.80 |
| 23 | DA | 2455 | G | C8-N9-C1' | -5.89 | 119.34 | 127.00 |
| 1 | AA | 1223 | C | N3-C2-O2 | -5.89 | 117.78 | 121.90 |
| 1 | AA | 1312 | G | C5-C6-N1 | 5.89 | 114.44 | 111.50 |
| 23 | BA | 2226 | C | C6-N1-C2 | 5.89 | 122.66 | 120.30 |
| 25 | BD | 229 | VAL | CB-CA-C | -5.89 | 100.22 | 111.40 |
| 23 | DA | 214 | G | C5-C6-O6 | -5.89 | 125.07 | 128.60 |
| 23 | BA | 2319 | G | C5-N7-C8 | -5.88 | 101.36 | 104.30 |
| 23 | BA | 2335 | A | N9-C4-C5 | -5.88 | 103.45 | 105.80 |
| 1 | CA | 721 | G | C6-C5-N7 | -5.88 | 126.87 | 130.40 |
| 23 | DA | 179 | G | N9-C4-C5 | -5.88 | 103.05 | 105.40 |
| 23 | DA | 1653 | G | N3-C4-N9 | 5.88 | 129.53 | 126.00 |
| 24 | DB | 81 | G | C5-N7-C8 | -5.88 | 101.36 | 104.30 |
| 23 | DA | 625 | G | C2-N3-C4 | -5.88 | 108.96 | 111.90 |
| 23 | DA | 1617 | C | C4-C5-C6 | 5.88 | 120.34 | 117.40 |
| 1 | AA | 1524 | C | C5-C6-N1 | -5.88 | 118.06 | 121.00 |
| 23 | BA | 1721 | G | C8-N9-C4 | -5.88 | 104.05 | 106.40 |
| 23 | BA | 240 | G | C5-C6-N1 | 5.88 | 114.44 | 111.50 |
| 23 | BA | 271(S) | G | N1-C6-O6 | 5.88 | 123.43 | 119.90 |
| 23 | DA | 1863 | G | C8-N9-C4 | 5.88 | 108.75 | 106.40 |
| 23 | BA | 667 | U | N3-C4-O4 | 5.88 | 123.51 | 119.40 |
| 23 | DA | 1464 | C | N3-C4-C5 | -5.88 | 119.55 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 256 | A | C8-N9-C4 | 5.88 | 108.15 | 105.80 |
| 23 | BA | 819 | A | N1-C6-N6 | -5.88 | 115.08 | 118.60 |
| 23 | BA | 1428 | C | C4-C5-C6 | 5.88 | 120.34 | 117.40 |
| 23 | BA | 1479 | G | N1-C6-O6 | 5.88 | 123.43 | 119.90 |
| 1 | CA | 1312 | G | C6-N1-C2 | 5.88 | 128.63 | 125.10 |
| 23 | DA | 242 | G | C4-N9-C1' | -5.88 | 118.86 | 126.50 |
| 23 | DA | 1298 | C | C2-N3-C4 | -5.88 | 116.96 | 119.90 |
| 1 | AA | 509 | A | C8-N9-C4 | -5.88 | 103.45 | 105.80 |
| 23 | BA | 2297 | C | C5-C4-N4 | 5.88 | 124.31 | 120.20 |
| 23 | BA | 2729 | G | C6-C5-N7 | -5.88 | 126.88 | 130.40 |
| 23 | DA | 1141 | U | C5-C4-O4 | 5.88 | 129.43 | 125.90 |
| 23 | DA | 1281 | G | N1-C6-O6 | 5.88 | 123.42 | 119.90 |
| 23 | DA | 1623 | G | C2-N3-C4 | -5.88 | 108.96 | 111.90 |
| 1 | AA | 610 | G | N3-C4-N9 | 5.87 | 129.53 | 126.00 |
| 1 | CA | 240 | C | C5-C6-N1 | -5.87 | 118.06 | 121.00 |
| 1 | CA | 1042 | G | N1-C2-N2 | 5.87 | 121.49 | 116.20 |
| 23 | DA | 1359 | A | C5-C6-N1 | 5.87 | 120.64 | 117.70 |
| 1 | AA | 1030 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 23 | BA | 209 | C | C4-C5-C6 | 5.87 | 120.34 | 117.40 |
| 23 | BA | 752 | A | P-O3'-C3' | 5.87 | 126.75 | 119.70 |
| 23 | BA | 2129 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 1 | CA | 1270 | C | C6-N1-C2 | -5.87 | 117.95 | 120.30 |
| 1 | AA | 1184 | G | C2-N3-C4 | 5.87 | 114.83 | 111.90 |
| 23 | DA | 2587 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 1 | AA | 1328 | C | C2-N1-C1' | -5.87 | 112.34 | 118.80 |
| 2 | CB | 129 | GLU | N-CA-C | -5.87 | 95.16 | 111.00 |
| 23 | DA | 448 | U | C4-C5-C6 | 5.87 | 123.22 | 119.70 |
| 23 | DA | 582 | G | C2-N3-C4 | -5.87 | 108.97 | 111.90 |
| 23 | DA | 629 | G | N3-C4-C5 | 5.87 | 131.53 | 128.60 |
| 23 | DA | 1257 | C | N3-C4-C5 | -5.87 | 119.55 | 121.90 |
| 23 | BA | 736 | C | N1-C2-O2 | -5.87 | 115.38 | 118.90 |
| 23 | BA | 1230 | C | C6-N1-C2 | 5.87 | 122.65 | 120.30 |
| 1 | AA | 286 | G | C5-C6-O6 | 5.86 | 132.12 | 128.60 |
| 1 | AA | 346 | G | N3-C4-N9 | 5.86 | 129.52 | 126.00 |
| 1 | AA | 1371 | G | C8-N9-C4 | 5.86 | 108.75 | 106.40 |
| 1 | AA | 1442 | G | N7-C8-N9 | -5.86 | 110.17 | 113.10 |
| 23 | BA | 610 | G | C8-N9-C4 | 5.86 | 108.75 | 106.40 |
| 23 | BA | 1128 | A | C5-C6-N1 | 5.86 | 120.63 | 117.70 |
| 23 | BA | 1926 | U | N3-C2-O2 | -5.86 | 118.09 | 122.20 |
| 1 | CA | 317 | G | N1-C6-O6 | 5.86 | 123.42 | 119.90 |
| 1 | CA | 1120 | G | N3-C2-N2 | -5.86 | 115.80 | 119.90 |
| 23 | DA | 2351 | G | C4-N9-C1' | 5.86 | 134.12 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 1265 | A | N1-C6-N6 | 5.86 | 122.12 | 118.60 |
| 23 | DA | 2464 | C | C4-C5-C6 | -5.86 | 114.47 | 117.40 |
| 23 | BA | 756 | C | N1-C2-O2 | -5.86 | 115.38 | 118.90 |
| 23 | BA | 1128 | A | N9-C4-C5 | 5.86 | 108.14 | 105.80 |
| 23 | DA | 1276 | A | N1-C6-N6 | 5.86 | 122.12 | 118.60 |
| 23 | BA | 330 | A | C5-C6-N1 | -5.86 | 114.77 | 117.70 |
| 23 | BA | 1951 | U | N3-C4-O4 | 5.86 | 123.50 | 119.40 |
| 1 | AA | 1038 | C | C5-C4-N4 | 5.86 | 124.30 | 120.20 |
| 1 | AA | 1239 | A | N9-C4-C5 | 5.86 | 108.14 | 105.80 |
| 23 | BA | 1405 | U | C5-C6-N1 | -5.86 | 119.77 | 122.70 |
| 23 | DA | 2510 | C | C4-C5-C6 | 5.86 | 120.33 | 117.40 |
| 23 | DA | 2626 | C | N3-C4-C5 | 5.86 | 124.24 | 121.90 |
| 23 | DA | 2805 | G | C5-C6-O6 | 5.86 | 132.12 | 128.60 |
| 1 | AA | 54 | C | N3-C2-O2 | 5.86 | 126.00 | 121.90 |
| 23 | BA | 845 | G | N3-C4-N9 | 5.86 | 129.51 | 126.00 |
| 23 | BA | 846 | C | C2-N3-C4 | -5.86 | 116.97 | 119.90 |
| 23 | BA | 1989 | G | C6-C5-N7 | -5.86 | 126.89 | 130.40 |
| 13 | CM | 70 | LEU | CA-CB-CG | 5.86 | 128.77 | 115.30 |
| 23 | DA | 1619 | G | C5-C6-N1 | 5.86 | 114.43 | 111.50 |
| 24 | DB | 4 | C | C6-N1-C2 | 5.86 | 122.64 | 120.30 |
| 23 | BA | 2260 | C | N1-C2-N3 | 5.85 | 123.30 | 119.20 |
| 1 | AA | 199 | G | C8-N9-C4 | 5.85 | 108.74 | 106.40 |
| 23 | BA | 751 | A | N7-C8-N9 | -5.85 | 110.87 | 113.80 |
| 23 | BA | 822 | U | N3-C2-O2 | -5.85 | 118.10 | 122.20 |
| 23 | BA | 1304 | C | C5-C6-N1 | -5.85 | 118.07 | 121.00 |
| 23 | BA | 2441 | C | C2-N3-C4 | -5.85 | 116.97 | 119.90 |
| 23 | BA | 2751 | G | C8-N9-C4 | -5.85 | 104.06 | 106.40 |
| 23 | BA | 2857 | G | N1-C6-O6 | 5.85 | 123.41 | 119.90 |
| 1 | CA | 357 | G | C8-N9-C4 | -5.85 | 104.06 | 106.40 |
| 1 | CA | 982 | U | C5-C6-N1 | 5.85 | 125.63 | 122.70 |
| 1 | CA | 1282 | C | C2-N1-C1' | 5.85 | 125.24 | 118.80 |
| 1 | AA | 1150 | U | N3-C4-O4 | -5.85 | 115.31 | 119.40 |
| 1 | AA | 1467 | G | C5-C6-O6 | 5.85 | 132.11 | 128.60 |
| 23 | BA | 679 | C | N1-C2-O2 | -5.85 | 115.39 | 118.90 |
| 23 | BA | 2201 | C | C2-N3-C4 | -5.85 | 116.97 | 119.90 |
| 1 | CA | 1030(A) | G | N3-C4-C5 | -5.85 | 125.67 | 128.60 |
| 23 | DA | 571 | A | N7-C8-N9 | -5.85 | 110.88 | 113.80 |
| 1 | AA | 754 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 1 | AA | 1256 | A | N7-C8-N9 | -5.85 | 110.88 | 113.80 |
| 23 | BA | 1677 | A | C2-N3-C4 | -5.85 | 107.68 | 110.60 |
| 23 | BA | 2004 | G | N7-C8-N9 | 5.85 | 116.02 | 113.10 |
| 1 | CA | 307 | C | C6-N1-C2 | -5.85 | 117.96 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 150 | C | C5-C6-N1 | 5.85 | 123.92 | 121.00 |
| 23 | BA | 1645 | G | N9-C4-C5 | 5.84 | 107.74 | 105.40 |
| 23 | DA | 1881 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 24 | DB | 64 | C | C6-N1-C2 | 5.84 | 122.64 | 120.30 |
| 1 | AA | 998 | G | C4-N9-C1' | -5.84 | 118.90 | 126.50 |
| 1 | CA | 880 | C | C6-N1-C2 | 5.84 | 122.64 | 120.30 |
| 23 | DA | 1252 | G | C8-N9-C4 | 5.84 | 108.74 | 106.40 |
| 23 | DA | 1946 | U | N3-C4-C5 | 5.84 | 118.11 | 114.60 |
| 1 | AA | 1523 | G | C4-C5-N7 | -5.84 | 108.46 | 110.80 |
| 23 | BA | 508 | G | C6-C5-N7 | -5.84 | 126.89 | 130.40 |
| 23 | BA | 1004 | C | C6-N1-C2 | -5.84 | 117.96 | 120.30 |
| 23 | BA | 1351 | C | N1-C2-O2 | -5.84 | 115.39 | 118.90 |
| 23 | BA | 1367 | A | N7-C8-N9 | -5.84 | 110.88 | 113.80 |
| 23 | BA | 2087 | G | C2-N3-C4 | -5.84 | 108.98 | 111.90 |
| 23 | BA | 2453 | A | N1-C6-N6 | -5.84 | 115.09 | 118.60 |
| 23 | DA | 1261 | C | C6-N1-C2 | 5.84 | 122.64 | 120.30 |
| 1 | AA | 204 | U | C5-C6-N1 | 5.84 | 125.62 | 122.70 |
| 23 | BA | 1290 | C | N3-C2-O2 | -5.84 | 117.81 | 121.90 |
| 23 | BA | 1382 | G | C8-N9-C4 | 5.84 | 108.74 | 106.40 |
| 23 | BA | 1653 | G | N3-C4-N9 | 5.84 | 129.50 | 126.00 |
| 23 | BA | 2740 | A | N1-C2-N3 | 5.84 | 132.22 | 129.30 |
| 1 | CA | 1367 | C | N1-C2-O2 | 5.84 | 122.40 | 118.90 |
| 1 | AA | 606 | G | N3-C4-C5 | -5.84 | 125.68 | 128.60 |
| 1 | CA | 577 | G | N3-C4-C5 | 5.84 | 131.52 | 128.60 |
| 1 | CA | 1351 | U | C6-N1-C2 | 5.84 | 124.50 | 121.00 |
| 23 | DA | 1751 | C | N1-C2-O2 | -5.84 | 115.40 | 118.90 |
| 1 | AA | 1037 | C | C2-N3-C4 | 5.84 | 122.82 | 119.90 |
| 23 | BA | 1297 | C | N1-C2-O2 | -5.84 | 115.40 | 118.90 |
| 23 | BA | 1519 | G | C8-N9-C4 | -5.84 | 104.07 | 106.40 |
| 23 | BA | 1779 | U | C5-C4-O4 | -5.84 | 122.40 | 125.90 |
| 23 | BA | 2546 | U | N3-C4-C5 | -5.84 | 111.10 | 114.60 |
| 1 | CA | 1008 | C | C5-C6-N1 | 5.84 | 123.92 | 121.00 |
| 23 | DA | 928 | G | C5-N7-C8 | -5.84 | 101.38 | 104.30 |
| 23 | BA | 793 | A | C5-C6-N6 | -5.83 | 119.03 | 123.70 |
| 23 | BA | 1211 | U | N3-C2-O2 | 5.83 | 126.28 | 122.20 |
| 23 | DA | 1654 | A | N9-C4-C5 | 5.83 | 108.13 | 105.80 |
| 23 | BA | 807 | U | N3-C4-O4 | 5.83 | 123.48 | 119.40 |
| 1 | CA | 1354 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 23 | DA | 300 | A | N9-C4-C5 | -5.83 | 103.47 | 105.80 |
| 23 | DA | 1231 | G | N1-C6-O6 | 5.83 | 123.40 | 119.90 |
| 23 | BA | 2044 | C | N3-C2-O2 | 5.83 | 125.98 | 121.90 |
| 23 | BA | 2455 | G | C5-C6-O6 | -5.83 | 125.10 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 34 | BQ | 87 | LYS | CD-CE-NZ | 5.83 | 125.11 | 111.70 |
| 1 | CA | 1064 | G | C8-N9-C4 | -5.83 | 104.07 | 106.40 |
| 1 | CA | 1254 | C | C4-C5-C6 | 5.83 | 120.32 | 117.40 |
| 13 | CM | 56 | LEU | CA-CB-CG | 5.83 | 128.71 | 115.30 |
| 23 | DA | 391 | G | C5-C6-O6 | -5.83 | 125.10 | 128.60 |
| 23 | DA | 624 | C | N3-C4-C5 | 5.83 | 124.23 | 121.90 |
| 23 | DA | 1776 | G | N3-C2-N2 | 5.83 | 123.98 | 119.90 |
| 23 | DA | 2464 | C | C2-N1-C1' | 5.83 | 125.22 | 118.80 |
| 23 | BA | 1271 | G | C5-C6-N1 | -5.83 | 108.58 | 111.50 |
| 1 | CA | 610 | G | C8-N9-C1' | -5.83 | 119.42 | 127.00 |
| 23 | DA | 529 | A | C5-N7-C8 | -5.83 | 100.98 | 103.90 |
| 23 | DA | 856 | C | C5-C6-N1 | 5.83 | 123.92 | 121.00 |
| 1 | AA | 1308 | U | N1-C2-O2 | 5.83 | 126.88 | 122.80 |
| 23 | BA | 848 | G | C4-N9-C1' | 5.83 | 134.08 | 126.50 |
| 23 | DA | 1292 | U | N3-C2-O2 | 5.83 | 126.28 | 122.20 |
| 23 | DA | 1618 | A | N1-C6-N6 | -5.83 | 115.10 | 118.60 |
| 23 | DA | 2499 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 23 | BA | 640 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 1 | AA | 749 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 1 | AA | 1456 | G | C2-N3-C4 | 5.83 | 114.81 | 111.90 |
| 23 | DA | 2843 | G | N3-C2-N2 | -5.83 | 115.82 | 119.90 |
| 23 | DA | 1435 | G | C5-C6-O6 | -5.82 | 125.11 | 128.60 |
| 23 | DA | 2425 | A | C5-N7-C8 | -5.82 | 100.99 | 103.90 |
| 23 | DA | 2617 | C | C6-N1-C2 | 5.82 | 122.63 | 120.30 |
| 1 | AA | 993 | G | C8-N9-C4 | -5.82 | 104.07 | 106.40 |
| 23 | BA | 2017 | U | C6-N1-C2 | -5.82 | 117.51 | 121.00 |
| 23 | DA | 1304 | C | N3-C4-C5 | 5.82 | 124.23 | 121.90 |
| 23 | BA | 1021 | A | C4-C5-N7 | 5.82 | 113.61 | 110.70 |
| 23 | BA | 2348 | U | N3-C4-C5 | 5.82 | 118.09 | 114.60 |
| 23 | BA | 2617 | C | C5-C6-N1 | -5.82 | 118.09 | 121.00 |
| 1 | CA | 1306 | A | C8-N9-C4 | -5.82 | 103.47 | 105.80 |
| 23 | DA | 1647 | G | N3-C4-C5 | 5.82 | 131.51 | 128.60 |
| 23 | DA | 2070 | G | N1-C2-N2 | -5.82 | 110.96 | 116.20 |
| 23 | BA | 1680 | U | C6-N1-C2 | -5.82 | 117.51 | 121.00 |
| 23 | BA | 2146 | C | N1-C2-O2 | 5.82 | 122.39 | 118.90 |
| 1 | AA | 187 | C | C5-C6-N1 | 5.82 | 123.91 | 121.00 |
| 1 | AA | 696 | A | N9-C4-C5 | 5.82 | 108.13 | 105.80 |
| 1 | AA | 1516 | G | C2-N3-C4 | -5.82 | 108.99 | 111.90 |
| 23 | BA | 968 | G | N7-C8-N9 | -5.82 | 110.19 | 113.10 |
| 23 | BA | 2746 | U | C5-C4-O4 | 5.82 | 129.39 | 125.90 |
| 1 | CA | 304 | U | C5-C4-O4 | 5.82 | 129.39 | 125.90 |
| 23 | DA | 1478 | G | N3-C4-N9 | 5.82 | 129.49 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 485 | G | C8-N9-C4 | 5.82 | 108.73 | 106.40 |
| 23 | BA | 141 | A | C5-C6-N6 | -5.82 | 119.05 | 123.70 |
| 23 | BA | 1432 | C | N3-C4-N4 | 5.82 | 122.07 | 118.00 |
| 23 | BA | 2049 | G | N3-C4-C5 | 5.82 | 131.51 | 128.60 |
| 1 | CA | 1306 | A | N7-C8-N9 | 5.82 | 116.71 | 113.80 |
| 1 | AA | 307 | C | C6-N1-C2 | -5.81 | 117.97 | 120.30 |
| 23 | BA | 1333 | C | N1-C2-O2 | -5.81 | 115.41 | 118.90 |
| 23 | DA | 938 | G | C8-N9-C4 | 5.81 | 108.73 | 106.40 |
| 1 | AA | 398 | C | C5-C6-N1 | -5.81 | 118.09 | 121.00 |
| 23 | DA | 60 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 23 | BA | 1359 | A | C4-C5-C6 | -5.81 | 114.09 | 117.00 |
| 1 | AA | 32 | A | N9-C4-C5 | 5.81 | 108.12 | 105.80 |
| 23 | BA | 746 | A | C5-N7-C8 | -5.81 | 101.00 | 103.90 |
| 23 | BA | 1207 | C | C4-C5-C6 | 5.81 | 120.31 | 117.40 |
| 23 | BA | 2849 | U | N1-C2-O2 | -5.81 | 118.73 | 122.80 |
| 23 | DA | 445 | C | C5-C6-N1 | -5.81 | 118.10 | 121.00 |
| 23 | DA | 750 | A | C5-C6-N1 | -5.81 | 114.80 | 117.70 |
| 23 | BA | 1387 | C | C6-N1-C2 | -5.81 | 117.98 | 120.30 |
| 23 | BA | 2304 | G | C5-C6-N1 | 5.81 | 114.40 | 111.50 |
| 23 | DA | 362 | U | C5-C4-O4 | -5.81 | 122.42 | 125.90 |
| 23 | DA | 1298 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 23 | DA | 1539 | G | C4-C5-N7 | 5.81 | 113.12 | 110.80 |
| 23 | DA | 1801 | G | C5-C6-O6 | -5.81 | 125.12 | 128.60 |
| 1 | AA | 1061 | G | C4-C5-N7 | -5.81 | 108.48 | 110.80 |
| 23 | BA | 1578 | U | N3-C2-O2 | -5.80 | 118.14 | 122.20 |
| 23 | BA | 2073 | C | C4-C5-C6 | 5.80 | 120.30 | 117.40 |
| 23 | DA | 304 | G | C5-C6-N1 | -5.80 | 108.60 | 111.50 |
| 23 | DA | 1373 | A | N7-C8-N9 | -5.80 | 110.90 | 113.80 |
| 23 | DA | 2038 | G | C5-N7-C8 | -5.80 | 101.40 | 104.30 |
| 1 | AA | 244 | U | C5-C6-N1 | -5.80 | 119.80 | 122.70 |
| 1 | CA | 1145 | C | C5-C4-N4 | 5.80 | 124.26 | 120.20 |
| 23 | DA | 1243 | G | C8-N9-C4 | 5.80 | 108.72 | 106.40 |
| 23 | DA | 2497 | A | C5-C6-N6 | -5.80 | 119.06 | 123.70 |
| 1 | AA | 1447 | A | C2-N3-C4 | 5.80 | 113.50 | 110.60 |
| 23 | BA | 446 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 23 | BA | 510 | C | C5-C4-N4 | 5.80 | 124.26 | 120.20 |
| 1 | CA | 1183 | A | C8-N9-C4 | -5.80 | 103.48 | 105.80 |
| 1 | CA | 1272 | G | N9-C4-C5 | -5.80 | 103.08 | 105.40 |
| 23 | DA | 656 | G | C8-N9-C4 | 5.80 | 108.72 | 106.40 |
| 23 | DA | 2413 | G | C2-N3-C4 | -5.80 | 109.00 | 111.90 |
| 1 | AA | 960 | U | C2-N1-C1' | 5.80 | 124.66 | 117.70 |
| 1 | AA | 960 | U | C5-C6-N1 | 5.80 | 125.60 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 1133 | G | N9-C4-C5 | 5.80 | 107.72 | 105.40 |
| 23 | BA | 115 | C | N1-C2-O2 | -5.80 | 115.42 | 118.90 |
| 23 | BA | 2230 | G | N1-C2-N2 | 5.80 | 121.42 | 116.20 |
| 1 | CA | 749 | C | C6-N1-C2 | -5.80 | 117.98 | 120.30 |
| 1 | CA | 993 | G | N3-C4-C5 | -5.80 | 125.70 | 128.60 |
| 1 | CA | 1031 | G | C8-N9-C4 | -5.80 | 104.08 | 106.40 |
| 1 | CA | 1405 | G | N3-C2-N2 | 5.80 | 123.96 | 119.90 |
| 23 | DA | 391 | G | C4-C5-N7 | 5.80 | 113.12 | 110.80 |
| 1 | CA | 1008 | C | C2-N1-C1' | 5.80 | 125.18 | 118.80 |
| 23 | BA | 1963 | U | C5-C6-N1 | 5.79 | 125.60 | 122.70 |
| 23 | BA | 2592 | G | N3-C4-C5 | -5.79 | 125.70 | 128.60 |
| 23 | BA | 723 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 23 | BA | 1938 | A | C8-N9-C4 | -5.79 | 103.48 | 105.80 |
| 23 | DA | 1200 | C | C5-C6-N1 | -5.79 | 118.10 | 121.00 |
| 23 | BA | 1142(A) | A | C6-C5-N7 | -5.79 | 128.25 | 132.30 |
| 23 | BA | 1769 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 23 | BA | 571 | A | C5-C6-N6 | -5.79 | 119.07 | 123.70 |
| 23 | BA | 1937 | A | C6-N1-C2 | -5.79 | 115.13 | 118.60 |
| 23 | DA | 644 | A | N1-C6-N6 | -5.79 | 115.13 | 118.60 |
| 23 | DA | 2077 | A | C2-N3-C4 | 5.79 | 113.50 | 110.60 |
| 23 | DA | 2672 | G | N1-C6-O6 | 5.79 | 123.37 | 119.90 |
| 1 | AA | 480 | U | C5-C6-N1 | -5.79 | 119.81 | 122.70 |
| 1 | AA | 1377 | A | C6-C5-N7 | -5.79 | 128.25 | 132.30 |
| 23 | BA | 475 | U | N1-C2-N3 | 5.79 | 118.37 | 114.90 |
| 23 | BA | 2273 | A | N7-C8-N9 | 5.79 | 116.69 | 113.80 |
| 1 | AA | 403 | C | N3-C4-C5 | -5.79 | 119.58 | 121.90 |
| 23 | BA | 188 | G | C8-N9-C4 | 5.79 | 108.71 | 106.40 |
| 23 | BA | 452 | G | C4-C5-N7 | -5.79 | 108.49 | 110.80 |
| 23 | DA | 792 | G | C8-N9-C1' | -5.79 | 119.48 | 127.00 |
| 23 | DA | 2323 | G | C4-C5-N7 | 5.79 | 113.11 | 110.80 |
| 23 | DA | 2395 | C | C6-N1-C2 | 5.79 | 122.61 | 120.30 |
| 1 | AA | 90 | U | N1-C2-O2 | 5.78 | 126.85 | 122.80 |
| 1 | AA | 1158 | C | C6-N1-C1' | -5.78 | 113.86 | 120.80 |
| 23 | BA | 496 | G | N9-C4-C5 | -5.78 | 103.09 | 105.40 |
| 23 | BA | 794 | G | N1-C2-N3 | 5.78 | 127.37 | 123.90 |
| 1 | CA | 610 | G | C4-N9-C1' | 5.78 | 134.02 | 126.50 |
| 1 | CA | 1024 | G | C5-N7-C8 | -5.78 | 101.41 | 104.30 |
| 23 | DA | 179 | G | N3-C4-C5 | 5.78 | 131.49 | 128.60 |
| 23 | DA | 825 | C | C5-C4-N4 | -5.78 | 116.15 | 120.20 |
| 23 | DA | 2221 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 1 | AA | 460 | G | N7-C8-N9 | 5.78 | 115.99 | 113.10 |
| 23 | DA | 129 | C | C5-C6-N1 | -5.78 | 118.11 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 774 | A | N7-C8-N9 | 5.78 | 116.69 | 113.80 |
| 1 | CA | 982 | U | C6-N1-C2 | -5.78 | 117.53 | 121.00 |
| 18 | CR | 85 | LEU | CA-CB-CG | 5.78 | 128.59 | 115.30 |
| 23 | DA | 2745 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 1 | AA | 517 | G | N3-C4-C5 | -5.78 | 125.71 | 128.60 |
| 23 | BA | 674 | G | C4-C5-N7 | 5.78 | 113.11 | 110.80 |
| 23 | BA | 1273 | U | C2-N3-C4 | -5.78 | 123.53 | 127.00 |
| 24 | BB | 15 | A | N1-C6-N6 | 5.78 | 122.07 | 118.60 |
| 1 | CA | 1160 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 1 | AA | 1040 | U | C5-C4-O4 | 5.78 | 129.37 | 125.90 |
| 23 | BA | 2054 | A | C5-C6-N6 | -5.78 | 119.08 | 123.70 |
| 23 | DA | 39 | C | C4-C5-C6 | 5.78 | 120.29 | 117.40 |
| 23 | DA | 1381 | G | C4-C5-N7 | -5.78 | 108.49 | 110.80 |
| 1 | AA | 402 | G | N1-C6-O6 | 5.77 | 123.36 | 119.90 |
| 1 | AA | 900 | A | N1-C2-N3 | -5.77 | 126.41 | 129.30 |
| 1 | AA | 1210 | C | C5-C4-N4 | -5.77 | 116.16 | 120.20 |
| 23 | BA | 2712(A) | A | N1-C6-N6 | 5.77 | 122.06 | 118.60 |
| 23 | DA | 2288 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 23 | DA | 2517 | C | C2-N3-C4 | -5.77 | 117.01 | 119.90 |
| 24 | DB | 27 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 1 | AA | 90 | U | C2-N3-C4 | 5.77 | 130.46 | 127.00 |
| 1 | AA | 1266 | G | C8-N9-C4 | -5.77 | 104.09 | 106.40 |
| 23 | BA | 1117 | G | C5-C6-O6 | -5.77 | 125.14 | 128.60 |
| 23 | BA | 2304 | G | C8-N9-C1' | 5.77 | 134.50 | 127.00 |
| 23 | BA | 2745 | C | C2-N1-C1' | 5.77 | 125.15 | 118.80 |
| 1 | CA | 1442(B) | A | N3-C4-N9 | 5.77 | 132.02 | 127.40 |
| 23 | DA | 1914 | C | C6-N1-C1' | 5.77 | 127.73 | 120.80 |
| 23 | DA | 1994 | C | N3-C4-N4 | -5.77 | 113.96 | 118.00 |
| 23 | DA | 2224 | G | C4-C5-N7 | 5.77 | 113.11 | 110.80 |
| 23 | BA | 991 | C | N1-C2-O2 | -5.77 | 115.44 | 118.90 |
| 24 | DB | 33 | G | N9-C4-C5 | -5.77 | 103.09 | 105.40 |
| 23 | BA | 2370 | G | N1-C6-O6 | -5.77 | 116.44 | 119.90 |
| 23 | DA | 327 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 23 | DA | 775 | G | N1-C6-O6 | -5.77 | 116.44 | 119.90 |
| 23 | DA | 1544 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 23 | DA | 1208 | C | C5-C4-N4 | -5.77 | 116.16 | 120.20 |
| 1 | AA | 55 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 22 | AX | 54 | LEU | CA-CB-CG | 5.77 | 128.56 | 115.30 |
| 1 | CA | 1442(B) | A | C6-N1-C2 | -5.77 | 115.14 | 118.60 |
| 23 | DA | 2254 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 23 | BA | 1266 | G | C4-C5-N7 | 5.76 | 113.11 | 110.80 |
| 23 | BA | 2609 | U | N1-C2-N3 | 5.76 | 118.36 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 23 | BA | 951 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 23 | BA | 2454 | G | C8-N9-C4 | 5.76 | 108.70 | 106.40 |
| 23 | BA | 2790 | A | C8-N9-C4 | -5.76 | 103.50 | 105.80 |
| 23 | DA | 208 | C | C6-N1-C2 | 5.76 | 122.61 | 120.30 |
| 23 | DA | 794 | G | N1-C2-N2 | -5.76 | 111.01 | 116.20 |
| 1 | AA | 534 | U | C5-C4-O4 | 5.76 | 129.36 | 125.90 |
| 23 | BA | 1180 | C | C5-C6-N1 | -5.76 | 118.12 | 121.00 |
| 23 | BA | 2298 | A | N1-C6-N6 | -5.76 | 115.14 | 118.60 |
| 1 | CA | 1273 | G | N7-C8-N9 | 5.76 | 115.98 | 113.10 |
| 1 | CA | 1350 | A | N7-C8-N9 | 5.76 | 116.68 | 113.80 |
| 23 | DA | 1304 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 23 | DA | 2705 | A | C2-N3-C4 | -5.76 | 107.72 | 110.60 |
| 1 | AA | 1261 | A | C4-C5-N7 | 5.76 | 113.58 | 110.70 |
| 1 | AA | 1351 | U | N1-C2-O2 | 5.76 | 126.83 | 122.80 |
| 23 | BA | 1022 | G | N3-C2-N2 | -5.76 | 115.87 | 119.90 |
| 23 | BA | 2430 | A | N1-C2-N3 | 5.76 | 132.18 | 129.30 |
| 1 | CA | 359 | U | C5-C6-N1 | -5.76 | 119.82 | 122.70 |
| 23 | DA | 2444 | G | N1-C6-O6 | -5.76 | 116.44 | 119.90 |
| 23 | DA | 1038 | C | N3-C2-O2 | -5.76 | 117.87 | 121.90 |
| 23 | BA | 1269 | A | C5-N7-C8 | -5.76 | 101.02 | 103.90 |
| 23 | BA | 2004 | G | C8-N9-C4 | -5.76 | 104.10 | 106.40 |
| 23 | BA | 1998 | G | C5-C6-N1 | -5.75 | 108.62 | 111.50 |
| 1 | CA | 998 | G | N3-C2-N2 | -5.75 | 115.87 | 119.90 |
| 23 | DA | 1261 | C | N3-C4-C5 | 5.75 | 124.20 | 121.90 |
| 23 | DA | 1695 | G | C6-C5-N7 | -5.75 | 126.95 | 130.40 |
| 23 | DA | 2490 | G | N1-C6-O6 | 5.75 | 123.35 | 119.90 |
| 1 | AA | 945 | G | C5-C6-O6 | -5.75 | 125.15 | 128.60 |
| 23 | BA | 633 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 23 | BA | 803 | U | C4-C5-C6 | 5.75 | 123.15 | 119.70 |
| 23 | BA | 1478 | G | N1-C2-N2 | -5.75 | 111.02 | 116.20 |
| 23 | BA | 1658 | C | N3-C4-N4 | 5.75 | 122.03 | 118.00 |
| 23 | BA | 2300 | G | N3-C4-C5 | -5.75 | 125.72 | 128.60 |
| 1 | CA | 1182 | G | N3-C4-N9 | -5.75 | 122.55 | 126.00 |
| 23 | DA | 2306 | C | N1-C2-O2 | 5.75 | 122.35 | 118.90 |
| 23 | DA | 2587 | A | C4-C5-C6 | 5.75 | 119.88 | 117.00 |
| 23 | BA | 13 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 23 | BA | 1398 | C | N1-C2-O2 | -5.75 | 115.45 | 118.90 |
| 23 | BA | 2322 | A | N3-C4-C5 | -5.75 | 122.77 | 126.80 |
| 1 | CA | 952 | U | C5-C4-O4 | 5.75 | 129.35 | 125.90 |
| 1 | CA | 1116 | C | N3-C4-N4 | -5.75 | 113.97 | 118.00 |
| 23 | DA | 2171 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 1 | AA | 569 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1760 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 23 | DA | 2597 | G | C8-N9-C1' | -5.75 | 119.53 | 127.00 |
| 1 | CA | 950 | U | N3-C2-O2 | -5.75 | 118.17 | 122.20 |
| 23 | DA | 2616 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 2 | AB | 129 | GLU | N-CA-C | -5.75 | 95.49 | 111.00 |
| 23 | BA | 1254 | A | N9-C4-C5 | 5.75 | 108.10 | 105.80 |
| 23 | BA | 2840 | C | C2-N3-C4 | -5.75 | 117.03 | 119.90 |
| 1 | CA | 1114 | C | N3-C2-O2 | -5.75 | 117.88 | 121.90 |
| 23 | DA | 2525 | G | C4-C5-N7 | 5.75 | 113.10 | 110.80 |
| 23 | DA | 243 | U | N3-C2-O2 | -5.75 | 118.18 | 122.20 |
| 23 | BA | 677 | A | C2-N3-C4 | -5.74 | 107.73 | 110.60 |
| 23 | DA | 1930 | G | C8-N9-C4 | 5.74 | 108.70 | 106.40 |
| 1 | AA | 1141 | C | N1-C2-O2 | -5.74 | 115.45 | 118.90 |
| 23 | BA | 193 | U | N1-C2-N3 | 5.74 | 118.34 | 114.90 |
| 23 | BA | 848 | G | C8-N9-C1' | -5.74 | 119.54 | 127.00 |
| 23 | DA | 265 | A | C5-C6-N1 | -5.74 | 114.83 | 117.70 |
| 23 | DA | 2506 | U | N3-C2-O2 | -5.74 | 118.18 | 122.20 |
| 1 | AA | 570 | G | C8-N9-C4 | -5.74 | 104.10 | 106.40 |
| 23 | BA | 1791 | A | C2-N3-C4 | -5.74 | 107.73 | 110.60 |
| 23 | BA | 2626 | C | N3-C4-C5 | 5.74 | 124.20 | 121.90 |
| 1 | CA | 292 | G | N3-C4-C5 | -5.74 | 125.73 | 128.60 |
| 1 | CA | 1293 | G | N9-C4-C5 | -5.74 | 103.10 | 105.40 |
| 23 | BA | 810 | U | N3-C2-O2 | 5.74 | 126.22 | 122.20 |
| 23 | BA | 1805 | U | N3-C4-O4 | 5.74 | 123.42 | 119.40 |
| 23 | BA | 2589 | A | C8-N9-C4 | 5.74 | 108.10 | 105.80 |
| 23 | DA | 1996 | C | C6-N1-C2 | 5.74 | 122.59 | 120.30 |
| 1 | AA | 339 | C | C5-C6-N1 | -5.74 | 118.13 | 121.00 |
| 1 | AA | 346 | G | C8-N9-C1' | -5.74 | 119.54 | 127.00 |
| 23 | BA | 1938 | A | C6-N1-C2 | -5.74 | 115.16 | 118.60 |
| 1 | CA | 1077 | G | N7-C8-N9 | -5.74 | 110.23 | 113.10 |
| 1 | CA | 1163 | C | C2-N3-C4 | 5.74 | 122.77 | 119.90 |
| 23 | DA | 2306 | C | C6-N1-C1' | -5.74 | 113.92 | 120.80 |
| 23 | BA | 510 | C | C4-C5-C6 | 5.74 | 120.27 | 117.40 |
| 23 | BA | 712 | G | C8-N9-C4 | 5.74 | 108.69 | 106.40 |
| 1 | CA | 1124 | G | C4-N9-C1' | 5.74 | 133.96 | 126.50 |
| 23 | DA | 216 | A | C8-N9-C4 | 5.74 | 108.09 | 105.80 |
| 23 | DA | 1005 | C | C5-C6-N1 | -5.74 | 118.13 | 121.00 |
| 1 | CA | 1353 | G | N3-C4-C5 | -5.73 | 125.73 | 128.60 |
| 23 | DA | 968 | G | C8-N9-C4 | 5.73 | 108.69 | 106.40 |
| 24 | BB | 97 | G | C5-N7-C8 | 5.73 | 107.17 | 104.30 |
| 1 | CA | 980 | C | N3-C4-N4 | -5.73 | 113.99 | 118.00 |
| 23 | DA | 1989 | G | C6-C5-N7 | -5.73 | 126.96 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2376 | A | N1-C6-N6 | 5.73 | 122.04 | 118.60 |
| 23 | DA | 2517 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 23 | BA | 2014 | A | N1-C6-N6 | 5.73 | 122.04 | 118.60 |
| 23 | BA | 2590 | A | C5-N7-C8 | -5.73 | 101.03 | 103.90 |
| 23 | BA | 2732 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |
| 23 | BA | 2785 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 23 | DA | 1320 | C | N3-C4-N4 | 5.73 | 122.01 | 118.00 |
| 23 | DA | 1428 | C | C2-N3-C4 | -5.73 | 117.03 | 119.90 |
| 23 | BA | 2442 | C | C5-C6-N1 | -5.73 | 118.14 | 121.00 |
| 24 | BB | 5 | C | C6-N1-C2 | 5.73 | 122.59 | 120.30 |
| 1 | CA | 67 | C | C6-N1-C2 | -5.73 | 118.01 | 120.30 |
| 1 | CA | 204 | U | C2-N1-C1' | 5.73 | 124.57 | 117.70 |
| 23 | DA | 1637 | A | N1-C6-N6 | -5.73 | 115.16 | 118.60 |
| 23 | DA | 2310 | A | N1-C6-N6 | 5.73 | 122.04 | 118.60 |
| 27 | DF | 45 | ARG | NE-CZ-NH1 | -5.73 | 117.44 | 120.30 |
| 1 | AA | 998 | G | N3-C4-C5 | 5.73 | 131.46 | 128.60 |
| 23 | DA | 2146 | C | N3-C2-O2 | -5.73 | 117.89 | 121.90 |
| 1 | AA | 946 | A | N9-C4-C5 | -5.72 | 103.51 | 105.80 |
| 23 | BA | 1801 | G | C5-C6-O6 | -5.72 | 125.17 | 128.60 |
| 23 | DA | 1313 | U | N3-C4-C5 | -5.72 | 111.17 | 114.60 |
| 23 | DA | 1380 | G | C2-N3-C4 | -5.72 | 109.04 | 111.90 |
| 23 | DA | 1471 | A | N1-C2-N3 | 5.72 | 132.16 | 129.30 |
| 23 | BA | 2260 | C | C2-N3-C4 | -5.72 | 117.04 | 119.90 |
| 1 | CA | 1054 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 1 | CA | 1352 | C | N1-C2-N3 | 5.72 | 123.20 | 119.20 |
| 23 | DA | 51 | G | C4-C5-N7 | -5.72 | 108.51 | 110.80 |
| 23 | DA | 695 | G | N1-C6-O6 | -5.72 | 116.47 | 119.90 |
| 23 | BA | 463 | G | N1-C6-O6 | -5.72 | 116.47 | 119.90 |
| 23 | DA | 2096 | U | C6-N1-C2 | -5.72 | 117.57 | 121.00 |
| 1 | AA | 418 | C | C6-N1-C2 | -5.72 | 118.01 | 120.30 |
| 23 | BA | 664 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 23 | BA | 2682 | U | C5-C4-O4 | -5.72 | 122.47 | 125.90 |
| 1 | CA | 1171 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 23 | DA | 1222 | C | C6-N1-C2 | 5.72 | 122.59 | 120.30 |
| 23 | DA | 2681 | C | N3-C2-O2 | -5.72 | 117.90 | 121.90 |
| 1 | AA | 1199 | U | N1-C2-O2 | 5.72 | 126.80 | 122.80 |
| 1 | CA | 357 | G | C2-N3-C4 | 5.72 | 114.76 | 111.90 |
| 1 | AA | 144 | G | N1-C6-O6 | 5.72 | 123.33 | 119.90 |
| 1 | AA | 1207 | G | N3-C4-C5 | 5.72 | 131.46 | 128.60 |
| 23 | BA | 1543 | C | N1-C2-O2 | 5.72 | 122.33 | 118.90 |
| 23 | BA | 2676 | C | C5-C6-N1 | -5.72 | 118.14 | 121.00 |
| 23 | DA | 728 | G | C5-N7-C8 | 5.72 | 107.16 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 398 | C | N3-C2-O2 | -5.71 | 117.90 | 121.90 |
| 23 | BA | 607 | U | C6-N1-C2 | 5.71 | 124.43 | 121.00 |
| 23 | DA | 1210 | A | C6-C5-N7 | -5.71 | 128.30 | 132.30 |
| 23 | DA | 1891 | G | C2-N3-C4 | -5.71 | 109.04 | 111.90 |
| 23 | DA | 2286 | A | C5-N7-C8 | -5.71 | 101.04 | 103.90 |
| 1 | AA | 1032 | G | C6-N1-C2 | 5.71 | 128.53 | 125.10 |
| 23 | BA | 2066 | C | C5-C6-N1 | 5.71 | 123.86 | 121.00 |
| 1 | CA | 691 | G | C5-C6-O6 | -5.71 | 125.17 | 128.60 |
| 1 | AA | 352 | C | C2-N1-C1' | 5.71 | 125.08 | 118.80 |
| 23 | BA | 324 | A | N7-C8-N9 | -5.71 | 110.94 | 113.80 |
| 23 | BA | 1225 | G | N3-C4-N9 | -5.71 | 122.57 | 126.00 |
| 23 | BA | 1858 | G | N3-C4-C5 | -5.71 | 125.75 | 128.60 |
| 23 | BA | 2694 | G | N3-C4-N9 | 5.71 | 129.43 | 126.00 |
| 41 | BX | 57 | LEU | CA-CB-CG | 5.71 | 128.43 | 115.30 |
| 1 | CA | 1284 | C | C2-N3-C4 | 5.71 | 122.75 | 119.90 |
| 23 | BA | 1261 | C | N1-C2-O2 | -5.71 | 115.47 | 118.90 |
| 1 | CA | 1493 | A | C8-N9-C4 | -5.71 | 103.52 | 105.80 |
| 23 | DA | 986 | C | N3-C2-O2 | -5.71 | 117.91 | 121.90 |
| 1 | AA | 1312 | G | N7-C8-N9 | 5.71 | 115.95 | 113.10 |
| 23 | BA | 2261 | C | N3-C4-C5 | -5.71 | 119.62 | 121.90 |
| 24 | BB | 61 | G | N1-C6-O6 | 5.71 | 123.32 | 119.90 |
| 23 | BA | 431 | U | C2-N1-C1' | 5.71 | 124.55 | 117.70 |
| 24 | BB | 14 | U | C5-C6-N1 | -5.71 | 119.85 | 122.70 |
| 23 | DA | 1999 | C | C5-C6-N1 | -5.71 | 118.15 | 121.00 |
| 23 | DA | 2023 | G | N1-C6-O6 | 5.71 | 123.32 | 119.90 |
| 1 | AA | 438 | G | N3-C4-C5 | -5.70 | 125.75 | 128.60 |
| 1 | CA | 323 | U | C5-C6-N1 | 5.70 | 125.55 | 122.70 |
| 23 | DA | 988 | A | C6-C5-N7 | -5.70 | 128.31 | 132.30 |
| 23 | DA | 1648 | C | N3-C2-O2 | -5.70 | 117.91 | 121.90 |
| 1 | AA | 1019 | C | N1-C2-O2 | 5.70 | 122.32 | 118.90 |
| 23 | BA | 841 | A | N1-C2-N3 | 5.70 | 132.15 | 129.30 |
| 23 | BA | 1341 | U | N3-C2-O2 | -5.70 | 118.21 | 122.20 |
| 23 | BA | 2764 | A | C5-C6-N6 | 5.70 | 128.26 | 123.70 |
| 23 | BA | 2883 | A | C8-N9-C4 | 5.70 | 108.08 | 105.80 |
| 1 | CA | 7 | G | N3-C4-C5 | 5.70 | 131.45 | 128.60 |
| 1 | CA | 972 | C | C2-N1-C1' | 5.70 | 125.07 | 118.80 |
| 1 | CA | 1017 | G | C5-C6-O6 | 5.70 | 132.02 | 128.60 |
| 1 | CA | 1367 | C | N3-C2-O2 | -5.70 | 117.91 | 121.90 |
| 23 | DA | 47 | C | C5-C6-N1 | -5.70 | 118.15 | 121.00 |
| 23 | DA | 1898 | U | C5-C4-O4 | 5.70 | 129.32 | 125.90 |
| 1 | AA | 789 | U | N3-C4-C5 | -5.70 | 111.18 | 114.60 |
| 23 | BA | 1125 | G | N3-C4-N9 | 5.70 | 129.42 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 24 | BB | 74 | U | N1-C2-N3 | 5.70 | 118.32 | 114.90 |
| 23 | DA | 1284 | A | C4-C5-N7 | 5.70 | 113.55 | 110.70 |
| 23 | BA | 2577 | A | C4-C5-C6 | -5.70 | 114.15 | 117.00 |
| 23 | DA | 2421 | G | C4-C5-N7 | 5.70 | 113.08 | 110.80 |
| 23 | BA | 48 | G | C5-C6-O6 | 5.70 | 132.02 | 128.60 |
| 23 | BA | 1828 | G | C8-N9-C4 | 5.70 | 108.68 | 106.40 |
| 23 | BA | 2189 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 23 | BA | 2491 | U | C6-N1-C2 | 5.70 | 124.42 | 121.00 |
| 1 | CA | 638 | G | C8-N9-C4 | 5.70 | 108.68 | 106.40 |
| 23 | DA | 141 | A | C2-N3-C4 | -5.70 | 107.75 | 110.60 |
| 23 | DA | 733 | G | N3-C2-N2 | 5.70 | 123.89 | 119.90 |
| 23 | BA | 1586 | A | N7-C8-N9 | 5.69 | 116.65 | 113.80 |
| 23 | DA | 1394 | U | N3-C2-O2 | -5.69 | 118.21 | 122.20 |
| 23 | BA | 734 | A | N1-C6-N6 | 5.69 | 122.02 | 118.60 |
| 23 | BA | 2893 | G | C8-N9-C1' | 5.69 | 134.40 | 127.00 |
| 1 | CA | 1443 | G | N3-C4-N9 | 5.69 | 129.41 | 126.00 |
| 23 | DA | 1843 | C | C6-N1-C2 | 5.69 | 122.58 | 120.30 |
| 23 | BA | 806 | C | N3-C4-C5 | 5.69 | 124.18 | 121.90 |
| 23 | BA | 1139 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 23 | BA | 1858 | G | C4-N9-C1' | 5.69 | 133.90 | 126.50 |
| 23 | BA | 2445 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 23 | BA | 2623 | G | N1-C6-O6 | -5.69 | 116.49 | 119.90 |
| 45 | B1 | 46 | LEU | CA-CB-CG | 5.69 | 128.39 | 115.30 |
| 23 | DA | 1319 | G | C8-N9-C1' | -5.69 | 119.60 | 127.00 |
| 23 | DA | 1926 | U | N3-C2-O2 | -5.69 | 118.22 | 122.20 |
| 23 | DA | 2300 | G | N3-C4-C5 | -5.69 | 125.75 | 128.60 |
| 1 | AA | 1308 | U | C2-N3-C4 | 5.69 | 130.41 | 127.00 |
| 1 | AA | 1327 | C | N3-C4-C5 | 5.69 | 124.18 | 121.90 |
| 23 | BA | 2086 | U | C5-C4-O4 | 5.69 | 129.31 | 125.90 |
| 23 | DA | 945 | A | C1'-O4'-C4' | -5.69 | 105.35 | 109.90 |
| 23 | DA | 1990 | C | N1-C2-O2 | -5.69 | 115.49 | 118.90 |
| 23 | DA | 2708 | G | C5-C6-O6 | 5.69 | 132.01 | 128.60 |
| 23 | BA | 194 | G | C2-N3-C4 | -5.69 | 109.06 | 111.90 |
| 23 | BA | 2832 | U | C6-N1-C1' | -5.69 | 113.24 | 121.20 |
| 1 | CA | 615 | C | C6-N1-C2 | -5.69 | 118.03 | 120.30 |
| 1 | CA | 979 | C | N3-C4-C5 | -5.69 | 119.62 | 121.90 |
| 1 | AA | 1210 | C | C6-N1-C1' | -5.69 | 113.98 | 120.80 |
| 23 | BA | 2186 | G | C5-C6-N1 | -5.69 | 108.66 | 111.50 |
| 23 | DA | 1554 | A | N1-C6-N6 | 5.69 | 122.01 | 118.60 |
| 1 | AA | 1267 | C | C2-N1-C1' | -5.68 | 112.55 | 118.80 |
| 23 | BA | 26 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 1 | CA | 1243 | C | C6-N1-C1' | 5.68 | 127.62 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 1249 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 23 | DA | 509 | C | N3-C2-O2 | -5.68 | 117.92 | 121.90 |
| 23 | DA | 932 | G | C4-N9-C1' | -5.68 | 119.11 | 126.50 |
| 23 | DA | 961 | C | C5-C4-N4 | -5.68 | 116.22 | 120.20 |
| 23 | DA | 1464 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 1 | AA | 39 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 1 | AA | 529 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 1 | AA | 1256 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 23 | BA | 508 | G | C4-C5-N7 | 5.68 | 113.07 | 110.80 |
| 23 | BA | 1368 | G | C8-N9-C4 | -5.68 | 104.13 | 106.40 |
| 23 | DA | 751 | A | C5-N7-C8 | 5.68 | 106.74 | 103.90 |
| 23 | DA | 1340 | U | C6-N1-C2 | 5.68 | 124.41 | 121.00 |
| 23 | DA | 1659 | U | C2-N3-C4 | -5.68 | 123.59 | 127.00 |
| 23 | DA | 2444 | G | C4-C5-N7 | -5.68 | 108.53 | 110.80 |
| 24 | DB | 9 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 1 | AA | 1037 | C | C5-C4-N4 | 5.68 | 124.18 | 120.20 |
| 23 | BA | 2597 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 1 | CA | 1378 | C | C5-C6-N1 | 5.68 | 123.84 | 121.00 |
| 1 | CA | 1514 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 23 | DA | 2100 | G | C6-C5-N7 | -5.68 | 126.99 | 130.40 |
| 23 | DA | 2287 | A | C2-N3-C4 | -5.68 | 107.76 | 110.60 |
| 23 | BA | 1244 | G | N3-C2-N2 | -5.68 | 115.92 | 119.90 |
| 24 | DB | 115 | G | C2-N3-C4 | -5.68 | 109.06 | 111.90 |
| 23 | BA | 870 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 23 | BA | 1443 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 23 | BA | 1998 | G | C2-N3-C4 | -5.68 | 109.06 | 111.90 |
| 23 | BA | 2338 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 23 | BA | 2499 | C | C6-N1-C2 | -5.68 | 118.03 | 120.30 |
| 1 | CA | 1232 | U | C5-C6-N1 | 5.68 | 125.54 | 122.70 |
| 23 | DA | 2596 | U | N1-C2-O2 | -5.68 | 118.83 | 122.80 |
| 23 | BA | 476 | G | C5-C6-N1 | -5.67 | 108.66 | 111.50 |
| 23 | BA | 528 | A | C6-N1-C2 | 5.67 | 122.00 | 118.60 |
| 23 | DA | 208 | C | N3-C2-O2 | 5.67 | 125.87 | 121.90 |
| 23 | DA | 1565 | C | C2-N1-C1' | -5.67 | 112.56 | 118.80 |
| 23 | DA | 2181 | G | N3-C4-N9 | -5.67 | 122.59 | 126.00 |
| 23 | DA | 2287 | A | N9-C4-C5 | -5.67 | 103.53 | 105.80 |
| 1 | AA | 1340 | A | C5-C6-N6 | 5.67 | 128.24 | 123.70 |
| 23 | BA | 512 | G | C4-C5-N7 | -5.67 | 108.53 | 110.80 |
| 23 | BA | 874 | G | N3-C4-C5 | 5.67 | 131.44 | 128.60 |
| 23 | BA | 938 | G | C8-N9-C4 | 5.67 | 108.67 | 106.40 |
| 23 | BA | 1586 | A | C4-C5-C6 | 5.67 | 119.84 | 117.00 |
| 1 | CA | 358 | U | N3-C4-O4 | -5.67 | 115.43 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 1467 | G | N9-C4-C5 | 5.67 | 107.67 | 105.40 |
| 23 | BA | 431 | U | N3-C4-O4 | 5.67 | 123.37 | 119.40 |
| 1 | CA | 403 | C | C2-N3-C4 | -5.67 | 117.06 | 119.90 |
| 23 | DA | 449 | A | N7-C8-N9 | 5.67 | 116.64 | 113.80 |
| 1 | AA | 1442(A) | G | N9-C4-C5 | -5.67 | 103.13 | 105.40 |
| 23 | BA | 363(E) | U | C6-N1-C2 | -5.67 | 117.60 | 121.00 |
| 23 | BA | 734 | A | C5-N7-C8 | -5.67 | 101.07 | 103.90 |
| 23 | BA | 2699 | C | C5-C4-N4 | -5.67 | 116.23 | 120.20 |
| 23 | DA | 2100 | G | C5-C6-O6 | -5.67 | 125.20 | 128.60 |
| 23 | DA | 2100 | G | C8-N9-C1' | -5.67 | 119.63 | 127.00 |
| 23 | BA | 2821 | A | N9-C4-C5 | -5.66 | 103.53 | 105.80 |
| 1 | CA | 53 | A | C6-N1-C2 | -5.66 | 115.20 | 118.60 |
| 23 | DA | 2826 | A | N1-C6-N6 | -5.66 | 115.20 | 118.60 |
| 23 | BA | 2182 | G | C4-C5-N7 | -5.66 | 108.53 | 110.80 |
| 23 | DA | 1325 | G | N3-C4-N9 | 5.66 | 129.40 | 126.00 |
| 1 | AA | 1518 | A | N9-C4-C5 | 5.66 | 108.06 | 105.80 |
| 23 | BA | 577 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 23 | BA | 1374 | G | N1-C6-O6 | 5.66 | 123.30 | 119.90 |
| 23 | BA | 2826 | A | C2-N3-C4 | -5.66 | 107.77 | 110.60 |
| 1 | CA | 1441 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 23 | DA | 1191 | G | N9-C4-C5 | -5.66 | 103.14 | 105.40 |
| 23 | BA | 1845 | G | C5-C6-O6 | 5.66 | 132.00 | 128.60 |
| 1 | CA | 1390 | U | N1-C2-O2 | -5.66 | 118.84 | 122.80 |
| 23 | DA | 509 | C | C2-N3-C4 | -5.66 | 117.07 | 119.90 |
| 23 | DA | 1635 | G | C6-C5-N7 | -5.66 | 127.00 | 130.40 |
| 23 | DA | 2318 | G | N7-C8-N9 | 5.66 | 115.93 | 113.10 |
| 1 | AA | 398 | C | C2-N3-C4 | -5.66 | 117.07 | 119.90 |
| 23 | DA | 1645 | G | N1-C2-N3 | 5.66 | 127.29 | 123.90 |
| 1 | AA | 932 | C | C6-N1-C2 | -5.66 | 118.04 | 120.30 |
| 23 | BA | 1459 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 23 | DA | 645 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 23 | DA | 926 | A | C5-C6-N6 | -5.66 | 119.18 | 123.70 |
| 23 | DA | 1359 | A | N9-C4-C5 | 5.66 | 108.06 | 105.80 |
| 23 | DA | 2861 | G | C8-N9-C4 | -5.66 | 104.14 | 106.40 |
| 1 | AA | 1030(B) | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 23 | BA | 1799 | G | P-O3'-C3' | 5.65 | 126.48 | 119.70 |
| 1 | CA | 1006 | C | N1-C2-O2 | -5.65 | 115.51 | 118.90 |
| 23 | BA | 1345 | C | N1-C2-O2 | -5.65 | 115.51 | 118.90 |
| 1 | CA | 455 | C | C5-C6-N1 | 5.65 | 123.83 | 121.00 |
| 23 | DA | 2052 | G | N3-C2-N2 | -5.65 | 115.94 | 119.90 |
| 23 | DA | 60 | G | N9-C4-C5 | -5.65 | 103.14 | 105.40 |
| 23 | DA | 2189 | U | N3-C2-O2 | -5.65 | 118.25 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 26 | DE | 119 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 23 | BA | 954 | G | N3-C4-C5 | -5.65 | 125.78 | 128.60 |
| 23 | BA | 1797 | C | C6-N1-C2 | 5.65 | 122.56 | 120.30 |
| 1 | AA | 1124 | G | N3-C2-N2 | 5.65 | 123.85 | 119.90 |
| 23 | BA | 577 | G | C5-C6-N1 | -5.65 | 108.68 | 111.50 |
| 23 | BA | 932 | G | N9-C4-C5 | 5.65 | 107.66 | 105.40 |
| 1 | CA | 694 | A | N1-C6-N6 | 5.65 | 121.99 | 118.60 |
| 1 | CA | 951 | G | N3-C4-N9 | 5.65 | 129.39 | 126.00 |
| 23 | DA | 1685 | C | C5-C4-N4 | -5.65 | 116.25 | 120.20 |
| 23 | BA | 1409 | C | C6-N1-C2 | 5.64 | 122.56 | 120.30 |
| 23 | BA | 1982 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 1 | CA | 940 | C | C6-N1-C2 | -5.64 | 118.04 | 120.30 |
| 23 | DA | 53 | A | C2-N3-C4 | -5.64 | 107.78 | 110.60 |
| 1 | AA | 1035 | A | N7-C8-N9 | 5.64 | 116.62 | 113.80 |
| 1 | AA | 1505 | G | C5-C6-N1 | -5.64 | 108.68 | 111.50 |
| 23 | BA | 99 | U | C6-N1-C2 | 5.64 | 124.39 | 121.00 |
| 23 | BA | 250 | G | C5-C6-O6 | -5.64 | 125.22 | 128.60 |
| 23 | BA | 1407 | C | N1-C2-O2 | -5.64 | 115.52 | 118.90 |
| 23 | BA | 2866 | U | C5-C4-O4 | 5.64 | 129.29 | 125.90 |
| 23 | BA | 1316 | U | N1-C2-O2 | 5.64 | 126.75 | 122.80 |
| 23 | DA | 692 | C | N3-C4-C5 | 5.64 | 124.16 | 121.90 |
| 1 | AA | 172 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 23 | BA | 1779 | U | C2-N1-C1' | 5.64 | 124.47 | 117.70 |
| 1 | CA | 1029 | C | N3-C4-C5 | -5.64 | 119.64 | 121.90 |
| 23 | DA | 308 | G | C4-N9-C1' | 5.64 | 133.83 | 126.50 |
| 23 | DA | 1315 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 23 | BA | 1992 | G | P-O3'-C3' | 5.64 | 126.47 | 119.70 |
| 1 | AA | 944 | G | C8-N9-C4 | -5.64 | 104.14 | 106.40 |
| 23 | DA | 141 | A | C8-N9-C4 | -5.64 | 103.55 | 105.80 |
| 23 | DA | 271(S) | G | C6-C5-N7 | -5.64 | 127.02 | 130.40 |
| 23 | DA | 1374 | G | N7-C8-N9 | 5.64 | 115.92 | 113.10 |
| 23 | DA | 2516 | G | N9-C4-C5 | 5.64 | 107.66 | 105.40 |
| 1 | AA | 888 | G | C8-N9-C4 | 5.63 | 108.65 | 106.40 |
| 23 | BA | 1758 | G | C5-C6-O6 | -5.63 | 125.22 | 128.60 |
| 1 | CA | 1165 | C | N1-C2-O2 | 5.63 | 122.28 | 118.90 |
| 23 | DA | 787 | U | N3-C4-O4 | -5.63 | 115.46 | 119.40 |
| 1 | AA | 250 | A | N1-C6-N6 | -5.63 | 115.22 | 118.60 |
| 23 | DA | 2581 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 23 | BA | 308 | G | C4-N9-C1' | 5.63 | 133.82 | 126.50 |
| 1 | CA | 1171 | G | N7-C8-N9 | 5.63 | 115.92 | 113.10 |
| 23 | DA | 195 | A | C4-C5-C6 | 5.63 | 119.81 | 117.00 |
| 23 | DA | 2049 | G | N3-C4-N9 | -5.63 | 122.62 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | BA | 1002 | G | C8-N9-C4 | -5.63 | 104.15 | 106.40 |
| 23 | BA | 2471 | C | N3-C2-O2 | -5.63 | 117.96 | 121.90 |
| 23 | BA | 1900 | A | C8-N9-C4 | -5.63 | 103.55 | 105.80 |
| 1 | CA | 361 | G | C5-C6-N1 | -5.63 | 108.69 | 111.50 |
| 1 | CA | 976 | G | C8-N9-C1' | 5.63 | 134.31 | 127.00 |
| 23 | DA | 122 | G | C4-C5-N7 | 5.63 | 113.05 | 110.80 |
| 24 | DB | 99 | G | N1-C6-O6 | 5.63 | 123.28 | 119.90 |
| 1 | AA | 1124 | G | N9-C4-C5 | -5.62 | 103.15 | 105.40 |
| 23 | DA | 2785 | C | C6-N1-C2 | -5.62 | 118.05 | 120.30 |
| 23 | BA | 185 | U | N1-C2-N3 | 5.62 | 118.27 | 114.90 |
| 23 | BA | 512 | G | O4'-C1'-N9 | 5.62 | 112.70 | 108.20 |
| 23 | BA | 1001 | A | C4-C5-C6 | -5.62 | 114.19 | 117.00 |
| 23 | BA | 2055 | C | C2-N1-C1' | -5.62 | 112.61 | 118.80 |
| 1 | CA | 1021 | G | C5-C6-O6 | -5.62 | 125.23 | 128.60 |
| 23 | DA | 816 | C | C5-C4-N4 | -5.62 | 116.26 | 120.20 |
| 23 | DA | 1008 | C | C6-N1-C2 | 5.62 | 122.55 | 120.30 |
| 23 | DA | 2087 | G | N3-C4-C5 | 5.62 | 131.41 | 128.60 |
| 23 | DA | 2510 | C | N3-C2-O2 | -5.62 | 117.96 | 121.90 |
| 1 | AA | 1183 | A | C8-N9-C4 | 5.62 | 108.05 | 105.80 |
| 23 | BA | 907 | U | N1-C2-O2 | 5.62 | 126.74 | 122.80 |
| 23 | DA | 251 | A | C5-C6-N1 | -5.62 | 114.89 | 117.70 |
| 23 | DA | 255 | A | C5-N7-C8 | -5.62 | 101.09 | 103.90 |
| 23 | DA | 1823 | G | N3-C4-C5 | 5.62 | 131.41 | 128.60 |
| 23 | BA | 201 | C | C2-N3-C4 | -5.62 | 117.09 | 119.90 |
| 23 | BA | 706 | A | N9-C4-C5 | -5.62 | 103.55 | 105.80 |
| 23 | BA | 1322 | A | N1-C2-N3 | -5.62 | 126.49 | 129.30 |
| 1 | CA | 986 | A | C5-C6-N6 | -5.62 | 119.20 | 123.70 |
| 23 | DA | 2297 | C | C6-N1-C1' | 5.62 | 127.54 | 120.80 |
| 23 | BA | 116 | C | C4-C5-C6 | 5.62 | 120.21 | 117.40 |
| 23 | BA | 1256 | G | C4-N9-C1' | 5.62 | 133.81 | 126.50 |
| 23 | BA | 1278 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 23 | BA | 2857 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 23 | DA | 250 | G | N1-C6-O6 | 5.62 | 123.27 | 119.90 |
| 1 | AA | 988 | G | C4-C5-N7 | -5.62 | 108.55 | 110.80 |
| 23 | DA | 821 | A | C4-C5-C6 | 5.62 | 119.81 | 117.00 |
| 23 | DA | 2351 | G | N3-C4-N9 | 5.62 | 129.37 | 126.00 |
| 1 | AA | 252 | U | C6-N1-C2 | 5.62 | 124.37 | 121.00 |
| 1 | AA | 988 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 23 | BA | 1187 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 23 | BA | 1797 | C | C5-C4-N4 | -5.62 | 116.27 | 120.20 |
| 23 | BA | 2055 | C | C6-N1-C1' | 5.62 | 127.54 | 120.80 |
| 1 | CA | 713 | G | C5-C6-N1 | 5.62 | 114.31 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 188 | G | C6-C5-N7 | -5.62 | 127.03 | 130.40 |
| 23 | DA | 940 | G | C5-C6-O6 | -5.62 | 125.23 | 128.60 |
| 1 | AA | 938 | A | C8-N9-C4 | -5.61 | 103.56 | 105.80 |
| 23 | BA | 58 | G | N1-C2-N3 | 5.61 | 127.27 | 123.90 |
| 23 | BA | 1824 | G | C5-N7-C8 | 5.61 | 107.11 | 104.30 |
| 23 | BA | 1916 | A | C8-N9-C4 | 5.61 | 108.05 | 105.80 |
| 23 | DA | 2286 | A | C4-C5-N7 | 5.61 | 113.51 | 110.70 |
| 23 | BA | 799 | G | N1-C2-N3 | 5.61 | 127.27 | 123.90 |
| 23 | BA | 1022 | G | N3-C4-N9 | -5.61 | 122.63 | 126.00 |
| 23 | DA | 936 | C | N1-C2-O2 | -5.61 | 115.53 | 118.90 |
| 23 | DA | 2125 | G | C8-N9-C4 | -5.61 | 104.16 | 106.40 |
| 23 | DA | 2707 | G | C4-C5-N7 | 5.61 | 113.05 | 110.80 |
| 1 | AA | 266 | G | C2-N3-C4 | -5.61 | 109.09 | 111.90 |
| 1 | AA | 1350 | A | N3-C4-C5 | -5.61 | 122.87 | 126.80 |
| 1 | AA | 1492 | A | C2-N3-C4 | 5.61 | 113.41 | 110.60 |
| 23 | BA | 1049 | C | N1-C2-O2 | 5.61 | 122.27 | 118.90 |
| 23 | BA | 1187 | G | C8-N9-C4 | -5.61 | 104.16 | 106.40 |
| 23 | BA | 1637 | A | C8-N9-C4 | -5.61 | 103.56 | 105.80 |
| 23 | BA | 1785 | A | C6-C5-N7 | -5.61 | 128.37 | 132.30 |
| 23 | DA | 229 | A | C8-N9-C4 | -5.61 | 103.56 | 105.80 |
| 23 | DA | 582 | G | C8-N9-C4 | 5.61 | 108.64 | 106.40 |
| 1 | AA | 1126 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 23 | DA | 739 | G | C5-N7-C8 | 5.61 | 107.10 | 104.30 |
| 23 | DA | 1619 | G | C4-C5-C6 | -5.61 | 115.44 | 118.80 |
| 1 | AA | 403 | C | N1-C2-O2 | -5.61 | 115.54 | 118.90 |
| 1 | AA | 1037 | C | C6-N1-C1' | 5.61 | 127.53 | 120.80 |
| 23 | BA | 271(W) | G | N1-C6-O6 | -5.61 | 116.54 | 119.90 |
| 23 | BA | 1298 | C | N3-C4-N4 | -5.61 | 114.08 | 118.00 |
| 23 | DA | 194 | G | N3-C2-N2 | -5.61 | 115.97 | 119.90 |
| 23 | DA | 786 | C | N3-C4-N4 | -5.61 | 114.08 | 118.00 |
| 23 | DA | 1968 | G | N3-C2-N2 | -5.61 | 115.98 | 119.90 |
| 23 | DA | 311 | A | N1-C6-N6 | 5.60 | 121.96 | 118.60 |
| 23 | DA | 1207 | C | N3-C2-O2 | 5.60 | 125.82 | 121.90 |
| 1 | AA | 1309 | G | C4-N9-C1' | -5.60 | 119.22 | 126.50 |
| 23 | BA | 739 | G | C5-C6-O6 | -5.60 | 125.24 | 128.60 |
| 23 | BA | 932 | G | N3-C4-N9 | -5.60 | 122.64 | 126.00 |
| 23 | BA | 1242 | A | N1-C6-N6 | 5.60 | 121.96 | 118.60 |
| 23 | BA | 1989 | G | C5-C6-O6 | -5.60 | 125.24 | 128.60 |
| 23 | BA | 2554 | U | N1-C2-O2 | -5.60 | 118.88 | 122.80 |
| 23 | BA | 2676 | C | C2-N3-C4 | -5.60 | 117.10 | 119.90 |
| 1 | CA | 438 | G | N3-C4-N9 | 5.60 | 129.36 | 126.00 |
| 1 | AA | 988 | G | C8-N9-C4 | -5.60 | 104.16 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2260 | C | C5-C6-N1 | -5.60 | 118.20 | 121.00 |
| 23 | DA | 2709 | G | C4-C5-N7 | 5.60 | 113.04 | 110.80 |
| 1 | AA | 346 | G | N3-C2-N2 | 5.60 | 123.82 | 119.90 |
| 1 | AA | 1341 | U | N1-C2-O2 | -5.60 | 118.88 | 122.80 |
| 23 | BA | 1170 | G | C6-C5-N7 | -5.60 | 127.04 | 130.40 |
| 23 | BA | 1333 | C | N3-C4-C5 | 5.60 | 124.14 | 121.90 |
| 23 | BA | 1374 | G | N3-C2-N2 | -5.60 | 115.98 | 119.90 |
| 1 | AA | 1047 | G | N1-C6-O6 | 5.60 | 123.26 | 119.90 |
| 23 | BA | 1829 | A | C2-N3-C4 | -5.60 | 107.80 | 110.60 |
| 24 | BB | 86 | G | C5-C6-O6 | -5.60 | 125.24 | 128.60 |
| 23 | DA | 188 | G | N9-C4-C5 | -5.60 | 103.16 | 105.40 |
| 23 | DA | 1261 | C | C2-N3-C4 | -5.60 | 117.10 | 119.90 |
| 1 | AA | 433 | C | C2-N3-C4 | -5.60 | 117.10 | 119.90 |
| 23 | BA | 1358 | G | C4-C5-N7 | -5.60 | 108.56 | 110.80 |
| 1 | CA | 150 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 1 | CA | 1362 | C | N1-C2-O2 | 5.60 | 122.26 | 118.90 |
| 23 | DA | 526 | A | N1-C6-N6 | -5.60 | 115.24 | 118.60 |
| 1 | AA | 795 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 18 | AR | 85 | LEU | CA-CB-CG | 5.59 | 128.17 | 115.30 |
| 23 | BA | 496 | G | C8-N9-C4 | 5.59 | 108.64 | 106.40 |
| 23 | BA | 729 | G | C5-C6-O6 | -5.59 | 125.24 | 128.60 |
| 1 | CA | 1457 | G | C5-C6-O6 | -5.59 | 125.24 | 128.60 |
| 23 | DA | 2395 | C | N3-C4-C5 | 5.59 | 124.14 | 121.90 |
| 23 | BA | 2550 | G | N3-C2-N2 | -5.59 | 115.98 | 119.90 |
| 23 | BA | 2610 | C | N3-C4-C5 | 5.59 | 124.14 | 121.90 |
| 1 | CA | 286 | G | N1-C6-O6 | -5.59 | 116.54 | 119.90 |
| 23 | DA | 2452 | C | N3-C4-N4 | 5.59 | 121.92 | 118.00 |
| 23 | DA | 2746 | U | N3-C4-O4 | -5.59 | 115.48 | 119.40 |
| 23 | BA | 509 | C | C4-C5-C6 | 5.59 | 120.19 | 117.40 |
| 23 | BA | 837 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 29 | BH | 71 | LEU | N-CA-C | -5.59 | 95.90 | 111.00 |
| 23 | DA | 130 | C | C5-C6-N1 | -5.59 | 118.20 | 121.00 |
| 23 | DA | 988 | A | C4-C5-N7 | 5.59 | 113.50 | 110.70 |
| 23 | DA | 2000 | G | C2-N3-C4 | -5.59 | 109.10 | 111.90 |
| 1 | AA | 1125 | U | N1-C2-O2 | -5.59 | 118.89 | 122.80 |
| 23 | BA | 959 | A | C4-C5-N7 | -5.59 | 107.91 | 110.70 |
| 23 | BA | 1022 | G | C8-N9-C1' | 5.59 | 134.27 | 127.00 |
| 1 | CA | 1420 | C | C6-N1-C2 | -5.59 | 118.06 | 120.30 |
| 23 | DA | 975 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 23 | DA | 2296 | U | C6-N1-C2 | 5.59 | 124.35 | 121.00 |
| 1 | AA | 93 | G | N1-C6-O6 | 5.59 | 123.25 | 119.90 |
| 23 | DA | 1808 | U | N1-C2-N3 | -5.59 | 111.55 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2021 | C | C5-C6-N1 | -5.59 | 118.21 | 121.00 |
| 23 | DA | 2828 | C | C5-C6-N1 | -5.59 | 118.21 | 121.00 |
| 1 | AA | 1357 | A | N1-C6-N6 | 5.59 | 121.95 | 118.60 |
| 23 | BA | 425 | G | C5-N7-C8 | 5.59 | 107.09 | 104.30 |
| 23 | BA | 1021 | A | C6-C5-N7 | -5.59 | 128.39 | 132.30 |
| 23 | BA | 2441 | C | C5-C6-N1 | -5.59 | 118.21 | 121.00 |
| 1 | CA | 998 | G | C6-C5-N7 | 5.59 | 133.75 | 130.40 |
| 1 | CA | 1032 | G | C5-C6-O6 | 5.59 | 131.95 | 128.60 |
| 23 | DA | 205 | G | N1-C6-O6 | 5.59 | 123.25 | 119.90 |
| 23 | DA | 1373 | A | C5-N7-C8 | 5.59 | 106.69 | 103.90 |
| 23 | BA | 1261 | C | N3-C4-C5 | -5.58 | 119.67 | 121.90 |
| 23 | BA | 2416 | C | N1-C2-O2 | -5.58 | 115.55 | 118.90 |
| 24 | BB | 97 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | CA | 1385 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 1 | CA | 1456 | G | N1-C2-N3 | -5.58 | 120.55 | 123.90 |
| 23 | DA | 1155 | A | N1-C6-N6 | 5.58 | 121.95 | 118.60 |
| 23 | DA | 2148 | G | C6-C5-N7 | 5.58 | 133.75 | 130.40 |
| 23 | BA | 2087 | G | C6-C5-N7 | -5.58 | 127.05 | 130.40 |
| 1 | CA | 1133 | G | N9-C4-C5 | 5.58 | 107.63 | 105.40 |
| 23 | DA | 403 | U | C5-C6-N1 | -5.58 | 119.91 | 122.70 |
| 1 | AA | 1217 | C | N3-C4-N4 | -5.58 | 114.09 | 118.00 |
| 1 | AA | 1327 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 23 | BA | 560 | C | C2-N3-C4 | -5.58 | 117.11 | 119.90 |
| 1 | CA | 1230 | C | N1-C2-O2 | 5.58 | 122.25 | 118.90 |
| 1 | CA | 1497 | G | C8-N9-C4 | -5.58 | 104.17 | 106.40 |
| 23 | DA | 961 | C | N3-C4-N4 | 5.58 | 121.91 | 118.00 |
| 23 | DA | 2075 | U | N1-C2-O2 | -5.58 | 118.89 | 122.80 |
| 23 | BA | 2179 | C | C2-N1-C1' | 5.58 | 124.94 | 118.80 |
| 23 | BA | 2733 | A | N1-C6-N6 | 5.58 | 121.95 | 118.60 |
| 23 | BA | 614(B) | G | C4-C5-N7 | -5.58 | 108.57 | 110.80 |
| 23 | BA | 746 | A | C4-C5-N7 | 5.58 | 113.49 | 110.70 |
| 23 | DA | 777 | A | C8-N9-C4 | -5.58 | 103.57 | 105.80 |
| 23 | DA | 1617 | C | C6-N1-C2 | 5.58 | 122.53 | 120.30 |
| 23 | DA | 2245 | U | N1-C2-O2 | -5.58 | 118.89 | 122.80 |
| 1 | AA | 1467 | G | C4-C5-N7 | -5.58 | 108.57 | 110.80 |
| 23 | BA | 13 | A | C5-C6-N6 | 5.58 | 128.16 | 123.70 |
| 23 | DA | 1539 | G | N7-C8-N9 | 5.58 | 115.89 | 113.10 |
| 1 | AA | 274 | A | N1-C6-N6 | -5.58 | 115.25 | 118.60 |
| 1 | AA | 365 | U | N3-C4-O4 | -5.58 | 115.50 | 119.40 |
| 23 | BA | 1349 | A | N1-C6-N6 | 5.58 | 121.94 | 118.60 |
| 1 | CA | 1232 | U | N3-C4-O4 | 5.58 | 123.30 | 119.40 |
| 23 | DA | 2026 | C | N3-C2-O2 | 5.58 | 125.80 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1779 | U | N3-C4-C5 | 5.57 | 117.94 | 114.60 |
| 23 | BA | 2593 | U | C5-C4-O4 | 5.57 | 129.24 | 125.90 |
| 23 | BA | 2661 | G | N3-C4-C5 | -5.57 | 125.81 | 128.60 |
| 1 | CA | 358 | U | C5-C4-O4 | 5.57 | 129.24 | 125.90 |
| 1 | CA | 571 | U | C5-C6-N1 | 5.57 | 125.49 | 122.70 |
| 23 | DA | 143 | G | C4-N9-C1' | -5.57 | 119.26 | 126.50 |
| 23 | DA | 2424 | C | C4-C5-C6 | 5.57 | 120.19 | 117.40 |
| 23 | DA | 2439 | A | C5-C6-N1 | -5.57 | 114.91 | 117.70 |
| 1 | AA | 1284 | C | C2-N1-C1' | 5.57 | 124.93 | 118.80 |
| 23 | BA | 1488 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | BA | 1653 | G | C4-C5-C6 | 5.57 | 122.14 | 118.80 |
| 52 | B8 | 34 | TRP | N-CA-C | -5.57 | 95.96 | 111.00 |
| 23 | DA | 205 | G | N3-C4-N9 | 5.57 | 129.34 | 126.00 |
| 23 | DA | 1125 | G | C4-N9-C1' | 5.57 | 133.74 | 126.50 |
| 23 | BA | 659 | C | C4-C5-C6 | 5.57 | 120.19 | 117.40 |
| 23 | BA | 1597 | A | N7-C8-N9 | -5.57 | 111.02 | 113.80 |
| 23 | BA | 1999 | C | N1-C2-O2 | -5.57 | 115.56 | 118.90 |
| 23 | DA | 713 | G | N1-C6-O6 | 5.57 | 123.24 | 119.90 |
| 23 | DA | 1022 | G | C6-C5-N7 | 5.57 | 133.74 | 130.40 |
| 23 | DA | 1116 | C | C6-N1-C2 | 5.57 | 122.53 | 120.30 |
| 23 | DA | 1819 | A | N1-C6-N6 | -5.57 | 115.26 | 118.60 |
| 23 | DA | 2129 | C | C5-C4-N4 | 5.57 | 124.10 | 120.20 |
| 25 | DD | 131 | LEU | CB-CG-CD2 | -5.57 | 101.53 | 111.00 |
| 23 | BA | 1193 | G | C8-N9-C4 | 5.57 | 108.63 | 106.40 |
| 23 | BA | 2351 | G | N3-C4-N9 | 5.57 | 129.34 | 126.00 |
| 23 | DA | 704 | G | C5-C6-O6 | -5.57 | 125.26 | 128.60 |
| 1 | CA | 485 | G | C4-N9-C1' | -5.57 | 119.26 | 126.50 |
| 1 | CA | 1317 | C | N1-C2-O2 | 5.57 | 122.24 | 118.90 |
| 23 | DA | 848 | G | N3-C4-N9 | 5.57 | 129.34 | 126.00 |
| 1 | AA | 971 | G | N9-C4-C5 | 5.57 | 107.63 | 105.40 |
| 23 | BA | 2696 | U | N3-C4-O4 | -5.57 | 115.50 | 119.40 |
| 1 | CA | 1177 | G | C8-N9-C4 | -5.57 | 104.17 | 106.40 |
| 23 | DA | 733 | G | N1-C2-N2 | -5.57 | 111.19 | 116.20 |
| 23 | DA | 1616 | A | C5-C6-N6 | -5.57 | 119.25 | 123.70 |
| 23 | BA | 2538 | C | C2-N3-C4 | -5.56 | 117.12 | 119.90 |
| 23 | BA | 2545 | G | N3-C2-N2 | -5.56 | 116.00 | 119.90 |
| 24 | BB | 64 | C | C2-N1-C1' | -5.56 | 112.68 | 118.80 |
| 1 | CA | 1343 | G | C4-N9-C1' | 5.56 | 133.73 | 126.50 |
| 23 | DA | 2607 | G | N3-C4-N9 | 5.56 | 129.34 | 126.00 |
| 1 | CA | 1241 | G | C6-C5-N7 | -5.56 | 127.06 | 130.40 |
| 1 | CA | 1254 | C | N1-C2-O2 | -5.56 | 115.56 | 118.90 |
| 23 | DA | 1137 | G | N3-C2-N2 | -5.56 | 116.01 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 1940 | U | N3-C4-O4 | 5.56 | 123.29 | 119.40 |
| 23 | DA | 2259 | G | C5-C6-N1 | -5.56 | 108.72 | 111.50 |
| 23 | DA | 2505 | G | N3-C4-C5 | 5.56 | 131.38 | 128.60 |
| 23 | BA | 1803 | A | C8-N9-C4 | -5.56 | 103.58 | 105.80 |
| 23 | DA | 2070 | G | N1-C6-O6 | -5.56 | 116.56 | 119.90 |
| 23 | BA | 2587 | A | N9-C4-C5 | -5.56 | 103.58 | 105.80 |
| 23 | DA | 440 | G | C5-C6-O6 | 5.56 | 131.94 | 128.60 |
| 23 | DA | 2034 | U | C5-C6-N1 | -5.56 | 119.92 | 122.70 |
| 1 | AA | 1034 | G | N9-C4-C5 | 5.56 | 107.62 | 105.40 |
| 23 | BA | 2342 | C | C5-C6-N1 | 5.56 | 123.78 | 121.00 |
| 23 | DA | 2321 | G | C5-C6-O6 | 5.56 | 131.93 | 128.60 |
| 1 | AA | 1035 | A | C8-N9-C4 | -5.56 | 103.58 | 105.80 |
| 1 | CA | 1163 | C | N3-C4-C5 | -5.56 | 119.68 | 121.90 |
| 23 | DA | 2363 | C | C5-C6-N1 | -5.56 | 118.22 | 121.00 |
| 24 | DB | 113 | G | C8-N9-C4 | 5.56 | 108.62 | 106.40 |
| 23 | BA | 496 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 23 | BA | 1204 | A | C4-C5-N7 | 5.55 | 113.48 | 110.70 |
| 23 | BA | 2297 | C | C6-N1-C1' | 5.55 | 127.47 | 120.80 |
| 23 | BA | 2641 | G | N7-C8-N9 | 5.55 | 115.88 | 113.10 |
| 23 | DA | 1645 | G | N9-C4-C5 | 5.55 | 107.62 | 105.40 |
| 1 | AA | 1309 | G | N3-C2-N2 | -5.55 | 116.01 | 119.90 |
| 23 | BA | 1021 | A | N3-C4-N9 | -5.55 | 122.96 | 127.40 |
| 23 | BA | 1939 | U | C4-C5-C6 | -5.55 | 116.37 | 119.70 |
| 23 | DA | 1779 | U | C2-N1-C1' | 5.55 | 124.36 | 117.70 |
| 23 | DA | 2447 | G | N9-C4-C5 | -5.55 | 103.18 | 105.40 |
| 1 | AA | 93 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |
| 23 | BA | 263 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 23 | BA | 1250 | G | C5-C6-O6 | -5.55 | 125.27 | 128.60 |
| 1 | AA | 1258 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 23 | BA | 2611 | U | C5-C4-O4 | -5.55 | 122.57 | 125.90 |
| 1 | CA | 901 | A | N1-C6-N6 | 5.55 | 121.93 | 118.60 |
| 23 | DA | 171 | G | C6-N1-C2 | 5.55 | 128.43 | 125.10 |
| 23 | DA | 1001 | A | N7-C8-N9 | -5.55 | 111.03 | 113.80 |
| 23 | DA | 2872 | G | N1-C6-O6 | 5.55 | 123.23 | 119.90 |
| 23 | BA | 1900 | A | C5-C6-N1 | 5.55 | 120.47 | 117.70 |
| 1 | CA | 1216 | G | C4-N9-C1' | -5.55 | 119.29 | 126.50 |
| 23 | DA | 190 | A | C2-N3-C4 | -5.55 | 107.83 | 110.60 |
| 23 | DA | 665 | C | C4-C5-C6 | -5.55 | 114.63 | 117.40 |
| 23 | DA | 822 | U | C5-C4-O4 | 5.55 | 129.23 | 125.90 |
| 23 | BA | 1403 | C | C2-N1-C1' | -5.55 | 112.70 | 118.80 |
| 23 | BA | 1822 | G | N7-C8-N9 | -5.55 | 110.33 | 113.10 |
| 23 | DA | 1041 | C | C6-N1-C2 | -5.55 | 118.08 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 1965 | C | N1-C2-O2 | 5.55 | 122.23 | 118.90 |
| 23 | BA | 90 | U | N1-C2-N3 | -5.54 | 111.57 | 114.90 |
| 1 | CA | 252 | U | C5-C6-N1 | -5.54 | 119.93 | 122.70 |
| 1 | AA | 356 | A | C2-N3-C4 | 5.54 | 113.37 | 110.60 |
| 1 | AA | 555 | C | N1-C2-O2 | -5.54 | 115.57 | 118.90 |
| 1 | AA | 1367 | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 1 | CA | 792 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 1 | CA | 1120 | G | N1-C2-N2 | 5.54 | 121.19 | 116.20 |
| 23 | DA | 1988 | C | C5-C4-N4 | -5.54 | 116.32 | 120.20 |
| 23 | BA | 1322 | A | N1-C6-N6 | 5.54 | 121.92 | 118.60 |
| 23 | BA | 2567 | G | N7-C8-N9 | -5.54 | 110.33 | 113.10 |
| 23 | BA | 2607 | G | N3-C2-N2 | 5.54 | 123.78 | 119.90 |
| 1 | CA | 946 | A | C5-C6-N1 | 5.54 | 120.47 | 117.70 |
| 1 | CA | 1328 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 23 | DA | 530 | G | C8-N9-C1' | 5.54 | 134.20 | 127.00 |
| 23 | DA | 1670 | C | C5-C4-N4 | 5.54 | 124.08 | 120.20 |
| 23 | DA | 1677 | A | N1-C6-N6 | 5.54 | 121.92 | 118.60 |
| 23 | DA | 2292 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 1 | AA | 313 | A | N1-C6-N6 | -5.54 | 115.28 | 118.60 |
| 23 | BA | 425 | G | N3-C4-N9 | 5.54 | 129.32 | 126.00 |
| 23 | BA | 966 | G | N3-C2-N2 | 5.54 | 123.78 | 119.90 |
| 23 | BA | 1816 | G | C4-C5-N7 | 5.54 | 113.02 | 110.80 |
| 23 | DA | 41 | C | C2-N3-C4 | -5.54 | 117.13 | 119.90 |
| 23 | DA | 956 | G | C4-C5-N7 | -5.54 | 108.58 | 110.80 |
| 23 | DA | 1315 | C | N1-C2-N3 | 5.54 | 123.08 | 119.20 |
| 23 | DA | 2056 | G | C6-C5-N7 | -5.54 | 127.08 | 130.40 |
| 23 | DA | 2504 | U | C6-N1-C2 | 5.54 | 124.32 | 121.00 |
| 1 | AA | 992 | U | P-O3'-C3' | 5.54 | 126.35 | 119.70 |
| 23 | BA | 2271 | G | N3-C4-N9 | 5.54 | 129.32 | 126.00 |
| 1 | CA | 1241 | G | C4-N9-C1' | 5.54 | 133.70 | 126.50 |
| 23 | DA | 383 | U | C4-C5-C6 | 5.54 | 123.02 | 119.70 |
| 23 | DA | 693 | C | N3-C4-C5 | 5.54 | 124.11 | 121.90 |
| 23 | BA | 1805 | U | C4-C5-C6 | 5.54 | 123.02 | 119.70 |
| 23 | BA | 154(A) | C | C5-C4-N4 | 5.54 | 124.07 | 120.20 |
| 23 | BA | 1581 | G | C4-N9-C1' | 5.54 | 133.69 | 126.50 |
| 23 | DA | 85 | G | C8-N9-C4 | 5.54 | 108.61 | 106.40 |
| 23 | DA | 756 | C | C4-C5-C6 | 5.54 | 120.17 | 117.40 |
| 23 | DA | 2048 | G | N7-C8-N9 | 5.54 | 115.87 | 113.10 |
| 23 | DA | 2287 | A | C8-N9-C4 | 5.54 | 108.01 | 105.80 |
| 23 | DA | 2819 | G | C8-N9-C4 | 5.54 | 108.61 | 106.40 |
| 23 | BA | 179 | G | N9-C4-C5 | -5.53 | 103.19 | 105.40 |
| 23 | BA | 1800 | C | N3-C4-C5 | -5.53 | 119.69 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | DA | 115 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 23 | DA | 2304 | G | C6-C5-N7 | 5.53 | 133.72 | 130.40 |
| 1 | CA | 942 | G | C4-C5-N7 | -5.53 | 108.59 | 110.80 |
| 1 | CA | 1283 | G | N7-C8-N9 | 5.53 | 115.87 | 113.10 |
| 23 | DA | 2615 | U | C4-C5-C6 | -5.53 | 116.38 | 119.70 |
| 23 | BA | 768 | G | N3-C4-N9 | 5.53 | 129.32 | 126.00 |
| 48 | B4 | 42 | PHE | C-N-CA | 5.53 | 135.53 | 121.70 |
| 23 | DA | 1193 | G | C8-N9-C4 | 5.53 | 108.61 | 106.40 |
| 23 | DA | 570 | G | N3-C2-N2 | 5.53 | 123.77 | 119.90 |
| 1 | AA | 1003 | G | C6-N1-C2 | 5.53 | 128.42 | 125.10 |
| 23 | BA | 2354 | G | C5-N7-C8 | -5.53 | 101.54 | 104.30 |
| 23 | DA | 742 | G | N1-C2-N2 | -5.53 | 111.22 | 116.20 |
| 23 | DA | 856 | C | C3'-C2'-C1' | -5.53 | 97.08 | 101.50 |
| 23 | DA | 2775 | A | C6-N1-C2 | 5.53 | 121.92 | 118.60 |
| 23 | BA | 830 | G | C5-N7-C8 | 5.53 | 107.06 | 104.30 |
| 23 | BA | 1489 | U | N1-C2-O2 | -5.53 | 118.93 | 122.80 |
| 23 | BA | 2430 | A | C8-N9-C4 | -5.53 | 103.59 | 105.80 |
| 23 | BA | 2605 | U | N1-C2-N3 | 5.53 | 118.22 | 114.90 |
| 1 | CA | 782 | A | C8-N9-C4 | -5.53 | 103.59 | 105.80 |
| 1 | CA | 1160 | G | C4-C5-N7 | 5.53 | 113.01 | 110.80 |
| 1 | CA | 1442 | G | N3-C4-N9 | 5.53 | 129.31 | 126.00 |
| 23 | DA | 2870 | C | C2-N3-C4 | -5.53 | 117.14 | 119.90 |
| 1 | AA | 1274 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 23 | BA | 648 | G | N3-C2-N2 | -5.52 | 116.03 | 119.90 |
| 23 | BA | 1391 | U | C6-N1-C1' | -5.52 | 113.47 | 121.20 |
| 23 | BA | 1530 | C | C5-C4-N4 | -5.52 | 116.33 | 120.20 |
| 23 | BA | 2314 | C | C2-N1-C1' | -5.52 | 112.72 | 118.80 |
| 23 | DA | 508 | G | N9-C4-C5 | -5.52 | 103.19 | 105.40 |
| 23 | BA | 1271 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 23 | BA | 1628 | G | N7-C8-N9 | 5.52 | 115.86 | 113.10 |
| 23 | BA | 1641 | A | N1-C2-N3 | 5.52 | 132.06 | 129.30 |
| 23 | BA | 2043 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 23 | BA | 2590 | A | N3-C4-C5 | 5.52 | 130.67 | 126.80 |
| 1 | CA | 171 | A | N9-C4-C5 | 5.52 | 108.01 | 105.80 |
| 23 | DA | 292 | C | C6-N1-C2 | 5.52 | 122.51 | 120.30 |
| 23 | DA | 803 | U | C5-C6-N1 | -5.52 | 119.94 | 122.70 |
| 1 | AA | 506 | G | N7-C8-N9 | 5.52 | 115.86 | 113.10 |
| 23 | BA | 2716 | U | N1-C2-O2 | 5.52 | 126.67 | 122.80 |
| 1 | CA | 809 | G | C8-N9-C4 | 5.52 | 108.61 | 106.40 |
| 23 | DA | 1021 | A | N3-C4-C5 | 5.52 | 130.66 | 126.80 |
| 23 | DA | 2026 | C | N3-C4-C5 | -5.52 | 119.69 | 121.90 |
| 1 | AA | 1012 | U | N3-C4-O4 | 5.52 | 123.26 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2252 | G | C8-N9-C4 | 5.52 | 108.61 | 106.40 |
| 24 | BB | 104 | U | N3-C4-C5 | 5.52 | 117.91 | 114.60 |
| 24 | BB | 104 | U | C6-N1-C2 | 5.52 | 124.31 | 121.00 |
| 1 | CA | 78 | G | N1-C6-O6 | 5.52 | 123.21 | 119.90 |
| 1 | CA | 359 | U | N1-C2-N3 | 5.52 | 118.21 | 114.90 |
| 1 | CA | 925 | G | N9-C4-C5 | -5.52 | 103.19 | 105.40 |
| 1 | CA | 1032 | G | N3-C4-C5 | 5.52 | 131.36 | 128.60 |
| 23 | DA | 252 | G | C8-N9-C4 | 5.52 | 108.61 | 106.40 |
| 23 | DA | 2126 | A | C2-N3-C4 | -5.52 | 107.84 | 110.60 |
| 23 | DA | 2293 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |
| 23 | DA | 2510 | C | C5-C6-N1 | -5.52 | 118.24 | 121.00 |
| 1 | AA | 455 | C | C5-C6-N1 | 5.52 | 123.76 | 121.00 |
| 23 | BA | 1405 | U | N3-C4-C5 | 5.52 | 117.91 | 114.60 |
| 23 | BA | 2225 | A | C5-C6-N1 | 5.52 | 120.46 | 117.70 |
| 23 | DA | 441 | U | C5-C4-O4 | -5.52 | 122.59 | 125.90 |
| 23 | DA | 1125 | G | C8-N9-C1' | -5.52 | 119.83 | 127.00 |
| 23 | DA | 1918 | A | C8-N9-C4 | 5.52 | 108.01 | 105.80 |
| 1 | AA | 948 | C | N3-C4-N4 | 5.52 | 121.86 | 118.00 |
| 23 | DA | 1328 | G | N9-C4-C5 | -5.52 | 103.19 | 105.40 |
| 23 | BA | 688 | U | C2-N3-C4 | -5.51 | 123.69 | 127.00 |
| 23 | BA | 990 | A | N9-C4-C5 | -5.51 | 103.59 | 105.80 |
| 23 | DA | 775 | G | N3-C2-N2 | 5.51 | 123.76 | 119.90 |
| 23 | BA | 2895 | U | C5-C6-N1 | 5.51 | 125.46 | 122.70 |
| 23 | DA | 1452 | A | C2-N3-C4 | -5.51 | 107.84 | 110.60 |
| 1 | CA | 1057 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 23 | DA | 308 | G | N7-C8-N9 | 5.51 | 115.86 | 113.10 |
| 23 | DA | 1890 | A | C8-N9-C4 | 5.51 | 108.00 | 105.80 |
| 23 | DA | 1896 | G | C5-C6-O6 | -5.51 | 125.29 | 128.60 |
| 41 | DX | 57 | LEU | CA-CB-CG | 5.51 | 127.98 | 115.30 |
| 1 | AA | 543 | C | C6-N1-C2 | -5.51 | 118.10 | 120.30 |
| 1 | AA | 824 | C | N1-C2-O2 | -5.51 | 115.60 | 118.90 |
| 23 | BA | 122 | G | C6-C5-N7 | -5.51 | 127.10 | 130.40 |
| 1 | CA | 1182 | G | C8-N9-C1' | 5.51 | 134.16 | 127.00 |
| 1 | CA | 1323 | G | N7-C8-N9 | 5.51 | 115.85 | 113.10 |
| 23 | DA | 1990 | C | C2-N3-C4 | -5.51 | 117.15 | 119.90 |
| 23 | DA | 2162 | G | N3-C4-C5 | -5.51 | 125.85 | 128.60 |
| 23 | BA | 1561 | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 23 | DA | 2326 | C | N3-C4-C5 | -5.50 | 119.70 | 121.90 |
| 23 | DA | 2522 | U | C2-N1-C1' | 5.50 | 124.31 | 117.70 |
| 23 | BA | 1752 | C | N3-C2-O2 | 5.50 | 125.75 | 121.90 |
| 23 | DA | 1340 | U | C5-C4-O4 | -5.50 | 122.60 | 125.90 |
| 23 | DA | 1790 | C | N3-C2-O2 | 5.50 | 125.75 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | AA | 1379 | G | N7-C8-N9 | 5.50 | 115.85 | 113.10 |
| 23 | BA | 1962 | C | C5-C6-N1 | 5.50 | 123.75 | 121.00 |
| 1 | AA | 365 | U | C2-N1-C1' | -5.50 | 111.10 | 117.70 |
| 1 | AA | 907 | A | C2-N3-C4 | -5.50 | 107.85 | 110.60 |
| 23 | BA | 675 | A | C5-N7-C8 | -5.50 | 101.15 | 103.90 |
| 23 | DA | 833 | U | N3-C4-C5 | -5.50 | 111.30 | 114.60 |
| 23 | DA | 1821 | A | C5-C6-N1 | 5.50 | 120.45 | 117.70 |
| 23 | BA | 33 | U | C5-C6-N1 | -5.50 | 119.95 | 122.70 |
| 23 | BA | 1912 | A | C8-N9-C4 | -5.50 | 103.60 | 105.80 |
| 23 | BA | 2623 | G | C8-N9-C4 | -5.50 | 104.20 | 106.40 |
| 1 | CA | 960 | U | C6-N1-C2 | -5.50 | 117.70 | 121.00 |
| 23 | DA | 514 | A | C6-N1-C2 | -5.50 | 115.30 | 118.60 |
| 23 | DA | 1459 | G | N3-C4-C5 | -5.50 | 125.85 | 128.60 |
| 23 | DA | 2354 | G | N7-C8-N9 | 5.50 | 115.85 | 113.10 |
| 23 | DA | 2447 | G | C8-N9-C4 | 5.50 | 108.60 | 106.40 |
| 23 | BA | 652(F) | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 23 | BA | 754 | C | N3-C4-N4 | 5.50 | 121.85 | 118.00 |
| 23 | BA | 1022 | G | C4-N9-C1' | -5.50 | 119.35 | 126.50 |
| 23 | BA | 2162 | G | N3-C4-N9 | 5.50 | 129.30 | 126.00 |
| 23 | DA | 2709 | G | N1-C6-O6 | 5.50 | 123.20 | 119.90 |
| 23 | BA | 2370 | G | C6-N1-C2 | -5.50 | 121.80 | 125.10 |
| 23 | BA | 2881 | C | N3-C2-O2 | 5.50 | 125.75 | 121.90 |
| 50 | D6 | 13 | CYS | CA-CB-SG | 5.50 | 123.89 | 114.00 |
| 23 | BA | 446 | G | C8-N9-C1' | -5.49 | 119.86 | 127.00 |
| 1 | CA | 1277 | C | C2-N3-C4 | 5.49 | 122.65 | 119.90 |
| 23 | DA | 732 | C | C6-N1-C2 | 5.49 | 122.50 | 120.30 |
| 23 | BA | 826 | U | C4-C5-C6 | 5.49 | 122.99 | 119.70 |
| 23 | BA | 2238 | G | N3-C4-C5 | -5.49 | 125.86 | 128.60 |
| 24 | BB | 47 | C | N3-C4-N4 | 5.49 | 121.84 | 118.00 |
| 23 | DA | 1192 | G | N7-C8-N9 | -5.49 | 110.36 | 113.10 |
| 23 | DA | 1219 | G | N1-C6-O6 | 5.49 | 123.19 | 119.90 |
| 1 | AA | 438 | G | N3-C4-N9 | 5.49 | 129.29 | 126.00 |
| 23 | BA | 2157 | G | N9-C4-C5 | 5.49 | 107.59 | 105.40 |
| 1 | CA | 569 | C | N1-C2-O2 | 5.49 | 122.19 | 118.90 |
| 1 | CA | 925 | G | N1-C6-O6 | 5.49 | 123.19 | 119.90 |
| 1 | CA | 1101 | A | N1-C6-N6 | -5.49 | 115.31 | 118.60 |
| 23 | DA | 33 | U | C2-N1-C1' | -5.49 | 111.11 | 117.70 |
| 23 | DA | 2447 | G | C4-C5-N7 | 5.49 | 113.00 | 110.80 |
| 1 | AA | 1424 | C | C2-N3-C4 | -5.49 | 117.16 | 119.90 |
| 23 | DA | 1193 | G | N1-C6-O6 | 5.49 | 123.19 | 119.90 |
| 23 | BA | 928 | G | C4-C5-N7 | 5.49 | 112.99 | 110.80 |
| 23 | BA | 945 | A | N1-C6-N6 | 5.49 | 121.89 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2496 | C | N3-C2-O2 | 5.49 | 125.74 | 121.90 |
| 1 | CA | 1032 | G | C6-N1-C2 | 5.49 | 128.39 | 125.10 |
| 23 | DA | 529 | A | C4-C5-N7 | 5.49 | 113.44 | 110.70 |
| 23 | DA | 952 | G | C5-C6-N1 | 5.49 | 114.24 | 111.50 |
| 23 | DA | 1211 | U | C6-N1-C2 | 5.49 | 124.29 | 121.00 |
| 23 | DA | 2007 | C | N3-C4-C5 | -5.49 | 119.71 | 121.90 |
| 23 | DA | 2443 | C | N1-C2-O2 | -5.49 | 115.61 | 118.90 |
| 23 | BA | 299 | A | N9-C4-C5 | 5.48 | 107.99 | 105.80 |
| 23 | BA | 1313 | U | N3-C2-O2 | -5.48 | 118.36 | 122.20 |
| 23 | DA | 1247 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 1 | AA | 916 | G | C4-N9-C1' | 5.48 | 133.63 | 126.50 |
| 1 | AA | 1518 | A | C8-N9-C4 | -5.48 | 103.61 | 105.80 |
| 23 | BA | 1626 | G | N1-C6-O6 | -5.48 | 116.61 | 119.90 |
| 1 | CA | 71 | C | C6-N1-C2 | -5.48 | 118.11 | 120.30 |
| 1 | CA | 1340 | A | N1-C6-N6 | -5.48 | 115.31 | 118.60 |
| 23 | BA | 1269 | A | C8-N9-C4 | 5.48 | 107.99 | 105.80 |
| 23 | BA | 1948 | G | N1-C6-O6 | -5.48 | 116.61 | 119.90 |
| 23 | DA | 205 | G | C6-C5-N7 | -5.48 | 127.11 | 130.40 |
| 23 | DA | 932 | G | C4-C5-N7 | -5.48 | 108.61 | 110.80 |
| 23 | DA | 1202 | C | C5-C6-N1 | -5.48 | 118.26 | 121.00 |
| 1 | AA | 21 | G | N3-C4-C5 | -5.48 | 125.86 | 128.60 |
| 23 | BA | 2590 | A | C4-C5-N7 | 5.48 | 113.44 | 110.70 |
| 23 | DA | 2485 | G | C4-C5-N7 | 5.48 | 112.99 | 110.80 |
| 23 | BA | 945 | A | N1-C2-N3 | 5.48 | 132.04 | 129.30 |
| 23 | BA | 1306 | C | N3-C4-C5 | 5.48 | 124.09 | 121.90 |
| 23 | BA | 1992 | G | C8-N9-C4 | -5.48 | 104.21 | 106.40 |
| 1 | AA | 1493 | A | C8-N9-C4 | -5.47 | 103.61 | 105.80 |
| 23 | BA | 230 | U | C2-N1-C1' | 5.47 | 124.27 | 117.70 |
| 23 | BA | 1942 | C | C6-N1-C1' | 5.47 | 127.37 | 120.80 |
| 23 | DA | 1038 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 23 | BA | 736 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 23 | BA | 1621 | U | N3-C4-O4 | 5.47 | 123.23 | 119.40 |
| 23 | BA | 2506 | U | N3-C2-O2 | -5.47 | 118.37 | 122.20 |
| 1 | CA | 1237 | C | C2-N3-C4 | 5.47 | 122.64 | 119.90 |
| 1 | CA | 1320 | C | N1-C2-O2 | 5.47 | 122.18 | 118.90 |
| 23 | DA | 449 | A | N1-C6-N6 | 5.47 | 121.88 | 118.60 |
| 23 | DA | 2723 | C | C6-N1-C2 | 5.47 | 122.49 | 120.30 |
| 23 | BA | 631 | A | N1-C6-N6 | 5.47 | 121.88 | 118.60 |
| 23 | DA | 1403 | C | C6-N1-C1' | 5.47 | 127.36 | 120.80 |
| 23 | DA | 2558 | C | C5-C6-N1 | -5.47 | 118.26 | 121.00 |
| 1 | AA | 1174 | G | C4-C5-C6 | -5.47 | 115.52 | 118.80 |
| 23 | BA | 488 | G | C5-N7-C8 | 5.47 | 107.03 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1275 | A | N1-C2-N3 | 5.47 | 132.03 | 129.30 |
| 23 | BA | 1330 | C | N3-C4-N4 | 5.47 | 121.83 | 118.00 |
| 1 | CA | 240 | C | C2-N3-C4 | -5.47 | 117.17 | 119.90 |
| 1 | CA | 1031 | G | C2-N3-C4 | 5.47 | 114.64 | 111.90 |
| 1 | CA | 1166 | G | N1-C6-O6 | -5.47 | 116.62 | 119.90 |
| 23 | DA | 1006 | C | C5-C4-N4 | 5.47 | 124.03 | 120.20 |
| 1 | CA | 1228 | C | C2-N3-C4 | 5.47 | 122.63 | 119.90 |
| 23 | DA | 657 | U | C5-C4-O4 | 5.47 | 129.18 | 125.90 |
| 23 | DA | 1763 | G | N3-C4-C5 | 5.47 | 131.33 | 128.60 |
| 23 | BA | 768 | G | N3-C4-C5 | -5.47 | 125.87 | 128.60 |
| 23 | BA | 1295 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 23 | BA | 1320 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 23 | BA | 1588 | C | C6-N1-C2 | -5.47 | 118.11 | 120.30 |
| 23 | BA | 2032 | G | C4-C5-C6 | 5.47 | 122.08 | 118.80 |
| 1 | AA | 204 | U | C2-N1-C1' | 5.46 | 124.26 | 117.70 |
| 23 | BA | 1553 | A | N9-C4-C5 | 5.46 | 107.99 | 105.80 |
| 23 | BA | 1624 | G | C5-C6-N1 | 5.46 | 114.23 | 111.50 |
| 23 | BA | 2804 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 1 | CA | 443 | C | N1-C2-O2 | 5.46 | 122.18 | 118.90 |
| 1 | CA | 896 | C | C5-C6-N1 | -5.46 | 118.27 | 121.00 |
| 1 | AA | 786 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 23 | BA | 1930 | G | C4-N9-C1' | -5.46 | 119.40 | 126.50 |
| 23 | BA | 2084 | C | C4-C5-C6 | 5.46 | 120.13 | 117.40 |
| 23 | DA | 2817 | G | N1-C6-O6 | 5.46 | 123.18 | 119.90 |
| 23 | BA | 2032 | G | N1-C6-O6 | 5.46 | 123.18 | 119.90 |
| 1 | CA | 356 | A | C2-N3-C4 | 5.46 | 113.33 | 110.60 |
| 1 | CA | 1305 | G | N3-C4-C5 | 5.46 | 131.33 | 128.60 |
| 23 | DA | 2294 | C | N3-C4-C5 | 5.46 | 124.08 | 121.90 |
| 23 | DA | 2711 | A | C8-N9-C4 | 5.46 | 107.98 | 105.80 |
| 23 | BA | 948 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 23 | BA | 1257 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 23 | BA | 139 | G | C8-N9-C4 | -5.46 | 104.22 | 106.40 |
| 23 | BA | 443 | A | C8-N9-C4 | -5.46 | 103.62 | 105.80 |
| 23 | BA | 1343 | G | C4-N9-C1' | 5.46 | 133.59 | 126.50 |
| 1 | CA | 105 | G | N9-C4-C5 | 5.46 | 107.58 | 105.40 |
| 1 | CA | 1326 | C | C2-N3-C4 | 5.46 | 122.63 | 119.90 |
| 23 | DA | 945 | A | C6-C5-N7 | -5.46 | 128.48 | 132.30 |
| 23 | DA | 2055 | C | C6-N1-C2 | 5.46 | 122.48 | 120.30 |
| 23 | BA | 835 | A | N1-C2-N3 | -5.46 | 126.57 | 129.30 |
| 23 | BA | 856 | C | C5-C6-N1 | 5.46 | 123.73 | 121.00 |
| 1 | CA | 28 | G | C5-C6-O6 | -5.46 | 125.33 | 128.60 |
| 1 | AA | 939 | G | C6-N1-C2 | 5.46 | 128.37 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | BA | 1653 | G | C8-N9-C1' | -5.46 | 119.91 | 127.00 |
| 23 | DA | 127 | A | C2-N3-C4 | -5.46 | 107.87 | 110.60 |
| 23 | DA | 413 | C | N3-C2-O2 | 5.46 | 125.72 | 121.90 |
| 23 | DA | 1807 | G | C8-N9-C4 | 5.46 | 108.58 | 106.40 |
| 23 | DA | 2857 | G | N1-C6-O6 | 5.46 | 123.17 | 119.90 |
| 1 | AA | 117 | G | C8-N9-C1' | -5.45 | 119.91 | 127.00 |
| 1 | AA | 1106 | G | C8-N9-C4 | -5.45 | 104.22 | 106.40 |
| 23 | BA | 885 | C | C5-C4-N4 | -5.45 | 116.38 | 120.20 |
| 23 | BA | 2373 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 23 | DA | 124 | G | C2-N3-C4 | -5.45 | 109.17 | 111.90 |
| 23 | DA | 1983 | C | C2-N3-C4 | -5.45 | 117.17 | 119.90 |
| 23 | DA | 512 | G | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 23 | DA | 2641 | G | C8-N9-C1' | -5.45 | 119.91 | 127.00 |
| 1 | AA | 605 | U | N3-C4-C5 | -5.45 | 111.33 | 114.60 |
| 1 | AA | 1423 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 1 | CA | 509 | A | C8-N9-C4 | -5.45 | 103.62 | 105.80 |
| 1 | AA | 28 | G | N3-C2-N2 | -5.45 | 116.09 | 119.90 |
| 11 | AK | 118 | GLY | N-CA-C | 5.45 | 126.72 | 113.10 |
| 23 | BA | 847 | U | C2-N3-C4 | -5.45 | 123.73 | 127.00 |
| 23 | BA | 928 | G | N7-C8-N9 | 5.45 | 115.82 | 113.10 |
| 23 | BA | 1140 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 23 | DA | 662 | G | N3-C4-C5 | -5.45 | 125.88 | 128.60 |
| 1 | AA | 1039 | C | N1-C2-O2 | 5.45 | 122.17 | 118.90 |
| 23 | BA | 1048 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 23 | BA | 1216 | G | N1-C2-N2 | -5.45 | 111.30 | 116.20 |
| 23 | BA | 1257 | C | N1-C2-N3 | 5.45 | 123.01 | 119.20 |
| 1 | CA | 1301 | U | N3-C4-C5 | -5.45 | 111.33 | 114.60 |
| 23 | DA | 1199 | U | N1-C2-N3 | 5.45 | 118.17 | 114.90 |
| 1 | AA | 1166 | G | C8-N9-C1' | 5.45 | 134.08 | 127.00 |
| 23 | DA | 351 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 23 | DA | 1609 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 23 | DA | 2032 | G | C5-C6-O6 | -5.45 | 125.33 | 128.60 |
| 23 | DA | 2587 | A | C2-N3-C4 | -5.45 | 107.88 | 110.60 |
| 23 | BA | 1316 | U | N3-C2-O2 | -5.44 | 118.39 | 122.20 |
| 23 | BA | 1829 | A | C8-N9-C4 | 5.44 | 107.98 | 105.80 |
| 1 | CA | 812 | C | C6-N1-C2 | 5.44 | 122.48 | 120.30 |
| 23 | DA | 512 | G | C5-C6-O6 | 5.44 | 131.87 | 128.60 |
| 23 | DA | 2435 | A | C4-C5-N7 | 5.44 | 113.42 | 110.70 |
| 23 | BA | 2307 | G | C5-N7-C8 | -5.44 | 101.58 | 104.30 |
| 23 | DA | 623 | G | C5-C6-O6 | -5.44 | 125.33 | 128.60 |
| 23 | DA | 1276 | A | N9-C4-C5 | -5.44 | 103.62 | 105.80 |
| 23 | BA | 454 | A | N1-C6-N6 | 5.44 | 121.86 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2035 | G | C8-N9-C4 | -5.44 | 104.22 | 106.40 |
| 1 | CA | 78 | G | C5-C6-N1 | -5.44 | 108.78 | 111.50 |
| 23 | DA | 308 | G | C6-C5-N7 | -5.44 | 127.14 | 130.40 |
| 23 | DA | 676 | A | N1-C6-N6 | 5.44 | 121.86 | 118.60 |
| 23 | DA | 915 | C | C2-N1-C1' | 5.44 | 124.78 | 118.80 |
| 23 | DA | 1428 | C | C5-C6-N1 | -5.44 | 118.28 | 121.00 |
| 1 | AA | 378 | G | C8-N9-C4 | 5.44 | 108.58 | 106.40 |
| 23 | BA | 528 | A | C4-C5-C6 | -5.44 | 114.28 | 117.00 |
| 23 | BA | 1204 | A | N3-C4-N9 | -5.44 | 123.05 | 127.40 |
| 23 | BA | 1348 | G | N1-C6-O6 | 5.44 | 123.16 | 119.90 |
| 23 | BA | 2358 | G | N1-C6-O6 | -5.44 | 116.64 | 119.90 |
| 1 | CA | 1241 | G | C8-N9-C4 | -5.44 | 104.22 | 106.40 |
| 1 | CA | 1322 | C | C5-C6-N1 | 5.44 | 123.72 | 121.00 |
| 23 | DA | 1938 | A | N1-C2-N3 | 5.44 | 132.02 | 129.30 |
| 23 | DA | 2149 | G | N1-C2-N2 | 5.44 | 121.09 | 116.20 |
| 23 | BA | 928 | G | C4-C5-C6 | 5.44 | 122.06 | 118.80 |
| 23 | BA | 2286 | A | C4-N9-C1' | 5.44 | 136.09 | 126.30 |
| 24 | BB | 6 | C | N1-C2-O2 | 5.44 | 122.16 | 118.90 |
| 23 | DA | 1377 | G | C2-N3-C4 | 5.44 | 114.62 | 111.90 |
| 1 | AA | 1328 | C | C6-N1-C1' | 5.44 | 127.32 | 120.80 |
| 23 | BA | 1049 | C | C4-C5-C6 | -5.44 | 114.68 | 117.40 |
| 23 | DA | 53 | A | N1-C2-N3 | 5.44 | 132.02 | 129.30 |
| 1 | AA | 333 | G | C5-C6-O6 | -5.43 | 125.34 | 128.60 |
| 1 | AA | 1338 | G | N3-C4-N9 | 5.43 | 129.26 | 126.00 |
| 23 | BA | 1845 | G | C4-C5-N7 | -5.43 | 108.63 | 110.80 |
| 23 | DA | 624 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 1 | AA | 25 | C | N3-C4-N4 | 5.43 | 121.80 | 118.00 |
| 23 | BA | 309 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 23 | BA | 645 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 23 | BA | 1547 | C | C5-C6-N1 | -5.43 | 118.28 | 121.00 |
| 23 | BA | 2251 | G | N1-C6-O6 | -5.43 | 116.64 | 119.90 |
| 43 | BZ | 151 | HIS | N-CA-C | 5.43 | 125.67 | 111.00 |
| 1 | CA | 936 | C | N3-C4-N4 | 5.43 | 121.80 | 118.00 |
| 23 | DA | 1112 | G | N3-C4-N9 | -5.43 | 122.74 | 126.00 |
| 23 | DA | 1123 | C | C2-N1-C1' | -5.43 | 112.83 | 118.80 |
| 1 | AA | 1195 | C | C6-N1-C2 | -5.43 | 118.13 | 120.30 |
| 23 | BA | 2000 | G | C8-N9-C4 | 5.43 | 108.57 | 106.40 |
| 23 | BA | 2264 | C | C5-C6-N1 | -5.43 | 118.28 | 121.00 |
| 23 | BA | 2769 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 1 | AA | 557 | G | C4-N9-C1' | 5.43 | 133.56 | 126.50 |
| 1 | AA | 1148 | U | C5-C6-N1 | 5.43 | 125.41 | 122.70 |
| 23 | BA | 2084 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 33 | BP | 148 | LEU | CA-CB-CG | 5.43 | 127.79 | 115.30 |
| 1 | CA | 77 | G | N9-C4-C5 | -5.43 | 103.23 | 105.40 |
| 23 | DA | 265 | A | C4-N9-C1' | 5.43 | 136.07 | 126.30 |
| 23 | DA | 546 | C | C2-N1-C1' | 5.43 | 124.77 | 118.80 |
| 23 | DA | 1371 | G | C6-C5-N7 | -5.43 | 127.14 | 130.40 |
| 23 | DA | 1432 | C | C6-N1-C2 | 5.43 | 122.47 | 120.30 |
| 23 | DA | 2434 | A | C8-N9-C4 | 5.43 | 107.97 | 105.80 |
| 1 | AA | 1468 | A | C5-C6-N6 | -5.43 | 119.36 | 123.70 |
| 23 | DA | 263 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 1 | AA | 149 | A | N1-C6-N6 | 5.43 | 121.86 | 118.60 |
| 1 | AA | 801 | U | C5-C6-N1 | -5.43 | 119.99 | 122.70 |
| 1 | AA | 1116 | C | N1-C2-O2 | 5.43 | 122.16 | 118.90 |
| 23 | BA | 2000 | G | C5-N7-C8 | 5.43 | 107.01 | 104.30 |
| 23 | DA | 1021 | A | C8-N9-C4 | -5.43 | 103.63 | 105.80 |
| 1 | AA | 1259 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 23 | BA | 663 | G | C8-N9-C4 | -5.42 | 104.23 | 106.40 |
| 23 | BA | 2271 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 23 | BA | 2866 | U | C4-C5-C6 | 5.42 | 122.95 | 119.70 |
| 23 | DA | 2338 | G | N9-C4-C5 | -5.42 | 103.23 | 105.40 |
| 23 | BA | 742 | G | N9-C4-C5 | -5.42 | 103.23 | 105.40 |
| 23 | DA | 652(R) | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 23 | BA | 147 | U | N1-C2-N3 | 5.42 | 118.15 | 114.90 |
| 23 | BA | 525 | U | N1-C2-N3 | 5.42 | 118.15 | 114.90 |
| 23 | BA | 2680 | C | C5-C4-N4 | -5.42 | 116.41 | 120.20 |
| 1 | CA | 553 | A | C8-N9-C4 | -5.42 | 103.63 | 105.80 |
| 23 | DA | 1566 | A | C2-N3-C4 | -5.42 | 107.89 | 110.60 |
| 23 | DA | 1995 | U | N1-C2-N3 | 5.42 | 118.15 | 114.90 |
| 23 | DA | 2728 | U | C5-C6-N1 | -5.42 | 119.99 | 122.70 |
| 23 | BA | 1233 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 23 | BA | 1785 | A | C4-C5-C6 | 5.42 | 119.71 | 117.00 |
| 23 | DA | 768 | G | C6-C5-N7 | -5.42 | 127.15 | 130.40 |
| 1 | AA | 21 | G | C5-C6-O6 | 5.42 | 131.85 | 128.60 |
| 1 | AA | 286 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 23 | BA | 1319 | G | N1-C2-N3 | 5.42 | 127.15 | 123.90 |
| 23 | BA | 1845 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 23 | DA | 529 | A | N3-C4-C5 | 5.42 | 130.59 | 126.80 |
| 23 | DA | 1266 | G | N3-C2-N2 | 5.42 | 123.69 | 119.90 |
| 23 | BA | 351 | G | C8-N9-C4 | 5.42 | 108.57 | 106.40 |
| 23 | BA | 1022 | G | N1-C6-O6 | -5.42 | 116.65 | 119.90 |
| 23 | BA | 1471 | A | N1-C2-N3 | 5.42 | 132.01 | 129.30 |
| 23 | DA | 2444 | G | C5-C6-O6 | 5.42 | 131.85 | 128.60 |
| 1 | AA | 352 | C | N3-C2-O2 | -5.42 | 118.11 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | AA | 1329 | A | N1-C6-N6 | -5.42 | 115.35 | 118.60 |
| 23 | BA | 195 | A | N9-C4-C5 | -5.42 | 103.63 | 105.80 |
| 23 | BA | 645 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 23 | BA | 1034 | G | C4-C5-N7 | -5.42 | 108.63 | 110.80 |
| 23 | BA | 2287 | A | N1-C2-N3 | 5.42 | 132.01 | 129.30 |
| 23 | BA | 2351 | G | N3-C4-C5 | -5.42 | 125.89 | 128.60 |
| 1 | CA | 1145 | C | C2-N3-C4 | 5.42 | 122.61 | 119.90 |
| 1 | CA | 1238 | A | C5-N7-C8 | 5.41 | 106.61 | 103.90 |
| 23 | DA | 1238 | G | C8-N9-C4 | 5.41 | 108.56 | 106.40 |
| 23 | DA | 2491 | U | C6-N1-C2 | 5.41 | 124.25 | 121.00 |
| 1 | AA | 1290 | G | C8-N9-C1' | -5.41 | 119.96 | 127.00 |
| 23 | DA | 1026 | U | N3-C2-O2 | -5.41 | 118.41 | 122.20 |
| 23 | BA | 2441 | C | N3-C4-C5 | 5.41 | 124.06 | 121.90 |
| 23 | DA | 1996 | C | N3-C4-N4 | -5.41 | 114.21 | 118.00 |
| 24 | DB | 70 | C | C6-N1-C2 | -5.41 | 118.14 | 120.30 |
| 23 | BA | 171 | G | C6-N1-C2 | 5.41 | 128.34 | 125.10 |
| 23 | BA | 178 | G | N1-C2-N3 | 5.41 | 127.15 | 123.90 |
| 23 | BA | 333 | G | C8-N9-C1' | -5.41 | 119.97 | 127.00 |
| 23 | BA | 2240 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 23 | BA | 2894 | G | C5-N7-C8 | -5.41 | 101.59 | 104.30 |
| 1 | CA | 610 | G | N3-C4-N9 | 5.41 | 129.25 | 126.00 |
| 23 | DA | 505 | A | C2-N3-C4 | -5.41 | 107.90 | 110.60 |
| 23 | DA | 614(B) | G | C6-C5-N7 | 5.41 | 133.65 | 130.40 |
| 23 | DA | 2283 | C | N3-C2-O2 | 5.41 | 125.69 | 121.90 |
| 23 | BA | 33 | U | C6-N1-C2 | 5.41 | 124.24 | 121.00 |
| 23 | BA | 1206 | G | N1-C2-N3 | 5.41 | 127.14 | 123.90 |
| 23 | DA | 1688 | U | N1-C2-O2 | -5.41 | 119.02 | 122.80 |
| 23 | DA | 2375 | G | C2-N3-C4 | -5.41 | 109.20 | 111.90 |
| 1 | AA | 1017 | G | C6-N1-C2 | 5.41 | 128.34 | 125.10 |
| 23 | BA | 915 | C | N3-C2-O2 | -5.41 | 118.12 | 121.90 |
| 1 | CA | 841 | U | C5-C6-N1 | 5.41 | 125.40 | 122.70 |
| 1 | CA | 1045 | C | C5-C6-N1 | 5.41 | 123.70 | 121.00 |
| 23 | BA | 2489 | G | N3-C4-C5 | -5.40 | 125.90 | 128.60 |
| 1 | CA | 1099 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 23 | DA | 2393 | A | N7-C8-N9 | 5.40 | 116.50 | 113.80 |
| 23 | DA | 2731 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 1 | AA | 1022 | G | C2-N3-C4 | 5.40 | 114.60 | 111.90 |
| 23 | BA | 800 | A | C6-N1-C2 | -5.40 | 115.36 | 118.60 |
| 23 | BA | 2628 | C | N3-C4-C5 | 5.40 | 124.06 | 121.90 |
| 1 | CA | 43 | C | C2-N3-C4 | 5.40 | 122.60 | 119.90 |
| 23 | DA | 1022 | G | C4-N9-C1' | -5.40 | 119.48 | 126.50 |
| 1 | AA | 21 | G | C4-C5-N7 | -5.40 | 108.64 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 23 | BA | 717 | G | N3-C4-C5 | 5.40 | 131.30 | 128.60 |
| 23 | BA | 1436 | G | C6-C5-N7 | -5.40 | 127.16 | 130.40 |
| 23 | DA | 268 | C | N3-C4-N4 | 5.40 | 121.78 | 118.00 |
| 23 | BA | 654 | A | C8-N9-C4 | 5.40 | 107.96 | 105.80 |
| 1 | CA | 261 | U | C2-N1-C1' | -5.40 | 111.22 | 117.70 |
| 23 | DA | 446 | G | N7-C8-N9 | -5.40 | 110.40 | 113.10 |
| 1 | AA | 274 | A | C5-C6-N1 | 5.40 | 120.40 | 117.70 |
| 23 | BA | 801 | G | N9-C4-C5 | 5.40 | 107.56 | 105.40 |
| 23 | BA | 2727 | G | C5-C6-O6 | -5.40 | 125.36 | 128.60 |
| 23 | DA | 40 | C | C6-N1-C2 | 5.40 | 122.46 | 120.30 |
| 23 | DA | 1006 | C | C6-N1-C1' | 5.40 | 127.28 | 120.80 |
| 23 | DA | 1530 | C | C5-C4-N4 | -5.40 | 116.42 | 120.20 |
| 23 | DA | 2151 | G | N1-C2-N2 | 5.40 | 121.06 | 116.20 |
| 23 | BA | 432 | A | C8-N9-C4 | -5.39 | 103.64 | 105.80 |
| 23 | BA | 1133 | U | N3-C4-C5 | 5.39 | 117.84 | 114.60 |
| 1 | AA | 171 | A | N9-C4-C5 | 5.39 | 107.96 | 105.80 |
| 1 | CA | 1246 | C | C2-N1-C1' | 5.39 | 124.73 | 118.80 |
| 23 | DA | 383 | U | N3-C4-C5 | -5.39 | 111.36 | 114.60 |
| 23 | DA | 2515 | C | C5-C4-N4 | -5.39 | 116.42 | 120.20 |
| 24 | DB | 55 | U | C6-N1-C2 | -5.39 | 117.76 | 121.00 |
| 23 | BA | 393 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 23 | BA | 1536 | C | N3-C4-C5 | -5.39 | 119.74 | 121.90 |
| 23 | DA | 1941 | C | N1-C2-O2 | -5.39 | 115.67 | 118.90 |
| 1 | AA | 433 | C | C5-C6-N1 | -5.39 | 118.31 | 121.00 |
| 23 | BA | 676 | A | C1'-O4'-C4' | -5.39 | 105.59 | 109.90 |
| 23 | BA | 763 | G | C5-N7-C8 | 5.39 | 106.99 | 104.30 |
| 23 | BA | 1231 | G | N1-C2-N3 | 5.39 | 127.13 | 123.90 |
| 23 | BA | 2276 | G | N3-C2-N2 | -5.39 | 116.13 | 119.90 |
| 23 | DA | 62 | C | N3-C4-C5 | 5.39 | 124.06 | 121.90 |
| 23 | DA | 826 | U | C4-C5-C6 | 5.39 | 122.93 | 119.70 |
| 23 | DA | 2547 | U | C6-N1-C2 | 5.39 | 124.23 | 121.00 |
| 1 | CA | 1361 | G | N3-C4-C5 | -5.39 | 125.91 | 128.60 |
| 23 | DA | 348 | G | C8-N9-C4 | 5.39 | 108.56 | 106.40 |
| 23 | DA | 2027 | G | N1-C2-N3 | 5.39 | 127.13 | 123.90 |
| 23 | DA | 2272 | U | N3-C2-O2 | -5.39 | 118.43 | 122.20 |
| 33 | DP | 148 | LEU | CA-CB-CG | 5.39 | 127.69 | 115.30 |
| 1 | AA | 322 | C | C5-C6-N1 | -5.39 | 118.31 | 121.00 |
| 23 | BA | 2894 | G | C5-C6-N1 | 5.39 | 114.19 | 111.50 |
| 23 | DA | 261 | G | N1-C6-O6 | 5.39 | 123.13 | 119.90 |
| 23 | DA | 565 | C | C4-C5-C6 | 5.39 | 120.09 | 117.40 |
| 23 | DA | 2330 | G | C8-N9-C4 | 5.39 | 108.55 | 106.40 |
| 1 | AA | 1342 | C | C2-N1-C1' | -5.38 | 112.88 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 776 | G | N1-C2-N3 | 5.38 | 127.13 | 123.90 |
| 23 | BA | 1324 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 23 | BA | 1448 | G | C8-N9-C4 | 5.38 | 108.55 | 106.40 |
| 1 | CA | 1467 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 23 | DA | 530 | G | C5-N7-C8 | -5.38 | 101.61 | 104.30 |
| 23 | DA | 1031 | G | C2-N3-C4 | -5.38 | 109.21 | 111.90 |
| 23 | DA | 2515 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 23 | DA | 2676 | C | N3-C4-C5 | 5.38 | 124.05 | 121.90 |
| 1 | AA | 1043 | C | C4-C5-C6 | 5.38 | 120.09 | 117.40 |
| 1 | CA | 791 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 23 | DA | 446 | G | C5-N7-C8 | 5.38 | 106.99 | 104.30 |
| 23 | BA | 941 | A | N1-C2-N3 | -5.38 | 126.61 | 129.30 |
| 23 | BA | 1448 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 23 | BA | 1490 | A | N7-C8-N9 | -5.38 | 111.11 | 113.80 |
| 23 | BA | 1681 | G | C5-N7-C8 | -5.38 | 101.61 | 104.30 |
| 23 | BA | 2031 | A | C5-C6-N6 | -5.38 | 119.39 | 123.70 |
| 23 | BA | 2129 | C | N3-C2-O2 | -5.38 | 118.13 | 121.90 |
| 23 | BA | 2515 | C | N3-C4-N4 | 5.38 | 121.77 | 118.00 |
| 23 | BA | 2762 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 1 | CA | 381 | C | N3-C4-C5 | -5.38 | 119.75 | 121.90 |
| 1 | CA | 1235 | U | N3-C2-O2 | -5.38 | 118.43 | 122.20 |
| 1 | CA | 1361 | G | N1-C6-O6 | -5.38 | 116.67 | 119.90 |
| 23 | DA | 312 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 23 | BA | 1189 | A | C4-C5-N7 | 5.38 | 113.39 | 110.70 |
| 23 | BA | 2790 | A | C2-N3-C4 | 5.38 | 113.29 | 110.60 |
| 1 | CA | 79 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 1 | CA | 1216 | G | C8-N9-C1' | 5.38 | 133.99 | 127.00 |
| 23 | BA | 1231 | G | C5-C6-N1 | -5.38 | 108.81 | 111.50 |
| 23 | BA | 2443 | C | C6-N1-C2 | -5.38 | 118.15 | 120.30 |
| 23 | BA | 2767 | C | C5-C6-N1 | -5.38 | 118.31 | 121.00 |
| 1 | CA | 226 | G | C8-N9-C4 | 5.38 | 108.55 | 106.40 |
| 23 | DA | 60 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 23 | DA | 1377 | G | C6-N1-C2 | -5.38 | 121.87 | 125.10 |
| 23 | DA | 2027 | G | C6-N1-C2 | -5.38 | 121.87 | 125.10 |
| 23 | BA | 2224 | G | C5-C6-O6 | -5.38 | 125.38 | 128.60 |
| 23 | BA | 2536 | G | N1-C2-N3 | 5.38 | 127.13 | 123.90 |
| 23 | DA | 585 | G | C8-N9-C4 | 5.38 | 108.55 | 106.40 |
| 23 | DA | 1653 | G | P-O3'-C3' | 5.38 | 126.15 | 119.70 |
| 23 | DA | 1654 | A | C5-C6-N6 | 5.38 | 128.00 | 123.70 |
| 1 | AA | 1068 | G | N3-C4-N9 | 5.38 | 129.22 | 126.00 |
| 23 | BA | 2346 | A | C5-C6-N6 | -5.38 | 119.40 | 123.70 |
| 23 | BA | 2590 | A | C2-N3-C4 | -5.38 | 107.91 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | CA | 260 | G | N3-C4-N9 | -5.38 | 122.78 | 126.00 |
| 23 | DA | 1912 | A | N7-C8-N9 | 5.38 | 116.49 | 113.80 |
| 23 | BA | 1428 | C | N1-C2-O2 | -5.37 | 115.68 | 118.90 |
| 23 | BA | 2319 | G | N3-C2-N2 | -5.37 | 116.14 | 119.90 |
| 1 | CA | 1182 | G | N1-C2-N2 | 5.37 | 121.03 | 116.20 |
| 23 | BA | 1276 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 23 | BA | 1905 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 23 | BA | 2740 | A | C4-C5-C6 | 5.37 | 119.69 | 117.00 |
| 1 | CA | 11 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 23 | DA | 2297 | C | N1-C2-O2 | -5.37 | 115.68 | 118.90 |
| 1 | AA | 738 | C | C6-N1-C2 | -5.37 | 118.15 | 120.30 |
| 23 | BA | 2517 | C | C2-N3-C4 | -5.37 | 117.22 | 119.90 |
| 23 | DA | 600 | G | N1-C6-O6 | 5.37 | 123.12 | 119.90 |
| 23 | DA | 1658 | C | C5-C6-N1 | 5.37 | 123.69 | 121.00 |
| 1 | AA | 975 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 23 | BA | 2105 | C | C5-C6-N1 | 5.37 | 123.68 | 121.00 |
| 23 | BA | 2430 | A | N7-C8-N9 | 5.37 | 116.48 | 113.80 |
| 23 | BA | 2453 | A | C5-C6-N1 | 5.37 | 120.39 | 117.70 |
| 1 | CA | 171 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 23 | DA | 682 | G | N3-C4-N9 | 5.37 | 129.22 | 126.00 |
| 23 | DA | 1785 | A | C6-C5-N7 | -5.37 | 128.54 | 132.30 |
| 1 | AA | 92 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 32 | BO | 8 | LEU | CA-CB-CG | 5.37 | 127.64 | 115.30 |
| 23 | DA | 1220 | A | C8-N9-C4 | 5.37 | 107.95 | 105.80 |
| 23 | DA | 2312 | U | N1-C2-O2 | 5.37 | 126.56 | 122.80 |
| 1 | AA | 946 | A | C4-C5-N7 | 5.36 | 113.38 | 110.70 |
| 23 | BA | 69 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 1 | CA | 1163 | C | C2-N1-C1' | 5.36 | 124.70 | 118.80 |
| 23 | DA | 743 | G | C5-C6-N1 | 5.36 | 114.18 | 111.50 |
| 23 | DA | 1381 | G | C5-C6-O6 | 5.36 | 131.82 | 128.60 |
| 23 | DA | 2296 | U | C3'-C2'-C1' | -5.36 | 97.21 | 101.50 |
| 23 | DA | 2455 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 1 | AA | 487 | A | N1-C6-N6 | 5.36 | 121.82 | 118.60 |
| 1 | AA | 754 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |
| 23 | BA | 874 | G | N1-C6-O6 | 5.36 | 123.12 | 119.90 |
| 23 | BA | 782 | A | C5-C6-N1 | 5.36 | 120.38 | 117.70 |
| 23 | BA | 874 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 23 | BA | 994 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 23 | BA | 1365 | A | C5-N7-C8 | -5.36 | 101.22 | 103.90 |
| 23 | BA | 2373 | G | C2-N3-C4 | -5.36 | 109.22 | 111.90 |
| 1 | CA | 346 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 23 | DA | 94 | C | N3-C2-O2 | -5.36 | 118.15 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 791 | C | C2-N3-C4 | -5.36 | 117.22 | 119.90 |
| 23 | DA | 2300 | G | C5-C6-O6 | -5.36 | 125.38 | 128.60 |
| 23 | DA | 2878 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 23 | BA | 730 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 1 | CA | 1231 | G | C8-N9-C4 | -5.36 | 104.26 | 106.40 |
| 1 | AA | 483 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 23 | BA | 476 | G | N1-C6-O6 | 5.36 | 123.11 | 119.90 |
| 23 | BA | 2335 | A | C4-C5-C6 | -5.36 | 114.32 | 117.00 |
| 23 | DA | 2442 | C | N1-C2-O2 | -5.36 | 115.69 | 118.90 |
| 23 | BA | 804 | A | N1-C6-N6 | 5.36 | 121.81 | 118.60 |
| 23 | BA | 2016 | U | N3-C2-O2 | 5.36 | 125.95 | 122.20 |
| 24 | BB | 8 | U | C5-C6-N1 | 5.36 | 125.38 | 122.70 |
| 23 | DA | 546 | C | C5-C6-N1 | 5.36 | 123.68 | 121.00 |
| 23 | DA | 1994 | C | C5-C4-N4 | 5.36 | 123.95 | 120.20 |
| 1 | AA | 1029 | C | C6-N1-C1' | 5.35 | 127.22 | 120.80 |
| 1 | AA | 1034 | G | C6-N1-C2 | 5.35 | 128.31 | 125.10 |
| 1 | AA | 1042 | G | C8-N9-C1' | 5.35 | 133.96 | 127.00 |
| 23 | BA | 702 | G | N1-C6-O6 | 5.35 | 123.11 | 119.90 |
| 23 | BA | 2694 | G | C4-N9-C1' | 5.35 | 133.46 | 126.50 |
| 23 | BA | 2820 | A | N1-C6-N6 | 5.35 | 121.81 | 118.60 |
| 25 | BD | 263 | ARG | NE-CZ-NH1 | -5.35 | 117.62 | 120.30 |
| 23 | DA | 236 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 23 | DA | 652(S) | C | C5-C6-N1 | 5.35 | 123.68 | 121.00 |
| 23 | DA | 1299 | G | N7-C8-N9 | 5.35 | 115.78 | 113.10 |
| 23 | DA | 2056 | G | C2-N3-C4 | -5.35 | 109.22 | 111.90 |
| 23 | DA | 2447 | G | N3-C4-C5 | 5.35 | 131.28 | 128.60 |
| 23 | BA | 762 | U | N1-C2-O2 | 5.35 | 126.55 | 122.80 |
| 23 | BA | 1558 | A | P-O3'-C3' | 5.35 | 126.12 | 119.70 |
| 23 | DA | 339 | U | C6-N1-C2 | 5.35 | 124.21 | 121.00 |
| 23 | DA | 2681 | C | N1-C2-N3 | 5.35 | 122.95 | 119.20 |
| 23 | BA | 380 | U | C6-N1-C2 | 5.35 | 124.21 | 121.00 |
| 23 | BA | 697 | C | N3-C4-N4 | 5.35 | 121.74 | 118.00 |
| 23 | BA | 1407 | C | N3-C4-C5 | -5.35 | 119.76 | 121.90 |
| 23 | BA | 1673 | U | C5-C6-N1 | -5.35 | 120.03 | 122.70 |
| 23 | BA | 1687 | G | C8-N9-C4 | -5.35 | 104.26 | 106.40 |
| 24 | BB | 95 | C | C6-N1-C2 | -5.35 | 118.16 | 120.30 |
| 1 | CA | 49 | U | C5-C6-N1 | -5.35 | 120.03 | 122.70 |
| 23 | DA | 2099 | U | C2-N1-C1' | 5.35 | 124.12 | 117.70 |
| 23 | DA | 2505 | G | C2-N3-C4 | -5.35 | 109.23 | 111.90 |
| 1 | AA | 217 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 1 | AA | 1395 | C | N1-C2-O2 | 5.35 | 122.11 | 118.90 |
| 23 | BA | 1010 | A | C8-N9-C4 | 5.35 | 107.94 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 1283 | G | N3-C4-C5 | -5.35 | 125.93 | 128.60 |
| 23 | DA | 2266 | A | C4-C5-N7 | 5.35 | 113.37 | 110.70 |
| 24 | DB | 64 | C | C2-N1-C1' | -5.35 | 112.92 | 118.80 |
| 23 | BA | 614(B) | G | C4-N9-C1' | -5.35 | 119.55 | 126.50 |
| 23 | DA | 2849 | U | C2-N3-C4 | -5.35 | 123.79 | 127.00 |
| 1 | AA | 71 | C | C2-N3-C4 | 5.34 | 122.57 | 119.90 |
| 1 | AA | 534 | U | N3-C4-O4 | -5.34 | 115.66 | 119.40 |
| 1 | AA | 1442(B) | A | N1-C2-N3 | 5.34 | 131.97 | 129.30 |
| 23 | BA | 1858 | G | C6-C5-N7 | -5.34 | 127.19 | 130.40 |
| 1 | CA | 370 | C | C6-N1-C2 | 5.34 | 122.44 | 120.30 |
| 23 | DA | 1899 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 23 | BA | 553 | G | C2-N3-C4 | -5.34 | 109.23 | 111.90 |
| 23 | BA | 2074 | U | N1-C2-O2 | 5.34 | 126.54 | 122.80 |
| 23 | DA | 2363 | C | C2-N1-C1' | -5.34 | 112.92 | 118.80 |
| 23 | DA | 2396 | G | C5-N7-C8 | -5.34 | 101.63 | 104.30 |
| 23 | DA | 2689 | U | N1-C2-N3 | 5.34 | 118.11 | 114.90 |
| 48 | D4 | 42 | PHE | C-N-CA | 5.34 | 135.06 | 121.70 |
| 1 | AA | 1284 | C | N1-C2-O2 | 5.34 | 122.11 | 118.90 |
| 23 | BA | 53 | A | C5-N7-C8 | -5.34 | 101.23 | 103.90 |
| 23 | BA | 185 | U | C2-N3-C4 | -5.34 | 123.80 | 127.00 |
| 23 | BA | 960 | A | N9-C4-C5 | -5.34 | 103.66 | 105.80 |
| 1 | CA | 1141 | C | N1-C2-O2 | -5.34 | 115.69 | 118.90 |
| 5 | CE | 71 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 23 | DA | 574 | C | N3-C4-N4 | -5.34 | 114.26 | 118.00 |
| 23 | DA | 1645 | G | C5-C6-O6 | 5.34 | 131.81 | 128.60 |
| 1 | AA | 940 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 23 | BA | 77 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |
| 23 | BA | 700 | G | N1-C2-N3 | 5.34 | 127.10 | 123.90 |
| 23 | BA | 733 | G | N7-C8-N9 | -5.34 | 110.43 | 113.10 |
| 23 | BA | 1573 | G | N3-C2-N2 | 5.34 | 123.64 | 119.90 |
| 23 | BA | 1653 | G | P-O3'-C3' | 5.34 | 126.11 | 119.70 |
| 23 | DA | 252 | G | N7-C8-N9 | -5.34 | 110.43 | 113.10 |
| 23 | DA | 1777 | U | C6-N1-C2 | 5.34 | 124.20 | 121.00 |
| 1 | AA | 670 | G | N1-C6-O6 | -5.34 | 116.70 | 119.90 |
| 23 | BA | 956 | G | C5-C6-N1 | -5.34 | 108.83 | 111.50 |
| 1 | CA | 1160 | G | C5-C6-N1 | 5.34 | 114.17 | 111.50 |
| 23 | DA | 1359 | A | C5-C6-N6 | 5.34 | 127.97 | 123.70 |
| 23 | BA | 568 | U | C5-C4-O4 | -5.33 | 122.70 | 125.90 |
| 23 | BA | 1721 | G | N7-C8-N9 | 5.33 | 115.77 | 113.10 |
| 23 | DA | 924 | C | C2-N3-C4 | -5.33 | 117.23 | 119.90 |
| 1 | AA | 458 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 23 | BA | 1613 | G | N1-C2-N2 | -5.33 | 111.40 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 2607 | G | C5-C6-N1 | -5.33 | 108.83 | 111.50 |
| 23 | DA | 60 | G | C5-C6-O6 | -5.33 | 125.40 | 128.60 |
| 23 | DA | 558 | G | C8-N9-C4 | 5.33 | 108.53 | 106.40 |
| 1 | AA | 809 | G | N3-C4-N9 | -5.33 | 122.80 | 126.00 |
| 23 | BA | 69 | C | C4-C5-C6 | 5.33 | 120.06 | 117.40 |
| 23 | BA | 130 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |
| 23 | BA | 1225 | G | N9-C4-C5 | 5.33 | 107.53 | 105.40 |
| 23 | BA | 1609 | A | C6-N1-C2 | -5.33 | 115.40 | 118.60 |
| 23 | BA | 2429 | G | N7-C8-N9 | 5.33 | 115.77 | 113.10 |
| 23 | BA | 2602 | A | C6-N1-C2 | -5.33 | 115.40 | 118.60 |
| 24 | BB | 60 | C | N3-C4-C5 | -5.33 | 119.77 | 121.90 |
| 23 | DA | 71 | A | C6-C5-N7 | -5.33 | 128.57 | 132.30 |
| 23 | DA | 271(A) | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 23 | DA | 1129 | A | N1-C6-N6 | -5.33 | 115.40 | 118.60 |
| 23 | DA | 2224 | G | C2-N3-C4 | -5.33 | 109.23 | 111.90 |
| 23 | DA | 2638 | G | C5-C6-N1 | -5.33 | 108.83 | 111.50 |
| 23 | DA | 956 | G | C5-N7-C8 | 5.33 | 106.97 | 104.30 |
| 1 | AA | 1104 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 23 | BA | 750 | A | N7-C8-N9 | 5.33 | 116.46 | 113.80 |
| 23 | BA | 1460 | A | C2-N3-C4 | 5.33 | 113.26 | 110.60 |
| 23 | BA | 2420 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | CA | 577 | G | N9-C4-C5 | -5.33 | 103.27 | 105.40 |
| 23 | DA | 2708 | G | N1-C2-N3 | 5.33 | 127.10 | 123.90 |
| 1 | AA | 59 | A | C5-C6-N6 | -5.33 | 119.44 | 123.70 |
| 1 | CA | 984 | C | N3-C4-N4 | 5.33 | 121.73 | 118.00 |
| 1 | AA | 470 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 23 | BA | 102 | G | C8-N9-C1' | -5.33 | 120.08 | 127.00 |
| 23 | BA | 1231 | G | N1-C6-O6 | 5.33 | 123.10 | 119.90 |
| 23 | BA | 1238 | G | C5-C6-O6 | -5.33 | 125.41 | 128.60 |
| 23 | BA | 1406 | U | C5-C6-N1 | 5.33 | 125.36 | 122.70 |
| 23 | BA | 1693 | U | C5-C6-N1 | -5.33 | 120.04 | 122.70 |
| 1 | CA | 1120 | G | C6-C5-N7 | 5.33 | 133.60 | 130.40 |
| 1 | AA | 317 | G | C6-C5-N7 | -5.32 | 127.21 | 130.40 |
| 23 | BA | 1983 | C | C5-C4-N4 | -5.32 | 116.47 | 120.20 |
| 1 | CA | 266 | G | C2-N3-C4 | -5.32 | 109.24 | 111.90 |
| 23 | DA | 818 | G | N7-C8-N9 | -5.32 | 110.44 | 113.10 |
| 23 | DA | 1142(A) | A | C6-C5-N7 | -5.32 | 128.57 | 132.30 |
| 23 | DA | 1639 | U | N3-C2-O2 | -5.32 | 118.47 | 122.20 |
| 23 | DA | 2028 | U | C5-C4-O4 | -5.32 | 122.71 | 125.90 |
| 23 | DA | 2157 | G | N9-C4-C5 | 5.32 | 107.53 | 105.40 |
| 23 | DA | 2379 | G | C8-N9-C4 | -5.32 | 104.27 | 106.40 |
| 1 | CA | 982 | U | N3-C4-O4 | 5.32 | 123.13 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 1031 | G | N3-C4-C5 | -5.32 | 125.94 | 128.60 |
| 23 | DA | 1380 | G | N3-C2-N2 | -5.32 | 116.17 | 119.90 |
| 23 | BA | 465 | G | C4-N9-C1' | 5.32 | 133.42 | 126.50 |
| 23 | BA | 1942 | C | C2-N1-C1' | -5.32 | 112.95 | 118.80 |
| 23 | DA | 509 | C | C5-C6-N1 | -5.32 | 118.34 | 121.00 |
| 1 | AA | 1037 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 23 | BA | 1661 | G | C6-N1-C2 | -5.32 | 121.91 | 125.10 |
| 23 | BA | 2331 | G | C5-C6-O6 | -5.32 | 125.41 | 128.60 |
| 23 | DA | 1265 | A | C4-C5-C6 | 5.32 | 119.66 | 117.00 |
| 23 | DA | 1380 | G | N3-C4-C5 | 5.32 | 131.26 | 128.60 |
| 1 | AA | 402 | G | C5-C6-N1 | -5.32 | 108.84 | 111.50 |
| 23 | BA | 1336 | A | C5-C6-N1 | 5.32 | 120.36 | 117.70 |
| 27 | BF | 168 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 14 | CN | 43 | CYS | CA-CB-SG | -5.32 | 104.43 | 114.00 |
| 23 | DA | 599 | G | C2-N3-C4 | -5.32 | 109.24 | 111.90 |
| 23 | DA | 1829 | A | N7-C8-N9 | -5.32 | 111.14 | 113.80 |
| 1 | AA | 1376 | U | N3-C2-O2 | 5.32 | 125.92 | 122.20 |
| 1 | AA | 1381 | U | C6-N1-C1' | -5.32 | 113.76 | 121.20 |
| 1 | CA | 1351 | U | C2-N1-C1' | -5.32 | 111.32 | 117.70 |
| 23 | DA | 2699 | C | N3-C4-C5 | 5.32 | 124.03 | 121.90 |
| 23 | DA | 2744 | G | C2-N3-C4 | -5.32 | 109.24 | 111.90 |
| 23 | BA | 787 | U | N1-C2-N3 | 5.31 | 118.09 | 114.90 |
| 23 | DA | 2237 | G | C8-N9-C4 | 5.31 | 108.53 | 106.40 |
| 1 | AA | 1017 | G | C5-C6-O6 | 5.31 | 131.79 | 128.60 |
| 23 | BA | 1130 | U | N3-C4-C5 | -5.31 | 111.41 | 114.60 |
| 23 | BA | 1632 | A | C5-C6-N6 | -5.31 | 119.45 | 123.70 |
| 23 | BA | 2312 | U | C6-N1-C2 | -5.31 | 117.81 | 121.00 |
| 23 | BA | 2356 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 23 | BA | 2587 | A | C2-N3-C4 | -5.31 | 107.94 | 110.60 |
| 23 | DA | 1284 | A | C5-N7-C8 | -5.31 | 101.24 | 103.90 |
| 23 | BA | 775 | G | N3-C2-N2 | 5.31 | 123.62 | 119.90 |
| 23 | BA | 1404 | C | N1-C2-O2 | 5.31 | 122.09 | 118.90 |
| 23 | DA | 2015 | A | C5-C6-N6 | 5.31 | 127.95 | 123.70 |
| 24 | DB | 104 | U | C2-N1-C1' | -5.31 | 111.33 | 117.70 |
| 1 | CA | 1000 | U | C6-N1-C2 | -5.31 | 117.81 | 121.00 |
| 1 | CA | 1468 | A | C8-N9-C4 | 5.31 | 107.92 | 105.80 |
| 23 | DA | 1181 | C | N1-C2-O2 | 5.31 | 122.08 | 118.90 |
| 23 | DA | 2622 | C | N3-C4-C5 | 5.31 | 124.02 | 121.90 |
| 1 | AA | 243 | A | C8-N9-C4 | -5.31 | 103.68 | 105.80 |
| 23 | BA | 2242 | G | N3-C4-N9 | -5.31 | 122.82 | 126.00 |
| 1 | CA | 150 | C | C2-N3-C4 | 5.31 | 122.55 | 119.90 |
| 1 | CA | 611 | A | N1-C6-N6 | -5.31 | 115.42 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 464 | U | C5-C4-O4 | 5.31 | 129.08 | 125.90 |
| 23 | DA | 1612 | C | N3-C4-N4 | 5.31 | 121.72 | 118.00 |
| 23 | DA | 2615 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 23 | DA | 2761 | G | C8-N9-C4 | -5.31 | 104.28 | 106.40 |
| 23 | BA | 982 | C | C6-N1-C2 | -5.31 | 118.18 | 120.30 |
| 23 | BA | 1414 | G | C8-N9-C4 | -5.31 | 104.28 | 106.40 |
| 23 | DA | 2547 | U | C5-C6-N1 | -5.31 | 120.05 | 122.70 |
| 23 | DA | 2675 | A | C5-C6-N6 | -5.31 | 119.46 | 123.70 |
| 1 | AA | 1042 | G | N3-C4-N9 | -5.30 | 122.82 | 126.00 |
| 1 | AA | 1307 | U | C5-C4-O4 | -5.30 | 122.72 | 125.90 |
| 23 | BA | 1631(A) | A | C8-N9-C4 | -5.30 | 103.68 | 105.80 |
| 23 | BA | 2067 | G | N3-C4-N9 | 5.30 | 129.18 | 126.00 |
| 23 | BA | 2287 | A | C4-C5-N7 | 5.30 | 113.35 | 110.70 |
| 1 | CA | 1060 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 23 | DA | 614(B) | G | C4-N9-C1' | -5.30 | 119.60 | 126.50 |
| 23 | DA | 2059 | A | C2-N3-C4 | -5.30 | 107.95 | 110.60 |
| 23 | BA | 1187 | G | N9-C4-C5 | 5.30 | 107.52 | 105.40 |
| 23 | DA | 2787 | C | N3-C2-O2 | -5.30 | 118.19 | 121.90 |
| 1 | AA | 1003 | G | N9-C4-C5 | 5.30 | 107.52 | 105.40 |
| 1 | AA | 1153 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 1 | AA | 1226 | C | N3-C4-N4 | -5.30 | 114.29 | 118.00 |
| 23 | BA | 452 | G | N1-C2-N3 | 5.30 | 127.08 | 123.90 |
| 1 | CA | 981 | U | N3-C4-O4 | 5.30 | 123.11 | 119.40 |
| 23 | DA | 2082 | A | N1-C6-N6 | 5.30 | 121.78 | 118.60 |
| 1 | AA | 286 | G | C8-N9-C4 | -5.30 | 104.28 | 106.40 |
| 1 | AA | 1435 | G | N1-C6-O6 | 5.30 | 123.08 | 119.90 |
| 23 | BA | 102 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 23 | BA | 757 | U | N3-C2-O2 | -5.30 | 118.49 | 122.20 |
| 23 | BA | 888 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 23 | BA | 1762 | A | N3-C4-C5 | -5.30 | 123.09 | 126.80 |
| 23 | BA | 2033 | A | N1-C6-N6 | -5.30 | 115.42 | 118.60 |
| 1 | CA | 7 | G | N3-C4-N9 | -5.30 | 122.82 | 126.00 |
| 1 | CA | 454 | C | C4-C5-C6 | 5.30 | 120.05 | 117.40 |
| 23 | DA | 463 | G | N3-C4-N9 | -5.30 | 122.82 | 126.00 |
| 23 | DA | 796 | C | C2-N3-C4 | -5.30 | 117.25 | 119.90 |
| 23 | DA | 1216 | G | N3-C4-N9 | 5.30 | 129.18 | 126.00 |
| 23 | DA | 1881 | C | C5-C6-N1 | 5.30 | 123.65 | 121.00 |
| 1 | AA | 855 | G | C8-N9-C4 | -5.30 | 104.28 | 106.40 |
| 23 | BA | 1618 | A | C5-C6-N6 | 5.30 | 127.94 | 123.70 |
| 23 | BA | 1845 | G | N1-C2-N2 | -5.30 | 111.43 | 116.20 |
| 1 | CA | 1258 | G | C6-N1-C2 | 5.30 | 128.28 | 125.10 |
| 1 | AA | 1034 | G | C6-C5-N7 | 5.30 | 133.58 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23 | BA | 207 | A | N3-C4-N9 | -5.30 | 123.16 | 127.40 |
| 23 | BA | 856 | C | N3-C4-C5 | -5.30 | 119.78 | 121.90 |
| 23 | BA | 949 | C | C6-N1-C2 | 5.30 | 122.42 | 120.30 |
| 23 | BA | 2080 | G | N7-C8-N9 | -5.30 | 110.45 | 113.10 |
| 23 | DA | 1452 | A | C8-N9-C4 | 5.30 | 107.92 | 105.80 |
| 23 | DA | 2334 | G | C8-N9-C4 | 5.30 | 108.52 | 106.40 |
| 1 | AA | 930 | C | N3-C4-N4 | -5.29 | 114.29 | 118.00 |
| 23 | BA | 889 | C | N1-C2-O2 | 5.29 | 122.08 | 118.90 |
| 23 | BA | 2348 | U | C6-N1-C2 | 5.29 | 124.18 | 121.00 |
| 1 | AA | 980 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 23 | BA | 796 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 23 | BA | 1657 | C | N3-C2-O2 | 5.29 | 125.61 | 121.90 |
| 47 | B3 | 56 | VAL | CB-CA-C | -5.29 | 101.34 | 111.40 |
| 1 | CA | 675 | A | N1-C6-N6 | 5.29 | 121.78 | 118.60 |
| 1 | CA | 927 | G | N1-C6-O6 | 5.29 | 123.08 | 119.90 |
| 23 | DA | 448 | U | N3-C4-C5 | -5.29 | 111.42 | 114.60 |
| 23 | DA | 723 | G | N9-C4-C5 | -5.29 | 103.28 | 105.40 |
| 1 | AA | 378 | G | N3-C4-C5 | 5.29 | 131.25 | 128.60 |
| 23 | BA | 266 | G | C8-N9-C4 | 5.29 | 108.52 | 106.40 |
| 23 | BA | 2613 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 23 | DA | 564 | C | C5-C6-N1 | -5.29 | 118.36 | 121.00 |
| 26 | DE | 119 | ARG | NE-CZ-NH2 | -5.29 | 117.65 | 120.30 |
| 23 | BA | 696 | G | C8-N9-C4 | 5.29 | 108.52 | 106.40 |
| 1 | CA | 1003 | G | C6-N1-C2 | 5.29 | 128.27 | 125.10 |
| 23 | DA | 530 | G | C8-N9-C4 | -5.29 | 104.28 | 106.40 |
| 23 | BA | 59 | U | N1-C2-N3 | 5.29 | 118.07 | 114.90 |
| 23 | BA | 645 | C | N3-C2-O2 | -5.29 | 118.20 | 121.90 |
| 23 | BA | 1204 | A | C3'-C2'-C1' | -5.29 | 97.27 | 101.50 |
| 23 | BA | 1318 | C | N1-C2-O2 | -5.29 | 115.73 | 118.90 |
| 1 | CA | 1150 | U | C5-C4-O4 | 5.29 | 129.07 | 125.90 |
| 23 | DA | 1581 | G | C4-N9-C1' | 5.29 | 133.38 | 126.50 |
| 24 | DB | 30 | C | N3-C4-N4 | 5.29 | 121.70 | 118.00 |
| 1 | AA | 1381 | U | N3-C2-O2 | -5.29 | 118.50 | 122.20 |
| 1 | AA | 1502 | A | C5-C6-N6 | -5.29 | 119.47 | 123.70 |
| 23 | BA | 2079 | U | C4-C5-C6 | 5.29 | 122.87 | 119.70 |
| 23 | DA | 401 | A | N1-C2-N3 | 5.29 | 131.94 | 129.30 |
| 1 | AA | 1022 | G | C5-C6-O6 | -5.29 | 125.43 | 128.60 |
| 1 | AA | 1294 | G | N3-C4-N9 | -5.29 | 122.83 | 126.00 |
| 23 | BA | 394 | A | C2-N3-C4 | -5.29 | 107.96 | 110.60 |
| 23 | BA | 652(T) | C | C5-C4-N4 | 5.29 | 123.90 | 120.20 |
| 23 | BA | 1222 | C | C6-N1-C2 | 5.29 | 122.41 | 120.30 |
| 1 | CA | 102 | G | N9-C4-C5 | 5.29 | 107.51 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 874 | G | N3-C4-C5 | 5.29 | 131.24 | 128.60 |
| 45 | D1 | 40 | ARG | NE-CZ-NH1 | 5.29 | 122.94 | 120.30 |
| 1 | AA | 1309 | G | C8-N9-C1' | 5.28 | 133.87 | 127.00 |
| 23 | BA | 389 | G | C8-N9-C1' | -5.28 | 120.13 | 127.00 |
| 23 | BA | 587 | C | N1-C2-N3 | 5.28 | 122.90 | 119.20 |
| 23 | BA | 966 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 23 | BA | 1608 | A | N3-C4-N9 | -5.28 | 123.17 | 127.40 |
| 1 | CA | 163 | C | C2-N1-C1' | 5.28 | 124.61 | 118.80 |
| 23 | DA | 1692 | U | C5-C6-N1 | -5.28 | 120.06 | 122.70 |
| 23 | DA | 1826 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 23 | DA | 2182 | G | C4-C5-N7 | -5.28 | 108.69 | 110.80 |
| 1 | AA | 1303 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 23 | BA | 884 | C | N3-C4-C5 | -5.28 | 119.79 | 121.90 |
| 23 | BA | 2764 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 23 | DA | 602 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 1 | AA | 1283 | G | C2-N3-C4 | 5.28 | 114.54 | 111.90 |
| 1 | AA | 1328 | C | N3-C4-N4 | -5.28 | 114.30 | 118.00 |
| 1 | AA | 1362 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 23 | BA | 108 | U | N1-C2-O2 | 5.28 | 126.50 | 122.80 |
| 23 | BA | 765 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 23 | BA | 839 | U | C6-N1-C2 | -5.28 | 117.83 | 121.00 |
| 23 | BA | 861 | A | N1-C2-N3 | -5.28 | 126.66 | 129.30 |
| 23 | BA | 2088 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 23 | DA | 171 | G | N3-C2-N2 | 5.28 | 123.60 | 119.90 |
| 23 | DA | 1612 | C | N3-C2-O2 | 5.28 | 125.60 | 121.90 |
| 23 | DA | 2822 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 1 | AA | 1249 | C | N1-C2-O2 | 5.28 | 122.07 | 118.90 |
| 23 | DA | 1124 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 23 | DA | 2359 | C | C4-C5-C6 | 5.28 | 120.04 | 117.40 |
| 1 | AA | 927 | G | N7-C8-N9 | -5.28 | 110.46 | 113.10 |
| 1 | AA | 993 | G | N3-C4-N9 | 5.28 | 129.17 | 126.00 |
| 23 | BA | 936 | C | C5-C6-N1 | -5.28 | 118.36 | 121.00 |
| 23 | BA | 1654 | A | C5-C6-N6 | 5.28 | 127.92 | 123.70 |
| 23 | BA | 2488 | A | N7-C8-N9 | -5.28 | 111.16 | 113.80 |
| 23 | DA | 737 | C | C5-C4-N4 | -5.28 | 116.50 | 120.20 |
| 23 | DA | 2235 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 23 | DA | 2379 | G | C5-N7-C8 | -5.28 | 101.66 | 104.30 |
| 23 | BA | 512 | G | N9-C4-C5 | 5.28 | 107.51 | 105.40 |
| 23 | BA | 607 | U | C5-C6-N1 | -5.28 | 120.06 | 122.70 |
| 23 | BA | 886 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 23 | BA | 2297 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 24 | BB | 70 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 24 | BB | 91 | C | C6-N1-C2 | 5.28 | 122.41 | 120.30 |
| 1 | CA | 1166 | G | C8-N9-C1' | 5.28 | 133.86 | 127.00 |
| 23 | DA | 127 | A | N1-C2-N3 | 5.28 | 131.94 | 129.30 |
| 23 | DA | 204 | A | C5-N7-C8 | -5.28 | 101.26 | 103.90 |
| 23 | DA | 1120 | G | C5-C6-O6 | 5.28 | 131.76 | 128.60 |
| 23 | DA | 1210 | A | N7-C8-N9 | 5.28 | 116.44 | 113.80 |
| 23 | DA | 1800 | C | N3-C4-C5 | 5.28 | 124.01 | 121.90 |
| 23 | DA | 2297 | C | C2-N1-C1' | -5.28 | 113.00 | 118.80 |
| 23 | DA | 652(T) | C | C5-C4-N4 | 5.27 | 123.89 | 120.20 |
| 23 | DA | 932 | G | N3-C4-C5 | 5.27 | 131.24 | 128.60 |
| 23 | DA | 1993 | U | N3-C2-O2 | 5.27 | 125.89 | 122.20 |
| 23 | DA | 2346 | A | N3-C4-C5 | -5.27 | 123.11 | 126.80 |
| 23 | BA | 2013 | A | C4-C5-N7 | 5.27 | 113.34 | 110.70 |
| 23 | BA | 2607 | G | N3-C4-N9 | 5.27 | 129.16 | 126.00 |
| 1 | CA | 78 | G | N3-C4-C5 | 5.27 | 131.24 | 128.60 |
| 1 | CA | 1009 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 24 | DB | 93 | G | C5-C6-O6 | -5.27 | 125.44 | 128.60 |
| 1 | AA | 139 | G | N7-C8-N9 | 5.27 | 115.74 | 113.10 |
| 23 | DA | 208 | C | N1-C2-O2 | -5.27 | 115.74 | 118.90 |
| 23 | BA | 351 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 23 | BA | 2398 | U | N3-C4-C5 | -5.27 | 111.44 | 114.60 |
| 1 | CA | 954 | G | N9-C4-C5 | -5.27 | 103.29 | 105.40 |
| 1 | CA | 1006 | C | N3-C4-N4 | 5.27 | 121.69 | 118.00 |
| 1 | CA | 1467 | G | N3-C4-C5 | -5.27 | 125.97 | 128.60 |
| 4 | CD | 26 | CYS | CA-CB-SG | 5.27 | 123.48 | 114.00 |
| 23 | DA | 195 | A | C6-C5-N7 | -5.27 | 128.61 | 132.30 |
| 23 | DA | 333 | G | C4-N9-C1' | 5.27 | 133.35 | 126.50 |
| 1 | AA | 979 | C | C6-N1-C2 | -5.27 | 118.19 | 120.30 |
| 23 | BA | 446 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 23 | BA | 2510 | C | N1-C2-N3 | 5.27 | 122.89 | 119.20 |
| 23 | DA | 2866 | U | C4-C5-C6 | 5.27 | 122.86 | 119.70 |
| 1 | CA | 419 | C | N3-C2-O2 | 5.27 | 125.59 | 121.90 |
| 1 | CA | 1333 | A | N7-C8-N9 | 5.27 | 116.43 | 113.80 |
| 23 | DA | 570 | G | N1-C2-N2 | -5.27 | 111.46 | 116.20 |
| 1 | AA | 1502 | A | N1-C2-N3 | 5.26 | 131.93 | 129.30 |
| 23 | BA | 32 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 23 | BA | 849 | A | N7-C8-N9 | -5.26 | 111.17 | 113.80 |
| 23 | BA | 1531 | C | C2-N1-C1' | 5.26 | 124.59 | 118.80 |
| 23 | BA | 2254 | C | C6-N1-C2 | 5.26 | 122.41 | 120.30 |
| 23 | DA | 2487 | G | C4-C5-N7 | 5.26 | 112.91 | 110.80 |
| 1 | AA | 913 | A | N9-C4-C5 | 5.26 | 107.91 | 105.80 |
| 23 | BA | 2114 | A | N7-C8-N9 | 5.26 | 116.43 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 727 | A | C4-C5-C6 | 5.26 | 119.63 | 117.00 |
| 23 | DA | 732 | C | C5-C4-N4 | -5.26 | 116.52 | 120.20 |
| 23 | DA | 1256 | G | C2-N3-C4 | -5.26 | 109.27 | 111.90 |
| 31 | DN | 20 | GLY | N-CA-C | -5.26 | 99.94 | 113.10 |
| 23 | BA | 60 | G | C6-C5-N7 | -5.26 | 127.24 | 130.40 |
| 23 | BA | 171 | G | N3-C2-N2 | 5.26 | 123.58 | 119.90 |
| 23 | BA | 363(B) | G | N9-C4-C5 | -5.26 | 103.30 | 105.40 |
| 23 | BA | 1487 | G | C8-N9-C4 | -5.26 | 104.30 | 106.40 |
| 23 | BA | 1965 | C | N1-C2-O2 | 5.26 | 122.06 | 118.90 |
| 23 | BA | 2487 | G | N9-C4-C5 | -5.26 | 103.30 | 105.40 |
| 1 | CA | 893 | C | C6-N1-C2 | 5.26 | 122.40 | 120.30 |
| 1 | CA | 1350 | A | C4-C5-C6 | 5.26 | 119.63 | 117.00 |
| 23 | DA | 1816 | G | C8-N9-C1' | -5.26 | 120.16 | 127.00 |
| 23 | DA | 1992 | G | C5-N7-C8 | 5.26 | 106.93 | 104.30 |
| 23 | DA | 2099 | U | C5-C6-N1 | 5.26 | 125.33 | 122.70 |
| 23 | BA | 548 | A | N9-C4-C5 | -5.26 | 103.70 | 105.80 |
| 23 | BA | 690 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 23 | DA | 2096 | U | C5-C6-N1 | 5.26 | 125.33 | 122.70 |
| 23 | DA | 2329 | G | C2-N3-C4 | -5.26 | 109.27 | 111.90 |
| 23 | DA | 2518 | A | C8-N9-C4 | -5.26 | 103.70 | 105.80 |
| 1 | AA | 39 | G | N1-C2-N2 | 5.26 | 120.93 | 116.20 |
| 23 | BA | 1187 | G | C2-N3-C4 | 5.26 | 114.53 | 111.90 |
| 23 | BA | 1241 | A | C2-N3-C4 | -5.26 | 107.97 | 110.60 |
| 23 | BA | 1994 | C | N3-C4-C5 | 5.26 | 124.00 | 121.90 |
| 23 | BA | 2048 | G | C5-C6-N1 | -5.26 | 108.87 | 111.50 |
| 23 | BA | 2157 | G | C8-N9-C1' | 5.26 | 133.83 | 127.00 |
| 1 | CA | 260 | G | N3-C4-C5 | 5.26 | 131.23 | 128.60 |
| 1 | CA | 1370 | G | N3-C4-N9 | -5.26 | 122.85 | 126.00 |
| 23 | DA | 2032 | G | C6-C5-N7 | -5.26 | 127.25 | 130.40 |
| 5 | AE | 71 | LEU | CA-CB-CG | 5.25 | 127.39 | 115.30 |
| 23 | BA | 2350 | C | N3-C4-N4 | 5.25 | 121.68 | 118.00 |
| 1 | CA | 413 | G | C4-C5-N7 | -5.25 | 108.70 | 110.80 |
| 1 | AA | 1001(A) | G | N9-C4-C5 | -5.25 | 103.30 | 105.40 |
| 1 | AA | 1006 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 23 | BA | 392 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 23 | BA | 1341 | U | N1-C2-O2 | 5.25 | 126.48 | 122.80 |
| 23 | BA | 2348 | U | N1-C2-O2 | 5.25 | 126.48 | 122.80 |
| 23 | DA | 1267 | U | N1-C2-O2 | 5.25 | 126.48 | 122.80 |
| 1 | AA | 457 | C | C6-N1-C2 | -5.25 | 118.20 | 120.30 |
| 23 | BA | 686 | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 23 | BA | 1688 | U | N1-C2-N3 | 5.25 | 118.05 | 114.90 |
| 23 | BA | 2303 | G | C8-N9-C4 | -5.25 | 104.30 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 2623 | G | N9-C4-C5 | 5.25 | 107.50 | 105.40 |
| 1 | CA | 631 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 1 | CA | 1185 | G | C2-N3-C4 | 5.25 | 114.53 | 111.90 |
| 1 | AA | 1226 | C | C2-N1-C1' | -5.25 | 113.03 | 118.80 |
| 23 | BA | 790 | C | N3-C2-O2 | 5.25 | 125.58 | 121.90 |
| 23 | BA | 2037 | G | C5-C6-O6 | 5.25 | 131.75 | 128.60 |
| 23 | BA | 2425 | A | C5-N7-C8 | -5.25 | 101.28 | 103.90 |
| 1 | CA | 1343 | G | N9-C4-C5 | -5.25 | 103.30 | 105.40 |
| 23 | DA | 990 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 23 | DA | 1775 | U | C5-C6-N1 | -5.25 | 120.08 | 122.70 |
| 23 | BA | 760 | G | C5-N7-C8 | -5.25 | 101.68 | 104.30 |
| 23 | BA | 1050 | A | C8-N9-C4 | -5.25 | 103.70 | 105.80 |
| 23 | BA | 2157 | G | N3-C4-N9 | -5.25 | 122.85 | 126.00 |
| 1 | CA | 1293 | G | C8-N9-C4 | 5.25 | 108.50 | 106.40 |
| 23 | DA | 557 | U | N1-C2-N3 | 5.25 | 118.05 | 114.90 |
| 24 | DB | 76 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 23 | BA | 1582 | C | N1-C2-O2 | 5.25 | 122.05 | 118.90 |
| 23 | BA | 1981 | A | N9-C4-C5 | 5.25 | 107.90 | 105.80 |
| 1 | CA | 982 | U | N3-C4-C5 | -5.25 | 111.45 | 114.60 |
| 1 | CA | 1492 | A | C2-N3-C4 | 5.25 | 113.22 | 110.60 |
| 23 | DA | 254 | G | N3-C4-C5 | 5.25 | 131.22 | 128.60 |
| 23 | DA | 1942 | C | C6-N1-C1' | 5.25 | 127.09 | 120.80 |
| 23 | DA | 2723 | C | C2-N1-C1' | -5.25 | 113.03 | 118.80 |
| 23 | BA | 1415 | U | N3-C4-O4 | -5.25 | 115.73 | 119.40 |
| 23 | DA | 39 | C | N1-C2-N3 | 5.25 | 122.87 | 119.20 |
| 23 | DA | 933 | A | N7-C8-N9 | 5.25 | 116.42 | 113.80 |
| 23 | DA | 2202 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |
| 1 | AA | 855 | G | C5-C6-O6 | 5.24 | 131.75 | 128.60 |
| 41 | BX | 54 | VAL | CB-CA-C | -5.24 | 101.44 | 111.40 |
| 45 | B1 | 21 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | CA | 190 | U | C5-C6-N1 | 5.24 | 125.32 | 122.70 |
| 23 | DA | 392 | C | C4-C5-C6 | -5.24 | 114.78 | 117.40 |
| 23 | DA | 412 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 23 | DA | 2010 | G | N3-C2-N2 | -5.24 | 116.23 | 119.90 |
| 1 | AA | 1028 | C | C5-C4-N4 | -5.24 | 116.53 | 120.20 |
| 1 | CA | 1014 | A | N7-C8-N9 | 5.24 | 116.42 | 113.80 |
| 1 | AA | 1475 | G | N1-C6-O6 | 5.24 | 123.04 | 119.90 |
| 23 | BA | 2261 | C | N3-C2-O2 | -5.24 | 118.23 | 121.90 |
| 1 | CA | 1330 | U | C6-N1-C2 | -5.24 | 117.86 | 121.00 |
| 23 | DA | 271(S) | G | C5-C6-N1 | -5.24 | 108.88 | 111.50 |
| 23 | DA | 1677 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 23 | DA | 1985 | G | C6-N1-C2 | -5.24 | 121.96 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | DA | 2011 | U | N1-C2-O2 | -5.24 | 119.13 | 122.80 |
| 1 | AA | 1267 | C | N1-C2-O2 | -5.24 | 115.76 | 118.90 |
| 23 | BA | 525 | U | N3-C4-C5 | -5.24 | 111.46 | 114.60 |
| 23 | BA | 1324 | G | C5-C6-O6 | -5.24 | 125.46 | 128.60 |
| 23 | BA | 2322 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 23 | BA | 2626 | C | C2-N3-C4 | -5.24 | 117.28 | 119.90 |
| 1 | CA | 984 | C | C5-C6-N1 | 5.24 | 123.62 | 121.00 |
| 1 | CA | 1293 | G | C6-N1-C2 | -5.24 | 121.96 | 125.10 |
| 23 | DA | 1539 | G | C5-N7-C8 | -5.24 | 101.68 | 104.30 |
| 23 | DA | 2105 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 23 | BA | 2081 | C | C4-C5-C6 | 5.24 | 120.02 | 117.40 |
| 23 | DA | 822 | U | N3-C4-O4 | -5.24 | 115.73 | 119.40 |
| 1 | AA | 944 | G | N7-C8-N9 | 5.24 | 115.72 | 113.10 |
| 23 | BA | 676 | A | O4'-C1'-N9 | 5.24 | 112.39 | 108.20 |
| 23 | BA | 2602 | A | C5-C6-N1 | 5.24 | 120.32 | 117.70 |
| 1 | CA | 981 | U | C5-C6-N1 | 5.24 | 125.32 | 122.70 |
| 23 | DA | 51 | G | C5-N7-C8 | 5.24 | 106.92 | 104.30 |
| 23 | DA | 827 | U | N3-C2-O2 | 5.24 | 125.86 | 122.20 |
| 23 | DA | 1655 | A | N7-C8-N9 | -5.24 | 111.18 | 113.80 |
| 1 | AA | 939 | G | N3-C4-C5 | 5.23 | 131.22 | 128.60 |
| 23 | BA | 124 | G | N3-C4-C5 | 5.23 | 131.22 | 128.60 |
| 23 | BA | 915 | C | C2-N1-C1' | 5.23 | 124.56 | 118.80 |
| 23 | DA | 1546 | C | C2-N1-C1' | 5.23 | 124.56 | 118.80 |
| 23 | BA | 2763 | G | C6-C5-N7 | -5.23 | 127.26 | 130.40 |
| 1 | CA | 484 | G | C5-C6-O6 | 5.23 | 131.74 | 128.60 |
| 23 | DA | 1021 | A | N3-C4-N9 | -5.23 | 123.21 | 127.40 |
| 23 | DA | 1311 | G | C6-C5-N7 | -5.23 | 127.26 | 130.40 |
| 23 | DA | 2084 | C | C5-C6-N1 | -5.23 | 118.38 | 121.00 |
| 1 | AA | 203 | U | C6-N1-C2 | -5.23 | 117.86 | 121.00 |
| 1 | AA | 934 | C | N3-C4-C5 | -5.23 | 119.81 | 121.90 |
| 23 | BA | 1308 | A | C4-C5-C6 | 5.23 | 119.62 | 117.00 |
| 23 | BA | 1490 | A | N1-C6-N6 | 5.23 | 121.74 | 118.60 |
| 23 | BA | 1586 | A | C8-N9-C4 | -5.23 | 103.71 | 105.80 |
| 23 | DA | 71 | A | N1-C2-N3 | 5.23 | 131.92 | 129.30 |
| 23 | BA | 747 | U | C2-N3-C4 | -5.23 | 123.86 | 127.00 |
| 23 | DA | 1988 | C | N3-C4-C5 | 5.23 | 123.99 | 121.90 |
| 23 | DA | 2055 | C | N1-C2-O2 | -5.23 | 115.76 | 118.90 |
| 1 | AA | 696 | A | C8-N9-C4 | -5.23 | 103.71 | 105.80 |
| 23 | BA | 1012 | U | N3-C2-O2 | -5.23 | 118.54 | 122.20 |
| 23 | DA | 448 | U | N3-C2-O2 | -5.23 | 118.54 | 122.20 |
| 23 | DA | 1424 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 1 | CA | 1165 | C | C6-N1-C1' | 5.23 | 127.07 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1112 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 23 | BA | 1283 | G | N1-C2-N2 | -5.22 | 111.50 | 116.20 |
| 23 | BA | 2065 | C | C4-C5-C6 | 5.22 | 120.01 | 117.40 |
| 1 | CA | 39 | G | C6-N1-C2 | -5.22 | 121.97 | 125.10 |
| 23 | DA | 54 | G | C8-N9-C4 | 5.22 | 108.49 | 106.40 |
| 23 | DA | 202 | U | N1-C2-N3 | -5.22 | 111.77 | 114.90 |
| 23 | DA | 702 | G | N3-C2-N2 | -5.22 | 116.24 | 119.90 |
| 23 | DA | 758 | C | N1-C2-O2 | -5.22 | 115.77 | 118.90 |
| 23 | DA | 839 | U | C5-C4-O4 | 5.22 | 129.03 | 125.90 |
| 1 | AA | 541 | G | C8-N9-C1' | 5.22 | 133.79 | 127.00 |
| 1 | AA | 736 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | AA | 1350 | A | C5-C6-N1 | 5.22 | 120.31 | 117.70 |
| 23 | BA | 2782 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 24 | BB | 87 | G | N7-C8-N9 | -5.22 | 110.49 | 113.10 |
| 23 | DA | 841 | A | N1-C2-N3 | 5.22 | 131.91 | 129.30 |
| 1 | CA | 1081 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 1 | CA | 1315 | U | C6-N1-C2 | -5.22 | 117.87 | 121.00 |
| 23 | BA | 182 | A | C8-N9-C4 | -5.22 | 103.71 | 105.80 |
| 23 | BA | 2273 | A | N1-C2-N3 | -5.22 | 126.69 | 129.30 |
| 23 | BA | 2558 | C | N3-C4-C5 | 5.22 | 123.99 | 121.90 |
| 24 | BB | 17 | C | C6-N1-C2 | 5.22 | 122.39 | 120.30 |
| 23 | DA | 154 | G | N9-C4-C5 | -5.22 | 103.31 | 105.40 |
| 23 | DA | 1021 | A | N1-C6-N6 | 5.22 | 121.73 | 118.60 |
| 23 | DA | 1381 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 23 | BA | 2152 | G | C4-N9-C1' | -5.22 | 119.72 | 126.50 |
| 23 | BA | 2335 | A | N7-C8-N9 | -5.22 | 111.19 | 113.80 |
| 23 | DA | 583 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 23 | DA | 821 | A | N1-C2-N3 | 5.22 | 131.91 | 129.30 |
| 23 | DA | 1930 | G | N7-C8-N9 | -5.22 | 110.49 | 113.10 |
| 1 | AA | 825 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 23 | BA | 391 | G | C8-N9-C1' | -5.22 | 120.22 | 127.00 |
| 23 | BA | 1974 | C | N3-C4-C5 | 5.22 | 123.99 | 121.90 |
| 23 | DA | 893 | C | C6-N1-C1' | -5.22 | 114.54 | 120.80 |
| 23 | DA | 1613 | G | N1-C2-N2 | -5.22 | 111.51 | 116.20 |
| 23 | DA | 2071 | A | C2-N3-C4 | 5.22 | 113.21 | 110.60 |
| 1 | AA | 1239 | A | C5-C6-N6 | 5.21 | 127.87 | 123.70 |
| 23 | BA | 2582 | G | C8-N9-C4 | -5.21 | 104.31 | 106.40 |
| 23 | DA | 2496 | C | C4-C5-C6 | -5.21 | 114.79 | 117.40 |
| 23 | DA | 2822 | G | C8-N9-C4 | 5.21 | 108.49 | 106.40 |
| 1 | AA | 1295 | G | C8-N9-C4 | -5.21 | 104.31 | 106.40 |
| 23 | BA | 1670 | C | C2-N3-C4 | -5.21 | 117.29 | 119.90 |
| 23 | BA | 2403 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2338 | G | C6-C5-N7 | -5.21 | 127.27 | 130.40 |
| 1 | AA | 1210 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 1 | AA | 1241 | G | N7-C8-N9 | 5.21 | 115.71 | 113.10 |
| 23 | BA | 571 | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 23 | BA | 592 | G | C5-C6-O6 | 5.21 | 131.73 | 128.60 |
| 23 | BA | 702 | G | N1-C2-N3 | 5.21 | 127.03 | 123.90 |
| 23 | BA | 1698 | A | C4-C5-C6 | 5.21 | 119.61 | 117.00 |
| 23 | BA | 2331 | G | N1-C6-O6 | 5.21 | 123.03 | 119.90 |
| 23 | BA | 2412 | A | N1-C6-N6 | -5.21 | 115.47 | 118.60 |
| 1 | CA | 776 | G | N3-C4-N9 | -5.21 | 122.87 | 126.00 |
| 23 | DA | 1170 | G | N3-C4-N9 | 5.21 | 129.13 | 126.00 |
| 23 | DA | 2609 | U | C4-C5-C6 | 5.21 | 122.83 | 119.70 |
| 23 | DA | 130 | C | N1-C2-O2 | 5.21 | 122.03 | 118.90 |
| 23 | DA | 1261 | C | N1-C2-O2 | -5.21 | 115.77 | 118.90 |
| 1 | AA | 106 | C | C5-C6-N1 | -5.21 | 118.40 | 121.00 |
| 23 | BA | 775 | G | N1-C2-N2 | -5.21 | 111.51 | 116.20 |
| 23 | BA | 1129 | A | C8-N9-C4 | -5.21 | 103.72 | 105.80 |
| 23 | DA | 188 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 23 | DA | 213 | A | N1-C6-N6 | 5.21 | 121.72 | 118.60 |
| 23 | DA | 1321 | A | N1-C2-N3 | 5.21 | 131.91 | 129.30 |
| 23 | BA | 469 | G | C5-C6-O6 | -5.21 | 125.48 | 128.60 |
| 23 | BA | 857 | C | N1-C2-N3 | 5.21 | 122.84 | 119.20 |
| 1 | CA | 361 | G | C6-N1-C2 | 5.21 | 128.22 | 125.10 |
| 23 | DA | 1270 | C | C4-C5-C6 | 5.21 | 120.00 | 117.40 |
| 23 | DA | 1530 | C | N3-C4-C5 | 5.21 | 123.98 | 121.90 |
| 23 | DA | 2351 | G | C8-N9-C1' | -5.21 | 120.23 | 127.00 |
| 23 | DA | 2362 | G | N3-C4-C5 | 5.21 | 131.20 | 128.60 |
| 23 | DA | 2672 | G | C2-N3-C4 | -5.21 | 109.30 | 111.90 |
| 35 | DR | 114 | VAL | CB-CA-C | -5.21 | 101.51 | 111.40 |
| 23 | BA | 190 | A | N1-C2-N3 | -5.21 | 126.70 | 129.30 |
| 23 | BA | 958 | U | C6-N1-C2 | -5.21 | 117.88 | 121.00 |
| 23 | BA | 1342 | A | C8-N9-C4 | -5.21 | 103.72 | 105.80 |
| 24 | BB | 60 | C | C6-N1-C2 | -5.21 | 118.22 | 120.30 |
| 23 | DA | 363(F) | A | C8-N9-C4 | 5.21 | 107.88 | 105.80 |
| 23 | BA | 1006 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 1 | CA | 1182 | G | N3-C2-N2 | -5.20 | 116.26 | 119.90 |
| 1 | CA | 1206 | G | C6-N1-C2 | -5.20 | 121.98 | 125.10 |
| 23 | DA | 527 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 23 | DA | 1816 | G | C4-N9-C1' | 5.20 | 133.27 | 126.50 |
| 27 | DF | 62 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 23 | DA | 303 | U | N3-C4-C5 | 5.20 | 117.72 | 114.60 |
| 23 | DA | 1216 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | AA | 681 | C | N3-C2-O2 | 5.20 | 125.54 | 121.90 |
| 23 | BA | 1822 | G | N1-C2-N3 | 5.20 | 127.02 | 123.90 |
| 23 | BA | 2602 | A | P-O3'-C3' | 5.20 | 125.94 | 119.70 |
| 23 | DA | 921 | G | C5-C6-O6 | 5.20 | 131.72 | 128.60 |
| 23 | DA | 2575 | C | N3-C4-C5 | -5.20 | 119.82 | 121.90 |
| 24 | DB | 87 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 1 | AA | 938 | A | C5-N7-C8 | -5.20 | 101.30 | 103.90 |
| 23 | BA | 1131 | G | C4-C5-N7 | 5.20 | 112.88 | 110.80 |
| 1 | CA | 823 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |
| 1 | CA | 1182 | G | C4-N9-C1' | -5.20 | 119.74 | 126.50 |
| 23 | DA | 229 | A | N7-C8-N9 | 5.20 | 116.40 | 113.80 |
| 23 | DA | 320 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 23 | BA | 2328 | A | C8-N9-C4 | 5.20 | 107.88 | 105.80 |
| 23 | DA | 271(M) | G | C8-N9-C4 | -5.20 | 104.32 | 106.40 |
| 23 | DA | 697 | C | C5-C4-N4 | -5.20 | 116.56 | 120.20 |
| 23 | DA | 952 | G | C2-N3-C4 | 5.20 | 114.50 | 111.90 |
| 1 | AA | 689 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 1 | AA | 1023 | G | C5-C6-N1 | -5.20 | 108.90 | 111.50 |
| 23 | BA | 996 | A | N1-C6-N6 | -5.20 | 115.48 | 118.60 |
| 23 | BA | 1254 | A | C4-C5-C6 | 5.20 | 119.60 | 117.00 |
| 23 | BA | 2421 | G | C6-C5-N7 | -5.20 | 127.28 | 130.40 |
| 23 | BA | 2487 | G | C6-C5-N7 | -5.20 | 127.28 | 130.40 |
| 23 | BA | 2681 | C | N3-C2-O2 | -5.20 | 118.26 | 121.90 |
| 1 | CA | 1120 | G | C4-C5-N7 | -5.20 | 108.72 | 110.80 |
| 1 | CA | 1350 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 23 | DA | 2383 | G | C5-C6-O6 | 5.20 | 131.72 | 128.60 |
| 23 | DA | 2574 | G | C2-N3-C4 | -5.20 | 109.30 | 111.90 |
| 24 | DB | 28 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 1 | CA | 1405 | G | N3-C4-N9 | 5.19 | 129.12 | 126.00 |
| 23 | DA | 1471 | A | N7-C8-N9 | 5.19 | 116.40 | 113.80 |
| 23 | DA | 2191 | G | C5-C6-O6 | -5.19 | 125.48 | 128.60 |
| 1 | AA | 991 | U | C6-N1-C2 | -5.19 | 117.89 | 121.00 |
| 1 | AA | 1378 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 23 | BA | 577 | G | C4-C5-N7 | 5.19 | 112.88 | 110.80 |
| 23 | BA | 1279 | G | C5-C6-N1 | 5.19 | 114.10 | 111.50 |
| 1 | CA | 96 | U | N1-C2-N3 | -5.19 | 111.78 | 114.90 |
| 1 | CA | 1262 | C | C6-N1-C1' | -5.19 | 114.57 | 120.80 |
| 23 | DA | 612 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 23 | DA | 752 | A | C8-N9-C4 | -5.19 | 103.72 | 105.80 |
| 23 | DA | 1391 | U | C6-N1-C1' | -5.19 | 113.93 | 121.20 |
| 23 | DA | 1983 | C | N3-C2-O2 | 5.19 | 125.53 | 121.90 |
| 23 | BA | 327 | G | N9-C4-C5 | -5.19 | 103.32 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2581 | G | C4-N9-C1' | 5.19 | 133.25 | 126.50 |
| 1 | CA | 502 | G | C8-N9-C4 | -5.19 | 104.32 | 106.40 |
| 23 | DA | 321 | G | C8-N9-C4 | 5.19 | 108.48 | 106.40 |
| 23 | DA | 984 | A | C5-C6-N1 | 5.19 | 120.30 | 117.70 |
| 23 | DA | 995 | C | C2-N1-C1' | -5.19 | 113.09 | 118.80 |
| 23 | DA | 2725 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 1 | AA | 185 | A | C8-N9-C4 | -5.19 | 103.72 | 105.80 |
| 23 | DA | 680 | G | N1-C2-N3 | 5.19 | 127.01 | 123.90 |
| 24 | DB | 7 | G | N1-C6-O6 | 5.19 | 123.01 | 119.90 |
| 23 | BA | 974 | G | C8-N9-C4 | -5.19 | 104.33 | 106.40 |
| 23 | BA | 988 | A | C5-N7-C8 | -5.19 | 101.31 | 103.90 |
| 23 | BA | 2689 | U | C2-N1-C1' | -5.19 | 111.48 | 117.70 |
| 1 | CA | 1187 | G | N1-C6-O6 | 5.19 | 123.01 | 119.90 |
| 24 | DB | 35 | U | N3-C4-O4 | -5.19 | 115.77 | 119.40 |
| 23 | BA | 147 | U | C2-N3-C4 | -5.19 | 123.89 | 127.00 |
| 23 | BA | 181 | A | N1-C6-N6 | -5.19 | 115.49 | 118.60 |
| 1 | CA | 240 | C | N3-C4-N4 | -5.19 | 114.37 | 118.00 |
| 1 | CA | 932 | C | N1-C2-O2 | 5.19 | 122.01 | 118.90 |
| 23 | DA | 1321 | A | C2-N3-C4 | -5.19 | 108.01 | 110.60 |
| 23 | DA | 1882 | C | C5-C6-N1 | 5.19 | 123.59 | 121.00 |
| 23 | BA | 528 | A | C4-N9-C1' | -5.18 | 116.97 | 126.30 |
| 23 | BA | 1265 | A | C6-N1-C2 | -5.18 | 115.49 | 118.60 |
| 23 | BA | 2144 | U | C6-N1-C2 | -5.18 | 117.89 | 121.00 |
| 23 | BA | 2641 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 1 | CA | 1093 | A | N9-C4-C5 | -5.18 | 103.73 | 105.80 |
| 23 | DA | 189 | G | C5-C6-O6 | -5.18 | 125.49 | 128.60 |
| 23 | DA | 287 | C | C5-C6-N1 | -5.18 | 118.41 | 121.00 |
| 23 | DA | 1967 | C | N1-C2-O2 | 5.18 | 122.01 | 118.90 |
| 1 | AA | 145 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 10 | AJ | 34 | VAL | N-CA-C | 5.18 | 125.00 | 111.00 |
| 23 | BA | 1128 | A | N1-C2-N3 | 5.18 | 131.89 | 129.30 |
| 23 | BA | 1553 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 23 | BA | 2040 | C | N1-C2-N3 | -5.18 | 115.57 | 119.20 |
| 23 | BA | 2451 | A | N9-C4-C5 | 5.18 | 107.87 | 105.80 |
| 27 | BF | 16 | GLY | N-CA-C | 5.18 | 126.06 | 113.10 |
| 4 | CD | 26 | CYS | N-CA-C | -5.18 | 97.00 | 111.00 |
| 23 | DA | 481 | G | P-O3'-C3' | 5.18 | 125.92 | 119.70 |
| 23 | DA | 2699 | C | C2-N3-C4 | -5.18 | 117.31 | 119.90 |
| 1 | CA | 1500 | A | C8-N9-C4 | -5.18 | 103.73 | 105.80 |
| 23 | DA | 58 | G | C4-N9-C1' | 5.18 | 133.24 | 126.50 |
| 23 | DA | 2049 | G | N3-C4-C5 | 5.18 | 131.19 | 128.60 |
| 7 | AG | 130 | GLY | N-CA-C | 5.18 | 126.05 | 113.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 1127 | G | C5-C6-O6 | 5.18 | 131.71 | 128.60 |
| 23 | DA | 1319 | G | C8-N9-C4 | 5.18 | 108.47 | 106.40 |
| 23 | DA | 2036 | C | N1-C2-N3 | 5.18 | 122.83 | 119.20 |
| 23 | DA | 2103 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 23 | DA | 2259 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 23 | DA | 2485 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 23 | DA | 2689 | U | N3-C4-C5 | 5.18 | 117.71 | 114.60 |
| 23 | DA | 254 | G | C2-N3-C4 | -5.18 | 109.31 | 111.90 |
| 23 | DA | 564 | C | C4-C5-C6 | 5.18 | 119.99 | 117.40 |
| 1 | AA | 217 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 1 | AA | 731 | G | N9-C4-C5 | 5.18 | 107.47 | 105.40 |
| 1 | AA | 959 | A | C2-N3-C4 | -5.18 | 108.01 | 110.60 |
| 23 | BA | 610 | G | N9-C4-C5 | -5.18 | 103.33 | 105.40 |
| 23 | BA | 1865 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 1 | CA | 324 | G | N3-C4-C5 | -5.18 | 126.01 | 128.60 |
| 1 | CA | 557 | G | N3-C4-N9 | 5.18 | 129.11 | 126.00 |
| 1 | CA | 1037 | C | N1-C2-N3 | -5.18 | 115.58 | 119.20 |
| 3 | CC | 175 | LEU | CA-CB-CG | 5.18 | 127.20 | 115.30 |
| 23 | DA | 972 | G | C4-C5-N7 | -5.18 | 108.73 | 110.80 |
| 1 | AA | 223 | U | C5-C6-N1 | 5.17 | 125.29 | 122.70 |
| 1 | AA | 1207 | G | N7-C8-N9 | -5.17 | 110.51 | 113.10 |
| 1 | AA | 1277 | C | N1-C2-N3 | -5.17 | 115.58 | 119.20 |
| 23 | BA | 579 | G | C5-C6-N1 | -5.17 | 108.91 | 111.50 |
| 23 | BA | 2250 | G | C5-C6-O6 | 5.17 | 131.70 | 128.60 |
| 23 | BA | 2705 | A | N7-C8-N9 | -5.17 | 111.21 | 113.80 |
| 1 | CA | 1120 | G | C8-N9-C1' | 5.17 | 133.73 | 127.00 |
| 23 | BA | 750 | A | N1-C2-N3 | 5.17 | 131.89 | 129.30 |
| 23 | BA | 1181 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 23 | DA | 2255 | G | C6-C5-N7 | 5.17 | 133.50 | 130.40 |
| 1 | AA | 610 | G | C4-N9-C1' | 5.17 | 133.22 | 126.50 |
| 23 | BA | 488 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 23 | BA | 1932 | A | N1-C6-N6 | 5.17 | 121.70 | 118.60 |
| 1 | CA | 1267 | C | C2-N3-C4 | 5.17 | 122.49 | 119.90 |
| 23 | DA | 124 | G | C4-C5-N7 | 5.17 | 112.87 | 110.80 |
| 23 | DA | 1313 | U | C5-C6-N1 | 5.17 | 125.29 | 122.70 |
| 23 | BA | 102 | G | C6-C5-N7 | -5.17 | 127.30 | 130.40 |
| 1 | CA | 543 | C | C2-N3-C4 | 5.17 | 122.48 | 119.90 |
| 1 | AA | 973 | G | C6-C5-N7 | 5.17 | 133.50 | 130.40 |
| 1 | AA | 1153 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 23 | BA | 526 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 23 | BA | 530 | G | N1-C2-N2 | 5.17 | 120.85 | 116.20 |
| 23 | BA | 729 | G | N3-C2-N2 | -5.17 | 116.28 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 2251 | G | C2-N3-C4 | 5.17 | 114.48 | 111.90 |
| 24 | BB | 54 | G | N1-C6-O6 | 5.17 | 123.00 | 119.90 |
| 1 | CA | 1325 | C | N3-C4-C5 | -5.17 | 119.83 | 121.90 |
| 23 | DA | 1779 | U | N1-C2-O2 | 5.17 | 126.42 | 122.80 |
| 1 | AA | 690 | G | N3-C2-N2 | 5.17 | 123.52 | 119.90 |
| 23 | BA | 494 | G | N3-C2-N2 | -5.17 | 116.28 | 119.90 |
| 23 | BA | 590 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 23 | BA | 1882 | C | C2-N1-C1' | 5.17 | 124.48 | 118.80 |
| 23 | BA | 2251 | G | C4-N9-C1' | 5.17 | 133.22 | 126.50 |
| 1 | CA | 1189 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |
| 1 | CA | 1382 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 23 | DA | 516 | C | N3-C2-O2 | -5.17 | 118.28 | 121.90 |
| 23 | DA | 823 | G | C2-N3-C4 | -5.17 | 109.32 | 111.90 |
| 23 | DA | 1113 | U | C5-C4-O4 | 5.17 | 129.00 | 125.90 |
| 23 | DA | 1302 | A | N9-C4-C5 | 5.17 | 107.87 | 105.80 |
| 23 | DA | 2672 | G | C6-C5-N7 | -5.17 | 127.30 | 130.40 |
| 23 | DA | 2682 | U | C5-C6-N1 | -5.17 | 120.12 | 122.70 |
| 24 | DB | 9 | G | N1-C2-N2 | 5.17 | 120.85 | 116.20 |
| 1 | AA | 815 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | AA | 839 | U | C6-N1-C1' | -5.17 | 113.97 | 121.20 |
| 23 | BA | 809 | G | C5-C6-O6 | 5.17 | 131.70 | 128.60 |
| 23 | BA | 1359 | A | C8-N9-C4 | -5.17 | 103.73 | 105.80 |
| 1 | CA | 1249 | C | C5-C6-N1 | 5.17 | 123.58 | 121.00 |
| 23 | DA | 1779 | U | C2-N3-C4 | -5.17 | 123.90 | 127.00 |
| 23 | DA | 2487 | G | C8-N9-C1' | -5.17 | 120.28 | 127.00 |
| 23 | DA | 2766 | G | C4-C5-N7 | 5.17 | 112.87 | 110.80 |
| 1 | AA | 1005 | A | C8-N9-C4 | -5.16 | 103.73 | 105.80 |
| 23 | BA | 99 | U | C5-C6-N1 | -5.16 | 120.12 | 122.70 |
| 24 | BB | 1 | U | C2-N1-C1' | 5.16 | 123.90 | 117.70 |
| 1 | CA | 936 | C | C5-C6-N1 | 5.16 | 123.58 | 121.00 |
| 23 | DA | 71 | A | P-O3'-C3' | 5.16 | 125.90 | 119.70 |
| 23 | DA | 845 | G | C4-N9-C1' | 5.16 | 133.21 | 126.50 |
| 23 | DA | 1180 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 23 | DA | 1428 | C | C4-C5-C6 | 5.16 | 119.98 | 117.40 |
| 23 | BA | 2090 | G | C8-N9-C4 | 5.16 | 108.47 | 106.40 |
| 1 | AA | 6 | G | N1-C6-O6 | -5.16 | 116.80 | 119.90 |
| 1 | AA | 654 | G | N3-C4-N9 | -5.16 | 122.90 | 126.00 |
| 1 | AA | 1446 | U | N1-C2-N3 | -5.16 | 111.80 | 114.90 |
| 1 | AA | 1516 | G | N3-C4-C5 | 5.16 | 131.18 | 128.60 |
| 23 | BA | 841 | A | N1-C6-N6 | -5.16 | 115.50 | 118.60 |
| 23 | BA | 2842 | G | C5-C6-O6 | -5.16 | 125.50 | 128.60 |
| 1 | CA | 1223 | C | N3-C4-C5 | -5.16 | 119.83 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 9 | CI | 96 | LEU | N-CA-C | 5.16 | 124.93 | 111.00 |
| 23 | DA | 196 | A | C5-C6-N6 | -5.16 | 119.57 | 123.70 |
| 23 | DA | 792 | G | N3-C2-N2 | 5.16 | 123.51 | 119.90 |
| 23 | DA | 1142(A) | A | N1-C2-N3 | 5.16 | 131.88 | 129.30 |
| 23 | DA | 1541 | G | N3-C4-C5 | -5.16 | 126.02 | 128.60 |
| 23 | DA | 2013 | A | N9-C4-C5 | -5.16 | 103.74 | 105.80 |
| 1 | AA | 260 | G | N3-C4-C5 | 5.16 | 131.18 | 128.60 |
| 1 | AA | 1095 | U | C2-N1-C1' | 5.16 | 123.89 | 117.70 |
| 1 | CA | 749 | C | C6-N1-C1' | 5.16 | 126.99 | 120.80 |
| 1 | CA | 966 | G | N7-C8-N9 | 5.16 | 115.68 | 113.10 |
| 1 | CA | 1443 | G | C5-C6-N1 | 5.16 | 114.08 | 111.50 |
| 23 | DA | 2157 | G | C4-C5-N7 | -5.16 | 108.74 | 110.80 |
| 23 | DA | 2157 | G | N3-C4-N9 | -5.16 | 122.90 | 126.00 |
| 1 | AA | 1174 | G | C8-N9-C1' | 5.16 | 133.70 | 127.00 |
| 23 | BA | 242 | G | C4-N9-C1' | -5.16 | 119.80 | 126.50 |
| 23 | BA | 652(B) | A | C2-N3-C4 | 5.16 | 113.18 | 110.60 |
| 23 | BA | 2489 | G | N3-C4-N9 | 5.16 | 129.09 | 126.00 |
| 23 | BA | 562 | U | C6-N1-C2 | -5.16 | 117.91 | 121.00 |
| 23 | BA | 732 | C | C5-C4-N4 | -5.16 | 116.59 | 120.20 |
| 23 | BA | 2026 | C | C4-C5-C6 | 5.16 | 119.98 | 117.40 |
| 24 | BB | 43 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 23 | DA | 254 | G | C5-C6-N1 | -5.16 | 108.92 | 111.50 |
| 23 | DA | 736 | C | N3-C4-C5 | 5.16 | 123.96 | 121.90 |
| 23 | DA | 2070 | G | N3-C4-C5 | -5.16 | 126.02 | 128.60 |
| 23 | DA | 2277 | G | C5-N7-C8 | 5.16 | 106.88 | 104.30 |
| 23 | DA | 2296 | U | C4-C5-C6 | 5.16 | 122.79 | 119.70 |
| 23 | DA | 268 | C | N3-C4-C5 | -5.15 | 119.84 | 121.90 |
| 23 | DA | 1772 | G | N3-C4-C5 | 5.15 | 131.18 | 128.60 |
| 23 | DA | 2627 | G | C5-C6-O6 | 5.15 | 131.69 | 128.60 |
| 1 | AA | 1120 | G | C4-C5-N7 | 5.15 | 112.86 | 110.80 |
| 23 | BA | 1184 | G | C5-C6-N1 | -5.15 | 108.92 | 111.50 |
| 23 | BA | 2763 | G | C8-N9-C4 | -5.15 | 104.34 | 106.40 |
| 23 | BA | 2856 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 1 | CA | 1312 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 23 | DA | 70 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 23 | DA | 665 | C | N1-C2-N3 | -5.15 | 115.59 | 119.20 |
| 23 | DA | 1039 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 23 | DA | 1950 | G | N3-C4-C5 | -5.15 | 126.02 | 128.60 |
| 23 | BA | 2010 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 23 | BA | 2086 | U | C4-C5-C6 | 5.15 | 122.79 | 119.70 |
| 1 | CA | 1284 | C | C5-C6-N1 | 5.15 | 123.58 | 121.00 |
| 23 | DA | 271(M) | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 692 | C | N1-C2-O2 | -5.15 | 115.81 | 118.90 |
| 23 | DA | 2760 | C | C6-N1-C2 | 5.15 | 122.36 | 120.30 |
| 23 | BA | 178 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 23 | BA | 2322 | A | C2-N3-C4 | 5.15 | 113.17 | 110.60 |
| 23 | DA | 607 | U | C2-N1-C1' | -5.15 | 111.52 | 117.70 |
| 23 | DA | 1300 | U | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 23 | DA | 1949 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 1 | AA | 713 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 23 | BA | 1029 | A | C8-N9-C4 | 5.15 | 107.86 | 105.80 |
| 23 | BA | 2191 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 23 | BA | 2522 | U | C2-N1-C1' | 5.15 | 123.88 | 117.70 |
| 23 | BA | 2669 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 1 | CA | 43 | C | N3-C2-O2 | 5.15 | 125.50 | 121.90 |
| 1 | CA | 1176 | A | N1-C6-N6 | -5.15 | 115.51 | 118.60 |
| 23 | DA | 196 | A | C4-C5-N7 | 5.15 | 113.27 | 110.70 |
| 23 | DA | 2591 | C | N1-C2-N3 | 5.15 | 122.80 | 119.20 |
| 23 | BA | 686 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 23 | BA | 1243 | G | C5-N7-C8 | -5.15 | 101.73 | 104.30 |
| 23 | DA | 260 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 23 | DA | 2020 | A | C6-N1-C2 | -5.15 | 115.51 | 118.60 |
| 23 | DA | 2116 | G | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 23 | DA | 2181 | G | C6-C5-N7 | 5.15 | 133.49 | 130.40 |
| 23 | DA | 2421 | G | N1-C6-O6 | 5.15 | 122.99 | 119.90 |
| 1 | AA | 7 | G | N3-C4-N9 | -5.14 | 122.91 | 126.00 |
| 23 | BA | 1325 | G | C6-C5-N7 | -5.14 | 127.31 | 130.40 |
| 23 | DA | 843 | G | N3-C4-N9 | -5.14 | 122.91 | 126.00 |
| 23 | DA | 1799 | G | P-O3'-C3' | 5.14 | 125.87 | 119.70 |
| 23 | BA | 541 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 23 | BA | 602 | G | N9-C4-C5 | -5.14 | 103.34 | 105.40 |
| 23 | BA | 2088 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 1 | CA | 1052 | U | N1-C2-N3 | -5.14 | 111.81 | 114.90 |
| 1 | CA | 1467 | G | N9-C4-C5 | 5.14 | 107.46 | 105.40 |
| 23 | DA | 652(E) | G | C4-C5-N7 | 5.14 | 112.86 | 110.80 |
| 23 | DA | 1477 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 23 | DA | 2232 | U | C5-C6-N1 | -5.14 | 120.13 | 122.70 |
| 23 | BA | 2700 | C | C5-C4-N4 | -5.14 | 116.60 | 120.20 |
| 23 | BA | 2769 | C | C2-N3-C4 | -5.14 | 117.33 | 119.90 |
| 23 | DA | 2550 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |
| 1 | AA | 189(D) | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 1 | AA | 1493 | A | N7-C8-N9 | 5.14 | 116.37 | 113.80 |
| 23 | BA | 234 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 23 | BA | 281 | G | C8-N9-C4 | 5.14 | 108.46 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 975 | C | N1-C2-N3 | 5.14 | 122.80 | 119.20 |
| 23 | BA | 1340 | U | C2-N3-C4 | -5.14 | 123.92 | 127.00 |
| 23 | BA | 1417 | C | N3-C4-C5 | -5.14 | 119.84 | 121.90 |
| 23 | BA | 1957 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 23 | BA | 2056 | G | N3-C4-N9 | 5.14 | 129.08 | 126.00 |
| 1 | CA | 986 | A | N3-C4-N9 | 5.14 | 131.51 | 127.40 |
| 23 | DA | 1570 | A | C6-N1-C2 | -5.14 | 115.52 | 118.60 |
| 23 | DA | 2039 | C | C6-N1-C2 | -5.14 | 118.24 | 120.30 |
| 23 | DA | 2567 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 23 | BA | 2116 | G | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 23 | BA | 2370 | G | N1-C2-N2 | -5.14 | 111.58 | 116.20 |
| 1 | CA | 304 | U | C6-N1-C2 | -5.14 | 117.92 | 121.00 |
| 1 | CA | 1206 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 23 | DA | 1309 | G | C8-N9-C4 | 5.14 | 108.45 | 106.40 |
| 23 | BA | 792 | G | C4-N9-C1' | 5.14 | 133.18 | 126.50 |
| 23 | BA | 1307 | A | C2-N3-C4 | -5.14 | 108.03 | 110.60 |
| 23 | BA | 1932 | A | C5-N7-C8 | -5.14 | 101.33 | 103.90 |
| 24 | BB | 12 | C | N3-C4-C5 | 5.14 | 123.95 | 121.90 |
| 23 | BA | 893 | C | N3-C2-O2 | -5.13 | 118.31 | 121.90 |
| 23 | BA | 1278 | A | C6-N1-C2 | -5.13 | 115.52 | 118.60 |
| 23 | BA | 2607 | G | C4-N9-C1' | 5.13 | 133.17 | 126.50 |
| 24 | BB | 29 | A | C5-N7-C8 | -5.13 | 101.33 | 103.90 |
| 1 | CA | 365 | U | N3-C4-O4 | -5.13 | 115.81 | 119.40 |
| 1 | CA | 575 | G | C8-N9-C4 | 5.13 | 108.45 | 106.40 |
| 23 | DA | 272(G) | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 1 | CA | 689 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | CA | 1270 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 1 | CA | 1330 | U | C5-C6-N1 | 5.13 | 125.27 | 122.70 |
| 23 | DA | 715 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 23 | DA | 755 | C | N3-C4-N4 | 5.13 | 121.59 | 118.00 |
| 23 | DA | 845 | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 23 | DA | 846 | C | N1-C2-O2 | -5.13 | 115.82 | 118.90 |
| 1 | AA | 59 | A | C4-C5-N7 | 5.13 | 113.27 | 110.70 |
| 1 | AA | 1012 | U | C5-C6-N1 | 5.13 | 125.27 | 122.70 |
| 23 | BA | 826 | U | N1-C2-N3 | 5.13 | 117.98 | 114.90 |
| 1 | CA | 44 | G | C5-C6-N1 | -5.13 | 108.93 | 111.50 |
| 1 | CA | 1108 | G | C5-N7-C8 | 5.13 | 106.86 | 104.30 |
| 1 | CA | 1241 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 23 | BA | 2572 | A | N1-C6-N6 | -5.13 | 115.52 | 118.60 |
| 1 | CA | 1442(A) | G | N9-C4-C5 | -5.13 | 103.35 | 105.40 |
| 23 | DA | 1845 | G | N3-C4-C5 | -5.13 | 126.03 | 128.60 |
| 23 | DA | 1975 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 1120 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 1 | AA | 1291 | G | C8-N9-C4 | -5.13 | 104.35 | 106.40 |
| 23 | BA | 1269 | A | C2-N3-C4 | -5.13 | 108.04 | 110.60 |
| 23 | BA | 2310 | A | N1-C6-N6 | 5.13 | 121.68 | 118.60 |
| 23 | DA | 188 | G | N3-C4-N9 | 5.13 | 129.08 | 126.00 |
| 23 | DA | 1368 | G | N9-C4-C5 | 5.13 | 107.45 | 105.40 |
| 23 | DA | 2107 | C | C5-C6-N1 | 5.13 | 123.56 | 121.00 |
| 23 | DA | 2314 | C | C2-N1-C1' | -5.13 | 113.16 | 118.80 |
| 1 | AA | 34 | C | N1-C2-O2 | -5.13 | 115.82 | 118.90 |
| 1 | AA | 732 | C | C6-N1-C2 | -5.13 | 118.25 | 120.30 |
| 1 | AA | 1138 | G | N3-C4-N9 | 5.13 | 129.07 | 126.00 |
| 23 | BA | 2362 | G | N3-C4-C5 | 5.13 | 131.16 | 128.60 |
| 23 | DA | 1021 | A | C4-C5-N7 | 5.13 | 113.26 | 110.70 |
| 23 | BA | 272(I) | U | C6-N1-C2 | -5.12 | 117.92 | 121.00 |
| 23 | BA | 330 | A | C4-C5-N7 | 5.12 | 113.26 | 110.70 |
| 23 | BA | 1669 | A | C5-N7-C8 | -5.12 | 101.34 | 103.90 |
| 1 | CA | 1442(B) | A | C2-N3-C4 | 5.12 | 113.16 | 110.60 |
| 23 | DA | 955 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 23 | DA | 2233 | U | C6-N1-C2 | 5.12 | 124.08 | 121.00 |
| 1 | AA | 1076 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 23 | BA | 1047 | G | C2-N3-C4 | 5.12 | 114.46 | 111.90 |
| 23 | BA | 1688 | U | N1-C2-O2 | -5.12 | 119.21 | 122.80 |
| 23 | BA | 1826 | G | C5-C6-O6 | 5.12 | 131.67 | 128.60 |
| 23 | BA | 2182 | G | C5-C6-N1 | -5.12 | 108.94 | 111.50 |
| 23 | BA | 2259 | G | C5-C6-N1 | -5.12 | 108.94 | 111.50 |
| 23 | BA | 2330 | G | N1-C2-N3 | 5.12 | 126.97 | 123.90 |
| 23 | BA | 2497 | A | N3-C4-N9 | 5.12 | 131.50 | 127.40 |
| 23 | BA | 2597 | G | C4-N9-C1' | 5.12 | 133.16 | 126.50 |
| 23 | DA | 62 | C | C2-N1-C1' | -5.12 | 113.16 | 118.80 |
| 23 | DA | 528 | A | C4-C5-C6 | -5.12 | 114.44 | 117.00 |
| 23 | DA | 790 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 23 | DA | 1372 | U | C5-C4-O4 | 5.12 | 128.97 | 125.90 |
| 23 | DA | 1577 | C | C5-C6-N1 | -5.12 | 118.44 | 121.00 |
| 23 | BA | 154(A) | C | N3-C4-C5 | 5.12 | 123.95 | 121.90 |
| 23 | BA | 2370 | G | C5-C6-N1 | 5.12 | 114.06 | 111.50 |
| 23 | BA | 2819 | G | N7-C8-N9 | -5.12 | 110.54 | 113.10 |
| 23 | DA | 1366 | A | N9-C4-C5 | -5.12 | 103.75 | 105.80 |
| 23 | DA | 2550 | G | N7-C8-N9 | 5.12 | 115.66 | 113.10 |
| 1 | AA | 290 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 23 | BA | 636 | G | C4-N9-C1' | 5.12 | 133.16 | 126.50 |
| 23 | BA | 1216 | G | C2-N3-C4 | -5.12 | 109.34 | 111.90 |
| 23 | BA | 1626 | G | C2-N3-C4 | -5.12 | 109.34 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 1687 | G | N7-C8-N9 | 5.12 | 115.66 | 113.10 |
| 23 | DA | 13 | A | C5-C6-N6 | 5.12 | 127.80 | 123.70 |
| 1 | AA | 988 | G | C5-C6-O6 | 5.12 | 131.67 | 128.60 |
| 1 | AA | 1505 | G | C6-N1-C2 | 5.12 | 128.17 | 125.10 |
| 23 | BA | 513 | A | C8-N9-C4 | -5.12 | 103.75 | 105.80 |
| 23 | BA | 676 | A | N1-C2-N3 | 5.12 | 131.86 | 129.30 |
| 23 | BA | 1781 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 23 | BA | 1816 | G | N3-C4-N9 | 5.12 | 129.07 | 126.00 |
| 23 | BA | 2351 | G | C6-C5-N7 | -5.12 | 127.33 | 130.40 |
| 23 | BA | 2712(A) | A | C5-C6-N1 | -5.12 | 115.14 | 117.70 |
| 1 | CA | 1028 | C | C5-C6-N1 | 5.12 | 123.56 | 121.00 |
| 23 | DA | 748 | G | C5-N7-C8 | 5.12 | 106.86 | 104.30 |
| 23 | DA | 2336 | A | C2-N3-C4 | 5.12 | 113.16 | 110.60 |
| 23 | DA | 2861 | G | N7-C8-N9 | 5.12 | 115.66 | 113.10 |
| 23 | BA | 774 | A | N7-C8-N9 | 5.12 | 116.36 | 113.80 |
| 23 | BA | 1214 | A | C5-C6-N6 | -5.12 | 119.61 | 123.70 |
| 23 | BA | 1914 | C | C6-N1-C1' | 5.12 | 126.94 | 120.80 |
| 23 | BA | 2327 | A | N7-C8-N9 | -5.12 | 111.24 | 113.80 |
| 1 | CA | 77 | G | C6-C5-N7 | -5.12 | 127.33 | 130.40 |
| 1 | CA | 357 | G | C6-C5-N7 | 5.12 | 133.47 | 130.40 |
| 1 | CA | 365 | U | C5-C4-O4 | 5.12 | 128.97 | 125.90 |
| 24 | DB | 33 | G | C4-C5-N7 | 5.12 | 112.85 | 110.80 |
| 23 | BA | 117 | G | N3-C2-N2 | 5.12 | 123.48 | 119.90 |
| 23 | BA | 1123 | C | C2-N1-C1' | -5.12 | 113.17 | 118.80 |
| 23 | BA | 2768 | C | N3-C4-N4 | -5.12 | 114.42 | 118.00 |
| 1 | CA | 1002 | G | C8-N9-C4 | -5.12 | 104.35 | 106.40 |
| 1 | AA | 73 | G | N1-C6-O6 | 5.11 | 122.97 | 119.90 |
| 1 | AA | 359 | U | N1-C2-N3 | 5.11 | 117.97 | 114.90 |
| 1 | AA | 1011 | G | N3-C4-C5 | 5.11 | 131.16 | 128.60 |
| 23 | BA | 1291 | C | N3-C4-N4 | -5.11 | 114.42 | 118.00 |
| 1 | CA | 1253 | G | C5-C6-O6 | 5.11 | 131.67 | 128.60 |
| 23 | DA | 526 | A | C2-N3-C4 | 5.11 | 113.16 | 110.60 |
| 23 | DA | 657 | U | C4-C5-C6 | 5.11 | 122.77 | 119.70 |
| 23 | DA | 1021 | A | C6-C5-N7 | -5.11 | 128.72 | 132.30 |
| 23 | DA | 1337 | G | C5-C6-N1 | 5.11 | 114.06 | 111.50 |
| 23 | DA | 2070 | G | N1-C2-N3 | 5.11 | 126.97 | 123.90 |
| 32 | DO | 8 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 23 | BA | 2791 | C | C2-N3-C4 | 5.11 | 122.46 | 119.90 |
| 1 | CA | 380 | G | N3-C4-N9 | -5.11 | 122.93 | 126.00 |
| 23 | DA | 1394 | U | C5-C4-O4 | 5.11 | 128.97 | 125.90 |
| 1 | AA | 1108 | G | N9-C4-C5 | 5.11 | 107.44 | 105.40 |
| 23 | BA | 286 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23 | BA | 773 | U | C5-C6-N1 | -5.11 | 120.14 | 122.70 |
| 23 | BA | 1498 | C | N3-C2-O2 | 5.11 | 125.48 | 121.90 |
| 23 | BA | 1941 | C | N1-C2-O2 | -5.11 | 115.83 | 118.90 |
| 23 | BA | 2296 | U | C3'-C2'-C1' | -5.11 | 97.41 | 101.50 |
| 23 | BA | 2613 | U | N1-C2-O2 | 5.11 | 126.38 | 122.80 |
| 1 | CA | 1277 | C | C6-N1-C1' | 5.11 | 126.93 | 120.80 |
| 1 | AA | 1185 | G | N3-C4-N9 | 5.11 | 129.06 | 126.00 |
| 23 | BA | 1043 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 23 | DA | 982 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 1 | AA | 372 | C | N1-C2-N3 | -5.11 | 115.62 | 119.20 |
| 23 | BA | 30 | G | N1-C6-O6 | -5.11 | 116.84 | 119.90 |
| 23 | BA | 799 | G | C4-C5-N7 | -5.11 | 108.76 | 110.80 |
| 23 | BA | 1658 | C | C6-N1-C2 | -5.11 | 118.26 | 120.30 |
| 23 | BA | 1827 | C | N3-C2-O2 | -5.11 | 118.32 | 121.90 |
| 1 | CA | 1116 | C | C5-C6-N1 | 5.11 | 123.55 | 121.00 |
| 1 | CA | 1160 | G | N3-C4-N9 | 5.11 | 129.06 | 126.00 |
| 1 | AA | 733 | A | C8-N9-C4 | 5.11 | 107.84 | 105.80 |
| 23 | BA | 652(E) | G | C5-C6-N1 | -5.11 | 108.95 | 111.50 |
| 23 | BA | 886 | C | C2-N3-C4 | 5.11 | 122.45 | 119.90 |
| 1 | CA | 681 | C | N1-C2-N3 | -5.11 | 115.63 | 119.20 |
| 1 | CA | 1004 | A | N3-C4-C5 | -5.11 | 123.23 | 126.80 |
| 1 | CA | 1301 | U | C5-C4-O4 | 5.11 | 128.96 | 125.90 |
| 23 | DA | 1543 | C | N1-C2-O2 | 5.11 | 121.96 | 118.90 |
| 23 | DA | 2844 | G | C5-C6-O6 | -5.11 | 125.54 | 128.60 |
| 23 | BA | 2356 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 1 | AA | 47 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 23 | BA | 2574 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 1 | CA | 1045 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | CA | 1241 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 23 | DA | 125 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 23 | DA | 761 | A | C5-N7-C8 | 5.10 | 106.45 | 103.90 |
| 23 | DA | 930 | U | N3-C2-O2 | 5.10 | 125.77 | 122.20 |
| 23 | DA | 2288 | A | N7-C8-N9 | 5.10 | 116.35 | 113.80 |
| 23 | BA | 411 | G | C5-C6-O6 | 5.10 | 131.66 | 128.60 |
| 23 | BA | 2346 | A | C4-C5-C6 | 5.10 | 119.55 | 117.00 |
| 23 | DA | 2061 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 1 | AA | 1015 | A | N7-C8-N9 | 5.10 | 116.35 | 113.80 |
| 23 | BA | 1790 | C | N3-C4-N4 | 5.10 | 121.57 | 118.00 |
| 23 | BA | 1819 | A | C6-N1-C2 | -5.10 | 115.54 | 118.60 |
| 1 | CA | 355 | C | N1-C2-O2 | -5.10 | 115.84 | 118.90 |
| 23 | DA | 583 | G | C4-C5-N7 | 5.10 | 112.84 | 110.80 |
| 1 | AA | 1066 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | BA | 1364 | G | N9-C4-C5 | -5.10 | 103.36 | 105.40 |
| 23 | BA | 2053 | G | C8-N9-C4 | 5.10 | 108.44 | 106.40 |
| 23 | BA | 2706 | G | C6-N1-C2 | -5.10 | 122.04 | 125.10 |
| 1 | CA | 618 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | CA | 1153 | C | C5-C6-N1 | -5.10 | 118.45 | 121.00 |
| 11 | CK | 118 | GLY | N-CA-C | 5.10 | 125.84 | 113.10 |
| 23 | DA | 928 | G | C4-C5-C6 | 5.10 | 121.86 | 118.80 |
| 23 | BA | 591 | C | N3-C4-C5 | -5.10 | 119.86 | 121.90 |
| 24 | BB | 9 | G | C2-N3-C4 | 5.10 | 114.45 | 111.90 |
| 23 | DA | 2610 | C | P-O3'-C3' | 5.10 | 125.81 | 119.70 |
| 1 | AA | 1295 | G | N1-C2-N2 | 5.09 | 120.79 | 116.20 |
| 23 | BA | 389 | G | C8-N9-C4 | 5.09 | 108.44 | 106.40 |
| 23 | BA | 420 | C | N1-C2-O2 | 5.09 | 121.96 | 118.90 |
| 1 | CA | 242 | C | N3-C2-O2 | 5.09 | 125.47 | 121.90 |
| 1 | CA | 1262 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 23 | BA | 208 | C | C5-C4-N4 | -5.09 | 116.64 | 120.20 |
| 23 | BA | 633 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 23 | BA | 1327 | C | N1-C2-O2 | -5.09 | 115.84 | 118.90 |
| 23 | BA | 2519 | U | N3-C2-O2 | 5.09 | 125.76 | 122.20 |
| 23 | BA | 2557 | G | C4-C5-N7 | 5.09 | 112.84 | 110.80 |
| 1 | CA | 697 | U | C5-C6-N1 | -5.09 | 120.15 | 122.70 |
| 1 | CA | 1297 | C | C6-N1-C2 | -5.09 | 118.26 | 120.30 |
| 23 | BA | 627 | A | C8-N9-C4 | 5.09 | 107.84 | 105.80 |
| 23 | BA | 1334 | G | C4-C5-N7 | -5.09 | 108.76 | 110.80 |
| 1 | CA | 60 | A | C8-N9-C4 | -5.09 | 103.76 | 105.80 |
| 1 | CA | 65 | U | C5-C6-N1 | 5.09 | 125.25 | 122.70 |
| 1 | CA | 204 | U | N1-C2-O2 | 5.09 | 126.36 | 122.80 |
| 23 | DA | 453 | C | N1-C2-O2 | 5.09 | 121.95 | 118.90 |
| 23 | DA | 1047 | G | N3-C4-C5 | -5.09 | 126.06 | 128.60 |
| 23 | DA | 1107 | G | C2-N3-C4 | 5.09 | 114.44 | 111.90 |
| 23 | DA | 1697 | G | N3-C2-N2 | -5.09 | 116.34 | 119.90 |
| 23 | DA | 2319 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 23 | DA | 2581 | G | C8-N9-C1' | -5.09 | 120.38 | 127.00 |
| 1 | AA | 355 | C | C6-N1-C1' | 5.09 | 126.91 | 120.80 |
| 23 | BA | 122 | G | C4-C5-C6 | 5.09 | 121.85 | 118.80 |
| 23 | BA | 1229 | G | C6-C5-N7 | -5.09 | 127.35 | 130.40 |
| 23 | DA | 325 | G | C8-N9-C4 | 5.09 | 108.44 | 106.40 |
| 23 | DA | 466 | A | N1-C2-N3 | 5.09 | 131.84 | 129.30 |
| 24 | DB | 27 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 23 | BA | 131 | G | C5-C6-N1 | 5.09 | 114.04 | 111.50 |
| 23 | BA | 676 | A | C6-C5-N7 | -5.09 | 128.74 | 132.30 |
| 23 | BA | 801 | G | N1-C2-N3 | 5.09 | 126.95 | 123.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 23 | BA | 2370 | G | N3-C4-C5 | -5.09 | 126.06 | 128.60 |
| 23 | BA | 2851 | A | C4-C5-C6 | 5.09 | 119.54 | 117.00 |
| 1 | CA | 390 | C | C2-N3-C4 | -5.09 | 117.36 | 119.90 |
| 23 | DA | 329 | G | C5-C6-N1 | 5.09 | 114.04 | 111.50 |
| 23 | DA | 1280 | G | N1-C6-O6 | 5.09 | 122.95 | 119.90 |
| 23 | DA | 1553 | A | C8-N9-C4 | -5.09 | 103.77 | 105.80 |
| 23 | DA | 1566 | A | C5-C6-N1 | -5.09 | 115.16 | 117.70 |
| 23 | DA | 1604 | C | C2-N3-C4 | -5.09 | 117.36 | 119.90 |
| 24 | DB | 74 | U | N3-C2-O2 | -5.09 | 118.64 | 122.20 |
| 1 | CA | 514 | C | C5-C6-N1 | 5.08 | 123.54 | 121.00 |
| 23 | DA | 1614 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 23 | DA | 2036 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 1 | AA | 40 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 23 | BA | 2354 | G | C4-C5-N7 | 5.08 | 112.83 | 110.80 |
| 23 | BA | 2495 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 23 | BA | 2552 | U | N1-C2-O2 | -5.08 | 119.24 | 122.80 |
| 1 | CA | 1124 | G | C8-N9-C1' | -5.08 | 120.39 | 127.00 |
| 23 | DA | 951 | C | N3-C4-C5 | 5.08 | 123.93 | 121.90 |
| 1 | AA | 1014 | A | C6-N1-C2 | -5.08 | 115.55 | 118.60 |
| 23 | BA | 955 | C | N3-C2-O2 | 5.08 | 125.46 | 121.90 |
| 23 | BA | 989 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 23 | BA | 1372 | U | N1-C2-O2 | 5.08 | 126.36 | 122.80 |
| 23 | BA | 2610 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 1 | CA | 1249 | C | N1-C2-O2 | 5.08 | 121.95 | 118.90 |
| 1 | CA | 1340 | A | N3-C4-C5 | -5.08 | 123.24 | 126.80 |
| 23 | DA | 2723 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 23 | BA | 975(A) | G | C5-C6-N1 | 5.08 | 114.04 | 111.50 |
| 23 | BA | 2230 | G | N3-C2-N2 | -5.08 | 116.34 | 119.90 |
| 23 | BA | 2440 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 1 | CA | 993 | G | N3-C4-N9 | 5.08 | 129.05 | 126.00 |
| 1 | AA | 733 | A | N9-C4-C5 | -5.08 | 103.77 | 105.80 |
| 1 | AA | 1489 | G | C8-N9-C4 | 5.08 | 108.43 | 106.40 |
| 23 | BA | 1020 | A | C5-C6-N1 | -5.08 | 115.16 | 117.70 |
| 23 | BA | 1990 | C | C4-C5-C6 | 5.08 | 119.94 | 117.40 |
| 23 | BA | 2225 | A | C2-N3-C4 | 5.08 | 113.14 | 110.60 |
| 23 | BA | 2242 | G | N1-C2-N2 | 5.08 | 120.77 | 116.20 |
| 23 | DA | 1653 | G | N3-C2-N2 | 5.08 | 123.45 | 119.90 |
| 23 | DA | 2559 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 1 | AA | 1440 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 23 | BA | 847 | U | N3-C2-O2 | -5.08 | 118.65 | 122.20 |
| 23 | BA | 1204 | A | C1'-O4'-C4' | -5.08 | 105.84 | 109.90 |
| 23 | BA | 2038 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 23 | DA | 2832 | U | C6-N1-C1' | -5.08 | 114.09 | 121.20 |
| 23 | BA | 555 | U | N1-C2-O2 | -5.08 | 119.25 | 122.80 |
| 23 | BA | 738 | G | N7-C8-N9 | 5.08 | 115.64 | 113.10 |
| 23 | BA | 1672 | C | C2-N3-C4 | -5.08 | 117.36 | 119.90 |
| 23 | BA | 2556 | C | C5-C4-N4 | -5.08 | 116.65 | 120.20 |
| 23 | BA | 2689 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 23 | DA | 2338 | G | C5-C6-O6 | -5.08 | 125.56 | 128.60 |
| 1 | AA | 961 | U | N3-C2-O2 | -5.07 | 118.65 | 122.20 |
| 1 | AA | 1057 | G | N9-C4-C5 | -5.07 | 103.37 | 105.40 |
| 23 | BA | 100 | G | C8-N9-C4 | 5.07 | 108.43 | 106.40 |
| 23 | BA | 2285 | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 23 | BA | 2315 | G | C8-N9-C4 | 5.07 | 108.43 | 106.40 |
| 1 | CA | 982 | U | C2-N1-C1' | 5.07 | 123.79 | 117.70 |
| 23 | DA | 1914 | C | C2-N1-C1' | -5.07 | 113.22 | 118.80 |
| 23 | DA | 2265 | U | C5-C6-N1 | 5.07 | 125.24 | 122.70 |
| 23 | DA | 2292 | C | N3-C4-N4 | -5.07 | 114.45 | 118.00 |
| 23 | BA | 1414 | G | N7-C8-N9 | 5.07 | 115.64 | 113.10 |
| 1 | AA | 1012 | U | C5-C4-O4 | -5.07 | 122.86 | 125.90 |
| 23 | BA | 116 | C | N1-C2-N3 | 5.07 | 122.75 | 119.20 |
| 23 | BA | 196 | A | C5-C6-N6 | -5.07 | 119.64 | 123.70 |
| 23 | BA | 1489 | U | C5-C4-O4 | 5.07 | 128.94 | 125.90 |
| 23 | BA | 1974 | C | C2-N3-C4 | -5.07 | 117.36 | 119.90 |
| 25 | BD | 60 | ARG | NE-CZ-NH1 | -5.07 | 117.77 | 120.30 |
| 1 | CA | 78 | G | C6-N1-C2 | 5.07 | 128.14 | 125.10 |
| 23 | DA | 1858 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 23 | DA | 2191 | G | C4-C5-N7 | 5.07 | 112.83 | 110.80 |
| 23 | DA | 2607 | G | C4-N9-C1' | 5.07 | 133.09 | 126.50 |
| 1 | AA | 43 | C | C2-N3-C4 | -5.07 | 117.37 | 119.90 |
| 1 | CA | 1416 | G | C5-C6-N1 | -5.07 | 108.97 | 111.50 |
| 23 | DA | 94 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 24 | DB | 89 | G | C4-C5-N7 | 5.07 | 112.83 | 110.80 |
| 23 | BA | 187 | G | C6-C5-N7 | -5.07 | 127.36 | 130.40 |
| 23 | BA | 934 | G | N7-C8-N9 | -5.07 | 110.57 | 113.10 |
| 23 | BA | 1041 | C | C2-N3-C4 | 5.07 | 122.43 | 119.90 |
| 23 | BA | 1256 | G | C6-C5-N7 | -5.07 | 127.36 | 130.40 |
| 23 | BA | 2273 | A | C4-C5-N7 | 5.07 | 113.23 | 110.70 |
| 23 | BA | 2376 | A | C4-C5-C6 | 5.07 | 119.53 | 117.00 |
| 1 | CA | 1008 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 1 | CA | 1505 | G | N3-C4-N9 | -5.07 | 122.96 | 126.00 |
| 23 | DA | 2594 | C | C2-N3-C4 | -5.07 | 117.37 | 119.90 |
| 23 | DA | 2644 | G | C2-N3-C4 | -5.07 | 109.37 | 111.90 |
| 1 | AA | 728 | A | N7-C8-N9 | 5.07 | 116.33 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1312 | G | C2-N3-C4 | 5.07 | 114.43 | 111.90 |
| 23 | BA | 765 | G | N1-C2-N2 | 5.07 | 120.76 | 116.20 |
| 23 | BA | 989 | G | C6-C5-N7 | -5.07 | 127.36 | 130.40 |
| 23 | BA | 1336 | A | C2-N3-C4 | 5.07 | 113.13 | 110.60 |
| 23 | BA | 1463 | C | N1-C2-O2 | 5.07 | 121.94 | 118.90 |
| 24 | BB | 27 | C | C2-N1-C1' | 5.07 | 124.37 | 118.80 |
| 24 | BB | 57 | A | C8-N9-C4 | 5.07 | 107.83 | 105.80 |
| 23 | DA | 1415 | U | C2-N1-C1' | -5.07 | 111.62 | 117.70 |
| 23 | DA | 1790 | C | C4-C5-C6 | 5.07 | 119.93 | 117.40 |
| 23 | DA | 1864 | U | C6-N1-C2 | 5.07 | 124.04 | 121.00 |
| 23 | DA | 1921 | G | C4-C5-N7 | 5.07 | 112.83 | 110.80 |
| 23 | DA | 2579 | C | C4-C5-C6 | 5.07 | 119.93 | 117.40 |
| 23 | BA | 2107 | C | C5-C6-N1 | 5.06 | 123.53 | 121.00 |
| 1 | AA | 916 | G | C2-N3-C4 | 5.06 | 114.43 | 111.90 |
| 23 | BA | 1597 | A | N1-C6-N6 | -5.06 | 115.56 | 118.60 |
| 23 | BA | 2874 | C | N3-C4-C5 | 5.06 | 123.92 | 121.90 |
| 1 | CA | 292 | G | N3-C4-N9 | 5.06 | 129.04 | 126.00 |
| 1 | CA | 487 | A | N1-C6-N6 | 5.06 | 121.64 | 118.60 |
| 23 | DA | 1290 | C | N3-C2-O2 | -5.06 | 118.36 | 121.90 |
| 23 | BA | 1211 | U | N1-C2-O2 | -5.06 | 119.26 | 122.80 |
| 23 | BA | 1745 | C | N3-C2-O2 | 5.06 | 125.44 | 121.90 |
| 23 | BA | 2330 | G | C2-N3-C4 | -5.06 | 109.37 | 111.90 |
| 1 | CA | 1124 | G | N3-C4-N9 | 5.06 | 129.04 | 126.00 |
| 1 | AA | 1371 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 1 | CA | 150 | C | N3-C4-C5 | -5.06 | 119.88 | 121.90 |
| 1 | CA | 922 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 1 | CA | 1017 | G | C2-N3-C4 | 5.06 | 114.43 | 111.90 |
| 23 | DA | 171 | G | N9-C4-C5 | -5.06 | 103.38 | 105.40 |
| 23 | DA | 770 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 23 | DA | 1802 | A | C2-N3-C4 | -5.06 | 108.07 | 110.60 |
| 23 | DA | 2241 | A | N1-C2-N3 | 5.06 | 131.83 | 129.30 |
| 23 | DA | 2304 | G | C4-C5-N7 | -5.06 | 108.78 | 110.80 |
| 23 | DA | 2876 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 1 | AA | 1324 | A | C8-N9-C4 | -5.06 | 103.78 | 105.80 |
| 23 | BA | 211 | A | N7-C8-N9 | -5.06 | 111.27 | 113.80 |
| 23 | BA | 2755 | C | C2-N3-C4 | 5.06 | 122.43 | 119.90 |
| 23 | BA | 2853 | C | C6-N1-C2 | 5.06 | 122.32 | 120.30 |
| 1 | CA | 992 | U | P-O3'-C3' | 5.06 | 125.77 | 119.70 |
| 1 | CA | 1364 | U | C2-N3-C4 | 5.06 | 130.03 | 127.00 |
| 23 | DA | 532 | A | C4-C5-N7 | 5.06 | 113.23 | 110.70 |
| 23 | DA | 1193 | G | N9-C4-C5 | -5.06 | 103.38 | 105.40 |
| 23 | DA | 2647 | U | C5-C6-N1 | -5.06 | 120.17 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 2743 | C | N1-C2-N3 | 5.06 | 122.74 | 119.20 |
| 1 | CA | 297 | G | C5-C6-O6 | 5.06 | 131.63 | 128.60 |
| 1 | CA | 662 | G | N1-C6-O6 | 5.06 | 122.93 | 119.90 |
| 23 | DA | 362 | U | N3-C4-O4 | 5.06 | 122.94 | 119.40 |
| 23 | DA | 662 | G | N1-C6-O6 | -5.06 | 116.87 | 119.90 |
| 23 | DA | 2447 | G | C6-C5-N7 | -5.06 | 127.37 | 130.40 |
| 23 | BA | 614(B) | G | N1-C6-O6 | -5.05 | 116.87 | 119.90 |
| 23 | BA | 2053 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 23 | BA | 2291 | U | N1-C2-N3 | 5.05 | 117.93 | 114.90 |
| 23 | BA | 2646 | C | C5-C6-N1 | -5.05 | 118.47 | 121.00 |
| 20 | CT | 97 | ALA | C-N-CD | -5.05 | 109.48 | 120.60 |
| 23 | DA | 1261 | C | C5-C6-N1 | -5.05 | 118.47 | 121.00 |
| 23 | DA | 1635 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 23 | DA | 2030 | A | N3-C4-C5 | 5.05 | 130.34 | 126.80 |
| 24 | DB | 15 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 23 | BA | 435 | C | C6-N1-C2 | 5.05 | 122.32 | 120.30 |
| 23 | BA | 1824 | G | N7-C8-N9 | -5.05 | 110.57 | 113.10 |
| 1 | CA | 1033 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 23 | DA | 235 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 1 | AA | 936 | C | C5-C6-N1 | -5.05 | 118.47 | 121.00 |
| 1 | AA | 959 | A | N9-C4-C5 | -5.05 | 103.78 | 105.80 |
| 23 | BA | 559 | G | C8-N9-C4 | -5.05 | 104.38 | 106.40 |
| 23 | BA | 607 | U | C2-N1-C1' | -5.05 | 111.64 | 117.70 |
| 23 | BA | 2050 | C | C2-N3-C4 | -5.05 | 117.37 | 119.90 |
| 23 | BA | 2382 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 23 | DA | 104 | U | C6-N1-C2 | 5.05 | 124.03 | 121.00 |
| 23 | DA | 1205 | U | C5-C6-N1 | -5.05 | 120.17 | 122.70 |
| 23 | DA | 2359 | C | N3-C4-C5 | -5.05 | 119.88 | 121.90 |
| 23 | BA | 1042 | G | C2-N3-C4 | 5.05 | 114.42 | 111.90 |
| 23 | BA | 1358 | G | C5-C6-O6 | 5.05 | 131.63 | 128.60 |
| 23 | BA | 1368 | G | C2-N3-C4 | 5.05 | 114.42 | 111.90 |
| 23 | BA | 2129 | C | C5-C4-N4 | 5.05 | 123.73 | 120.20 |
| 23 | DA | 1526 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 40 | DW | 17 | VAL | CB-CA-C | -5.05 | 101.81 | 111.40 |
| 1 | AA | 1199 | U | N3-C2-O2 | -5.05 | 118.67 | 122.20 |
| 23 | BA | 686 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 23 | BA | 1422 | G | C4-C5-N7 | -5.05 | 108.78 | 110.80 |
| 23 | BA | 2025 | C | N1-C2-O2 | -5.05 | 115.87 | 118.90 |
| 23 | BA | 2042 | A | C8-N9-C4 | -5.05 | 103.78 | 105.80 |
| 23 | BA | 2601 | C | N3-C4-C5 | -5.05 | 119.88 | 121.90 |
| 23 | DA | 1481 | U | C5-C4-O4 | 5.05 | 128.93 | 125.90 |
| 23 | BA | 1256 | G | C6-N1-C2 | -5.05 | 122.07 | 125.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | BA | 2603 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 1 | CA | 358 | U | C2-N3-C4 | -5.05 | 123.97 | 127.00 |
| 1 | CA | 1447 | A | C2-N3-C4 | 5.05 | 113.12 | 110.60 |
| 23 | DA | 1315 | C | C4-C5-C6 | 5.05 | 119.92 | 117.40 |
| 23 | DA | 1926 | U | C5-C4-O4 | 5.05 | 128.93 | 125.90 |
| 23 | DA | 2548 | G | N7-C8-N9 | -5.05 | 110.58 | 113.10 |
| 23 | BA | 179 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 1 | CA | 1435 | G | N1-C6-O6 | 5.04 | 122.93 | 119.90 |
| 23 | DA | 2013 | A | C2-N3-C4 | -5.04 | 108.08 | 110.60 |
| 23 | DA | 2292 | C | C2-N3-C4 | -5.04 | 117.38 | 119.90 |
| 23 | DA | 2477 | C | C5-C6-N1 | -5.04 | 118.48 | 121.00 |
| 23 | BA | 124 | G | N1-C6-O6 | 5.04 | 122.93 | 119.90 |
| 1 | CA | 54 | C | N1-C2-N3 | 5.04 | 122.73 | 119.20 |
| 1 | CA | 987 | G | N1-C6-O6 | 5.04 | 122.93 | 119.90 |
| 23 | DA | 2275 | C | N1-C2-O2 | 5.04 | 121.93 | 118.90 |
| 23 | DA | 2711 | A | C4-C5-C6 | -5.04 | 114.48 | 117.00 |
| 23 | DA | 2744 | G | N3-C2-N2 | -5.04 | 116.37 | 119.90 |
| 1 | AA | 973 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 23 | BA | 465 | G | C5-C6-N1 | -5.04 | 108.98 | 111.50 |
| 23 | BA | 1603 | A | C8-N9-C4 | -5.04 | 103.78 | 105.80 |
| 1 | CA | 1258 | G | C5-C6-O6 | 5.04 | 131.62 | 128.60 |
| 23 | DA | 181 | A | N9-C4-C5 | 5.04 | 107.82 | 105.80 |
| 23 | DA | 728 | G | C8-N9-C1' | -5.04 | 120.45 | 127.00 |
| 23 | DA | 1802 | A | C6-N1-C2 | -5.04 | 115.58 | 118.60 |
| 1 | AA | 1072 | G | C4-C5-N7 | -5.04 | 108.78 | 110.80 |
| 23 | BA | 48 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 23 | BA | 1472 | A | N1-C6-N6 | -5.04 | 115.58 | 118.60 |
| 24 | BB | 6 | C | C6-N1-C2 | 5.04 | 122.32 | 120.30 |
| 23 | DA | 2429 | G | C8-N9-C4 | -5.04 | 104.38 | 106.40 |
| 1 | AA | 1442(B) | A | C4-C5-C6 | 5.04 | 119.52 | 117.00 |
| 23 | BA | 729 | G | C6-C5-N7 | -5.04 | 127.38 | 130.40 |
| 23 | BA | 2237 | G | C8-N9-C4 | 5.04 | 108.42 | 106.40 |
| 23 | BA | 2510 | C | C6-N1-C2 | -5.04 | 118.28 | 120.30 |
| 1 | CA | 776 | G | N3-C4-C5 | 5.04 | 131.12 | 128.60 |
| 23 | DA | 1238 | G | N7-C8-N9 | -5.04 | 110.58 | 113.10 |
| 1 | AA | 814 | A | C8-N9-C4 | 5.04 | 107.81 | 105.80 |
| 23 | BA | 2182 | G | N3-C4-C5 | 5.04 | 131.12 | 128.60 |
| 23 | BA | 2563 | U | N3-C4-C5 | -5.04 | 111.58 | 114.60 |
| 1 | AA | 17 | U | C2-N1-C1' | 5.04 | 123.74 | 117.70 |
| 1 | AA | 584 | G | N1-C6-O6 | 5.04 | 122.92 | 119.90 |
| 23 | BA | 745 | G | C4-C5-N7 | 5.04 | 112.81 | 110.80 |
| 23 | BA | 1901 | A | C5-C6-N6 | 5.04 | 127.73 | 123.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 23 | BA | 2751 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 1 | CA | 818 | G | C5-N7-C8 | 5.04 | 106.82 | 104.30 |
| 1 | CA | 1340 | A | C5-C6-N6 | 5.04 | 127.73 | 123.70 |
| 23 | DA | 1257 | C | C5-C6-N1 | -5.04 | 118.48 | 121.00 |
| 23 | DA | 2439 | A | C2-N3-C4 | -5.04 | 108.08 | 110.60 |
| 23 | BA | 425 | G | N7-C8-N9 | -5.03 | 110.58 | 113.10 |
| 23 | BA | 844 | C | C2-N3-C4 | -5.03 | 117.38 | 119.90 |
| 23 | BA | 988 | A | N7-C8-N9 | 5.03 | 116.32 | 113.80 |
| 1 | CA | 1122 | U | C5-C6-N1 | 5.03 | 125.22 | 122.70 |
| 23 | DA | 531 | C | C5-C6-N1 | -5.03 | 118.48 | 121.00 |
| 1 | AA | 531 | U | C2-N1-C1' | -5.03 | 111.66 | 117.70 |
| 1 | AA | 1068 | G | C5-C6-N1 | 5.03 | 114.02 | 111.50 |
| 23 | BA | 1298 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 23 | BA | 2842 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 24 | BB | 61 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |
| 1 | CA | 98 | G | N7-C8-N9 | 5.03 | 115.62 | 113.10 |
| 23 | DA | 608 | A | C5-N7-C8 | -5.03 | 101.38 | 103.90 |
| 23 | DA | 1596 | A | N1-C6-N6 | -5.03 | 115.58 | 118.60 |
| 1 | AA | 1176 | A | N7-C8-N9 | 5.03 | 116.31 | 113.80 |
| 23 | BA | 1427 | A | N1-C2-N3 | 5.03 | 131.81 | 129.30 |
| 1 | CA | 986 | A | N3-C4-C5 | -5.03 | 123.28 | 126.80 |
| 1 | CA | 1379 | G | N1-C2-N2 | -5.03 | 111.67 | 116.20 |
| 23 | DA | 18 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 23 | DA | 45 | C | C4-C5-C6 | 5.03 | 119.92 | 117.40 |
| 23 | DA | 682 | G | C8-N9-C1' | -5.03 | 120.46 | 127.00 |
| 23 | DA | 819 | A | C5-N7-C8 | -5.03 | 101.38 | 103.90 |
| 23 | DA | 1121 | C | C4-C5-C6 | 5.03 | 119.92 | 117.40 |
| 1 | AA | 1186 | G | N3-C4-N9 | 5.03 | 129.02 | 126.00 |
| 1 | AA | 1380 | U | C5-C4-O4 | 5.03 | 128.92 | 125.90 |
| 23 | BA | 908 | C | C5-C4-N4 | -5.03 | 116.68 | 120.20 |
| 1 | CA | 1442 | G | C4-C5-N7 | -5.03 | 108.79 | 110.80 |
| 23 | DA | 1677 | A | N9-C4-C5 | -5.03 | 103.79 | 105.80 |
| 1 | AA | 1028 | C | N1-C2-O2 | 5.03 | 121.92 | 118.90 |
| 1 | AA | 1344 | C | C2-N3-C4 | 5.03 | 122.41 | 119.90 |
| 1 | AA | 1442(A) | G | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 23 | BA | 48 | G | N3-C4-C5 | 5.03 | 131.11 | 128.60 |
| 23 | BA | 272(A) | U | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 23 | BA | 735 | A | C5-N7-C8 | 5.03 | 106.41 | 103.90 |
| 23 | BA | 748 | G | C6-N1-C2 | -5.03 | 122.08 | 125.10 |
| 23 | BA | 1221(A) | C | N3-C4-C5 | 5.03 | 123.91 | 121.90 |
| 23 | BA | 1617 | C | N3-C4-N4 | 5.03 | 121.52 | 118.00 |
| 1 | CA | 951 | G | C8-N9-C4 | -5.03 | 104.39 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 23 | DA | 154 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 23 | DA | 363(B) | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 23 | DA | 1016 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 23 | DA | 1546 | C | C6-N1-C1' | -5.03 | 114.77 | 120.80 |
| 23 | DA | 1695 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 23 | DA | 2417 | C | C4-C5-C6 | 5.03 | 119.91 | 117.40 |
| 23 | DA | 2487 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 1 | AA | 945 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 23 | BA | 393 | C | N1-C2-N3 | 5.03 | 122.72 | 119.20 |
| 23 | BA | 1815 | A | N9-C4-C5 | 5.03 | 107.81 | 105.80 |
| 23 | DA | 2445 | G | N1-C6-O6 | -5.03 | 116.89 | 119.90 |
| 23 | DA | 2602 | A | P-O3'-C3' | 5.03 | 125.73 | 119.70 |
| 24 | DB | 7 | G | N9-C4-C5 | -5.03 | 103.39 | 105.40 |
| 1 | AA | 935 | A | C5-C6-N6 | 5.02 | 127.72 | 123.70 |
| 23 | BA | 848 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 23 | BA | 1283 | G | C4-C5-N7 | -5.02 | 108.79 | 110.80 |
| 23 | BA | 2713 | A | N1-C6-N6 | -5.02 | 115.58 | 118.60 |
| 23 | DA | 1231 | G | C2-N3-C4 | -5.02 | 109.39 | 111.90 |
| 1 | AA | 1408 | A | N9-C4-C5 | 5.02 | 107.81 | 105.80 |
| 23 | BA | 108 | U | N3-C2-O2 | -5.02 | 118.69 | 122.20 |
| 23 | BA | 179 | G | C6-C5-N7 | -5.02 | 127.39 | 130.40 |
| 23 | BA | 1970 | A | N9-C4-C5 | -5.02 | 103.79 | 105.80 |
| 23 | BA | 2623 | G | C4-N9-C1' | 5.02 | 133.03 | 126.50 |
| 23 | DA | 2444 | G | N1-C2-N3 | 5.02 | 126.91 | 123.90 |
| 1 | AA | 1457 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 23 | BA | 1330 | C | C5-C4-N4 | -5.02 | 116.69 | 120.20 |
| 1 | CA | 1190 | G | N3-C4-C5 | 5.02 | 131.11 | 128.60 |
| 1 | AA | 1000 | U | N1-C2-N3 | -5.02 | 111.89 | 114.90 |
| 23 | BA | 265 | A | C4-N9-C1' | 5.02 | 135.33 | 126.30 |
| 23 | BA | 928 | G | C5-N7-C8 | -5.02 | 101.79 | 104.30 |
| 23 | BA | 1754 | C | N1-C2-N3 | 5.02 | 122.71 | 119.20 |
| 23 | BA | 1963 | U | C6-N1-C1' | -5.02 | 114.17 | 121.20 |
| 23 | BA | 2028 | U | C4-C5-C6 | -5.02 | 116.69 | 119.70 |
| 23 | BA | 2762 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 1 | CA | 839 | U | C6-N1-C1' | -5.02 | 114.17 | 121.20 |
| 1 | CA | 1442(B) | A | C8-N9-C1' | -5.02 | 118.67 | 127.70 |
| 23 | DA | 760 | G | N9-C4-C5 | -5.02 | 103.39 | 105.40 |
| 23 | DA | 1325 | G | C5-N7-C8 | -5.02 | 101.79 | 104.30 |
| 23 | DA | 1526 | G | N9-C4-C5 | -5.02 | 103.39 | 105.40 |
| 1 | AA | 150 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 23 | BA | 102 | G | P-O3'-C3' | 5.02 | 125.72 | 119.70 |
| 23 | BA | 767 | U | C6-N1-C2 | -5.02 | 117.99 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | BA | 1348 | G | C5-C6-O6 | -5.02 | 125.59 | 128.60 |
| 1 | CA | 1524 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 23 | DA | 2373 | G | N1-C6-O6 | 5.02 | 122.91 | 119.90 |
| 23 | DA | 2568 | C | N1-C2-O2 | -5.02 | 115.89 | 118.90 |
| 1 | AA | 1155 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 23 | BA | 983 | A | C8-N9-C4 | 5.02 | 107.81 | 105.80 |
| 23 | BA | 1808 | U | N1-C2-O2 | 5.02 | 126.31 | 122.80 |
| 23 | BA | 1914 | C | C2-N1-C1' | -5.02 | 113.28 | 118.80 |
| 1 | AA | 1215 | G | N7-C8-N9 | 5.01 | 115.61 | 113.10 |
| 23 | BA | 205 | G | C4-C5-N7 | 5.01 | 112.81 | 110.80 |
| 23 | BA | 607 | U | N3-C4-O4 | -5.01 | 115.89 | 119.40 |
| 23 | DA | 85 | G | N3-C4-C5 | 5.01 | 131.11 | 128.60 |
| 23 | DA | 1688 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |
| 23 | DA | 2023 | G | C8-N9-C4 | -5.01 | 104.39 | 106.40 |
| 23 | DA | 2502 | G | C5-N7-C8 | -5.01 | 101.79 | 104.30 |
| 23 | DA | 2669 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 23 | DA | 476 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 23 | DA | 691 | C | C2-N1-C1' | -5.01 | 113.28 | 118.80 |
| 23 | DA | 727 | A | C5-C6-N6 | -5.01 | 119.69 | 123.70 |
| 1 | AA | 455 | C | C4-C5-C6 | -5.01 | 114.89 | 117.40 |
| 23 | BA | 77 | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 23 | BA | 1452 | A | N1-C2-N3 | 5.01 | 131.81 | 129.30 |
| 23 | BA | 1539 | G | C4-N9-C1' | 5.01 | 133.01 | 126.50 |
| 23 | BA | 2778 | A | N1-C2-N3 | 5.01 | 131.81 | 129.30 |
| 1 | CA | 740 | U | C5-C4-O4 | 5.01 | 128.91 | 125.90 |
| 23 | DA | 932 | G | C8-N9-C1' | 5.01 | 133.52 | 127.00 |
| 23 | DA | 1049 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 23 | DA | 1368 | G | C4-C5-N7 | -5.01 | 108.80 | 110.80 |
| 23 | DA | 1772 | G | C4-N9-C1' | -5.01 | 119.99 | 126.50 |
| 23 | DA | 2417 | C | N1-C2-N3 | 5.01 | 122.71 | 119.20 |
| 1 | AA | 955 | U | C5-C4-O4 | 5.01 | 128.91 | 125.90 |
| 1 | AA | 1221 | G | N1-C6-O6 | 5.01 | 122.91 | 119.90 |
| 23 | BA | 225 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 23 | BA | 267 | C | N3-C4-C5 | 5.01 | 123.90 | 121.90 |
| 23 | BA | 652(R) | C | C5-C6-N1 | 5.01 | 123.50 | 121.00 |
| 23 | BA | 2070 | G | N1-C2-N2 | -5.01 | 111.69 | 116.20 |
| 23 | BA | 2148 | G | C6-C5-N7 | 5.01 | 133.41 | 130.40 |
| 23 | BA | 2573 | C | C6-N1-C2 | 5.01 | 122.30 | 120.30 |
| 24 | BB | 103 | G | N3-C2-N2 | -5.01 | 116.39 | 119.90 |
| 1 | CA | 1377 | A | N1-C6-N6 | -5.01 | 115.59 | 118.60 |
| 23 | DA | 1236 | G | C2-N3-C4 | -5.01 | 109.40 | 111.90 |
| 23 | DA | 1256 | G | C4-N9-C1' | 5.01 | 133.01 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 23 | DA | 2379 | G | C6-C5-N7 | -5.01 | 127.39 | 130.40 |
| 23 | DA | 2395 | C | N3-C2-O2 | 5.01 | 125.41 | 121.90 |
| 23 | BA | 1233 | C | C6-N1-C2 | -5.01 | 118.30 | 120.30 |
| 23 | BA | 2425 | A | N7-C8-N9 | 5.01 | 116.30 | 113.80 |
| 23 | DA | 2056 | G | N9-C4-C5 | -5.01 | 103.40 | 105.40 |
| 1 | AA | 1292 | U | C6-N1-C1' | -5.01 | 114.19 | 121.20 |
| 23 | BA | 334 | C | N1-C2-O2 | -5.01 | 115.90 | 118.90 |
| 23 | BA | 723 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |
| 23 | BA | 754 | C | C2-N3-C4 | -5.01 | 117.40 | 119.90 |
| 23 | BA | 1121 | C | N1-C2-O2 | -5.01 | 115.90 | 118.90 |
| 23 | BA | 1752 | C | C2-N1-C1' | -5.01 | 113.29 | 118.80 |
| 23 | BA | 1777 | U | C5-C6-N1 | -5.01 | 120.20 | 122.70 |
| 23 | BA | 1896 | G | C5-C6-O6 | -5.01 | 125.60 | 128.60 |
| 23 | BA | 2201 | C | C5-C6-N1 | -5.01 | 118.50 | 121.00 |
| 1 | CA | 60 | A | N9-C4-C5 | 5.01 | 107.80 | 105.80 |
| 23 | DA | 272(H) | C | C2-N1-C1' | 5.01 | 124.31 | 118.80 |
| 23 | DA | 452 | G | N7-C8-N9 | 5.01 | 115.60 | 113.10 |
| 23 | DA | 2607 | G | C5-N7-C8 | 5.01 | 106.80 | 104.30 |
| 23 | BA | 2038 | G | C5-N7-C8 | -5.00 | 101.80 | 104.30 |
| 23 | DA | 1943 | U | C4-C5-C6 | 5.00 | 122.70 | 119.70 |
| 1 | AA | 801 | U | N3-C4-O4 | -5.00 | 115.90 | 119.40 |
| 23 | BA | 570 | G | C5-C6-N1 | 5.00 | 114.00 | 111.50 |
| 23 | BA | 975(A) | G | C2-N3-C4 | 5.00 | 114.40 | 111.90 |
| 23 | BA | 1938 | A | N3-C4-C5 | -5.00 | 123.30 | 126.80 |
| 1 | CA | 1101 | A | N7-C8-N9 | -5.00 | 111.30 | 113.80 |
| 23 | DA | 1036 | G | N1-C2-N3 | 5.00 | 126.90 | 123.90 |
| 23 | DA | 1050 | A | C8-N9-C4 | -5.00 | 103.80 | 105.80 |
| 23 | DA | 1372 | U | N3-C4-O4 | -5.00 | 115.90 | 119.40 |
| 1 | AA | 836 | G | N1-C6-O6 | 5.00 | 122.90 | 119.90 |
| 23 | BA | 33 | U | N3-C4-O4 | -5.00 | 115.90 | 119.40 |
| 23 | BA | 569 | U | C5-C4-O4 | -5.00 | 122.90 | 125.90 |
| 23 | BA | 1606 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 23 | BA | 2303 | G | N3-C2-N2 | -5.00 | 116.40 | 119.90 |
| 1 | CA | 1216 | G | C4-C5-C6 | -5.00 | 115.80 | 118.80 |
| 23 | DA | 678 | C | C5-C6-N1 | -5.00 | 118.50 | 121.00 |
| 23 | DA | 819 | A | N7-C8-N9 | 5.00 | 116.30 | 113.80 |
| 23 | DA | 1639 | U | C5-C6-N1 | -5.00 | 120.20 | 122.70 |
| 23 | DA | 2020 | A | C4-C5-C6 | 5.00 | 119.50 | 117.00 |

There are no chirality outliers.

All (56) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 2 | AB | 129 | GLU | Peptide |
| 2 | AB | 14 | GLY | Peptide |
| 2 | AB | 71 | VAL | Peptide |
| 3 | AC | 147 | LYS | Peptide |
| 3 | AC | 19 | GLU | Peptide |
| 3 | AC | 51 | GLY | Peptide |
| 4 | AD | 29 | PRO | Peptide |
| 9 | AI | 117 | HIS | Peptide |
| 10 | AJ | 56 | HIS | Peptide |
| 10 | AJ | 86 | MET | Peptide |
| 13 | AM | 105 | THR | Peptide |
| 13 | AM | 40 | ASN | Peptide |
| 13 | AM | 85 | GLY | Peptide |
| 13 | AM | 86 | CYS | Peptide |
| 14 | AN | 12 | ARG | Peptide |
| 15 | AO | 75 | PRO | Peptide |
| 17 | AQ | 96 | GLU | Peptide |
| 19 | AS | 12 | ASP | Peptide |
| 20 | AT | 48 | LYS | Peptide |
| 45 | B1 | 83 | GLU | Peptide |
| 48 | B4 | 43 | TYR | Peptide |
| 23 | BA | 2335 | A | Sidechain |
| 26 | BE | 72 | VAL | Peptide |
| 34 | BQ | 18 | LYS | Peptide |
| 36 | BS | 82 | ILE | Peptide |
| 41 | BX | 93 | GLU | Peptide |
| 43 | BZ | 159 | PRO | Peptide |
| 43 | BZ | 191 | VAL | Peptide |
| 43 | BZ | 199 | LYS | Peptide |
| 2 | CB | 129 | GLU | Peptide |
| 2 | CB | 130 | ARG | Peptide |
| 2 | CB | 14 | GLY | Peptide |
| 2 | CB | 71 | VAL | Peptide |
| 3 | CC | 160 | ALA | Peptide |
| 4 | CD | 29 | PRO | Peptide |
| 7 | CG | 146 | GLU | Peptide |
| 7 | CG | 7 | ALA | Peptide |
| 9 | CI | 102 | LEU | Peptide |
| 10 | CJ | 21 | GLN | Peptide |
| 10 | CJ | 92 | THR | Peptide |
| 13 | CM | 65 | LYS | Peptide |
| 13 | CM | 86 | CYS | Peptide |
| 15 | CO | 75 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 17 | CQ | 96 | GLU | Peptide |
| 19 | CS | 76 | PRO | Peptide |
| 20 | CT | 48 | LYS | Peptide |
| 45 | D1 | 83 | GLU | Peptide |
| 48 | D4 | 43 | TYR | Peptide |
| 23 | DA | 2335 | A | Sidechain |
| 26 | DE | 72 | VAL | Peptide |
| 27 | DF | 85 | GLY | Peptide |
| 30 | DI | 86 | THR | Peptide |
| 34 | DQ | 18 | LYS | Peptide |
| 36 | DS | 82 | ILE | Peptide |
| 41 | DX | 93 | GLU | Peptide |
| 43 | DZ | 191 | VAL | Peptide |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32270 | 0 | 16286 | 1214 | 0 |
| 1 | CA | 32185 | 0 | 16244 | 1267 | 1 |
| 2 | AB | 1787 | 0 | 1752 | 122 | 0 |
| 2 | CB | 1775 | 0 | 1743 | 121 | 0 |
| 3 | AC | 1450 | 0 | 1314 | 92 | 0 |
| 3 | CC | 1450 | 0 | 1314 | 123 | 0 |
| 4 | AD | 1526 | 0 | 1415 | 71 | 0 |
| 4 | CD | 1526 | 0 | 1415 | 85 | 0 |
| 5 | AE | 1105 | 0 | 1130 | 56 | 0 |
| 5 | CE | 1105 | 0 | 1130 | 60 | 0 |
| 6 | AF | 777 | 0 | 737 | 31 | 0 |
| 6 | CF | 777 | 0 | 737 | 35 | 0 |
| 7 | AG | 1164 | 0 | 1106 | 87 | 0 |
| 7 | CG | 1164 | 0 | 1106 | 99 | 0 |
| 8 | AH | 1045 | 0 | 1033 | 48 | 0 |
| 8 | CH | 1045 | 0 | 1033 | 51 | 0 |
| 9 | AI | 852 | 0 | 742 | 83 | 0 |
| 9 | CI | 852 | 0 | 742 | 79 | 0 |
| 10 | AJ | 663 | 0 | 558 | 56 | 0 |
| 10 | CJ | 663 | 0 | 558 | 70 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11 | AK | 828 | 0 | 822 | 29 | 0 |
| 11 | CK | 828 | 0 | 822 | 28 | 0 |
| 12 | AL | 905 | 0 | 916 | 41 | 0 |
| 12 | CL | 905 | 0 | 916 | 32 | 0 |
| 13 | AM | 804 | 0 | 752 | 58 | 0 |
| 13 | CM | 804 | 0 | 752 | 60 | 0 |
| 14 | AN | 478 | 0 | 497 | 33 | 0 |
| 14 | CN | 478 | 0 | 496 | 58 | 0 |
| 15 | AO | 724 | 0 | 749 | 34 | 0 |
| 15 | CO | 724 | 0 | 749 | 31 | 0 |
| 16 | AP | 651 | 0 | 638 | 31 | 0 |
| 16 | CP | 651 | 0 | 638 | 36 | 0 |
| 17 | AQ | 823 | 0 | 891 | 43 | 0 |
| 17 | CQ | 823 | 0 | 891 | 47 | 0 |
| 18 | AR | 514 | 0 | 530 | 25 | 0 |
| 18 | CR | 514 | 0 | 530 | 21 | 0 |
| 19 | AS | 560 | 0 | 466 | 46 | 0 |
| 19 | CS | 560 | 0 | 466 | 40 | 0 |
| 20 | AT | 665 | 0 | 731 | 34 | 0 |
| 20 | CT | 713 | 0 | 766 | 39 | 0 |
| 21 | AU | 199 | 0 | 208 | 31 | 0 |
| 21 | CU | 199 | 0 | 208 | 23 | 0 |
| 22 | AX | 631 | 0 | 540 | 20 | 0 |
| 22 | CX | 601 | 0 | 485 | 16 | 0 |
| 23 | BA | 61112 | 0 | 30809 | 1210 | 1 |
| 23 | DA | 60621 | 0 | 30566 | 1219 | 0 |
| 24 | BB | 2573 | 0 | 1306 | 56 | 0 |
| 24 | DB | 2573 | 0 | 1306 | 55 | 0 |
| 25 | BD | 2135 | 0 | 2214 | 73 | 0 |
| 25 | DD | 2136 | 0 | 2218 | 79 | 0 |
| 26 | BE | 1555 | 0 | 1607 | 52 | 0 |
| 26 | DE | 1555 | 0 | 1607 | 56 | 0 |
| 27 | BF | 1580 | 0 | 1621 | 63 | 0 |
| 27 | DF | 1580 | 0 | 1621 | 63 | 0 |
| 28 | BG | 1368 | 0 | 1324 | 74 | 0 |
| 28 | DG | 1368 | 0 | 1324 | 86 | 0 |
| 29 | BH | 1317 | 0 | 1376 | 35 | 0 |
| 29 | DH | 1317 | 0 | 1376 | 36 | 0 |
| 30 | BI | 1037 | 0 | 1036 | 54 | 1 |
| 30 | DI | 953 | 0 | 858 | 38 | 0 |
| 31 | BN | 1112 | 0 | 1180 | 33 | 0 |
| 31 | DN | 1112 | 0 | 1180 | 44 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | BO | 923 | 0 | 981 | 26 | 0 |
| 32 | DO | 923 | 0 | 981 | 28 | 0 |
| 33 | BP | 1131 | 0 | 1201 | 45 | 0 |
| 33 | DP | 1131 | 0 | 1201 | 55 | 0 |
| 34 | BQ | 1122 | 0 | 1179 | 46 | 0 |
| 34 | DQ | 1122 | 0 | 1179 | 49 | 0 |
| 35 | BR | 968 | 0 | 1033 | 32 | 0 |
| 35 | DR | 968 | 0 | 1033 | 36 | 0 |
| 36 | BS | 865 | 0 | 905 | 50 | 0 |
| 36 | DS | 865 | 0 | 905 | 50 | 0 |
| 37 | BT | 1063 | 0 | 1103 | 42 | 0 |
| 37 | DT | 1063 | 0 | 1103 | 43 | 0 |
| 38 | BU | 959 | 0 | 1019 | 34 | 0 |
| 38 | DU | 959 | 0 | 1019 | 35 | 0 |
| 39 | BV | 771 | 0 | 830 | 23 | 0 |
| 39 | DV | 771 | 0 | 830 | 25 | 0 |
| 40 | BW | 881 | 0 | 935 | 21 | 0 |
| 40 | DW | 881 | 0 | 935 | 31 | 0 |
| 41 | BX | 742 | 0 | 799 | 23 | 0 |
| 41 | DX | 742 | 0 | 799 | 26 | 0 |
| 42 | BY | 785 | 0 | 828 | 23 | 0 |
| 42 | DY | 785 | 0 | 828 | 23 | 0 |
| 43 | BZ | 1536 | 0 | 1518 | 52 | 0 |
| 43 | DZ | 1522 | 0 | 1511 | 65 | 0 |
| 44 | B0 | 594 | 0 | 604 | 16 | 0 |
| 44 | D0 | 594 | 0 | 604 | 17 | 0 |
| 45 | B1 | 745 | 0 | 804 | 21 | 0 |
| 45 | D1 | 745 | 0 | 804 | 24 | 0 |
| 46 | B2 | 588 | 0 | 643 | 16 | 0 |
| 46 | D2 | 588 | 0 | 643 | 19 | 0 |
| 47 | B3 | 458 | 0 | 503 | 8 | 0 |
| 47 | D3 | 458 | 0 | 503 | 13 | 0 |
| 48 | B4 | 349 | 0 | 336 | 23 | 0 |
| 48 | D4 | 349 | 0 | 336 | 28 | 0 |
| 49 | B5 | 455 | 0 | 472 | 13 | 0 |
| 49 | D5 | 455 | 0 | 472 | 14 | 0 |
| 50 | B6 | 449 | 0 | 462 | 18 | 0 |
| 50 | D6 | 449 | 0 | 462 | 15 | 0 |
| 51 | B7 | 418 | 0 | 467 | 14 | 0 |
| 51 | D7 | 418 | 0 | 467 | 18 | 0 |
| 52 | B8 | 509 | 0 | 565 | 18 | 0 |
| 52 | D8 | 509 | 0 | 565 | 22 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 53 | B9 | 297 | 0 | 316 | 9 | 0 |
| 53 | D9 | 297 | 0 | 316 | 9 | 0 |
| 54 | AA | 135 | 0 | 0 | 0 | 0 |
| 54 | AC | 1 | 0 | 0 | 0 | 0 |
| 54 | AD | 1 | 0 | 0 | 0 | 0 |
| 54 | AF | 1 | 0 | 0 | 0 | 0 |
| 54 | AQ | 1 | 0 | 0 | 0 | 0 |
| 54 | B0 | 3 | 0 | 0 | 0 | 0 |
| 54 | B1 | 1 | 0 | 0 | 0 | 0 |
| 54 | B2 | 1 | 0 | 0 | 0 | 0 |
| 54 | B3 | 1 | 0 | 0 | 0 | 0 |
| 54 | B5 | 2 | 0 | 0 | 0 | 0 |
| 54 | B8 | 2 | 0 | 0 | 0 | 0 |
| 54 | B9 | 1 | 0 | 0 | 0 | 0 |
| 54 | BA | 660 | 0 | 0 | 0 | 0 |
| 54 | BB | 23 | 0 | 0 | 0 | 0 |
| 54 | BD | 3 | 0 | 0 | 0 | 0 |
| 54 | BE | 5 | 0 | 0 | 0 | 0 |
| 54 | BF | 2 | 0 | 0 | 0 | 0 |
| 54 | BG | 1 | 0 | 0 | 0 | 0 |
| 54 | BP | 1 | 0 | 0 | 0 | 0 |
| 54 | BQ | 4 | 0 | 0 | 0 | 0 |
| 54 | BR | 1 | 0 | 0 | 0 | 0 |
| 54 | BS | 1 | 0 | 0 | 0 | 0 |
| 54 | BT | 2 | 0 | 0 | 0 | 0 |
| 54 | BV | 1 | 0 | 0 | 0 | 0 |
| 54 | BW | 2 | 0 | 0 | 0 | 0 |
| 54 | BZ | 1 | 0 | 0 | 0 | 0 |
| 54 | CA | 162 | 0 | 0 | 0 | 0 |
| 54 | CE | 1 | 0 | 0 | 0 | 0 |
| 54 | CQ | 1 | 0 | 0 | 0 | 0 |
| 54 | D0 | 2 | 0 | 0 | 0 | 0 |
| 54 | D1 | 1 | 0 | 0 | 0 | 0 |
| 54 | D5 | 1 | 0 | 0 | 0 | 0 |
| 54 | D8 | 2 | 0 | 0 | 0 | 0 |
| 54 | DA | 598 | 0 | 0 | 0 | 0 |
| 54 | DB | 8 | 0 | 0 | 0 | 0 |
| 54 | DD | 2 | 0 | 0 | 0 | 0 |
| 54 | DE | 4 | 0 | 0 | 0 | 0 |
| 54 | DF | 1 | 0 | 0 | 0 | 0 |
| 54 | DO | 2 | 0 | 0 | 0 | 0 |
| 54 | DP | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54 | DQ | 2 | 0 | 0 | 0 | 0 |
| 54 | DR | 3 | 0 | 0 | 0 | 0 |
| 55 | AD | 1 | 0 | 0 | 0 | 0 |
| 55 | AN | 1 | 0 | 0 | 0 | 0 |
| 55 | B4 | 1 | 0 | 0 | 0 | 0 |
| 55 | B5 | 1 | 0 | 0 | 0 | 0 |
| 55 | B6 | 1 | 0 | 0 | 0 | 0 |
| 55 | B9 | 1 | 0 | 0 | 0 | 0 |
| 55 | BY | 1 | 0 | 0 | 0 | 0 |
| 55 | CD | 1 | 0 | 0 | 0 | 0 |
| 55 | CN | 1 | 0 | 0 | 0 | 0 |
| 55 | D4 | 1 | 0 | 0 | 0 | 0 |
| 55 | D5 | 1 | 0 | 0 | 0 | 0 |
| 55 | D6 | 1 | 0 | 0 | 0 | 0 |
| 55 | D9 | 1 | 0 | 0 | 0 | 0 |
| 55 | DY | 1 | 0 | 0 | 0 | 0 |
| 56 | AA | 268 | 0 | 0 | 32 | 0 |
| 56 | AE | 1 | 0 | 0 | 0 | 0 |
| 56 | AL | 1 | 0 | 0 | 0 | 0 |
| 56 | AO | 1 | 0 | 0 | 0 | 0 |
| 56 | AP | 1 | 0 | 0 | 0 | 0 |
| 56 | AT | 1 | 0 | 0 | 0 | 0 |
| 56 | AX | 1 | 0 | 0 | 0 | 0 |
| 56 | B0 | 8 | 0 | 0 | 0 | 0 |
| 56 | B1 | 2 | 0 | 0 | 0 | 0 |
| 56 | B3 | 1 | 0 | 0 | 0 | 0 |
| 56 | B5 | 3 | 0 | 0 | 0 | 0 |
| 56 | B6 | 1 | 0 | 0 | 1 | 0 |
| 56 | B7 | 5 | 0 | 0 | 0 | 0 |
| 56 | B8 | 10 | 0 | 0 | 0 | 0 |
| 56 | B9 | 1 | 0 | 0 | 1 | 0 |
| 56 | BA | 1694 | 0 | 0 | 169 | 0 |
| 56 | BB | 57 | 0 | 0 | 3 | 1 |
| 56 | BD | 20 | 0 | 0 | 3 | 0 |
| 56 | BE | 11 | 0 | 0 | 0 | 0 |
| 56 | BF | 6 | 0 | 0 | 1 | 0 |
| 56 | BH | 1 | 0 | 0 | 0 | 0 |
| 56 | BN | 2 | 0 | 0 | 0 | 0 |
| 56 | BO | 2 | 0 | 0 | 0 | 0 |
| 56 | BP | 11 | 0 | 0 | 2 | 0 |
| 56 | BQ | 5 | 0 | 0 | 0 | 0 |
| 56 | BR | 6 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56 | BT | 1 | 0 | 0 | 0 | 0 |
| 56 | BU | 3 | 0 | 0 | 0 | 0 |
| 56 | BV | 3 | 0 | 0 | 0 | 0 |
| 56 | BW | 3 | 0 | 0 | 0 | 0 |
| 56 | BX | 2 | 0 | 0 | 0 | 0 |
| 56 | BY | 4 | 0 | 0 | 0 | 0 |
| 56 | CA | 265 | 0 | 0 | 25 | 0 |
| 56 | CC | 1 | 0 | 0 | 2 | 0 |
| 56 | CD | 1 | 0 | 0 | 0 | 0 |
| 56 | CE | 2 | 0 | 0 | 0 | 0 |
| 56 | CK | 1 | 0 | 0 | 1 | 0 |
| 56 | CL | 2 | 0 | 0 | 1 | 0 |
| 56 | CN | 1 | 0 | 0 | 0 | 0 |
| 56 | CP | 1 | 0 | 0 | 0 | 0 |
| 56 | CQ | 1 | 0 | 0 | 0 | 0 |
| 56 | CT | 1 | 0 | 0 | 0 | 0 |
| 56 | CX | 1 | 0 | 0 | 0 | 0 |
| 56 | D0 | 1 | 0 | 0 | 0 | 0 |
| 56 | D1 | 5 | 0 | 0 | 0 | 0 |
| 56 | D3 | 1 | 0 | 0 | 0 | 0 |
| 56 | D4 | 1 | 0 | 0 | 0 | 0 |
| 56 | D7 | 3 | 0 | 0 | 0 | 0 |
| 56 | D8 | 1 | 0 | 0 | 0 | 0 |
| 56 | DA | 1174 | 0 | 0 | 171 | 0 |
| 56 | DB | 17 | 0 | 0 | 0 | 0 |
| 56 | DD | 8 | 0 | 0 | 2 | 0 |
| 56 | DE | 11 | 0 | 0 | 2 | 0 |
| 56 | DF | 7 | 0 | 0 | 1 | 0 |
| 56 | DN | 1 | 0 | 0 | 0 | 0 |
| 56 | DO | 5 | 0 | 0 | 1 | 0 |
| 56 | DP | 10 | 0 | 0 | 1 | 0 |
| 56 | DQ | 3 | 0 | 0 | 0 | 0 |
| 56 | DR | 2 | 0 | 0 | 1 | 0 |
| 56 | DT | 2 | 0 | 0 | 0 | 0 |
| 56 | DU | 5 | 0 | 0 | 0 | 0 |
| 56 | DV | 2 | 0 | 0 | 1 | 0 |
| 56 | DW | 2 | 0 | 0 | 0 | 0 |
| 56 | DX | 1 | 0 | 0 | 1 | 0 |
| 56 | DY | 2 | 0 | 0 | 0 | 0 |
| All | All | 286308 | 0 | 187082 | 8298 | 2 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (8298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AA:1441:G:H2' | 1:AA:1459:C:N4 | 1.20 | 1.46 |
| 1:AA:1459:C:C5 | 1:AA:1460:A:N6 | 1.79 | 1.44 |
| 1:AA:1441:G:C2' | 1:AA:1459:C:N4 | 1.88 | 1.36 |
| 1:AA:1441:G:C2' | 1:AA:1459:C:H41 | 1.44 | 1.29 |
| 1:CA:1441:G:H2' | 1:CA:1459:C:N4 | 1.50 | 1.25 |
| 1:CA:1441:G:C2' | 1:CA:1459:C:H41 | 1.54 | 1.19 |
| 23:BA:2296:U:O4 | 23:BA:2335:A:N6 | 1.76 | 1.19 |
| 23:DA:2296:U:O4 | 23:DA:2335:A:N6 | 1.77 | 1.15 |
| 1:CA:989:C:N4 | 1:CA:1216:G:H1 | 1.46 | 1.14 |
| 23:BA:885:C:C4 | 23:BA:890:A:N6 | 2.20 | 1.10 |
| 1:AA:1007:C:N4 | 1:AA:1022:G:H1 | 1.49 | 1.08 |
| 23:BA:885:C:N4 | 23:BA:890:A:C6 | 2.22 | 1.08 |
| 23:BA:2820:A:OP2 | 35:BR:2:ARG:NH2 | 1.87 | 1.07 |
| 23:DA:2820:A:OP2 | 35:DR:2:ARG:NH2 | 1.88 | 1.06 |
| 7:AG:88:PRO:HB3 | 7:AG:145:ALA:HA | 1.38 | 1.05 |
| 23:DA:2711:A:OP2 | 56:DA:3992:HOH:O | 1.73 | 1.04 |
| 1:AA:1003:G:H2' | 1:AA:1004:A:H4' | 1.41 | 1.03 |
| 23:BA:2036:C:OP1 | 56:BA:4559:HOH:O | 1.77 | 1.02 |
| 1:AA:1010:G:H1 | 1:AA:1019:C:N4 | 1.57 | 1.02 |
| 23:DA:847:U:O4 | 23:DA:933:A:N6 | 1.92 | 1.02 |
| 23:BA:847:U:O4 | 23:BA:933:A:N6 | 1.92 | 1.02 |
| 1:CA:1441:G:C2' | 1:CA:1459:C:N4 | 2.17 | 1.01 |
| 4:AD:9:CYS:SG | 4:AD:22:LYS:NZ | 2.34 | 1.01 |
| 23:DA:1439:A:OP1 | 56:DA:4126:HOH:O | 1.79 | 1.01 |
| 1:AA:1459:C:C3' | 1:AA:1460:A:C8 | 2.44 | 1.00 |
| 1:CA:949:A:H61 | 1:CA:1232:U:H3 | 1.05 | 1.00 |
| 23:DA:527:C:OP1 | 56:DA:4533:HOH:O | 1.77 | 1.00 |
| 1:CA:1089:G:H1 | 1:CA:1096:C:N4 | 1.58 | 1.00 |
| 23:DA:1671:U:OP2 | 56:DA:3807:HOH:O | 1.78 | 0.99 |
| 1:CA:1459:C:C5 | 1:CA:1460:A:N6 | 2.30 | 0.98 |
| 1:AA:839:U:H5' | 1:AA:840:C:H5 | 1.28 | 0.98 |
| 1:AA:1459:C:H3' | 1:AA:1460:A:N7 | 1.77 | 0.98 |
| 1:AA:1051:C:N4 | 1:AA:1207:G:N1 | 2.11 | 0.97 |
| 1:AA:1457:G:H2' | 1:AA:1458:G:H8 | 1.24 | 0.97 |
| 23:BA:463:G:OP1 | 56:BA:3949:HOH:O | 1.79 | 0.97 |
| 23:BA:2122:U:H3 | 23:BA:2176:A:H61 | 1.00 | 0.97 |
| 48:D4:42:PHE:HB3 | 48:D4:43:TYR:HB2 | 1.45 | 0.96 |
| 23:DA:563:G:OP2 | 56:DA:4622:HOH:O | 1.83 | 0.96 |
| 1:CA:1459:C:C3' | 1:CA:1460:A:C8 | 2.48 | 0.96 |
| 10:CJ:50:ILE:HA | 10:CJ:60:ARG:HG2 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AA:1151:A:HO2' | 1:AA:1152:A:H8 | 0.99 | 0.96 |
| 23:BA:631:A:OP1 | 33:BP:65:ARG:NH1 | 1.98 | 0.96 |
| 23:BA:450:G:O6 | 56:BA:4578:HOH:O | 1.84 | 0.96 |
| 1:CA:1459:C:H3' | 1:CA:1460:A:N7 | 1.81 | 0.95 |
| 1:AA:1458:G:OP1 | 20:AT:35:THR:OG1 | 1.85 | 0.95 |
| 1:AA:1459:C:H5 | 1:AA:1460:A:H62 | 1.02 | 0.95 |
| 1:AA:1168:A:H2' | 1:AA:1169:A:H8 | 1.27 | 0.95 |
| 1:CA:839:U:H5' | 1:CA:840:C:H5 | 1.28 | 0.95 |
| 1:CA:1457:G:H2' | 1:CA:1458:G:H8 | 1.27 | 0.95 |
| 1:AA:1051:C:N4 | 1:AA:1207:G:H1 | 1.63 | 0.95 |
| 1:AA:1168:A:H2' | 1:AA:1169:A:C8 | 2.01 | 0.95 |
| 8:AH:6:ILE:HB | 8:AH:85:ARG:HH12 | 1.28 | 0.95 |
| 7:AG:88:PRO:HG3 | 7:AG:149:ARG:HA | 1.44 | 0.95 |
| 23:DA:2122:U:H3 | 23:DA:2176:A:N6 | 1.64 | 0.94 |
| 23:DA:2227:A:OP2 | 56:DA:4145:HOH:O | 1.85 | 0.94 |
| 8:CH:6:ILE:HB | 8:CH:85:ARG:HH12 | 1.29 | 0.94 |
| 1:CA:950:U:H3 | 1:CA:1231:G:H1 | 1.05 | 0.94 |
| 1:AA:984:C:H42 | 1:AA:1221:G:H1 | 1.05 | 0.94 |
| 13:CM:3:ARG:HE | 13:CM:45:VAL:HG12 | 1.29 | 0.94 |
| 1:AA:986:A:H61 | 1:AA:1219:U:H3 | 0.97 | 0.94 |
| 1:CA:1089:G:H1 | 1:CA:1096:C:H42 | 0.96 | 0.94 |
| 23:BA:1359:A:N6 | 23:BA:1372:U:O4 | 1.99 | 0.94 |
| 1:CA:1113:C:N4 | 1:CA:1187:G:H1 | 1.64 | 0.94 |
| 1:CA:1128:C:H42 | 1:CA:1143:G:H1 | 1.11 | 0.93 |
| 13:CM:19:LEU:HB3 | 13:CM:25:ILE:HG21 | 1.47 | 0.93 |
| 2:CB:88:ALA:HB2 | 2:CB:219:VAL:HG13 | 1.50 | 0.93 |
| 1:AA:559:A:H4' | 1:AA:560:U:H3' | 1.50 | 0.93 |
| 1:CA:939:G:H1 | 1:CA:1344:C:H42 | 1.15 | 0.93 |
| 23:BA:2228:G:OP1 | 25:BD:261:LYS:NZ | 2.01 | 0.93 |
| 1:CA:1350:A:H61 | 1:CA:1372:U:H3 | 1.11 | 0.93 |
| 48:B4:42:PHE:HB3 | 48:B4:43:TYR:HB2 | 1.48 | 0.93 |
| 1:CA:932:C:N4 | 1:CA:1385:G:H1 | 1.66 | 0.93 |
| 2:AB:20:GLU:O | 2:AB:40:HIS:N | 2.01 | 0.93 |
| 1:AA:79:G:H2' | 1:AA:80:G:H8 | 1.32 | 0.93 |
| 37:DT:16:ARG:NH2 | 37:DT:83:ILE:O | 2.02 | 0.93 |
| 2:AB:88:ALA:HB2 | 2:AB:219:VAL:HG13 | 1.48 | 0.93 |
| 3:AC:121:ALA:HB2 | 3:AC:187:ALA:HB1 | 1.48 | 0.93 |
| 1:AA:1459:C:C6 | 1:AA:1460:A:N6 | 2.36 | 0.93 |
| 1:CA:1262:C:H42 | 1:CA:1273:G:H1 | 1.16 | 0.93 |
| 23:BA:1689:A:H62 | 23:BA:1698:A:H2 | 1.14 | 0.93 |
| 1:CA:1113:C:H42 | 1:CA:1187:G:H1 | 0.93 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1349:A:N7 | 1:CA:1373:G:N2 | 2.15 | 0.92 |
| 23:BA:271(I):G:H1 | 23:BA:271(O):C:H42 | 0.97 | 0.92 |
| 2:CB:20:GLU:O | 2:CB:40:HIS:N | 2.02 | 0.92 |
| 23:DA:271(I):G:H1 | 23:DA:271(O):C:H42 | 0.94 | 0.92 |
| 1:CA:954:G:N2 | 1:CA:1227:A:N7 | 2.17 | 0.92 |
| 1:AA:1343:G:H4' | 9:AI:122:ALA:HB3 | 1.52 | 0.92 |
| 2:AB:50:GLU:O | 2:AB:54:THR:OG1 | 1.88 | 0.92 |
| 23:DA:271(I):G:H1 | 23:DA:271(O):C:N4 | 1.68 | 0.92 |
| 1:CA:932:C:N4 | 1:CA:1385:G:N1 | 2.17 | 0.92 |
| 6:CF:15:ASP:HB2 | 6:CF:18:GLN:H | 1.34 | 0.92 |
| 1:CA:1441:G:H2' | 1:CA:1459:C:H41 | 0.76 | 0.92 |
| 1:CA:1262:C:N4 | 1:CA:1273:G:H1 | 1.67 | 0.91 |
| 23:DA:1970:A:OP1 | 56:DA:4210:HOH:O | 1.88 | 0.91 |
| 1:AA:1239:A:N6 | 1:AA:1299:A:H62 | 1.68 | 0.91 |
| 23:DA:2036:C:OP1 | 56:DA:4431:HOH:O | 1.88 | 0.91 |
| 1:CA:1006:C:H42 | 1:CA:1024:G:H21 | 1.09 | 0.91 |
| 1:AA:1246:C:N4 | 1:AA:1291:G:H1 | 1.67 | 0.91 |
| 1:AA:963:G:H1 | 1:AA:972:C:H42 | 1.09 | 0.91 |
| 1:CA:1443:G:O6 | 1:CA:1459:C:O2 | 1.89 | 0.91 |
| 2:AB:19:HIS:ND1 | 2:AB:189:ASP:OD2 | 2.03 | 0.91 |
| 1:CA:581:G:OP2 | 56:CA:2043:HOH:O | 1.87 | 0.91 |
| 1:CA:949:A:N6 | 1:CA:1232:U:H3 | 1.68 | 0.91 |
| 1:AA:1128:C:H42 | 1:AA:1143:G:H1 | 1.17 | 0.91 |
| 1:AA:993:G:H2' | 1:AA:995:C:H41 | 1.35 | 0.91 |
| 16:AP:19:ILE:HG22 | 16:AP:36:ILE:HG13 | 1.52 | 0.90 |
| 23:DA:631:A:OP1 | 33:DP:65:ARG:NH1 | 2.03 | 0.90 |
| 23:BA:583:G:N7 | 56:BA:5068:HOH:O | 2.03 | 0.90 |
| 23:BA:676:A:H8 | 23:BA:2069:G:H21 | 1.17 | 0.90 |
| 1:AA:1486:G:N7 | 56:AA:1839:HOH:O | 2.03 | 0.90 |
| 23:BA:1533:G:H21 | 23:BA:1536:C:H5 | 1.19 | 0.90 |
| 1:CA:1055:A:N7 | 1:CA:1200:C:N4 | 2.17 | 0.90 |
| 23:BA:271(I):G:H1 | 23:BA:271(O):C:N4 | 1.69 | 0.90 |
| 6:AF:15:ASP:HB2 | 6:AF:18:GLN:H | 1.36 | 0.90 |
| 23:DA:2304:G:H1 | 23:DA:2312:U:H3 | 1.19 | 0.90 |
| 1:CA:1346:A:OP1 | 9:CI:120:ARG:NH1 | 2.05 | 0.90 |
| 33:BP:39:LYS:HB2 | 33:BP:45:LEU:HG | 1.53 | 0.90 |
| 28:BG:63:ILE:HA | 28:BG:143:GLU:HG3 | 1.54 | 0.90 |
| 23:BA:2322:A:H61 | 23:BA:2335:A:N6 | 1.70 | 0.90 |
| 23:BA:1210:A:H5'' | 23:BA:1210:A:H8 | 1.35 | 0.90 |
| 1:AA:986:A:N6 | 1:AA:1219:U:H3 | 1.69 | 0.90 |
| 6:CF:81:ILE:HD11 | 25:DD:125:ILE:HB | 1.51 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 11:CK:29:ILE:HG23 | 11:CK:44:SER:HB3 | 1.51 | 0.90 |
| 1:CA:1502:A:OP1 | 56:CA:2034:HOH:O | 1.88 | 0.90 |
| 23:DA:330:A:H2 | 23:DA:1210:A:H2' | 1.36 | 0.89 |
| 1:CA:1371:G:H5'' | 9:CI:69:GLY:H | 1.35 | 0.89 |
| 23:BA:1189:A:OP2 | 56:BA:4525:HOH:O | 1.88 | 0.89 |
| 23:DA:407:G:OP2 | 56:DA:4603:HOH:O | 1.89 | 0.89 |
| 1:CA:1170:A:H3' | 1:CA:1171:G:H8 | 1.37 | 0.89 |
| 23:DA:1359:A:N6 | 23:DA:1372:U:O4 | 2.06 | 0.89 |
| 1:AA:1025:U:O2 | 1:AA:1036:G:O6 | 1.90 | 0.89 |
| 23:DA:2036:C:H6 | 23:DA:2036:C:H5' | 1.37 | 0.89 |
| 2:CB:19:HIS:ND1 | 2:CB:189:ASP:OD2 | 2.04 | 0.89 |
| 23:BA:2406:U:OP1 | 56:BA:4498:HOH:O | 1.90 | 0.89 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:H62 | 0.89 | 0.89 |
| 1:CA:955:U:H1' | 1:CA:1227:A:H61 | 1.36 | 0.89 |
| 1:AA:1459:C:H3' | 1:AA:1460:A:C8 | 2.07 | 0.89 |
| 1:CA:673:G:H2' | 1:CA:674:G:C8 | 2.07 | 0.89 |
| 23:DA:2122:U:H3 | 23:DA:2176:A:H61 | 0.91 | 0.88 |
| 37:BT:16:ARG:NH2 | 37:BT:83:ILE:O | 2.05 | 0.88 |
| 1:CA:989:C:N3 | 1:CA:1216:G:N2 | 2.22 | 0.88 |
| 1:CA:937:A:N6 | 1:CA:1345:U:O4 | 2.06 | 0.88 |
| 28:DG:41:GLN:HB3 | 28:DG:43:LEU:HD13 | 1.52 | 0.88 |
| 1:AA:1441:G:C2' | 1:AA:1459:C:H42 | 1.86 | 0.88 |
| 23:DA:1376:C:OP2 | 56:DA:3934:HOH:O | 1.90 | 0.88 |
| 23:BA:2366:A:OP1 | 56:BA:4104:HOH:O | 1.90 | 0.88 |
| 2:CB:50:GLU:O | 2:CB:54:THR:OG1 | 1.89 | 0.88 |
| 1:CA:1444:C:N4 | 1:CA:1459:C:O2 | 2.07 | 0.88 |
| 23:DA:2228:G:OP1 | 25:DD:261:LYS:NZ | 2.05 | 0.88 |
| 33:DP:39:LYS:HB2 | 33:DP:45:LEU:HG | 1.55 | 0.88 |
| 1:CA:1130:A:H61 | 1:CA:1144:G:H1' | 1.39 | 0.88 |
| 45:B1:82:LEU:HA | 45:B1:85:LEU:HD23 | 1.53 | 0.88 |
| 23:DA:785:G:OP2 | 56:DA:4113:HOH:O | 1.92 | 0.87 |
| 23:DA:1019:U:H3 | 23:DA:1142(A):A:H62 | 1.21 | 0.87 |
| 23:DA:2322:A:H61 | 23:DA:2335:A:N6 | 1.72 | 0.87 |
| 1:AA:1111:A:H61 | 3:AC:177:THR:HA | 1.39 | 0.87 |
| 23:BA:974:G:N7 | 56:BA:4207:HOH:O | 2.08 | 0.87 |
| 23:DA:927:G:N7 | 56:DA:4233:HOH:O | 2.08 | 0.87 |
| 23:BA:2122:U:H3 | 23:BA:2176:A:N6 | 1.71 | 0.87 |
| 23:BA:2304:G:H1 | 23:BA:2312:U:H3 | 1.22 | 0.87 |
| 23:DA:1865:G:N7 | 56:DA:4472:HOH:O | 2.06 | 0.87 |
| 1:AA:1279:A:OP2 | 10:AJ:9:ARG:NH1 | 2.07 | 0.87 |
| 1:AA:984:C:N4 | 1:AA:1221:G:H1 | 1.70 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:860:A:OP2 | 56:CA:1871:HOH:O | 1.91 | 0.87 |
| 1:CA:559:A:H4' | 1:CA:560:U:H3' | 1.57 | 0.87 |
| 1:CA:986:A:N3 | 19:CS:52:TYR:OH | 2.07 | 0.86 |
| 23:DA:1689:A:H62 | 23:DA:1698:A:H2 | 1.19 | 0.86 |
| 1:CA:758:G:N7 | 56:CA:2044:HOH:O | 2.06 | 0.86 |
| 23:BA:1284:A:N7 | 56:BA:5015:HOH:O | 2.06 | 0.86 |
| 23:DA:1352:U:OP2 | 56:DA:3935:HOH:O | 1.94 | 0.86 |
| 1:CA:953:G:O6 | 1:CA:1228:C:N3 | 2.09 | 0.86 |
| 23:DA:1345:C:OP2 | 56:DA:3943:HOH:O | 1.92 | 0.86 |
| 1:CA:1030:C:N4 | 1:CA:1031:G:C6 | 2.43 | 0.86 |
| 23:DA:1204:A:H2 | 23:DA:1241:A:H62 | 1.23 | 0.86 |
| 1:CA:949:A:H1' | 1:CA:1364:U:N3 | 1.91 | 0.86 |
| 1:AA:1237:C:O2' | 1:AA:1300:G:N2 | 2.08 | 0.86 |
| 1:AA:1246:C:H42 | 1:AA:1291:G:H1 | 0.89 | 0.86 |
| 23:BA:883:G:H2' | 23:BA:884:C:H5'' | 1.57 | 0.86 |
| 1:AA:1141:C:H2' | 1:AA:1142:G:H8 | 1.39 | 0.86 |
| 23:BA:1530:C:O2' | 23:BA:1531:C:O5' | 1.94 | 0.86 |
| 23:DA:2287:A:N6 | 23:DA:2344:U:H3 | 1.73 | 0.86 |
| 45:D1:82:LEU:HA | 45:D1:85:LEU:HD23 | 1.58 | 0.86 |
| 23:BA:558:G:N7 | 56:BA:4943:HOH:O | 2.09 | 0.86 |
| 1:AA:1086:U:H2' | 1:AA:1087:G:H8 | 1.41 | 0.85 |
| 23:BA:745:G:O6 | 56:BA:5274:HOH:O | 1.94 | 0.85 |
| 7:CG:123:GLU:HA | 7:CG:126:ASP:HB2 | 1.56 | 0.85 |
| 1:AA:1007:C:N3 | 1:AA:1022:G:N2 | 2.24 | 0.85 |
| 3:AC:152:ILE:HB | 3:AC:199:LYS:HB2 | 1.57 | 0.85 |
| 28:DG:63:ILE:HA | 28:DG:143:GLU:HG3 | 1.58 | 0.85 |
| 23:BA:1474:C:N4 | 56:BA:4420:HOH:O | 2.10 | 0.85 |
| 1:AA:1459:C:C4 | 1:AA:1460:A:N6 | 2.44 | 0.85 |
| 1:CA:782:A:OP1 | 56:CA:1947:HOH:O | 1.93 | 0.85 |
| 1:CA:1459:C:O3' | 1:CA:1460:A:C8 | 2.30 | 0.85 |
| 19:CS:16:LEU:HA | 19:CS:20:LEU:HB2 | 1.59 | 0.85 |
| 23:BA:2639:A:OP2 | 56:BA:4119:HOH:O | 1.94 | 0.85 |
| 23:BA:885:C:N4 | 23:BA:890:A:N6 | 2.22 | 0.85 |
| 23:DA:1641:A:OP2 | 56:DA:4176:HOH:O | 1.94 | 0.85 |
| 28:DG:15:VAL:HG13 | 28:DG:175:LEU:HB3 | 1.57 | 0.85 |
| 27:BF:101:LEU:O | 27:BF:106:ARG:NH1 | 2.10 | 0.85 |
| 1:AA:1459:C:O3' | 1:AA:1460:A:C8 | 2.30 | 0.84 |
| 1:CA:932:C:N3 | 1:CA:1385:G:N2 | 2.25 | 0.84 |
| 23:BA:2317:C:H2' | 23:BA:2318:G:H5' | 1.58 | 0.84 |
| 23:DA:2526:G:O6 | 56:DA:4287:HOH:O | 1.95 | 0.84 |
| 5:CE:122:GLU:O | 5:CE:126:ARG:NH1 | 2.09 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:AK:29:ILE:HG23 | 11:AK:44:SER:HB3 | 1.57 | 0.84 |
| 1:CA:1458:G:C2 | 1:CA:1459:C:O4' | 2.30 | 0.84 |
| 23:BA:1177:A:O2' | 23:BA:1178:C:O4' | 1.95 | 0.84 |
| 33:BP:126:VAL:HG12 | 33:BP:148:LEU:HD22 | 1.60 | 0.84 |
| 23:BA:242:G:OP1 | 56:BA:4242:HOH:O | 1.94 | 0.84 |
| 30:BI:3:VAL:HG12 | 30:BI:38:LEU:HA | 1.57 | 0.84 |
| 23:DA:1980:G:O2' | 23:DA:1982:C:OP2 | 1.95 | 0.84 |
| 1:AA:673:G:H2' | 1:AA:674:G:C8 | 2.13 | 0.84 |
| 23:DA:833:U:O2 | 33:DP:55:ARG:NH2 | 2.09 | 0.84 |
| 1:CA:1327:C:OP1 | 21:CU:20:LYS:N | 2.11 | 0.84 |
| 23:BA:510:C:OP1 | 56:BA:3896:HOH:O | 1.94 | 0.84 |
| 23:DA:2808:U:O2 | 23:DA:2892:A:N6 | 2.10 | 0.84 |
| 23:DA:1530:C:O2' | 23:DA:1531:C:O5' | 1.96 | 0.84 |
| 1:CA:1466:C:OP2 | 56:CA:1864:HOH:O | 1.94 | 0.84 |
| 23:DA:1271:G:OP2 | 56:DA:3848:HOH:O | 1.96 | 0.84 |
| 1:CA:1356:G:H2' | 1:CA:1357:A:C8 | 2.12 | 0.84 |
| 1:CA:1459:C:H3' | 1:CA:1460:A:C8 | 2.11 | 0.84 |
| 16:CP:19:ILE:HG22 | 16:CP:36:ILE:HG13 | 1.59 | 0.84 |
| 10:AJ:91:PRO:HG2 | 10:AJ:94:VAL:HB | 1.60 | 0.84 |
| 9:CI:16:ARG:HB2 | 9:CI:64:THR:HG23 | 1.57 | 0.83 |
| 23:DA:2161:C:C5 | 23:DA:2161:C:OP2 | 2.30 | 0.83 |
| 23:BA:2036:C:H5' | 23:BA:2036:C:H6 | 1.42 | 0.83 |
| 23:BA:330:A:H2 | 23:BA:1210:A:H2' | 1.43 | 0.83 |
| 10:CJ:8:LEU:HD11 | 10:CJ:20:ALA:HB2 | 1.59 | 0.83 |
| 1:AA:1118:C:H42 | 1:AA:1155:G:H1 | 1.26 | 0.83 |
| 23:BA:805:G:OP1 | 56:BA:4504:HOH:O | 1.95 | 0.83 |
| 23:DA:2298:A:H62 | 23:DA:2318:G:H8 | 1.24 | 0.83 |
| 1:CA:1300:G:H1 | 1:CA:1334:G:H2' | 1.43 | 0.83 |
| 1:AA:1158:C:H4' | 2:AB:133:LYS:HD2 | 1.60 | 0.83 |
| 25:BD:118:VAL:H | 25:BD:129:ASN:HD22 | 1.25 | 0.83 |
| 1:CA:973:G:H3' | 1:CA:974:A:H5" | 1.59 | 0.83 |
| 23:DA:2385:C:OP1 | 56:DA:4159:HOH:O | 1.95 | 0.83 |
| 1:CA:1368:G:H5" | 9:CI:112:LYS:HB3 | 1.60 | 0.83 |
| 23:BA:1210:A:H5" | 23:BA:1210:A:C8 | 2.13 | 0.83 |
| 23:BA:2134:A:O2' | 23:BA:2159:G:N2 | 2.12 | 0.83 |
| 1:CA:48:C:OP2 | 56:CA:1850:HOH:O | 1.95 | 0.83 |
| 23:DA:2161:C:C6 | 23:DA:2161:C:OP2 | 2.31 | 0.83 |
| 31:BN:20:GLY:HA2 | 31:BN:61:ARG:HG3 | 1.60 | 0.82 |
| 7:CG:14:PRO:HG3 | 7:CG:21:VAL:HG12 | 1.61 | 0.82 |
| 1:AA:1130:A:H61 | 1:AA:1144:G:H1' | 1.43 | 0.82 |
| 1:AA:1186:G:N2 | 14:AN:61:TRP:O | 2.10 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:624:C:OP1 | 56:BA:4243:HOH:O | 1.96 | 0.82 |
| 3:CC:20:SER:HB3 | 3:CC:22:TRP:HE1 | 1.43 | 0.82 |
| 1:CA:1508:G:OP1 | 56:CA:2021:HOH:O | 1.97 | 0.82 |
| 20:AT:10:LEU:HG | 20:AT:12:ALA:H | 1.45 | 0.82 |
| 1:AA:1051:C:N3 | 1:AA:1207:G:N2 | 2.27 | 0.82 |
| 5:AE:122:GLU:O | 5:AE:126:ARG:NH1 | 2.12 | 0.82 |
| 23:DA:2694:G:N7 | 56:DA:4770:HOH:O | 2.12 | 0.82 |
| 30:DI:3:VAL:HG12 | 30:DI:38:LEU:HA | 1.60 | 0.82 |
| 1:CA:390:C:O3' | 16:CP:28:ARG:NH2 | 2.12 | 0.82 |
| 33:DP:126:VAL:HG12 | 33:DP:148:LEU:HD22 | 1.61 | 0.82 |
| 23:DA:2074:U:OP1 | 56:DA:4301:HOH:O | 1.97 | 0.82 |
| 23:DA:2194:G:N7 | 56:DA:4551:HOH:O | 2.13 | 0.82 |
| 23:BA:1667:G:O6 | 56:BA:4985:HOH:O | 1.95 | 0.82 |
| 1:AA:977:A:O2' | 1:AA:981:U:N3 | 2.12 | 0.82 |
| 1:AA:963:G:H1 | 1:AA:972:C:N4 | 1.77 | 0.82 |
| 1:AA:893:C:O2 | 56:AA:1809:HOH:O | 1.98 | 0.82 |
| 1:CA:1156:G:H21 | 1:CA:1179:A:H61 | 1.24 | 0.82 |
| 23:BA:922:U:O4 | 56:BA:4369:HOH:O | 1.98 | 0.82 |
| 1:AA:812:C:N3 | 56:AA:1914:HOH:O | 2.13 | 0.82 |
| 23:DA:810:U:OP1 | 56:DA:4451:HOH:O | 1.96 | 0.82 |
| 31:DN:130:HIS:HB3 | 31:DN:133:GLN:HE21 | 1.43 | 0.82 |
| 31:BN:130:HIS:HB3 | 31:BN:133:GLN:HE21 | 1.43 | 0.81 |
| 9:CI:28:VAL:HB | 9:CI:36:TYR:HB3 | 1.59 | 0.81 |
| 1:AA:97:G:HO2' | 1:AA:98:G:H8 | 1.28 | 0.81 |
| 23:BA:578:A:OP2 | 56:BA:4057:HOH:O | 1.97 | 0.81 |
| 1:CA:1457:G:C4 | 1:CA:1458:G:C8 | 2.68 | 0.81 |
| 1:CA:1288:A:N1 | 1:CA:1371:G:H1' | 1.94 | 0.81 |
| 28:BG:41:GLN:HB3 | 28:BG:43:LEU:HD13 | 1.60 | 0.81 |
| 1:AA:1457:G:H2' | 1:AA:1458:G:C8 | 2.14 | 0.81 |
| 23:DA:2317:C:H2' | 23:DA:2318:G:H5' | 1.62 | 0.81 |
| 1:CA:1251:A:N6 | 1:CA:1285:A:N1 | 2.27 | 0.81 |
| 1:AA:642:A:N3 | 8:AH:113:SER:OG | 2.14 | 0.81 |
| 38:BU:28:ARG:NH1 | 38:BU:38:THR:OG1 | 2.12 | 0.81 |
| 1:AA:1065:U:H6 | 1:AA:1190:G:H21 | 1.23 | 0.81 |
| 23:BA:2033:A:OP1 | 56:BA:4596:HOH:O | 1.97 | 0.81 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:H8 | 1.44 | 0.81 |
| 1:CA:1422:G:H5' | 32:DO:48:PRO:HB3 | 1.63 | 0.81 |
| 1:CA:427:U:OP1 | 4:CD:13:ARG:NH2 | 2.14 | 0.81 |
| 23:DA:676:A:H8 | 23:DA:2069:G:H21 | 1.25 | 0.81 |
| 1:AA:1121:U:H3 | 1:AA:1152:A:H61 | 1.24 | 0.81 |
| 23:BA:1320:C:OP2 | 56:BA:5012:HOH:O | 1.99 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:BV:62:LEU:HD11 | 39:BV:95:LEU:HB2 | 1.63 | 0.81 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:N6 | 1.75 | 0.81 |
| 1:CA:1237:C:O2' | 1:CA:1300:G:N2 | 2.11 | 0.81 |
| 3:CC:137:ALA:HA | 3:CC:140:ARG:HD3 | 1.62 | 0.81 |
| 1:CA:1009:G:O6 | 1:CA:1020:U:O2 | 1.98 | 0.81 |
| 10:AJ:61:GLU:OE1 | 14:AN:58:LYS:NZ | 2.14 | 0.81 |
| 1:AA:768:A:N7 | 56:AA:1907:HOH:O | 2.14 | 0.81 |
| 23:DA:1303:G:OP1 | 56:DA:4525:HOH:O | 1.97 | 0.81 |
| 23:BA:1173:G:N1 | 23:BA:1176:G:OP2 | 2.11 | 0.80 |
| 1:CA:977:A:HO2' | 1:CA:981:U:H3 | 1.26 | 0.80 |
| 1:CA:581:G:N7 | 56:CA:2044:HOH:O | 2.14 | 0.80 |
| 28:BG:15:VAL:HG13 | 28:BG:175:LEU:HB3 | 1.63 | 0.80 |
| 23:DA:2134:A:O2' | 23:DA:2159:G:N2 | 2.15 | 0.80 |
| 1:CA:940:C:H42 | 1:CA:1343:G:H1 | 1.25 | 0.80 |
| 1:AA:1119:C:H2' | 1:AA:1120:G:H8 | 1.46 | 0.80 |
| 1:AA:1457:G:C4 | 1:AA:1458:G:C8 | 2.70 | 0.80 |
| 23:DA:271(A):A:N7 | 23:DA:271(W):G:N2 | 2.30 | 0.80 |
| 23:BA:2287:A:N6 | 23:BA:2344:U:H3 | 1.80 | 0.80 |
| 8:AH:4:ASP:OD1 | 8:AH:85:ARG:NH1 | 2.14 | 0.80 |
| 1:CA:1235:U:H5'' | 21:CU:3:LYS:HB2 | 1.63 | 0.80 |
| 23:DA:1022:G:H22 | 23:DA:1142(A):A:H2 | 1.29 | 0.80 |
| 7:CG:42:ILE:HA | 7:CG:45:ASP:HB2 | 1.63 | 0.80 |
| 23:BA:1541:G:O6 | 56:BA:4734:HOH:O | 1.98 | 0.80 |
| 23:BA:300:A:N6 | 56:BA:3924:HOH:O | 2.13 | 0.80 |
| 23:DA:71:A:C2 | 41:DX:31:HIS:HE1 | 1.99 | 0.80 |
| 23:BA:2161:C:C5 | 23:BA:2161:C:OP2 | 2.34 | 0.80 |
| 1:CA:1027:C:C2 | 1:CA:1034:G:N2 | 2.47 | 0.80 |
| 1:CA:1050:G:O6 | 1:CA:1208:C:N3 | 2.15 | 0.80 |
| 23:BA:561:G:N7 | 56:BA:5347:HOH:O | 2.15 | 0.79 |
| 52:D8:33:ASN:HA | 52:D8:36:LYS:HD2 | 1.63 | 0.79 |
| 1:AA:148:G:H2' | 1:AA:149:A:H8 | 1.47 | 0.79 |
| 7:CG:42:ILE:HB | 7:CG:116:ALA:HB3 | 1.64 | 0.79 |
| 13:AM:72:ALA:HA | 13:AM:75:ALA:HB3 | 1.64 | 0.79 |
| 23:DA:1403:C:H5'' | 23:DA:1471:A:H1' | 1.65 | 0.79 |
| 1:AA:1236:A:OP2 | 21:AU:3:LYS:NZ | 2.14 | 0.79 |
| 13:CM:86:CYS:HB3 | 13:CM:89:GLY:H | 1.44 | 0.79 |
| 27:DF:178:PRO:HB2 | 27:DF:201:VAL:HG11 | 1.64 | 0.79 |
| 6:CF:61:LEU:HB3 | 6:CF:63:TYR:HE2 | 1.46 | 0.79 |
| 1:AA:1013:G:H21 | 1:AA:1016:A:H8 | 1.30 | 0.79 |
| 23:DA:2472:G:H5' | 23:DA:2473:U:H5'' | 1.65 | 0.79 |
| 1:AA:942:G:H2' | 1:AA:943:U:H6 | 1.45 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:DA:80:G:N7 | 56:DA:4050:HOH:O | 2.15 | 0.79 |
| 1:CA:1350:A:N6 | 1:CA:1372:U:H3 | 1.81 | 0.79 |
| 23:BA:1517:G:O6 | 56:BA:4420:HOH:O | 2.00 | 0.79 |
| 1:CA:977:A:O2' | 1:CA:981:U:N3 | 2.12 | 0.79 |
| 1:CA:90:U:H2' | 1:CA:91:C:C6 | 2.18 | 0.79 |
| 23:BA:1888:G:N7 | 56:BA:4835:HOH:O | 2.15 | 0.79 |
| 23:BA:1607:C:N4 | 23:BA:1622:G:OP2 | 2.16 | 0.79 |
| 23:BA:2296:U:O4 | 23:BA:2335:A:C6 | 2.36 | 0.79 |
| 23:BA:885:C:C4 | 23:BA:890:A:C6 | 2.69 | 0.79 |
| 40:DW:25:ARG:NH2 | 40:DW:74:ALA:O | 2.16 | 0.79 |
| 1:CA:1457:G:H2' | 1:CA:1458:G:C8 | 2.17 | 0.79 |
| 25:BD:239:ARG:N | 56:BD:410:HOH:O | 2.15 | 0.79 |
| 1:AA:1268:A:N3 | 1:AA:1326:C:O2' | 2.15 | 0.79 |
| 23:BA:2298:A:H62 | 23:BA:2318:G:H8 | 1.27 | 0.79 |
| 23:DA:1604:C:OP1 | 56:DA:3790:HOH:O | 2.01 | 0.79 |
| 1:CA:1075:C:OP1 | 2:CB:179:LYS:NZ | 2.13 | 0.79 |
| 28:BG:105:LYS:NZ | 48:B4:25:TYR:O | 2.16 | 0.79 |
| 19:AS:46:GLY:HA2 | 19:AS:61:TYR:HE1 | 1.47 | 0.78 |
| 23:BA:1664:A:OP1 | 56:BA:4771:HOH:O | 2.00 | 0.78 |
| 23:BA:1019:U:H3 | 23:BA:1142(A):A:H62 | 1.29 | 0.78 |
| 1:AA:1010:G:H1 | 1:AA:1019:C:H42 | 0.82 | 0.78 |
| 2:CB:87:ARG:HE | 2:CB:233:SER:HB2 | 1.47 | 0.78 |
| 23:BA:784:A:OP1 | 56:BA:4425:HOH:O | 2.00 | 0.78 |
| 10:AJ:48:THR:HA | 10:AJ:62:HIS:HB3 | 1.63 | 0.78 |
| 1:AA:166:G:H2' | 1:AA:167:G:H8 | 1.48 | 0.78 |
| 1:CA:839:U:H5' | 1:CA:840:C:C5 | 2.18 | 0.78 |
| 1:CA:1128:C:N4 | 1:CA:1143:G:H1 | 1.80 | 0.78 |
| 2:AB:87:ARG:HE | 2:AB:233:SER:HB2 | 1.48 | 0.78 |
| 1:AA:12:U:O4 | 56:AA:1980:HOH:O | 2.02 | 0.78 |
| 1:CA:1170:A:H3' | 1:CA:1171:G:C8 | 2.18 | 0.78 |
| 8:CH:4:ASP:OD1 | 8:CH:85:ARG:NH1 | 2.16 | 0.78 |
| 20:AT:10:LEU:HD21 | 20:AT:12:ALA:HB3 | 1.65 | 0.78 |
| 1:CA:1179:A:H4' | 9:CI:103:THR:HA | 1.66 | 0.78 |
| 8:CH:29:SER:HB3 | 8:CH:32:LYS:HG3 | 1.65 | 0.78 |
| 1:AA:1103:C:H5'' | 2:AB:98:LEU:HD13 | 1.64 | 0.78 |
| 17:CQ:76:LEU:HD11 | 17:CQ:79:SER:HB2 | 1.62 | 0.78 |
| 37:DT:95:ARG:HG2 | 37:DT:95:ARG:HH11 | 1.47 | 0.78 |
| 1:AA:977:A:HO2' | 1:AA:981:U:H3 | 1.30 | 0.78 |
| 1:CA:1377:A:H2' | 7:CG:7:ALA:HB1 | 1.64 | 0.78 |
| 1:AA:1327:C:OP1 | 21:AU:20:LYS:N | 2.14 | 0.78 |
| 23:BA:1639:U:H2' | 23:BA:1640:C:H5'' | 1.64 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:DG:138:GLN:HG3 | 28:DG:144:ILE:HG21 | 1.64 | 0.78 |
| 23:BA:1970:A:N1 | 56:BA:5040:HOH:O | 2.16 | 0.78 |
| 43:BZ:82:ARG:HH21 | 43:BZ:82:ARG:HB3 | 1.48 | 0.78 |
| 23:BA:778:G:O6 | 56:BA:3910:HOH:O | 2.02 | 0.78 |
| 23:DA:1670:C:OP1 | 56:DA:3807:HOH:O | 2.01 | 0.78 |
| 23:DA:1022:G:O2' | 56:DA:3688:HOH:O | 2.01 | 0.78 |
| 23:BA:1022:G:H22 | 23:BA:1142(A):A:H2 | 1.31 | 0.78 |
| 1:AA:235:C:H5' | 17:AQ:70:ARG:HG2 | 1.66 | 0.78 |
| 23:BA:31:C:OP1 | 56:BA:3883:HOH:O | 2.01 | 0.78 |
| 1:AA:770:C:OP1 | 56:AA:1879:HOH:O | 2.00 | 0.78 |
| 3:CC:43:LEU:HD23 | 3:CC:47:LEU:HD13 | 1.65 | 0.78 |
| 1:AA:1259:C:O2' | 1:AA:1283:G:N3 | 2.17 | 0.77 |
| 1:AA:1294:G:H2' | 1:AA:1295:G:C8 | 2.19 | 0.77 |
| 23:BA:154(A):C:N4 | 23:BA:171:G:H1 | 1.83 | 0.77 |
| 9:CI:13:ALA:HB1 | 9:CI:73:GLN:HG3 | 1.66 | 0.77 |
| 2:CB:71:VAL:HG13 | 2:CB:93:VAL:HG23 | 1.66 | 0.77 |
| 23:BA:2161:C:C6 | 23:BA:2161:C:OP2 | 2.38 | 0.77 |
| 23:DA:1416:G:O6 | 56:DA:4489:HOH:O | 2.02 | 0.77 |
| 1:CA:176:C:OP1 | 20:CT:29:LYS:NZ | 2.15 | 0.77 |
| 27:DF:101:LEU:O | 27:DF:106:ARG:NH1 | 2.18 | 0.77 |
| 40:BW:25:ARG:NH2 | 40:BW:74:ALA:O | 2.16 | 0.77 |
| 13:AM:108:ARG:HD2 | 13:AM:113:PRO:HA | 1.65 | 0.77 |
| 23:DA:945:A:N7 | 56:DA:3684:HOH:O | 2.17 | 0.77 |
| 23:DA:411:G:OP1 | 56:DA:4065:HOH:O | 2.02 | 0.77 |
| 23:BA:1468:C:OP1 | 56:BA:4172:HOH:O | 2.02 | 0.77 |
| 23:DA:574:C:OP1 | 56:DA:3903:HOH:O | 2.03 | 0.77 |
| 23:DA:1639:U:OP1 | 56:DA:3985:HOH:O | 2.02 | 0.77 |
| 7:CG:16:LEU:HD22 | 9:CI:45:ALA:H | 1.49 | 0.77 |
| 23:BA:2285:C:OP2 | 50:B6:6:ARG:NH1 | 2.17 | 0.77 |
| 1:CA:1349:A:H2' | 1:CA:1350:A:H8 | 1.50 | 0.77 |
| 23:BA:2472:G:H5' | 23:BA:2473:U:H5'' | 1.66 | 0.77 |
| 1:AA:750:G:N3 | 15:AO:23:GLY:HA3 | 1.99 | 0.77 |
| 1:AA:352:C:OP2 | 56:AA:1847:HOH:O | 2.01 | 0.77 |
| 2:AB:71:VAL:HG13 | 2:AB:93:VAL:HG23 | 1.66 | 0.77 |
| 23:BA:1840:G:N7 | 56:BA:4640:HOH:O | 2.17 | 0.77 |
| 23:DA:2206:G:H5' | 23:DA:2207:G:N7 | 1.99 | 0.77 |
| 1:AA:1162:C:H42 | 1:AA:1174:G:H1 | 1.28 | 0.77 |
| 1:AA:1459:C:C3' | 1:AA:1460:A:N7 | 2.46 | 0.77 |
| 14:CN:32:SER:HB3 | 14:CN:41:ARG:HB3 | 1.67 | 0.77 |
| 1:CA:266:G:O2' | 1:CA:267:C:OP2 | 2.02 | 0.77 |
| 1:AA:266:G:O2' | 1:AA:267:C:OP2 | 2.01 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:1971:A:OP1 | 56:DA:4210:HOH:O | 2.02 | 0.77 |
| 1:CA:1237:C:N4 | 1:CA:1337:G:H1 | 1.82 | 0.77 |
| 1:CA:235:C:H5' | 17:CQ:70:ARG:HG2 | 1.64 | 0.77 |
| 1:CA:953:G:N1 | 1:CA:1228:C:O2 | 2.17 | 0.76 |
| 23:DA:452:G:OP2 | 56:DA:4034:HOH:O | 2.01 | 0.76 |
| 6:CF:7:ASN:HD21 | 18:CR:34:TYR:HE1 | 1.31 | 0.76 |
| 1:AA:773:G:OP1 | 56:AA:1808:HOH:O | 2.02 | 0.76 |
| 10:AJ:50:ILE:HA | 10:AJ:60:ARG:HG2 | 1.65 | 0.76 |
| 1:CA:1235:U:O2' | 1:CA:1305:G:OP1 | 2.03 | 0.76 |
| 23:DA:1639:U:H2' | 23:DA:1640:C:H5'' | 1.66 | 0.76 |
| 23:BA:1535:A:OP2 | 23:BA:1535:A:H3' | 1.84 | 0.76 |
| 1:CA:547:A:OP1 | 56:CA:1986:HOH:O | 2.04 | 0.76 |
| 24:DB:66:A:H61 | 24:DB:109:C:H5' | 1.49 | 0.76 |
| 25:BD:118:VAL:H | 25:BD:129:ASN:ND2 | 1.83 | 0.76 |
| 1:CA:1222:G:OP2 | 1:CA:1322:C:N4 | 2.19 | 0.76 |
| 7:CG:46:ALA:HA | 7:CG:121:ALA:HB2 | 1.68 | 0.76 |
| 17:AQ:76:LEU:HD11 | 17:AQ:79:SER:HB2 | 1.68 | 0.76 |
| 31:DN:20:GLY:HA2 | 31:DN:61:ARG:HG3 | 1.66 | 0.76 |
| 13:AM:23:TYR:HD1 | 13:AM:67:GLU:HG2 | 1.51 | 0.76 |
| 1:CA:1005:A:H1' | 1:CA:1036:G:H22 | 1.50 | 0.76 |
| 1:AA:942:G:H2' | 1:AA:943:U:C6 | 2.20 | 0.76 |
| 23:BA:2408:U:OP2 | 56:BA:4497:HOH:O | 2.04 | 0.76 |
| 1:AA:1030(C):G:O6 | 1:AA:1031:G:N2 | 2.19 | 0.76 |
| 23:BA:2439:A:O2' | 56:BA:4426:HOH:O | 2.03 | 0.76 |
| 15:AO:54:ARG:HG2 | 15:AO:58:MET:HE2 | 1.67 | 0.76 |
| 23:DA:2296:U:O4 | 23:DA:2335:A:C6 | 2.38 | 0.76 |
| 23:DA:2136:C:H42 | 23:DA:2155:G:H1 | 1.33 | 0.76 |
| 1:CA:1130:A:H4' | 9:CI:3:GLN:HE22 | 1.51 | 0.76 |
| 1:CA:1273:G:H3' | 1:CA:1274:G:H8 | 1.50 | 0.76 |
| 1:CA:1254:C:H42 | 1:CA:1283:G:H1 | 1.33 | 0.76 |
| 23:BA:2206:G:H5' | 23:BA:2207:G:N7 | 2.01 | 0.76 |
| 23:BA:2070:G:OP2 | 56:BA:3863:HOH:O | 2.04 | 0.76 |
| 1:AA:1244:C:H2' | 1:AA:1245:A:C8 | 2.21 | 0.75 |
| 2:AB:197:VAL:O | 8:AH:68:ARG:NH2 | 2.19 | 0.75 |
| 23:DA:1236:G:OP1 | 56:DA:4251:HOH:O | 2.04 | 0.75 |
| 13:AM:19:LEU:HA | 13:AM:22:ILE:HG13 | 1.69 | 0.75 |
| 23:BA:744:G:OP1 | 56:BA:4604:HOH:O | 2.03 | 0.75 |
| 1:AA:345:C:P | 37:BT:39:ARG:HH22 | 2.09 | 0.75 |
| 23:BA:2365:G:OP1 | 56:BA:4102:HOH:O | 2.03 | 0.75 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:H8 | 1.52 | 0.75 |
| 23:BA:1790:C:N3 | 56:BA:3738:HOH:O | 2.18 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 23:BA:990:A:OP2 | 56:BA:4518:HOH:O | 2.04 | 0.75 |
| 1:CA:1004:A:N6 | 1:CA:1035:A:N7 | 2.34 | 0.75 |
| 23:DA:1607:C:N4 | 23:DA:1622:G:OP2 | 2.19 | 0.75 |
| 23:BA:188:G:N7 | 56:BA:4302:HOH:O | 2.18 | 0.75 |
| 23:DA:2407:G:OP1 | 56:DA:4068:HOH:O | 2.04 | 0.75 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:H8 | 1.49 | 0.75 |
| 23:BA:1319:G:OP2 | 56:BA:3806:HOH:O | 2.04 | 0.75 |
| 1:CA:177:C:OP1 | 20:CT:65:LYS:NZ | 2.19 | 0.75 |
| 23:BA:380:U:OP1 | 56:BA:4338:HOH:O | 2.05 | 0.75 |
| 11:CK:79:SER:HA | 11:CK:104:GLN:HB2 | 1.68 | 0.75 |
| 2:CB:54:THR:HG23 | 2:CB:199:TYR:HB3 | 1.69 | 0.75 |
| 23:BA:942:G:O6 | 56:BA:4958:HOH:O | 2.04 | 0.75 |
| 23:DA:386:G:O3' | 56:DA:4075:HOH:O | 2.03 | 0.75 |
| 1:CA:1251:A:N6 | 1:CA:1354:C:O2' | 2.17 | 0.75 |
| 23:DA:2005:A:OP1 | 56:DA:3802:HOH:O | 2.03 | 0.75 |
| 23:DA:1268:A:OP1 | 56:DA:3880:HOH:O | 2.04 | 0.75 |
| 23:BA:2147:G:H2' | 23:BA:2148:G:O4' | 1.86 | 0.75 |
| 1:CA:750:G:N3 | 15:CO:23:GLY:HA3 | 2.01 | 0.75 |
| 7:CG:69:VAL:HG21 | 7:CG:104:LEU:HD13 | 1.69 | 0.75 |
| 23:DA:1226:A:OP1 | 39:DV:84:LYS:NZ | 2.18 | 0.75 |
| 2:AB:54:THR:HG23 | 2:AB:199:TYR:HB3 | 1.69 | 0.75 |
| 23:DA:399:G:OP2 | 56:DA:4081:HOH:O | 2.04 | 0.75 |
| 23:DA:853:G:O6 | 56:DA:4226:HOH:O | 2.04 | 0.75 |
| 23:DA:1376:C:OP2 | 56:DA:3933:HOH:O | 2.05 | 0.75 |
| 23:BA:1900:A:OP2 | 56:BA:4627:HOH:O | 2.05 | 0.75 |
| 24:BB:31:C:O2' | 24:BB:53:A:N6 | 2.20 | 0.75 |
| 2:CB:197:VAL:O | 8:CH:68:ARG:NH2 | 2.20 | 0.75 |
| 23:BA:1980:G:O2' | 23:BA:1982:C:OP2 | 2.04 | 0.75 |
| 23:DA:2296:U:OP2 | 36:DS:9:ARG:NH2 | 2.18 | 0.75 |
| 3:CC:17:ASP:O | 3:CC:54:ARG:NH2 | 2.19 | 0.75 |
| 4:AD:159:ARG:O | 4:AD:163:GLU:N | 2.16 | 0.75 |
| 50:B6:22:ALA:O | 56:B6:201:HOH:O | 2.05 | 0.75 |
| 9:CI:15:ALA:HB2 | 9:CI:65:VAL:HG23 | 1.69 | 0.74 |
| 19:CS:36:ARG:NH1 | 19:CS:75:ALA:O | 2.19 | 0.74 |
| 1:CA:166:G:H2' | 1:CA:167:G:H8 | 1.52 | 0.74 |
| 31:DN:47:ALA:HB2 | 31:DN:112:LEU:HD11 | 1.68 | 0.74 |
| 23:DA:1817:G:OP1 | 25:DD:88:ARG:NH2 | 2.19 | 0.74 |
| 1:CA:192:U:H2' | 1:CA:193:C:H6 | 1.51 | 0.74 |
| 1:CA:1459:C:O3' | 1:CA:1460:A:H8 | 1.67 | 0.74 |
| 1:CA:1262:C:N3 | 1:CA:1273:G:N2 | 2.34 | 0.74 |
| 1:AA:1304:G:O2' | 1:AA:1333:A:N6 | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 7:CG:73:MET:HG2 | 7:CG:145:ALA:HB1 | 1.69 | 0.74 |
| 23:DA:2147:G:H2' | 23:DA:2148:G:O4' | 1.87 | 0.74 |
| 30:DI:87:LYS:H | 30:DI:122:GLU:HA | 1.52 | 0.74 |
| 11:AK:79:SER:HA | 11:AK:104:GLN:HB2 | 1.68 | 0.74 |
| 23:BA:2371:G:O6 | 56:BA:4873:HOH:O | 2.05 | 0.74 |
| 1:CA:1457:G:C5 | 1:CA:1458:G:N7 | 2.55 | 0.74 |
| 23:DA:2712:U:O2' | 23:DA:2712(A):A:OP2 | 2.06 | 0.74 |
| 1:AA:839:U:H5' | 1:AA:840:C:C5 | 2.18 | 0.74 |
| 1:AA:1060:C:H2' | 1:AA:1061:G:H8 | 1.52 | 0.74 |
| 1:CA:1010:G:H2' | 1:CA:1011:G:H8 | 1.52 | 0.74 |
| 23:BA:71:A:C2 | 41:BX:31:HIS:HE1 | 2.05 | 0.74 |
| 4:AD:57:ARG:HE | 4:AD:202:LEU:HD22 | 1.53 | 0.74 |
| 1:AA:1219:U:OP1 | 14:AN:19:ARG:NH2 | 2.20 | 0.74 |
| 23:BA:1190:G:N7 | 56:BA:4525:HOH:O | 2.20 | 0.74 |
| 25:BD:234:GLY:O | 56:BD:415:HOH:O | 2.04 | 0.74 |
| 1:AA:1005:A:OP1 | 1:AA:1024:G:N2 | 2.20 | 0.74 |
| 1:CA:949:A:H1' | 1:CA:1364:U:H3 | 1.50 | 0.74 |
| 13:CM:86:CYS:HB3 | 13:CM:89:GLY:N | 2.01 | 0.74 |
| 1:AA:1156:G:H21 | 1:AA:1179:A:H61 | 1.36 | 0.74 |
| 23:BA:910:A:OP2 | 56:BA:4357:HOH:O | 2.04 | 0.74 |
| 28:DG:76:SER:HA | 28:DG:83:ARG:HA | 1.69 | 0.74 |
| 1:CA:1006:C:H2' | 1:CA:1007:C:C2 | 2.23 | 0.74 |
| 1:CA:437:U:H5'' | 4:CD:155:LEU:HD11 | 1.69 | 0.74 |
| 25:DD:118:VAL:H | 25:DD:129:ASN:HD22 | 1.36 | 0.74 |
| 1:CA:447:G:OP2 | 56:CA:1821:HOH:O | 2.05 | 0.74 |
| 23:DA:528:A:O2' | 56:DA:4767:HOH:O | 2.04 | 0.74 |
| 23:DA:1637:A:OP2 | 56:DA:3960:HOH:O | 2.06 | 0.74 |
| 1:CA:946:A:H61 | 1:CA:1235:U:H3 | 1.35 | 0.74 |
| 23:DA:1913:A:OP2 | 23:DA:1913:A:H3' | 1.86 | 0.74 |
| 1:CA:1346:A:H2 | 1:CA:1347:G:H21 | 1.33 | 0.74 |
| 48:D4:18:CYS:SG | 48:D4:39:CYS:HB3 | 2.28 | 0.74 |
| 9:CI:4:TYR:CZ | 9:CI:88:TYR:HB2 | 2.23 | 0.74 |
| 1:AA:1457:G:OP1 | 20:AT:39:LYS:NZ | 2.21 | 0.74 |
| 1:CA:1030:C:N3 | 1:CA:1031:G:C2 | 2.56 | 0.74 |
| 1:AA:1243:C:H42 | 1:AA:1294:G:H1 | 1.33 | 0.74 |
| 4:CD:159:ARG:O | 4:CD:163:GLU:N | 2.18 | 0.74 |
| 23:BA:833:U:O2 | 33:BP:55:ARG:NH2 | 2.20 | 0.74 |
| 1:AA:1321:C:H5' | 1:AA:1322:C:H5'' | 1.70 | 0.73 |
| 23:DA:71:A:H2 | 41:DX:31:HIS:HE1 | 1.36 | 0.73 |
| 24:BB:60:C:N4 | 56:BB:316:HOH:O | 2.19 | 0.73 |
| 23:DA:346:A:OP2 | 56:DA:4507:HOH:O | 2.05 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:1030:G:OP1 | 56:BA:4411:HOH:O | 2.05 | 0.73 |
| 1:CA:1444:C:H42 | 1:CA:1458:G:H1 | 1.36 | 0.73 |
| 23:BA:883:G:H1 | 23:BA:893:C:H42 | 1.35 | 0.73 |
| 1:AA:1169:A:H2' | 1:AA:1170:A:C8 | 2.22 | 0.73 |
| 1:AA:1128:C:N4 | 1:AA:1143:G:H1 | 1.86 | 0.73 |
| 23:BA:1171:G:H1' | 23:BA:1173:G:H5' | 1.69 | 0.73 |
| 43:DZ:10:ARG:NH2 | 43:DZ:26:GLY:O | 2.20 | 0.73 |
| 9:AI:26:VAL:HB | 9:AI:33:PHE:HA | 1.69 | 0.73 |
| 23:BA:2296:U:OP2 | 36:BS:9:ARG:NH2 | 2.21 | 0.73 |
| 23:BA:271(A):A:N7 | 23:BA:271(W):G:N2 | 2.35 | 0.73 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:H8 | 1.51 | 0.73 |
| 24:BB:86:G:O6 | 56:BB:339:HOH:O | 2.06 | 0.73 |
| 23:BA:1047:G:H2' | 23:BA:1110:G:H22 | 1.53 | 0.73 |
| 1:AA:1442:G:N7 | 1:AA:1442(A):G:C6 | 2.57 | 0.73 |
| 1:CA:940:C:N4 | 1:CA:1343:G:H1 | 1.84 | 0.73 |
| 2:AB:219:VAL:HA | 2:AB:222:ILE:HD12 | 1.71 | 0.73 |
| 23:DA:1377:G:OP2 | 56:DA:3929:HOH:O | 2.06 | 0.73 |
| 23:DA:607:U:OP1 | 27:DF:102:PRO:HA | 1.88 | 0.73 |
| 7:CG:43:PHE:HA | 7:CG:46:ALA:HB3 | 1.70 | 0.73 |
| 52:B8:33:ASN:HA | 52:B8:36:LYS:HD2 | 1.69 | 0.73 |
| 23:BA:1913:A:H3' | 23:BA:1913:A:OP2 | 1.88 | 0.73 |
| 23:BA:2109:U:H3 | 23:BA:2180:U:H3 | 1.36 | 0.73 |
| 7:CG:88:PRO:HG2 | 7:CG:152:ALA:HA | 1.70 | 0.73 |
| 23:DA:271(F):C:H2' | 23:DA:271(G):C:H6 | 1.51 | 0.73 |
| 23:DA:278:A:O2' | 23:DA:279:C:OP1 | 2.06 | 0.73 |
| 37:BT:95:ARG:HG2 | 37:BT:95:ARG:HH11 | 1.53 | 0.73 |
| 49:D5:16:ARG:HG2 | 49:D5:16:ARG:HH11 | 1.52 | 0.73 |
| 1:AA:1442(B):A:N7 | 37:BT:118:ARG:NH2 | 2.35 | 0.73 |
| 1:AA:1294:G:H2' | 1:AA:1295:G:H8 | 1.53 | 0.73 |
| 9:AI:71:SER:HA | 9:AI:74:ILE:HG22 | 1.69 | 0.73 |
| 23:DA:154(A):C:N4 | 23:DA:171:G:H1 | 1.85 | 0.73 |
| 1:AA:484:G:O2' | 1:AA:485:G:OP2 | 2.07 | 0.73 |
| 23:DA:141:A:H8 | 23:DA:1408:C:HO2' | 1.32 | 0.73 |
| 23:BA:531:C:OP1 | 23:BA:561:G:N2 | 2.20 | 0.73 |
| 23:BA:1845:G:N7 | 56:BA:5140:HOH:O | 2.22 | 0.73 |
| 23:DA:29:U:H2' | 23:DA:30:G:C8 | 2.22 | 0.73 |
| 14:CN:7:ILE:HG22 | 14:CN:23:ARG:HE | 1.52 | 0.73 |
| 6:AF:7:ASN:HD21 | 18:AR:34:TYR:HE1 | 1.34 | 0.73 |
| 1:CA:1376:U:H2' | 1:CA:1377:A:C8 | 2.24 | 0.73 |
| 1:CA:484:G:O2' | 1:CA:485:G:OP2 | 2.06 | 0.73 |
| 23:DA:1250:G:N7 | 33:DP:18:ARG:NH2 | 2.37 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:DI:40:THR:O | 30:DI:44:LEU:N | 2.17 | 0.73 |
| 1:AA:1457:G:C5 | 1:AA:1458:G:N7 | 2.56 | 0.73 |
| 37:DT:118:ARG:CZ | 37:DT:118:ARG:HA | 2.19 | 0.73 |
| 1:CA:1324:A:H5' | 1:CA:1363:C:H5'' | 1.71 | 0.73 |
| 14:CN:16:PHE:H | 14:CN:19:ARG:HB2 | 1.54 | 0.73 |
| 1:AA:1441:G:O2' | 1:AA:1459:C:N4 | 2.21 | 0.73 |
| 1:CA:1165:C:N4 | 1:CA:1171:G:H1 | 1.86 | 0.73 |
| 2:CB:60:ASP:O | 2:CB:64:ARG:HG3 | 1.89 | 0.73 |
| 23:BA:2534:A:N7 | 56:BA:5059:HOH:O | 2.21 | 0.73 |
| 1:AA:192:U:H2' | 1:AA:193:C:H6 | 1.53 | 0.73 |
| 3:AC:11:ARG:HE | 3:AC:180:ALA:HB3 | 1.53 | 0.72 |
| 1:AA:993:G:N2 | 1:AA:996:A:H61 | 1.86 | 0.72 |
| 23:BA:2136:C:H42 | 23:BA:2155:G:H1 | 1.36 | 0.72 |
| 23:BA:2706:G:O6 | 56:BA:4852:HOH:O | 2.06 | 0.72 |
| 1:AA:251:G:N7 | 56:AA:1924:HOH:O | 2.22 | 0.72 |
| 7:CG:138:LYS:NZ | 7:CG:142:GLU:OE1 | 2.20 | 0.72 |
| 11:AK:31:THR:HG22 | 11:AK:42:TRP:HB2 | 1.71 | 0.72 |
| 23:DA:768:G:N7 | 56:DA:3978:HOH:O | 2.21 | 0.72 |
| 23:DA:2526:G:H21 | 53:D9:2:LYS:HG2 | 1.54 | 0.72 |
| 1:AA:222:U:H2' | 1:AA:223:U:C6 | 2.24 | 0.72 |
| 23:DA:1721:G:H8 | 23:DA:1741:A:H62 | 1.37 | 0.72 |
| 1:CA:1442:G:N7 | 1:CA:1442(A):G:C6 | 2.57 | 0.72 |
| 1:CA:427:U:OP2 | 4:CD:36:ARG:NH2 | 2.22 | 0.72 |
| 23:BA:2287:A:H62 | 23:BA:2344:U:H3 | 1.36 | 0.72 |
| 1:AA:1075:C:OP1 | 2:AB:179:LYS:NZ | 2.15 | 0.72 |
| 23:BA:1817:G:OP1 | 25:BD:88:ARG:NH2 | 2.23 | 0.72 |
| 23:BA:674:G:OP2 | 56:BA:3870:HOH:O | 2.07 | 0.72 |
| 43:BZ:10:ARG:NH2 | 43:BZ:26:GLY:O | 2.22 | 0.72 |
| 1:CA:1147:C:O2 | 9:CI:16:ARG:NH2 | 2.23 | 0.72 |
| 1:AA:1118:C:H2' | 1:AA:1119:C:C6 | 2.25 | 0.72 |
| 23:BA:1022:G:O2' | 56:BA:3731:HOH:O | 2.05 | 0.72 |
| 23:BA:1721:G:H8 | 23:BA:1741:A:H62 | 1.37 | 0.72 |
| 28:BG:76:SER:HA | 28:BG:83:ARG:HA | 1.71 | 0.72 |
| 15:AO:39:LEU:HB3 | 15:AO:56:LEU:HD23 | 1.71 | 0.72 |
| 1:CA:1443:G:O6 | 1:CA:1459:C:C2 | 2.42 | 0.72 |
| 23:DA:1019:U:HO2' | 23:DA:1021:A:H2 | 1.37 | 0.72 |
| 23:DA:1237:A:OP1 | 56:DA:4018:HOH:O | 2.06 | 0.72 |
| 36:DS:11:LYS:HG3 | 36:DS:91:PRO:HD3 | 1.72 | 0.72 |
| 34:DQ:58:PHE:HB3 | 34:DQ:61:GLY:HA3 | 1.72 | 0.72 |
| 19:CS:46:GLY:HA2 | 19:CS:61:TYR:CE1 | 2.25 | 0.72 |
| 1:AA:1377:A:H8 | 1:AA:1377:A:H3' | 1.55 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:36:ASP:HA | 3:CC:39:ILE:HD12 | 1.70 | 0.72 |
| 23:DA:411:G:H5'' | 56:DA:4065:HOH:O | 1.90 | 0.72 |
| 5:AE:80:ILE:HG13 | 5:AE:91:LEU:HB2 | 1.72 | 0.72 |
| 1:AA:735:C:H2' | 1:AA:736:C:H6 | 1.53 | 0.72 |
| 25:DD:17:THR:O | 25:DD:211:ARG:NH2 | 2.21 | 0.72 |
| 15:CO:16:ALA:HB1 | 15:CO:21:ASP:HB3 | 1.72 | 0.72 |
| 37:DT:64:ARG:NH1 | 37:DT:103:ARG:HA | 2.05 | 0.72 |
| 23:DA:404:C:OP1 | 56:DA:4250:HOH:O | 2.06 | 0.72 |
| 1:CA:1231:G:N2 | 1:CA:1232:U:H1' | 2.05 | 0.72 |
| 1:AA:993:G:H21 | 1:AA:996:A:H61 | 1.37 | 0.72 |
| 1:CA:964:A:H2' | 1:CA:969:A:H1' | 1.71 | 0.72 |
| 30:BI:83:ALA:HB2 | 30:BI:88:ILE:HA | 1.70 | 0.72 |
| 1:CA:97:G:HO2' | 1:CA:98:G:H8 | 1.37 | 0.72 |
| 23:BA:1429:G:H2' | 23:BA:1430:C:C6 | 2.25 | 0.72 |
| 1:AA:1441:G:N2 | 1:AA:1459:C:C5 | 2.57 | 0.72 |
| 2:CB:87:ARG:HH21 | 2:CB:233:SER:H | 1.37 | 0.72 |
| 10:AJ:8:LEU:HD22 | 10:AJ:96:ILE:HG22 | 1.71 | 0.72 |
| 23:BA:607:U:OP1 | 27:BF:102:PRO:HA | 1.90 | 0.72 |
| 7:CG:41:ARG:NH2 | 9:CI:39:GLY:O | 2.23 | 0.72 |
| 23:DA:1394:U:OP1 | 56:DA:3790:HOH:O | 2.08 | 0.72 |
| 23:DA:1507:A:O2' | 23:DA:1508:A:H8 | 1.72 | 0.72 |
| 1:CA:148:G:H2' | 1:CA:149:A:H8 | 1.54 | 0.72 |
| 3:CC:13:GLY:HA3 | 14:CN:57:ARG:HH22 | 1.55 | 0.72 |
| 23:BA:2117:A:H61 | 23:BA:2166:G:H22 | 1.38 | 0.72 |
| 1:CA:1131:G:H1 | 1:CA:1143:G:H21 | 1.38 | 0.71 |
| 23:BA:243:U:OP1 | 52:B8:6:THR:OG1 | 2.08 | 0.71 |
| 1:CA:939:G:H1 | 1:CA:1344:C:N4 | 1.87 | 0.71 |
| 23:DA:2287:A:H62 | 23:DA:2344:U:H3 | 1.37 | 0.71 |
| 23:DA:2126:A:N6 | 23:DA:2163:C:H5' | 2.05 | 0.71 |
| 23:DA:1332:G:OP1 | 56:DA:3783:HOH:O | 2.08 | 0.71 |
| 20:CT:10:LEU:HG | 20:CT:12:ALA:H | 1.54 | 0.71 |
| 28:DG:105:LYS:NZ | 48:D4:25:TYR:O | 2.22 | 0.71 |
| 1:AA:1329:A:H5'' | 13:AM:25:ILE:HA | 1.72 | 0.71 |
| 23:BA:882:G:H1 | 23:BA:894:C:H42 | 1.38 | 0.71 |
| 2:CB:137:ARG:HH11 | 2:CB:137:ARG:HB2 | 1.55 | 0.71 |
| 1:CA:976:G:N2 | 1:CA:1363(A):A:OP1 | 2.23 | 0.71 |
| 30:BI:130:TYR:HB3 | 30:BI:138:ILE:HB | 1.70 | 0.71 |
| 23:BA:1324:G:O6 | 56:BA:4953:HOH:O | 2.07 | 0.71 |
| 23:BA:2322:A:N6 | 23:BA:2335:A:H61 | 1.87 | 0.71 |
| 23:DA:2268:A:OP1 | 56:DA:4335:HOH:O | 2.08 | 0.71 |
| 23:BA:1634:A:N1 | 56:BA:4325:HOH:O | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:DV:62:LEU:HD11 | 39:DV:95:LEU:HB2 | 1.72 | 0.71 |
| 23:DA:2109:U:H3 | 23:DA:2180:U:H3 | 1.38 | 0.71 |
| 23:BA:1370:C:OP1 | 56:BA:4694:HOH:O | 2.08 | 0.71 |
| 13:CM:71:ARG:HA | 13:CM:74:VAL:HB | 1.71 | 0.71 |
| 1:CA:642:A:N3 | 8:CH:113:SER:OG | 2.22 | 0.71 |
| 23:DA:1495:A:OP2 | 56:DA:4274:HOH:O | 2.07 | 0.71 |
| 23:DA:2226:C:OP2 | 56:DA:4146:HOH:O | 2.07 | 0.71 |
| 1:AA:1220:G:H2' | 1:AA:1221:G:O4' | 1.91 | 0.71 |
| 1:AA:1118:C:N4 | 1:AA:1155:G:H1 | 1.86 | 0.71 |
| 23:BA:1045:A:N3 | 23:BA:1045:A:H2' | 2.04 | 0.71 |
| 13:CM:70:LEU:O | 13:CM:74:VAL:N | 2.24 | 0.71 |
| 2:AB:167:PRO:O | 2:AB:171:ALA:N | 2.24 | 0.71 |
| 7:AG:74:GLU:O | 7:AG:89:MET:N | 2.23 | 0.71 |
| 23:DA:2646:C:OP2 | 23:DA:2732:G:O2' | 2.07 | 0.71 |
| 2:AB:60:ASP:O | 2:AB:64:ARG:HG3 | 1.91 | 0.71 |
| 23:BA:1235:G:OP1 | 56:BA:4227:HOH:O | 2.08 | 0.71 |
| 13:AM:86:CYS:HB3 | 13:AM:89:GLY:HA3 | 1.72 | 0.71 |
| 1:CA:538:G:H5'' | 12:CL:114:LYS:HB2 | 1.72 | 0.71 |
| 3:CC:6:HIS:HD2 | 3:CC:7:PRO:HD2 | 1.55 | 0.71 |
| 23:BA:269:U:OP1 | 56:BA:5071:HOH:O | 2.07 | 0.71 |
| 1:CA:576:G:OP1 | 56:CA:1944:HOH:O | 2.08 | 0.71 |
| 43:DZ:110:GLY:HA3 | 43:DZ:174:VAL:HG11 | 1.71 | 0.71 |
| 23:DA:1560:G:OP1 | 56:DA:4341:HOH:O | 2.08 | 0.71 |
| 1:CA:1156:G:H21 | 1:CA:1179:A:N6 | 1.88 | 0.71 |
| 23:BA:1665:A:OP2 | 56:BA:4771:HOH:O | 2.09 | 0.71 |
| 39:DV:56:SER:H | 39:DV:100:ARG:HB2 | 1.53 | 0.71 |
| 50:D6:3:SER:OG | 50:D6:4:GLU:N | 2.24 | 0.71 |
| 23:DA:392:C:OP1 | 56:DA:4594:HOH:O | 2.07 | 0.71 |
| 7:CG:15:ASP:N | 7:CG:20:ASP:O | 2.18 | 0.71 |
| 1:AA:1224:G:N1 | 1:AA:1363:C:O2 | 2.24 | 0.71 |
| 10:CJ:8:LEU:O | 10:CJ:69:ASN:HA | 1.89 | 0.71 |
| 9:AI:3:GLN:NE2 | 9:AI:4:TYR:O | 2.23 | 0.71 |
| 1:CA:1176:A:H2' | 1:CA:1177:G:C8 | 2.26 | 0.71 |
| 1:CA:735:C:H2' | 1:CA:736:C:H6 | 1.54 | 0.71 |
| 23:BA:1204:A:H2 | 23:BA:1241:A:H62 | 1.37 | 0.71 |
| 28:DG:56:ALA:HB2 | 28:DG:153:ARG:HE | 1.56 | 0.71 |
| 23:DA:2042:A:OP1 | 56:DA:3616:HOH:O | 2.09 | 0.71 |
| 14:CN:24:CYS:HB2 | 14:CN:40:CYS:N | 2.06 | 0.71 |
| 11:CK:31:THR:HG22 | 11:CK:42:TRP:HB2 | 1.72 | 0.71 |
| 1:CA:903:G:OP1 | 56:CA:1954:HOH:O | 2.09 | 0.71 |
| 2:AB:137:ARG:HB2 | 2:AB:137:ARG:HH11 | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:1047:G:H2' | 23:DA:1110:G:H22 | 1.54 | 0.71 |
| 4:AD:108:LEU:HD11 | 4:AD:174:LEU:HD22 | 1.72 | 0.71 |
| 23:DA:1313:U:OP1 | 56:DA:3775:HOH:O | 2.09 | 0.71 |
| 13:CM:15:VAL:HG22 | 13:CM:41:PRO:HA | 1.72 | 0.71 |
| 1:CA:1347:G:N2 | 1:CA:1374:A:O5' | 2.24 | 0.71 |
| 23:BA:2126:A:N6 | 23:BA:2163:C:H5' | 2.06 | 0.71 |
| 1:AA:352:C:O2' | 1:AA:354:G:OP1 | 2.07 | 0.71 |
| 6:AF:61:LEU:HB3 | 6:AF:63:TYR:HE2 | 1.55 | 0.71 |
| 39:BV:72:VAL:HG13 | 39:BV:85:LYS:HB3 | 1.71 | 0.71 |
| 1:CA:1342:C:H2' | 1:CA:1343:G:C8 | 2.25 | 0.70 |
| 23:DA:2747:G:N7 | 56:DA:4479:HOH:O | 2.24 | 0.70 |
| 28:BG:56:ALA:HB2 | 28:BG:153:ARG:HE | 1.56 | 0.70 |
| 29:DH:56:SER:OG | 29:DH:61:HIS:ND1 | 2.24 | 0.70 |
| 13:CM:3:ARG:NH2 | 13:CM:45:VAL:O | 2.21 | 0.70 |
| 1:AA:73:G:H1 | 1:AA:96:U:H3 | 1.39 | 0.70 |
| 3:AC:78:GLY:HA3 | 3:AC:83:ARG:H | 1.56 | 0.70 |
| 1:CA:1499:A:OP2 | 56:CA:1857:HOH:O | 2.08 | 0.70 |
| 34:BQ:58:PHE:HB3 | 34:BQ:61:GLY:HA3 | 1.74 | 0.70 |
| 3:AC:186:PHE:CE2 | 3:AC:188:LEU:HB2 | 2.26 | 0.70 |
| 23:DA:1914:C:H2' | 23:DA:1915:U:C6 | 2.26 | 0.70 |
| 3:CC:150:LYS:HB2 | 3:CC:173:VAL:HG21 | 1.73 | 0.70 |
| 1:CA:605:U:H2' | 1:CA:606:G:C8 | 2.26 | 0.70 |
| 1:AA:1441:G:H2' | 1:AA:1459:C:H41 | 0.83 | 0.70 |
| 2:CB:219:VAL:HA | 2:CB:222:ILE:HD12 | 1.73 | 0.70 |
| 23:DA:1210:A:H5'' | 23:DA:1210:A:C8 | 2.26 | 0.70 |
| 27:BF:178:PRO:HB2 | 27:BF:201:VAL:HG11 | 1.72 | 0.70 |
| 1:AA:519:C:OP2 | 12:AL:50:SER:OG | 2.08 | 0.70 |
| 15:CO:54:ARG:HG2 | 15:CO:58:MET:HE2 | 1.70 | 0.70 |
| 26:BE:47:VAL:HG11 | 26:BE:86:PRO:HD2 | 1.73 | 0.70 |
| 1:AA:48:C:O2 | 56:AA:1897:HOH:O | 2.07 | 0.70 |
| 34:BQ:111:GLU:OE1 | 34:BQ:133:ARG:NH2 | 2.24 | 0.70 |
| 23:DA:370:G:OP2 | 56:DA:4078:HOH:O | 2.08 | 0.70 |
| 1:CA:1273:G:H3' | 1:CA:1274:G:C8 | 2.27 | 0.70 |
| 1:CA:1301:U:OP1 | 13:CM:21:TYR:OH | 2.07 | 0.70 |
| 1:CA:1286:A:H2 | 21:CU:22:ARG:HH21 | 1.37 | 0.70 |
| 28:BG:16:ARG:HE | 28:BG:31:VAL:HG21 | 1.57 | 0.70 |
| 1:AA:1367:C:OP1 | 9:AI:115:GLY:N | 2.23 | 0.70 |
| 23:DA:882:G:H1 | 23:DA:894:C:H42 | 1.38 | 0.70 |
| 10:CJ:79:ARG:O | 10:CJ:81:THR:N | 2.21 | 0.70 |
| 1:CA:1173:G:H2' | 1:CA:1174:G:H8 | 1.55 | 0.70 |
| 1:AA:262:A:H2' | 1:AA:263:A:C8 | 2.25 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 26:DE:175:VAL:HG23 | 26:DE:177:PRO:HD3 | 1.73 | 0.70 |
| 30:DI:83:ALA:HA | 30:DI:89:TYR:CE2 | 2.27 | 0.70 |
| 1:AA:365:U:H5'' | 1:AA:366:C:OP1 | 1.91 | 0.70 |
| 1:AA:1444:C:H42 | 1:AA:1458:G:H1 | 1.38 | 0.70 |
| 1:CA:1237:C:H42 | 1:CA:1337:G:H1 | 1.39 | 0.70 |
| 23:DA:2781:A:H5'' | 23:DA:2782:G:H5' | 1.71 | 0.70 |
| 29:BH:154:PRO:HB3 | 29:BH:163:TYR:CZ | 2.27 | 0.70 |
| 23:DA:1186:G:OP1 | 56:DA:4637:HOH:O | 2.09 | 0.70 |
| 3:AC:70:VAL:HG12 | 3:AC:71:ALA:H | 1.56 | 0.70 |
| 23:DA:2115:G:H4' | 23:DA:2167:U:H4' | 1.74 | 0.70 |
| 23:BA:2600:A:OP2 | 56:BA:4426:HOH:O | 2.09 | 0.70 |
| 1:CA:222:U:H2' | 1:CA:223:U:C6 | 2.27 | 0.70 |
| 23:DA:531:C:OP1 | 23:DA:561:G:N2 | 2.24 | 0.70 |
| 24:DB:31:C:O2' | 24:DB:53:A:N6 | 2.24 | 0.70 |
| 3:CC:182:ILE:HG12 | 3:CC:203:PHE:HA | 1.73 | 0.70 |
| 3:CC:134:ILE:HG23 | 3:CC:151:VAL:HB | 1.74 | 0.70 |
| 1:CA:1231:G:N1 | 1:CA:1232:U:O2 | 2.25 | 0.70 |
| 1:AA:986:A:H1' | 19:AS:55:LYS:HA | 1.73 | 0.70 |
| 1:AA:382:A:H2' | 1:AA:383:A:C8 | 2.26 | 0.70 |
| 23:DA:2285:C:OP2 | 50:D6:6:ARG:NH1 | 2.24 | 0.70 |
| 40:BW:13:SER:HB3 | 40:BW:16:LYS:HD2 | 1.72 | 0.70 |
| 43:DZ:82:ARG:HB3 | 43:DZ:82:ARG:HH21 | 1.56 | 0.70 |
| 23:BA:453:C:OP1 | 56:BA:4578:HOH:O | 2.09 | 0.70 |
| 23:DA:2130:U:HO2' | 23:DA:2133:G:HO2' | 1.38 | 0.70 |
| 41:DX:56:THR:O | 56:DX:101:HOH:O | 2.09 | 0.70 |
| 39:DV:72:VAL:HG13 | 39:DV:85:LYS:HB3 | 1.73 | 0.70 |
| 4:CD:104:VAL:HA | 4:CD:107:ARG:HB2 | 1.73 | 0.70 |
| 3:AC:127:ARG:HB3 | 3:AC:127:ARG:HH11 | 1.55 | 0.70 |
| 4:CD:57:ARG:HE | 4:CD:202:LEU:HD22 | 1.57 | 0.70 |
| 30:BI:1:MET:N | 30:BI:21:VAL:O | 2.24 | 0.70 |
| 28:DG:16:ARG:HE | 28:DG:31:VAL:HG21 | 1.57 | 0.69 |
| 2:CB:167:PRO:O | 2:CB:171:ALA:N | 2.25 | 0.69 |
| 23:DA:1364:G:OP2 | 45:D1:3:LYS:HG2 | 1.92 | 0.69 |
| 18:AR:35:ARG:HB3 | 18:AR:35:ARG:NH1 | 2.07 | 0.69 |
| 23:BA:2322:A:H61 | 23:BA:2335:A:H61 | 1.39 | 0.69 |
| 1:AA:1131:G:H1 | 1:AA:1143:G:H21 | 1.40 | 0.69 |
| 36:DS:10:ARG:HH21 | 36:DS:91:PRO:HB2 | 1.57 | 0.69 |
| 23:DA:89:G:H3' | 23:DA:90:U:H5'' | 1.74 | 0.69 |
| 23:BA:2637:U:H5'' | 26:BE:82:ARG:HH21 | 1.57 | 0.69 |
| 13:CM:86:CYS:O | 19:CS:73:GLU:HB3 | 1.91 | 0.69 |
| 23:DA:1778:U:OP2 | 56:DA:4141:HOH:O | 2.10 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:DA:842:G:N7 | 56:DA:4657:HOH:O | 2.24 | 0.69 |
| 25:BD:17:THR:O | 25:BD:211:ARG:NH2 | 2.23 | 0.69 |
| 23:BA:2781:A:H5'' | 23:BA:2782:G:H5' | 1.74 | 0.69 |
| 4:CD:9:CYS:HA | 4:CD:12:CYS:HB2 | 1.73 | 0.69 |
| 23:BA:1997:G:OP2 | 56:BA:4618:HOH:O | 2.10 | 0.69 |
| 1:CA:1161:C:H2' | 1:CA:1162:C:C6 | 2.27 | 0.69 |
| 1:AA:1077:G:N2 | 1:AA:1080:A:OP2 | 2.20 | 0.69 |
| 23:BA:1507:A:O2' | 23:BA:1508:A:H8 | 1.74 | 0.69 |
| 23:DA:2887:U:H2' | 23:DA:2888:C:C6 | 2.27 | 0.69 |
| 23:BA:517:C:OP1 | 49:B5:16:ARG:NH2 | 2.24 | 0.69 |
| 1:CA:1442(B):A:N7 | 37:DT:118:ARG:NH1 | 2.41 | 0.69 |
| 23:BA:29:U:H2' | 23:BA:30:G:C8 | 2.27 | 0.69 |
| 1:CA:1154:G:H2' | 1:CA:1155:G:C8 | 2.28 | 0.69 |
| 30:BI:83:ALA:HA | 30:BI:89:TYR:CE2 | 2.27 | 0.69 |
| 23:BA:1364:G:OP2 | 45:B1:3:LYS:HG2 | 1.91 | 0.69 |
| 23:BA:278:A:O2' | 23:BA:279:C:OP1 | 2.04 | 0.69 |
| 23:BA:2306:C:H3' | 23:BA:2307:G:C8 | 2.27 | 0.69 |
| 23:DA:15:G:OP2 | 56:DA:4618:HOH:O | 2.09 | 0.69 |
| 23:DA:1266:G:O5' | 40:DW:15:ARG:NH2 | 2.24 | 0.69 |
| 23:DA:1380:G:OP2 | 56:DA:4635:HOH:O | 2.09 | 0.69 |
| 10:CJ:44:VAL:HG13 | 10:CJ:66:ARG:HG2 | 1.75 | 0.69 |
| 43:BZ:110:GLY:HA3 | 43:BZ:174:VAL:HG11 | 1.72 | 0.69 |
| 1:AA:1240:U:O4 | 7:AG:30:ILE:HG22 | 1.92 | 0.69 |
| 10:CJ:8:LEU:HD13 | 10:CJ:16:LEU:HG | 1.73 | 0.69 |
| 1:CA:1242:C:O2' | 1:CA:1303:C:OP1 | 2.11 | 0.69 |
| 7:CG:139:GLU:O | 7:CG:143:ARG:NE | 2.25 | 0.69 |
| 4:AD:104:VAL:HA | 4:AD:107:ARG:HB2 | 1.74 | 0.69 |
| 7:AG:71:PRO:HG3 | 7:AG:138:LYS:HG3 | 1.74 | 0.69 |
| 38:DU:92:ARG:HA | 38:DU:95:LEU:HB2 | 1.75 | 0.69 |
| 43:DZ:45:ASP:OD2 | 43:DZ:49:ARG:NH1 | 2.25 | 0.69 |
| 1:AA:1225:A:OP1 | 13:AM:103:THR:N | 2.24 | 0.69 |
| 23:BA:956:G:OP2 | 34:BQ:14:ARG:NH2 | 2.25 | 0.69 |
| 23:DA:1026:U:O2' | 23:DA:1027:A:O5' | 2.10 | 0.69 |
| 1:CA:1089:G:N2 | 1:CA:1096:C:N3 | 2.36 | 0.69 |
| 1:AA:1246:C:N3 | 1:AA:1291:G:N2 | 2.40 | 0.69 |
| 23:DA:2117:A:H61 | 23:DA:2166:G:H22 | 1.37 | 0.69 |
| 28:DG:124:SER:HB2 | 28:DG:131:TYR:CE1 | 2.28 | 0.69 |
| 23:BA:1914:C:H2' | 23:BA:1915:U:C6 | 2.28 | 0.69 |
| 42:BY:23:ARG:HG2 | 42:BY:42:VAL:HG22 | 1.75 | 0.69 |
| 30:DI:126:TYR:HB2 | 30:DI:142:VAL:HG23 | 1.75 | 0.69 |
| 1:CA:405:U:O4 | 4:CD:2:GLY:N | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:B7:24:THR:HG23 | 51:B7:27:GLY:H | 1.55 | 0.69 |
| 10:CJ:50:ILE:HD12 | 10:CJ:50:ILE:H | 1.57 | 0.69 |
| 23:BA:1359:A:N6 | 23:BA:1372:U:C4 | 2.58 | 0.69 |
| 1:CA:1376:U:H5' | 7:CG:102:ARG:HH22 | 1.57 | 0.69 |
| 1:AA:1300:G:O2' | 1:AA:1301:U:O5' | 2.08 | 0.69 |
| 23:BA:2115:G:H4' | 23:BA:2167:U:H4' | 1.74 | 0.69 |
| 23:DA:1434:A:H61 | 23:DA:1558:A:N6 | 1.90 | 0.69 |
| 23:DA:2002:G:O6 | 56:DA:3873:HOH:O | 2.11 | 0.69 |
| 23:DA:1828:G:OP2 | 56:DA:3773:HOH:O | 2.10 | 0.69 |
| 23:DA:587:C:OP2 | 33:DP:21:ARG:NH2 | 2.26 | 0.69 |
| 1:AA:1262:C:H42 | 1:AA:1273:G:H1 | 1.41 | 0.69 |
| 27:DF:53:THR:HG23 | 27:DF:55:GLY:H | 1.57 | 0.69 |
| 23:BA:94:C:H5' | 23:BA:94(A):G:OP2 | 1.93 | 0.69 |
| 23:BA:438:G:O6 | 56:BA:4813:HOH:O | 2.09 | 0.69 |
| 1:AA:1459:C:H6 | 1:AA:1460:A:N7 | 1.90 | 0.69 |
| 1:CA:1460:A:P | 1:CA:1460:A:H8 | 2.15 | 0.69 |
| 1:AA:1222:G:H5'' | 19:AS:78:ARG:NE | 2.08 | 0.69 |
| 23:BA:580:C:H2' | 23:BA:581:C:H6 | 1.57 | 0.69 |
| 23:BA:2588:G:OP1 | 56:BA:4425:HOH:O | 2.10 | 0.69 |
| 3:CC:40:ARG:HA | 3:CC:43:LEU:HD12 | 1.75 | 0.69 |
| 15:CO:39:LEU:HB3 | 15:CO:56:LEU:HD23 | 1.75 | 0.69 |
| 23:BA:392:C:OP1 | 56:BA:3960:HOH:O | 2.11 | 0.69 |
| 26:DE:28:ALA:HB3 | 26:DE:93:VAL:HG12 | 1.74 | 0.69 |
| 5:CE:50:GLU:HB2 | 5:CE:53:LEU:HD22 | 1.74 | 0.69 |
| 23:DA:2322:A:N6 | 23:DA:2335:A:H61 | 1.91 | 0.69 |
| 1:AA:1333:A:H3' | 1:AA:1334:G:H8 | 1.59 | 0.69 |
| 1:AA:1073:U:H2' | 1:AA:1074:G:C8 | 2.28 | 0.69 |
| 23:DA:1495:A:OP2 | 56:DA:4271:HOH:O | 2.11 | 0.69 |
| 11:AK:27:ASN:OD1 | 11:AK:28:THR:N | 2.26 | 0.69 |
| 1:AA:1123:A:H61 | 1:AA:1150:U:H3 | 1.40 | 0.69 |
| 1:AA:1104:G:O3' | 2:AB:111:ARG:NH2 | 2.26 | 0.69 |
| 3:CC:103:VAL:HG12 | 3:CC:104:GLN:H | 1.58 | 0.69 |
| 1:AA:724:G:OP2 | 56:AA:1871:HOH:O | 2.09 | 0.69 |
| 23:BA:1226:A:OP1 | 39:BV:84:LYS:NZ | 2.25 | 0.69 |
| 1:CA:434:U:H2' | 1:CA:435:C:C6 | 2.27 | 0.69 |
| 1:AA:1459:C:O3' | 1:AA:1460:A:H8 | 1.76 | 0.68 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:N1 | 1.92 | 0.68 |
| 23:BA:1266:G:O5' | 40:BW:15:ARG:NH2 | 2.26 | 0.68 |
| 1:AA:377:G:H2' | 1:AA:378:G:C8 | 2.28 | 0.68 |
| 33:DP:59:LEU:HD11 | 52:D8:10:ALA:HB2 | 1.75 | 0.68 |
| 44:B0:53:MET:HG3 | 44:B0:59:LEU:HD23 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1259:C:N4 | 1:AA:1260:C:O2 | 2.26 | 0.68 |
| 1:CA:426:G:OP1 | 4:CD:38:TYR:OH | 2.12 | 0.68 |
| 1:CA:977:A:N6 | 1:CA:1224:G:OP1 | 2.26 | 0.68 |
| 10:CJ:39:PRO:HA | 10:CJ:70:ARG:HG2 | 1.75 | 0.68 |
| 1:CA:952:U:H3 | 1:CA:1229:A:H61 | 1.39 | 0.68 |
| 43:DZ:33:LEU:HD23 | 43:DZ:90:VAL:HG21 | 1.75 | 0.68 |
| 28:DG:106:LEU:HD12 | 28:DG:110:ALA:HB3 | 1.75 | 0.68 |
| 23:BA:1529:G:C6 | 23:BA:1530:C:N4 | 2.61 | 0.68 |
| 23:BA:804:A:OP1 | 56:BA:4505:HOH:O | 2.10 | 0.68 |
| 1:AA:244:U:O2 | 56:AA:1809:HOH:O | 2.07 | 0.68 |
| 28:BG:101:ILE:HD13 | 48:B4:25:TYR:HB2 | 1.76 | 0.68 |
| 23:BA:271(V):G:N7 | 56:BA:4906:HOH:O | 2.26 | 0.68 |
| 27:BF:185:ASP:HA | 27:BF:188:ARG:HD3 | 1.75 | 0.68 |
| 40:DW:84:ARG:HG3 | 40:DW:98:LYS:HD2 | 1.76 | 0.68 |
| 23:DA:1950:G:OP2 | 56:DA:3603:HOH:O | 2.11 | 0.68 |
| 23:DA:2134:A:C2 | 23:DA:2159:G:H1' | 2.28 | 0.68 |
| 23:BA:2010:G:N7 | 56:BA:5219:HOH:O | 2.27 | 0.68 |
| 23:DA:2773:C:H5'' | 26:DE:164:ARG:HG2 | 1.75 | 0.68 |
| 1:AA:434:U:H2' | 1:AA:435:C:C6 | 2.28 | 0.68 |
| 23:DA:2760:C:H2' | 23:DA:2761:G:H5'' | 1.74 | 0.68 |
| 7:AG:48:LYS:O | 7:AG:52:GLU:HG2 | 1.93 | 0.68 |
| 2:CB:135:GLN:HA | 2:CB:138:LEU:HD12 | 1.73 | 0.68 |
| 23:BA:450:G:OP2 | 56:BA:4582:HOH:O | 2.12 | 0.68 |
| 1:CA:223:U:H2' | 1:CA:224:C:H6 | 1.58 | 0.68 |
| 23:DA:248:G:OP1 | 56:DA:4076:HOH:O | 2.10 | 0.68 |
| 1:CA:1002:G:H22 | 1:CA:1039:C:H1' | 1.58 | 0.68 |
| 2:AB:135:GLN:HA | 2:AB:138:LEU:HD12 | 1.75 | 0.68 |
| 30:BI:93:THR:HG23 | 30:BI:96:ASP:H | 1.58 | 0.68 |
| 23:BA:975:C:OP2 | 56:BA:4205:HOH:O | 2.10 | 0.68 |
| 23:BA:1250:G:N7 | 33:BP:18:ARG:NH2 | 2.42 | 0.68 |
| 1:CA:975:A:O3' | 1:CA:1358:U:O2' | 2.12 | 0.68 |
| 1:CA:1238:A:N1 | 1:CA:1241:G:N2 | 2.33 | 0.68 |
| 7:CG:66:VAL:HG22 | 7:CG:100:ALA:HB1 | 1.74 | 0.68 |
| 24:DB:48:A:H4' | 36:DS:95:HIS:HD2 | 1.58 | 0.68 |
| 23:BA:379:G:O6 | 56:BA:4400:HOH:O | 2.11 | 0.68 |
| 23:BA:2786:U:O2' | 26:BE:62:PRO:O | 2.07 | 0.68 |
| 27:DF:7:TYR:H | 27:DF:22:ALA:HB3 | 1.59 | 0.68 |
| 1:CA:1444:C:N4 | 1:CA:1458:G:H1 | 1.92 | 0.68 |
| 1:AA:1004:A:H61 | 1:AA:1034:G:H2' | 1.58 | 0.68 |
| 49:B5:16:ARG:NH1 | 49:B5:17:ASP:OD1 | 2.26 | 0.68 |
| 47:D3:23:LEU:HD13 | 47:D3:50:VAL:HG11 | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-------------------|--------------------------|-------------------|
| 27:DF:185:ASP:HA | 27:DF:188:ARG:HD3 | 1.75 | 0.68 |
| 40:DW:18:ARG:HG3 | 40:DW:76:VAL:HB | 1.75 | 0.68 |
| 5:CE:80:ILE:HG13 | 5:CE:91:LEU:HB2 | 1.76 | 0.68 |
| 50:B6:13:CYS:SG | 50:B6:47:THR:HG21 | 2.33 | 0.68 |
| 18:CR:35:ARG:HB3 | 18:CR:35:ARG:NH1 | 2.09 | 0.68 |
| 23:DA:1120:G:O6 | 56:DA:4641:HOH:O | 2.08 | 0.68 |
| 1:CA:1459:C:C3' | 1:CA:1460:A:N7 | 2.52 | 0.68 |
| 2:AB:222:ILE:O | 2:AB:226:ARG:HG2 | 1.92 | 0.68 |
| 23:BA:271(I):G:N2 | 23:BA:271(O):C:N3 | 2.38 | 0.68 |
| 23:DA:1355:G:O6 | 56:DA:4120:HOH:O | 2.10 | 0.68 |
| 3:CC:20:SER:HB3 | 3:CC:22:TRP:NE1 | 2.08 | 0.68 |
| 1:AA:768:A:OP2 | 56:AA:1910:HOH:O | 2.12 | 0.68 |
| 1:CA:959:A:H61 | 19:CS:78:ARG:HA | 1.59 | 0.68 |
| 23:BA:1484:G:N7 | 56:BA:4165:HOH:O | 2.26 | 0.68 |
| 23:BA:1157:G:OP1 | 56:BA:4196:HOH:O | 2.12 | 0.68 |
| 1:AA:1366:C:O2' | 10:AJ:60:ARG:NH1 | 2.27 | 0.68 |
| 23:BA:2712(A):A:H5'' | 23:BA:2713:A:OP2 | 1.93 | 0.68 |
| 23:DA:1763:G:OP1 | 23:DA:1763:G:H4' | 1.94 | 0.68 |
| 23:BA:2833:G:H3' | 23:BA:2834:G:H5' | 1.75 | 0.68 |
| 1:CA:1165:C:H42 | 1:CA:1171:G:H1 | 1.40 | 0.67 |
| 39:DV:35:LEU:HB2 | 39:DV:57:VAL:HG13 | 1.74 | 0.67 |
| 23:BA:1352:U:OP2 | 56:BA:3914:HOH:O | 2.12 | 0.67 |
| 25:DD:108:PRO:HB3 | 25:DD:143:HIS:CE1 | 2.29 | 0.67 |
| 23:BA:821:A:N1 | 56:BA:5237:HOH:O | 2.27 | 0.67 |
| 17:AQ:6:LEU:HD23 | 17:AQ:23:VAL:HG11 | 1.74 | 0.67 |
| 23:DA:1670:C:H5'' | 56:DA:3807:HOH:O | 1.95 | 0.67 |
| 23:DA:2206:G:H5' | 23:DA:2207:G:C5 | 2.29 | 0.67 |
| 1:CA:73:G:H1 | 1:CA:96:U:H3 | 1.41 | 0.67 |
| 1:AA:1249:C:H42 | 1:AA:1287:A:H3' | 1.59 | 0.67 |
| 1:CA:1150:U:O4 | 1:CA:1151:A:N6 | 2.27 | 0.67 |
| 13:AM:91:ARG:O | 13:AM:110:ARG:NH1 | 2.28 | 0.67 |
| 1:AA:1224:G:O6 | 1:AA:1363:C:N3 | 2.27 | 0.67 |
| 23:DA:1529:G:C6 | 23:DA:1530:C:N4 | 2.61 | 0.67 |
| 1:AA:1226:C:C4 | 13:AM:104:ARG:HA | 2.30 | 0.67 |
| 4:CD:133:VAL:HG11 | 4:CD:138:TYR:HD1 | 1.58 | 0.67 |
| 2:CB:157:ARG:NH2 | 2:CB:160:ASP:OD1 | 2.23 | 0.67 |
| 1:AA:22:G:O6 | 56:AA:1983:HOH:O | 2.09 | 0.67 |
| 37:BT:118:ARG:HA | 37:BT:118:ARG:CZ | 2.25 | 0.67 |
| 10:AJ:16:LEU:HD13 | 10:AJ:70:ARG:HG2 | 1.77 | 0.67 |
| 1:CA:1158:C:N3 | 1:CA:1181:G:N2 | 2.42 | 0.67 |
| 23:BA:271(F):C:H2' | 23:BA:271(G):C:H6 | 1.59 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:59:A:H5'' | 1:AA:60:A:H5'' | 1.75 | 0.67 |
| 36:BS:11:LYS:HG3 | 36:BS:91:PRO:HD3 | 1.75 | 0.67 |
| 1:AA:316:G:OP2 | 1:AA:351:G:O2' | 2.12 | 0.67 |
| 23:BA:2336:A:H61 | 44:B0:43:THR:HG22 | 1.60 | 0.67 |
| 23:BA:885:C:C5 | 23:BA:890:A:N6 | 2.61 | 0.67 |
| 23:DA:1045:A:H2' | 23:DA:1045:A:N3 | 2.08 | 0.67 |
| 5:CE:57:LYS:HG2 | 5:CE:61:TYR:CE2 | 2.30 | 0.67 |
| 23:DA:2322:A:H61 | 23:DA:2335:A:H61 | 1.43 | 0.67 |
| 1:AA:1316:G:H22 | 1:AA:1319:A:H5'' | 1.58 | 0.67 |
| 7:CG:142:GLU:HB3 | 7:CG:143:ARG:HH21 | 1.60 | 0.67 |
| 9:AI:118:LYS:O | 9:AI:120:ARG:N | 2.27 | 0.67 |
| 35:DR:11:ASN:ND2 | 56:DR:302:HOH:O | 2.27 | 0.67 |
| 1:CA:548:G:OP1 | 56:CA:1988:HOH:O | 2.13 | 0.67 |
| 4:AD:30:LYS:HA | 4:AD:35:ARG:HD2 | 1.76 | 0.67 |
| 23:BA:2249:U:O2' | 56:BA:4487:HOH:O | 2.13 | 0.67 |
| 23:BA:1403:C:H5'' | 23:BA:1471:A:H1' | 1.77 | 0.67 |
| 23:BA:620:G:H5'' | 23:BA:620:G:N3 | 2.10 | 0.67 |
| 1:AA:1109:C:P | 3:AC:176:HIS:HD1 | 2.17 | 0.67 |
| 2:CB:222:ILE:O | 2:CB:226:ARG:HG2 | 1.94 | 0.67 |
| 3:CC:36:ASP:O | 3:CC:39:ILE:HB | 1.94 | 0.67 |
| 23:DA:27:G:O2' | 23:DA:28:A:OP2 | 2.09 | 0.67 |
| 23:BA:271(M):G:OP2 | 30:BI:57:ARG:NH2 | 2.28 | 0.67 |
| 23:DA:2519:U:OP2 | 56:DA:4292:HOH:O | 2.13 | 0.67 |
| 23:DA:2431:U:O4 | 56:DA:3998:HOH:O | 2.10 | 0.67 |
| 23:BA:885:C:H4' | 23:BA:885:C:OP1 | 1.92 | 0.67 |
| 1:CA:1144:G:H21 | 1:CA:1146:A:N6 | 1.92 | 0.67 |
| 1:CA:1309:G:OP1 | 13:CM:92:HIS:NE2 | 2.28 | 0.67 |
| 3:CC:11:ARG:HB2 | 3:CC:11:ARG:HH11 | 1.59 | 0.67 |
| 23:DA:1014:U:H2' | 23:DA:1015:G:H8 | 1.60 | 0.67 |
| 29:BH:86:GLU:OE2 | 29:BH:132:ARG:NH1 | 2.28 | 0.67 |
| 1:AA:973:G:H3' | 1:AA:974:A:H5'' | 1.77 | 0.67 |
| 16:AP:49:LEU:HD11 | 16:AP:51:VAL:HG23 | 1.76 | 0.67 |
| 1:AA:1442(A):G:N3 | 1:AA:1442(B):A:H2' | 2.10 | 0.67 |
| 1:AA:1010:G:N2 | 1:AA:1019:C:N3 | 2.40 | 0.67 |
| 48:D4:42:PHE:CB | 48:D4:43:TYR:HB2 | 2.25 | 0.67 |
| 1:CA:1351:U:H2' | 1:CA:1352:C:H6 | 1.60 | 0.67 |
| 1:CA:1030(A):G:O2' | 1:CA:1030(C):G:N7 | 2.27 | 0.67 |
| 23:DA:2427:C:OP2 | 56:DA:4447:HOH:O | 2.12 | 0.67 |
| 1:AA:1157:A:H61 | 1:AA:1178:G:H1' | 1.58 | 0.67 |
| 1:AA:1372:U:H5'' | 9:AI:71:SER:HB3 | 1.77 | 0.67 |
| 1:CA:330:C:O2 | 56:CA:1861:HOH:O | 2.11 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:2243:U:H2' | 23:BA:2244:U:C6 | 2.30 | 0.67 |
| 8:AH:29:SER:HB3 | 8:AH:32:LYS:HG3 | 1.76 | 0.67 |
| 23:DA:1351:C:OP2 | 56:DA:3930:HOH:O | 2.12 | 0.67 |
| 23:BA:1186:G:OP2 | 56:BA:4518:HOH:O | 2.11 | 0.67 |
| 25:DD:71:ASP:HB3 | 25:DD:103:ARG:HH22 | 1.60 | 0.67 |
| 23:DA:365:C:OP2 | 56:DA:4247:HOH:O | 2.12 | 0.67 |
| 23:DA:2199:A:H3' | 23:DA:2200:C:H6 | 1.58 | 0.67 |
| 4:AD:133:VAL:HG11 | 4:AD:138:TYR:HD1 | 1.60 | 0.67 |
| 45:D1:50:ARG:HG2 | 45:D1:59:THR:HG22 | 1.76 | 0.67 |
| 1:AA:401:C:OP1 | 4:AD:73:ARG:NH2 | 2.27 | 0.67 |
| 1:AA:1007:C:H42 | 1:AA:1022:G:H1 | 0.74 | 0.66 |
| 10:AJ:16:LEU:O | 10:AJ:20:ALA:N | 2.26 | 0.66 |
| 23:BA:2134:A:C2 | 23:BA:2159:G:H1' | 2.30 | 0.66 |
| 3:CC:32:LEU:HD11 | 3:CC:59:ARG:HD2 | 1.76 | 0.66 |
| 3:CC:157:ILE:O | 3:CC:164:ARG:NH2 | 2.28 | 0.66 |
| 23:DA:856:C:H5' | 44:D0:27:GLU:OE2 | 1.94 | 0.66 |
| 44:D0:53:MET:HG3 | 44:D0:59:LEU:HD23 | 1.77 | 0.66 |
| 1:CA:1084:G:H21 | 1:CA:1102:A:N6 | 1.93 | 0.66 |
| 28:BG:138:GLN:HG3 | 28:BG:144:ILE:HG21 | 1.75 | 0.66 |
| 1:CA:425:G:O3' | 4:CD:45:GLN:NE2 | 2.28 | 0.66 |
| 23:BA:862:G:OP2 | 56:BA:4352:HOH:O | 2.13 | 0.66 |
| 1:AA:605:U:H2' | 1:AA:606:G:C8 | 2.29 | 0.66 |
| 5:AE:71:LEU:HD11 | 5:AE:74:GLY:H | 1.60 | 0.66 |
| 23:DA:1132:A:OP2 | 56:DA:3690:HOH:O | 2.13 | 0.66 |
| 1:CA:976:G:P | 14:CN:32:SER:H | 2.19 | 0.66 |
| 1:AA:1121:U:H3 | 1:AA:1152:A:N6 | 1.93 | 0.66 |
| 23:BA:1434:A:H61 | 23:BA:1558:A:N6 | 1.93 | 0.66 |
| 23:BA:587:C:OP2 | 33:BP:21:ARG:NH2 | 2.28 | 0.66 |
| 1:AA:142:G:H2' | 1:AA:143:A:H8 | 1.59 | 0.66 |
| 23:DA:2022:U:OP1 | 56:DA:3884:HOH:O | 2.13 | 0.66 |
| 27:BF:7:TYR:H | 27:BF:22:ALA:HB3 | 1.60 | 0.66 |
| 40:BW:4:LYS:HB2 | 40:BW:106:ILE:HG12 | 1.77 | 0.66 |
| 9:AI:46:ALA:HB1 | 9:AI:77:ILE:HB | 1.77 | 0.66 |
| 23:BA:885:C:C2 | 23:BA:886:C:H1' | 2.31 | 0.66 |
| 1:AA:1299:A:H4' | 1:AA:1300:G:OP1 | 1.95 | 0.66 |
| 1:CA:1297:C:H4' | 1:CA:1298:C:H5' | 1.76 | 0.66 |
| 1:AA:1268:A:H4' | 21:AU:20:LYS:HA | 1.78 | 0.66 |
| 15:CO:8:LYS:HG2 | 15:CO:12:ILE:HD11 | 1.78 | 0.66 |
| 9:AI:7:THR:H | 9:AI:83:ARG:HD3 | 1.60 | 0.66 |
| 1:CA:1435:G:H2' | 1:CA:1436:U:C6 | 2.30 | 0.66 |
| 37:BT:24:PRO:HA | 37:BT:49:VAL:HG22 | 1.75 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DY:9:LYS:NZ | 42:DY:28:LYS:O | 2.28 | 0.66 |
| 23:BA:105:C:OP1 | 56:BA:3776:HOH:O | 2.13 | 0.66 |
| 26:DE:47:VAL:HG11 | 26:DE:86:PRO:HD2 | 1.77 | 0.66 |
| 31:BN:47:ALA:HB2 | 31:BN:112:LEU:HD11 | 1.76 | 0.66 |
| 1:AA:1457:G:C4 | 1:AA:1458:G:N7 | 2.63 | 0.66 |
| 1:CA:1231:G:C2 | 1:CA:1232:U:H1' | 2.31 | 0.66 |
| 1:CA:1381:U:H3' | 1:CA:1382:C:H6 | 1.61 | 0.66 |
| 2:AB:87:ARG:HH21 | 2:AB:233:SER:H | 1.42 | 0.66 |
| 16:AP:28:ARG:HG2 | 16:AP:28:ARG:HH11 | 1.61 | 0.66 |
| 1:AA:1225:A:N3 | 1:AA:1225:A:H2' | 2.09 | 0.66 |
| 1:CA:1067:A:N3 | 1:CA:1068:G:H1' | 2.11 | 0.66 |
| 23:BA:1265:A:OP2 | 56:BA:4992:HOH:O | 2.12 | 0.66 |
| 23:DA:512:G:N7 | 56:DA:3836:HOH:O | 2.29 | 0.66 |
| 3:CC:156:ARG:NE | 3:CC:161:GLU:OE2 | 2.28 | 0.66 |
| 15:CO:70:LEU:HG | 15:CO:78:TYR:HB2 | 1.77 | 0.66 |
| 23:BA:1026:U:O2' | 23:BA:1027:A:O5' | 2.13 | 0.66 |
| 1:CA:382:A:H2' | 1:CA:383:A:C8 | 2.30 | 0.66 |
| 23:DA:674:G:H1' | 27:DF:74:ARG:HD3 | 1.78 | 0.66 |
| 23:BA:2318:G:N2 | 36:BS:3:ARG:HD3 | 2.10 | 0.66 |
| 4:CD:32:ALA:HA | 4:CD:35:ARG:HB2 | 1.77 | 0.66 |
| 23:DA:2130:U:O2' | 23:DA:2133:G:O2' | 2.10 | 0.66 |
| 9:AI:65:VAL:O | 9:AI:73:GLN:NE2 | 2.28 | 0.66 |
| 1:CA:365:U:H5'' | 1:CA:366:C:OP1 | 1.95 | 0.66 |
| 39:BV:35:LEU:HB2 | 39:BV:57:VAL:HG13 | 1.77 | 0.66 |
| 24:BB:66:A:H61 | 24:BB:109:C:H5' | 1.60 | 0.66 |
| 15:CO:3:ILE:H | 15:CO:3:ILE:HD13 | 1.61 | 0.66 |
| 31:DN:15:LEU:HB2 | 31:DN:135:PRO:HB2 | 1.77 | 0.66 |
| 22:CX:4:ASN:HB2 | 22:CX:38:TYR:HA | 1.78 | 0.66 |
| 10:AJ:31:GLY:HA3 | 10:AJ:78:ASN:CB | 2.25 | 0.66 |
| 1:CA:1046:A:H3' | 1:CA:1047:G:H8 | 1.60 | 0.66 |
| 23:DA:1970:A:H4' | 56:DA:4210:HOH:O | 1.95 | 0.66 |
| 23:BA:1171:G:O2' | 23:BA:1173:G:OP2 | 2.06 | 0.66 |
| 1:CA:1073:U:H2' | 1:CA:1074:G:C8 | 2.29 | 0.66 |
| 19:CS:46:GLY:N | 19:CS:62:ILE:O | 2.28 | 0.66 |
| 1:CA:171:A:H2' | 1:CA:172:A:C8 | 2.29 | 0.66 |
| 23:DA:2786:U:O2' | 26:DE:62:PRO:O | 2.07 | 0.66 |
| 23:BA:1379:A:H4' | 23:BA:1380:G:OP2 | 1.95 | 0.66 |
| 23:BA:1561:G:OP2 | 56:BA:4362:HOH:O | 2.14 | 0.66 |
| 4:CD:157:LEU:O | 4:CD:161:ASN:ND2 | 2.20 | 0.66 |
| 1:AA:1417:G:O6 | 56:AA:1843:HOH:O | 2.12 | 0.66 |
| 1:AA:242:C:OP1 | 56:AA:1818:HOH:O | 2.12 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1457:G:N3 | 1:CA:1458:G:C8 | 2.63 | 0.66 |
| 1:CA:1457:G:C4 | 1:CA:1458:G:N7 | 2.64 | 0.66 |
| 1:AA:1378:C:H1' | 1:AA:1379:G:O5' | 1.95 | 0.66 |
| 1:CA:1112:C:N3 | 3:CC:178:LEU:HB2 | 2.10 | 0.66 |
| 23:DA:1315:C:OP2 | 56:DA:3783:HOH:O | 2.14 | 0.66 |
| 20:CT:10:LEU:HD21 | 20:CT:12:ALA:HB3 | 1.76 | 0.66 |
| 23:BA:1778:U:H2' | 23:BA:1784:A:N6 | 2.10 | 0.66 |
| 5:AE:57:LYS:HG2 | 5:AE:61:TYR:CE2 | 2.30 | 0.66 |
| 28:BG:122:PRO:HG3 | 28:BG:180:PHE:HB3 | 1.78 | 0.66 |
| 1:AA:1459:C:C6 | 1:AA:1460:A:N7 | 2.64 | 0.66 |
| 23:BA:631:A:OP2 | 52:B8:47:LYS:NZ | 2.22 | 0.66 |
| 1:AA:1304:G:N2 | 1:AA:1332:A:OP2 | 2.28 | 0.66 |
| 1:AA:1377:A:C8 | 1:AA:1377:A:H3' | 2.31 | 0.66 |
| 23:BA:563:G:OP2 | 56:BA:4466:HOH:O | 2.14 | 0.66 |
| 23:BA:2705:A:OP2 | 56:BA:4854:HOH:O | 2.13 | 0.66 |
| 29:DH:86:GLU:OE2 | 29:DH:132:ARG:NH1 | 2.29 | 0.66 |
| 1:AA:186:C:H2' | 1:AA:187:C:C6 | 2.31 | 0.66 |
| 1:AA:1441:G:H21 | 1:AA:1459:C:H5 | 1.43 | 0.66 |
| 1:CA:1106:G:H5'' | 3:CC:172:ARG:HD3 | 1.77 | 0.66 |
| 11:AK:41:THR:HG21 | 11:AK:71:LYS:HD2 | 1.78 | 0.66 |
| 4:AD:32:ALA:HA | 4:AD:35:ARG:HB2 | 1.77 | 0.66 |
| 1:AA:1285:A:H4' | 1:AA:1286:A:O5' | 1.95 | 0.66 |
| 1:AA:662:G:O2' | 1:AA:836:G:OP1 | 2.13 | 0.66 |
| 23:BA:1016:G:N7 | 56:BA:5119:HOH:O | 2.28 | 0.66 |
| 23:DA:123:G:OP1 | 56:DA:3622:HOH:O | 2.13 | 0.66 |
| 1:AA:1296:C:OP2 | 1:AA:1297:C:N4 | 2.27 | 0.65 |
| 1:AA:1120:G:N2 | 1:AA:1154:G:H1' | 2.11 | 0.65 |
| 21:AU:15:ARG:HG3 | 21:AU:17:THR:HG23 | 1.79 | 0.65 |
| 36:BS:10:ARG:HH21 | 36:BS:91:PRO:HB2 | 1.60 | 0.65 |
| 34:BQ:54:MET:HE3 | 34:BQ:64:ILE:HD13 | 1.77 | 0.65 |
| 23:DA:910:A:C5 | 34:DQ:13:GLN:HG3 | 2.31 | 0.65 |
| 23:DA:552:G:O6 | 56:DA:4483:HOH:O | 2.13 | 0.65 |
| 37:DT:56:GLY:O | 37:DT:59:THR:HG22 | 1.95 | 0.65 |
| 23:DA:1405:U:H2' | 23:DA:1406:U:C6 | 2.30 | 0.65 |
| 1:CA:1211:U:H4' | 1:CA:1212:U:OP2 | 1.96 | 0.65 |
| 1:AA:243:A:H4' | 1:AA:244:U:O5' | 1.97 | 0.65 |
| 1:AA:174:C:H2' | 1:AA:175:C:H6 | 1.61 | 0.65 |
| 4:AD:155:LEU:HB3 | 4:AD:158:ILE:HB | 1.79 | 0.65 |
| 17:CQ:6:LEU:HD23 | 17:CQ:23:VAL:HG11 | 1.77 | 0.65 |
| 1:CA:1245:A:H61 | 1:CA:1292:U:H3 | 1.43 | 0.65 |
| 1:AA:41:G:H2' | 1:AA:42:G:C8 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:BA:376:C:OP2 | 56:BA:3961:HOH:O | 2.13 | 0.65 |
| 21:CU:17:THR:OG1 | 21:CU:18:TYR:N | 2.29 | 0.65 |
| 5:AE:50:GLU:HB2 | 5:AE:53:LEU:HD22 | 1.76 | 0.65 |
| 23:DA:688:U:O4 | 56:DA:3974:HOH:O | 2.11 | 0.65 |
| 1:AA:1128:C:H5' | 9:AI:16:ARG:NH2 | 2.11 | 0.65 |
| 1:CA:1332:A:H2' | 1:CA:1333:A:C8 | 2.31 | 0.65 |
| 23:BA:2319:G:N2 | 36:BS:3:ARG:HD2 | 2.11 | 0.65 |
| 23:DA:154(A):C:N4 | 23:DA:171:G:N1 | 2.45 | 0.65 |
| 23:BA:639:U:H2' | 23:BA:640:C:C6 | 2.32 | 0.65 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:H1 | 1.42 | 0.65 |
| 23:BA:856:C:H5' | 44:B0:27:GLU:OE2 | 1.96 | 0.65 |
| 47:B3:23:LEU:HD13 | 47:B3:50:VAL:HG11 | 1.78 | 0.65 |
| 5:CE:12:LEU:HB3 | 5:CE:31:LEU:HB3 | 1.78 | 0.65 |
| 23:DA:1838:C:O2' | 56:DA:4310:HOH:O | 2.13 | 0.65 |
| 1:AA:1221:G:H5' | 19:AS:36:ARG:HD3 | 1.79 | 0.65 |
| 1:CA:1306:A:H3' | 1:CA:1307:U:H6 | 1.62 | 0.65 |
| 1:CA:1078:U:H1' | 5:CE:130:ASN:HD21 | 1.61 | 0.65 |
| 28:DG:11:TYR:CE2 | 28:DG:16:ARG:HD3 | 2.31 | 0.65 |
| 1:AA:1120:G:H22 | 1:AA:1154:G:H1' | 1.60 | 0.65 |
| 1:CA:1028:C:N3 | 1:CA:1033:G:C6 | 2.65 | 0.65 |
| 21:AU:12:LYS:HE3 | 21:AU:19:GLY:HA3 | 1.79 | 0.65 |
| 23:BA:2712:U:O2' | 23:BA:2712(A):A:OP2 | 2.14 | 0.65 |
| 1:CA:1258:G:H2' | 1:CA:1259:C:C6 | 2.32 | 0.65 |
| 22:CX:17:ARG:HA | 22:CX:20:VAL:HG12 | 1.78 | 0.65 |
| 51:B7:34:ARG:NH1 | 51:B7:41:ARG:O | 2.30 | 0.65 |
| 23:DA:1423:G:H2' | 23:DA:1424:G:H8 | 1.62 | 0.65 |
| 23:BA:2533:A:OP2 | 56:BA:5056:HOH:O | 2.14 | 0.65 |
| 15:AO:16:ALA:HB1 | 15:AO:21:ASP:HB3 | 1.78 | 0.65 |
| 26:DE:11:MET:HG2 | 26:DE:24:THR:HB | 1.79 | 0.65 |
| 37:BT:60:THR:HG22 | 37:BT:77:PRO:HA | 1.79 | 0.65 |
| 1:AA:1218:C:H2' | 1:AA:1219:U:C6 | 2.32 | 0.65 |
| 21:CU:10:ARG:HA | 21:CU:10:ARG:HE | 1.61 | 0.65 |
| 28:BG:11:TYR:CE2 | 28:BG:16:ARG:HD3 | 2.31 | 0.65 |
| 1:AA:166:G:H2' | 1:AA:167:G:C8 | 2.31 | 0.65 |
| 25:DD:118:VAL:H | 25:DD:129:ASN:ND2 | 1.94 | 0.65 |
| 1:AA:974:A:OP1 | 1:AA:974:A:H8 | 1.80 | 0.65 |
| 2:CB:115:LEU:HD13 | 2:CB:145:LEU:HB3 | 1.78 | 0.65 |
| 23:BA:606:U:H4' | 23:BA:658:C:H4' | 1.79 | 0.65 |
| 23:BA:504:U:OP2 | 56:BA:4934:HOH:O | 2.13 | 0.65 |
| 11:AK:13:GLN:N | 11:AK:75:TYR:O | 2.28 | 0.65 |
| 5:CE:43:LEU:O | 5:CE:65:ASN:ND2 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1423:G:H2' | 23:BA:1424:G:H8 | 1.62 | 0.65 |
| 1:CA:1377:A:H2' | 7:CG:7:ALA:CB | 2.27 | 0.65 |
| 23:DA:1352:U:OP2 | 56:DA:3932:HOH:O | 2.14 | 0.65 |
| 23:DA:71:A:H2 | 41:DX:31:HIS:CE1 | 2.15 | 0.65 |
| 7:CG:43:PHE:HD1 | 7:CG:46:ALA:HB3 | 1.61 | 0.65 |
| 4:CD:108:LEU:HD11 | 4:CD:174:LEU:HD22 | 1.79 | 0.65 |
| 43:BZ:45:ASP:OD2 | 43:BZ:49:ARG:NH1 | 2.29 | 0.65 |
| 51:D7:24:THR:HG23 | 51:D7:27:GLY:H | 1.61 | 0.65 |
| 1:CA:1015:A:N3 | 1:CA:1218:C:O2' | 2.27 | 0.65 |
| 37:BT:64:ARG:NH1 | 37:BT:103:ARG:HA | 2.11 | 0.65 |
| 1:AA:324:G:OP1 | 20:AT:70:SER:HB2 | 1.96 | 0.65 |
| 23:DA:301:G:OP2 | 42:DY:84:ARG:NH2 | 2.29 | 0.65 |
| 1:AA:1435:G:H2' | 1:AA:1436:U:C6 | 2.31 | 0.65 |
| 32:DO:25:LEU:HD21 | 32:DO:40:VAL:HG23 | 1.79 | 0.65 |
| 1:AA:1443:G:O6 | 1:AA:1459:C:HI' | 1.96 | 0.65 |
| 23:DA:2319:G:N2 | 36:DS:3:ARG:HD2 | 2.11 | 0.65 |
| 23:DA:1379:A:H4' | 23:DA:1380:G:OP2 | 1.95 | 0.65 |
| 1:CA:186:C:H2' | 1:CA:187:C:C6 | 2.32 | 0.65 |
| 23:BA:2887:U:H2' | 23:BA:2888:C:C6 | 2.32 | 0.65 |
| 23:BA:1587:A:H2' | 23:BA:1588:C:C6 | 2.31 | 0.65 |
| 1:CA:1373:G:H5' | 7:CG:36:LYS:HG3 | 1.79 | 0.65 |
| 23:BA:154(A):C:N4 | 23:BA:171:G:N1 | 2.44 | 0.65 |
| 23:DA:1914:C:H2' | 23:DA:1915:U:H6 | 1.61 | 0.65 |
| 28:DG:122:PRO:HG3 | 28:DG:180:PHE:HB3 | 1.79 | 0.65 |
| 1:AA:1442(A):G:C2 | 1:AA:1442(B):A:H2' | 2.32 | 0.65 |
| 1:AA:1460:A:H8 | 1:AA:1460:A:P | 2.19 | 0.65 |
| 23:DA:2322:A:N6 | 23:DA:2335:A:N6 | 2.44 | 0.65 |
| 1:AA:1003:G:N2 | 1:AA:1037:C:C2 | 2.64 | 0.65 |
| 1:CA:1502:A:H2 | 1:CA:1505:G:H1 | 1.42 | 0.65 |
| 1:CA:1500:A:OP1 | 56:CA:2021:HOH:O | 2.15 | 0.65 |
| 5:CE:71:LEU:HD11 | 5:CE:74:GLY:H | 1.62 | 0.65 |
| 23:BA:1833:U:H2' | 23:BA:1834:U:H6 | 1.60 | 0.65 |
| 23:DA:484:C:H2' | 23:DA:485:C:C6 | 2.32 | 0.65 |
| 23:DA:252:G:OP2 | 33:DP:50:ARG:NH1 | 2.30 | 0.65 |
| 1:AA:559:A:OP1 | 5:AE:126:ARG:NH2 | 2.25 | 0.65 |
| 23:DA:1359:A:N6 | 23:DA:1372:U:C4 | 2.63 | 0.65 |
| 23:BA:1174:A:H5' | 23:BA:1177:A:H62 | 1.61 | 0.65 |
| 9:AI:8:GLY:HA3 | 9:AI:76:ALA:HB1 | 1.78 | 0.65 |
| 30:DI:120:ILE:HG21 | 30:DI:126:TYR:CE1 | 2.31 | 0.65 |
| 23:BA:1560:G:OP1 | 56:BA:4362:HOH:O | 2.13 | 0.65 |
| 1:AA:1502:A:H2 | 1:AA:1505:G:N1 | 1.94 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:696:G:N7 | 56:BA:5334:HOH:O | 2.29 | 0.65 |
| 22:AX:87:LYS:O | 22:AX:91:LYS:HG3 | 1.97 | 0.65 |
| 23:DA:639:U:H2' | 23:DA:640:C:C6 | 2.32 | 0.65 |
| 4:CD:20:TYR:HA | 4:CD:26:CYS:SG | 2.36 | 0.65 |
| 23:BA:886:C:H2' | 23:BA:889:C:H41 | 1.62 | 0.64 |
| 23:DA:2122:U:H2' | 23:DA:2123:G:C8 | 2.32 | 0.64 |
| 1:AA:1221:G:OP1 | 1:AA:1320:C:N4 | 2.30 | 0.64 |
| 21:AU:13:ILE:HA | 21:AU:22:ARG:NH1 | 2.12 | 0.64 |
| 23:BA:1174:A:H4' | 23:BA:1175:U:OP1 | 1.97 | 0.64 |
| 1:AA:1378:C:O2' | 1:AA:1379:G:H8 | 1.80 | 0.64 |
| 1:AA:382:A:H2' | 1:AA:383:A:H8 | 1.61 | 0.64 |
| 23:DA:250:G:OP2 | 52:D8:13:ARG:NH2 | 2.29 | 0.64 |
| 1:CA:996:A:H2' | 1:CA:997:U:C6 | 2.32 | 0.64 |
| 40:DW:4:LYS:HB2 | 40:DW:106:ILE:HG12 | 1.79 | 0.64 |
| 14:AN:29:ARG:HD2 | 14:AN:31:ARG:HB2 | 1.78 | 0.64 |
| 23:DA:2305:A:H5'' | 28:DG:134:GLY:HA3 | 1.79 | 0.64 |
| 26:DE:112:GLY:O | 26:DE:159:HIS:HA | 1.97 | 0.64 |
| 23:BA:314:A:N6 | 56:BA:5256:HOH:O | 2.21 | 0.64 |
| 23:BA:2721:A:OP2 | 56:BA:4075:HOH:O | 2.14 | 0.64 |
| 1:AA:1458:G:C2 | 1:AA:1459:C:O4' | 2.50 | 0.64 |
| 1:CA:1128:C:H4' | 9:CI:16:ARG:HH22 | 1.62 | 0.64 |
| 1:CA:1142:G:C6 | 1:CA:1143:G:H1' | 2.32 | 0.64 |
| 49:D5:16:ARG:NH1 | 49:D5:17:ASP:OD1 | 2.31 | 0.64 |
| 14:CN:24:CYS:SG | 14:CN:27:CYS:N | 2.70 | 0.64 |
| 42:BY:23:ARG:HB2 | 42:BY:23:ARG:HH11 | 1.61 | 0.64 |
| 27:BF:53:THR:HG23 | 27:BF:55:GLY:H | 1.62 | 0.64 |
| 1:CA:1210:C:H3' | 1:CA:1211:U:H5'' | 1.80 | 0.64 |
| 1:AA:1128:C:H1' | 1:AA:1146:A:H61 | 1.61 | 0.64 |
| 17:AQ:67:LYS:HA | 17:AQ:70:ARG:HH12 | 1.62 | 0.64 |
| 1:AA:1030(A):G:H2' | 1:AA:1030(C):G:OP2 | 1.96 | 0.64 |
| 1:CA:538:G:OP2 | 12:CL:115:LYS:HB2 | 1.97 | 0.64 |
| 9:AI:27:THR:HB | 9:AI:62:TYR:HA | 1.80 | 0.64 |
| 23:DA:96:G:H4' | 46:D2:48:HIS:CD2 | 2.31 | 0.64 |
| 35:DR:117:VAL:HG12 | 35:DR:118:GLU:H | 1.62 | 0.64 |
| 5:AE:43:LEU:O | 5:AE:65:ASN:ND2 | 2.30 | 0.64 |
| 23:BA:2305:A:H5'' | 28:BG:134:GLY:HA3 | 1.80 | 0.64 |
| 27:DF:129:PHE:CD2 | 27:DF:163:VAL:HG21 | 2.32 | 0.64 |
| 34:DQ:111:GLU:OE1 | 34:DQ:133:ARG:NH2 | 2.30 | 0.64 |
| 41:DX:27:THR:HG23 | 41:DX:80:ILE:HG13 | 1.79 | 0.64 |
| 1:AA:1444:C:N4 | 1:AA:1458:G:H1 | 1.95 | 0.64 |
| 1:AA:1243:C:N4 | 1:AA:1294:G:H1 | 1.95 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:674:G:H1' | 27:BF:74:ARG:HD3 | 1.78 | 0.64 |
| 23:DA:1778:U:H2' | 23:DA:1784:A:N6 | 2.12 | 0.64 |
| 38:DU:76:TYR:HH | 38:DU:92:ARG:HH11 | 1.43 | 0.64 |
| 12:AL:27:LEU:O | 12:AL:29:GLY:N | 2.31 | 0.64 |
| 23:BA:459:U:H5'' | 51:B7:40:TRP:CD2 | 2.33 | 0.64 |
| 23:DA:816:C:OP2 | 56:DA:4440:HOH:O | 2.14 | 0.64 |
| 1:CA:1111:A:N1 | 3:CC:177:THR:HG23 | 2.12 | 0.64 |
| 9:CI:22:GLY:HA3 | 9:CI:60:ASP:HB2 | 1.79 | 0.64 |
| 48:B4:16:CYS:SG | 48:B4:20:ASN:HB3 | 2.38 | 0.64 |
| 23:BA:2526:G:H21 | 53:B9:2:LYS:HG2 | 1.63 | 0.64 |
| 1:AA:1444:C:N4 | 1:AA:1459:C:O2 | 2.30 | 0.64 |
| 23:BA:2322:A:N6 | 23:BA:2335:A:N6 | 2.42 | 0.64 |
| 1:AA:946:A:H2' | 1:AA:947:G:C8 | 2.33 | 0.64 |
| 3:CC:54:ARG:HH11 | 3:CC:56:ASP:HB2 | 1.63 | 0.64 |
| 14:CN:7:ILE:HG22 | 14:CN:23:ARG:NE | 2.12 | 0.64 |
| 36:DS:14:VAL:O | 36:DS:18:ILE:HG12 | 1.97 | 0.64 |
| 11:CK:41:THR:HG21 | 11:CK:71:LYS:HD2 | 1.79 | 0.64 |
| 30:DI:83:ALA:HB2 | 30:DI:88:ILE:HA | 1.77 | 0.64 |
| 23:DA:910:A:H62 | 34:DQ:12:GLN:HA | 1.61 | 0.64 |
| 1:AA:41:G:H2' | 1:AA:42:G:H8 | 1.62 | 0.64 |
| 33:DP:50:ARG:HD3 | 52:D8:7:HIS:CD2 | 2.32 | 0.64 |
| 40:BW:18:ARG:HG3 | 40:BW:76:VAL:HB | 1.80 | 0.64 |
| 23:DA:2637:U:H5'' | 26:DE:82:ARG:HH21 | 1.62 | 0.64 |
| 26:BE:28:ALA:HB3 | 26:BE:93:VAL:HG12 | 1.78 | 0.64 |
| 23:DA:1429:G:H2' | 23:DA:1430:C:C6 | 2.32 | 0.64 |
| 27:DF:116:ASP:OD1 | 27:DF:119:ARG:NH2 | 2.31 | 0.64 |
| 38:BU:44:ASN:ND2 | 39:BV:75:PHE:O | 2.24 | 0.64 |
| 2:AB:157:ARG:NH2 | 2:AB:160:ASP:OD1 | 2.21 | 0.64 |
| 23:DA:526:A:OP1 | 56:DA:4533:HOH:O | 2.15 | 0.64 |
| 2:CB:87:ARG:HD2 | 2:CB:219:VAL:HG11 | 1.77 | 0.64 |
| 1:AA:1142:G:C6 | 1:AA:1143:G:H1' | 2.33 | 0.64 |
| 23:DA:1210:A:H8 | 23:DA:1210:A:H5'' | 1.62 | 0.64 |
| 23:BA:1176:G:H1' | 23:BA:1177:A:OP1 | 1.96 | 0.64 |
| 28:DG:101:ILE:HD13 | 48:D4:25:TYR:HB2 | 1.80 | 0.64 |
| 23:BA:2808:U:H5' | 23:BA:2891:G:O6 | 1.97 | 0.64 |
| 7:AG:99:LEU:HA | 7:AG:102:ARG:NH2 | 2.13 | 0.64 |
| 25:BD:71:ASP:HB3 | 25:BD:103:ARG:HH22 | 1.63 | 0.64 |
| 36:BS:58:LEU:HB2 | 36:BS:59:LYS:HB2 | 1.78 | 0.64 |
| 23:BA:492:A:OP2 | 56:BA:4859:HOH:O | 2.15 | 0.64 |
| 23:BA:90:U:H2' | 23:BA:92:A:C8 | 2.32 | 0.64 |
| 23:DA:188:G:H1 | 23:DA:208:C:H42 | 1.44 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1381:U:H3' | 1:CA:1382:C:C6 | 2.33 | 0.64 |
| 1:CA:1181:G:H4' | 1:CA:1184:G:H5' | 1.78 | 0.64 |
| 1:AA:102:G:H2' | 1:AA:103:C:H6 | 1.60 | 0.64 |
| 23:DA:8:A:OP1 | 31:DN:121:LYS:NZ | 2.30 | 0.64 |
| 14:AN:29:ARG:HG3 | 14:AN:31:ARG:H | 1.63 | 0.64 |
| 23:DA:1786:A:H1' | 23:DA:1938:A:N6 | 2.13 | 0.64 |
| 23:BA:2492:U:H2' | 23:BA:2493:U:C6 | 2.32 | 0.64 |
| 23:DA:2833:G:H3' | 23:DA:2834:G:H5' | 1.79 | 0.64 |
| 1:AA:814:A:H2' | 1:AA:816:A:H5'' | 1.78 | 0.64 |
| 23:BA:787:U:OP1 | 56:BA:4569:HOH:O | 2.15 | 0.64 |
| 23:BA:1176:G:H21 | 23:BA:1178:C:P | 2.21 | 0.64 |
| 20:AT:63:ILE:HD12 | 20:AT:81:LYS:HG2 | 1.79 | 0.64 |
| 33:BP:25:SER:O | 56:BP:304:HOH:O | 2.15 | 0.64 |
| 23:DA:467:G:OP1 | 51:D7:33:ARG:NH1 | 2.31 | 0.64 |
| 1:CA:59:A:H5'' | 1:CA:60:A:H5'' | 1.80 | 0.64 |
| 23:DA:1650:G:O6 | 56:DA:4754:HOH:O | 2.11 | 0.64 |
| 15:AO:70:LEU:HG | 15:AO:78:TYR:HB2 | 1.80 | 0.64 |
| 23:BA:2122:U:H2' | 23:BA:2123:G:C8 | 2.32 | 0.64 |
| 23:BA:271(J):C:O2' | 23:BA:271(K):U:H5' | 1.98 | 0.64 |
| 45:D1:3:LYS:HB2 | 45:D1:61:ARG:HH11 | 1.63 | 0.64 |
| 30:BI:12:LEU:HD22 | 30:BI:19:VAL:HG21 | 1.79 | 0.64 |
| 27:BF:123:LEU:HD13 | 27:BF:192:LEU:HD13 | 1.80 | 0.64 |
| 11:CK:73:MET:HG3 | 11:CK:103:LEU:HD21 | 1.80 | 0.64 |
| 3:AC:137:ALA:O | 3:AC:140:ARG:HB3 | 1.96 | 0.64 |
| 1:AA:1457:G:N3 | 1:AA:1458:G:C8 | 2.66 | 0.64 |
| 1:CA:1130:A:N6 | 1:CA:1144:G:H1' | 2.11 | 0.64 |
| 1:AA:1144:G:H21 | 1:AA:1146:A:N6 | 1.96 | 0.64 |
| 23:DA:2206:G:O2' | 23:DA:2207:G:OP1 | 2.15 | 0.64 |
| 23:BA:2206:G:O2' | 23:BA:2207:G:OP1 | 2.13 | 0.64 |
| 1:AA:49:U:O4 | 1:AA:365:U:H5 | 1.81 | 0.64 |
| 23:DA:553:G:O6 | 56:DA:4483:HOH:O | 2.14 | 0.64 |
| 1:CA:1326:C:H5'' | 21:CU:18:TYR:O | 1.98 | 0.64 |
| 23:BA:89:G:H3' | 23:BA:90:U:H5'' | 1.79 | 0.64 |
| 20:CT:97:ALA:HB3 | 20:CT:99:LEU:H | 1.62 | 0.64 |
| 26:BE:128:SER:OG | 26:BE:129:HIS:N | 2.27 | 0.64 |
| 25:BD:142:VAL:HG23 | 25:BD:193:VAL:HA | 1.79 | 0.64 |
| 23:BA:1288:U:C2 | 23:BA:1327:C:O2 | 2.51 | 0.64 |
| 9:CI:17:VAL:HG11 | 9:CI:81:ILE:HA | 1.80 | 0.64 |
| 1:CA:991:U:H3' | 1:CA:1212:U:H3 | 1.62 | 0.63 |
| 23:DA:271(J):C:O2' | 23:DA:271(K):U:H5' | 1.97 | 0.63 |
| 1:CA:1027:C:N1 | 1:CA:1034:G:N2 | 2.45 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1019:U:HO2' | 23:BA:1021:A:H2 | 1.44 | 0.63 |
| 23:BA:1639:U:C2' | 23:BA:1640:C:H5'' | 2.28 | 0.63 |
| 5:AE:98:THR:HG22 | 5:AE:99:GLY:H | 1.61 | 0.63 |
| 20:AT:33:ILE:O | 20:AT:37:SER:OG | 2.14 | 0.63 |
| 27:DF:68:LYS:HB3 | 27:DF:69:HIS:ND1 | 2.13 | 0.63 |
| 29:DH:70:THR:HA | 29:DH:73:ALA:HB3 | 1.80 | 0.63 |
| 23:BA:994:C:H3' | 38:BU:54:LYS:HE3 | 1.81 | 0.63 |
| 23:BA:2115:G:C2 | 23:BA:2117:A:N7 | 2.66 | 0.63 |
| 50:B6:3:SER:OG | 50:B6:4:GLU:N | 2.28 | 0.63 |
| 25:DD:237:GLU:OE1 | 56:DD:407:HOH:O | 2.15 | 0.63 |
| 1:CA:926:G:H21 | 22:CX:94:GLN:HE22 | 1.44 | 0.63 |
| 1:CA:1387:G:H2' | 1:CA:1388:C:C6 | 2.33 | 0.63 |
| 30:BI:62:LYS:HG2 | 30:BI:133:HIS:CE1 | 2.33 | 0.63 |
| 1:AA:1521:G:H2' | 1:AA:1522:U:C6 | 2.34 | 0.63 |
| 23:DA:2602:A:H4' | 23:DA:2603:G:OP1 | 1.98 | 0.63 |
| 9:CI:9:ARG:HH11 | 9:CI:104:ARG:HE | 1.45 | 0.63 |
| 23:BA:1536:C:H4' | 23:BA:1537:G:OP1 | 1.97 | 0.63 |
| 1:AA:1059:C:OP1 | 3:AC:199:LYS:NZ | 2.30 | 0.63 |
| 23:BA:301:G:OP2 | 42:BY:84:ARG:NH2 | 2.31 | 0.63 |
| 25:DD:5:LYS:HA | 25:DD:17:THR:HG22 | 1.81 | 0.63 |
| 1:CA:171:A:H2' | 1:CA:172:A:H8 | 1.63 | 0.63 |
| 23:DA:90:U:H2' | 23:DA:92:A:C8 | 2.33 | 0.63 |
| 23:DA:1784:A:OP1 | 56:DA:4604:HOH:O | 2.15 | 0.63 |
| 23:DA:2306:C:H3' | 23:DA:2307:G:C8 | 2.33 | 0.63 |
| 23:DA:1011:G:OP2 | 38:DU:66:ASN:ND2 | 2.28 | 0.63 |
| 1:CA:102:G:H2' | 1:CA:103:C:H6 | 1.62 | 0.63 |
| 1:AA:1400:C:N3 | 22:AX:63:ALA:HA | 2.13 | 0.63 |
| 11:CK:84:VAL:HG11 | 11:CK:91:ARG:HD2 | 1.80 | 0.63 |
| 23:DA:83:G:OP1 | 42:DY:95:LYS:NZ | 2.31 | 0.63 |
| 23:DA:2336:A:H61 | 44:D0:43:THR:HG22 | 1.64 | 0.63 |
| 3:AC:187:ALA:HB3 | 3:AC:198:VAL:HB | 1.80 | 0.63 |
| 28:BG:56:ALA:HA | 28:BG:153:ARG:HH21 | 1.63 | 0.63 |
| 1:CA:1121:U:O4 | 1:CA:1152:A:N1 | 2.31 | 0.63 |
| 8:AH:120:THR:H | 8:AH:123:GLU:HB2 | 1.64 | 0.63 |
| 5:CE:98:THR:HG22 | 5:CE:99:GLY:H | 1.63 | 0.63 |
| 38:DU:28:ARG:NH1 | 38:DU:38:THR:OG1 | 2.31 | 0.63 |
| 9:AI:28:VAL:HG21 | 9:AI:37:PHE:HE2 | 1.63 | 0.63 |
| 1:AA:1441:G:C3' | 1:AA:1459:C:H42 | 2.12 | 0.63 |
| 1:AA:1009:G:O6 | 1:AA:1020:U:O2 | 2.17 | 0.63 |
| 13:CM:89:GLY:HA2 | 13:CM:92:HIS:CD2 | 2.33 | 0.63 |
| 33:DP:38:GLN:HA | 33:DP:41:ARG:HG2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1086:U:H2' | 1:AA:1087:G:C8 | 2.29 | 0.63 |
| 14:CN:23:ARG:NH1 | 14:CN:30:ALA:HB2 | 2.14 | 0.63 |
| 23:DA:668:G:H5'' | 23:DA:669:G:OP2 | 1.97 | 0.63 |
| 1:CA:1243:C:H5'' | 21:CU:8:THR:HG21 | 1.80 | 0.63 |
| 1:AA:533:A:OP2 | 56:AA:1816:HOH:O | 2.15 | 0.63 |
| 1:CA:989:C:H42 | 1:CA:1216:G:H1 | 0.72 | 0.63 |
| 1:CA:952:U:H3 | 1:CA:1229:A:N6 | 1.97 | 0.63 |
| 43:BZ:82:ARG:NH2 | 43:BZ:82:ARG:HB3 | 2.14 | 0.63 |
| 25:DD:108:PRO:HG2 | 25:DD:111:LEU:HG | 1.80 | 0.63 |
| 26:DE:9:VAL:HG22 | 26:DE:25:VAL:HB | 1.81 | 0.63 |
| 17:AQ:13:ASP:CG | 17:AQ:14:LYS:H | 2.02 | 0.63 |
| 23:DA:2592:G:OP1 | 56:DA:3768:HOH:O | 2.15 | 0.63 |
| 23:DA:68:G:O6 | 56:DA:4046:HOH:O | 2.15 | 0.63 |
| 32:BO:25:LEU:HD21 | 32:BO:40:VAL:HG23 | 1.81 | 0.63 |
| 33:BP:127:ALA:O | 33:BP:148:LEU:HD23 | 1.98 | 0.63 |
| 23:BA:910:A:H62 | 34:BQ:12:GLN:HA | 1.63 | 0.63 |
| 23:BA:314:A:C2' | 23:BA:315:G:H5' | 2.28 | 0.63 |
| 23:DA:546:C:H2' | 23:DA:547:A:H5' | 1.80 | 0.63 |
| 30:DI:1:MET:N | 30:DI:21:VAL:O | 2.31 | 0.63 |
| 23:BA:1968:G:OP1 | 56:BA:3899:HOH:O | 2.15 | 0.63 |
| 23:DA:95:G:O2' | 46:D2:46:GLN:HA | 1.99 | 0.63 |
| 1:AA:174:C:H2' | 1:AA:175:C:C6 | 2.33 | 0.63 |
| 49:B5:16:ARG:HG2 | 49:B5:16:ARG:HH11 | 1.62 | 0.63 |
| 23:BA:1278:A:OP1 | 35:BR:36:THR:HG23 | 1.98 | 0.63 |
| 29:BH:3:ARG:CZ | 29:BH:4:ILE:H | 2.12 | 0.63 |
| 23:BA:570:G:H5'' | 56:BA:4144:HOH:O | 1.98 | 0.63 |
| 23:BA:484:C:H2' | 23:BA:485:C:C6 | 2.34 | 0.63 |
| 20:CT:33:ILE:O | 20:CT:37:SER:OG | 2.12 | 0.63 |
| 53:B9:4:ARG:NH1 | 56:B9:201:HOH:O | 2.32 | 0.63 |
| 23:BA:249:C:OP1 | 56:BA:4502:HOH:O | 2.15 | 0.63 |
| 23:DA:2243:U:H2' | 23:DA:2244:U:C6 | 2.34 | 0.63 |
| 23:BA:1532:C:H2' | 23:BA:1533:G:O4' | 1.99 | 0.63 |
| 1:AA:1340:A:H2' | 1:AA:1341:U:O4' | 1.97 | 0.63 |
| 1:AA:1310:G:H2' | 1:AA:1311:G:C8 | 2.34 | 0.63 |
| 23:BA:1566:A:OP1 | 25:BD:211:ARG:NH1 | 2.32 | 0.63 |
| 29:BH:70:THR:HA | 29:BH:73:ALA:HB3 | 1.81 | 0.63 |
| 3:AC:47:LEU:HB3 | 3:AC:52:LEU:HD13 | 1.78 | 0.63 |
| 13:AM:40:ASN:O | 13:AM:42:ALA:N | 2.26 | 0.63 |
| 2:AB:17:PHE:H | 2:AB:17:PHE:HD2 | 1.46 | 0.63 |
| 23:BA:240:G:O6 | 56:BA:4246:HOH:O | 2.12 | 0.63 |
| 23:BA:2646:C:OP2 | 23:BA:2732:G:O2' | 2.15 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:AQ:50:LYS:HD3 | 17:AQ:51:TYR:CE1 | 2.34 | 0.63 |
| 1:AA:79:G:H2' | 1:AA:80:G:C8 | 2.24 | 0.62 |
| 23:DA:1140:C:O3' | 31:DN:25:ARG:NH1 | 2.31 | 0.62 |
| 16:CP:29:ASP:OD2 | 16:CP:29:ASP:N | 2.31 | 0.62 |
| 1:CA:352:C:O2' | 1:CA:354:G:OP1 | 2.12 | 0.62 |
| 23:DA:1485:G:H1 | 23:DA:1504:C:H42 | 1.47 | 0.62 |
| 7:CG:111:ARG:NH1 | 7:CG:119:ARG:O | 2.32 | 0.62 |
| 19:CS:80:TYR:O | 19:CS:81:ARG:HG3 | 1.99 | 0.62 |
| 23:DA:993:G:OP1 | 38:DU:50:ARG:NH2 | 2.31 | 0.62 |
| 23:BA:1171:G:O2' | 23:BA:1173:G:H2' | 2.00 | 0.62 |
| 4:CD:30:LYS:HA | 4:CD:35:ARG:HD2 | 1.80 | 0.62 |
| 1:AA:169:C:H2' | 1:AA:170:U:H6 | 1.65 | 0.62 |
| 1:AA:171:A:H2' | 1:AA:172:A:C8 | 2.34 | 0.62 |
| 1:AA:1378:C:HO2' | 1:AA:1379:G:H8 | 1.45 | 0.62 |
| 36:DS:58:LEU:HB2 | 36:DS:59:LYS:HB2 | 1.80 | 0.62 |
| 7:AG:65:ALA:HB2 | 7:AG:124:LEU:HD23 | 1.81 | 0.62 |
| 17:AQ:65:ILE:HD13 | 17:AQ:69:LYS:HE2 | 1.79 | 0.62 |
| 7:AG:139:GLU:O | 7:AG:143:ARG:N | 2.32 | 0.62 |
| 1:CA:920:U:H2' | 1:CA:921:U:C6 | 2.34 | 0.62 |
| 23:DA:459:U:H5'' | 51:D7:40:TRP:CD2 | 2.33 | 0.62 |
| 40:DW:13:SER:HB3 | 40:DW:16:LYS:HD2 | 1.80 | 0.62 |
| 1:CA:324:G:OP1 | 20:CT:70:SER:HB2 | 1.99 | 0.62 |
| 1:AA:1459:C:C6 | 1:AA:1460:A:C6 | 2.87 | 0.62 |
| 1:CA:1444:C:N3 | 1:CA:1459:C:H1' | 2.14 | 0.62 |
| 1:AA:1237:C:H2' | 1:AA:1335:C:H5' | 1.81 | 0.62 |
| 1:CA:1359:C:OP2 | 14:CN:35:ARG:HD2 | 1.99 | 0.62 |
| 23:BA:1047:G:H2' | 23:BA:1110:G:H1 | 1.64 | 0.62 |
| 3:AC:140:ARG:HB2 | 3:AC:140:ARG:NH1 | 2.14 | 0.62 |
| 3:AC:43:LEU:HD22 | 3:AC:47:LEU:HB2 | 1.81 | 0.62 |
| 23:DA:2394:C:OP1 | 52:D8:30:ARG:NH1 | 2.32 | 0.62 |
| 23:DA:644:A:H4' | 23:DA:645:C:C5 | 2.34 | 0.62 |
| 23:BA:2562:U:H1' | 32:BO:23:ARG:HH11 | 1.63 | 0.62 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:C8 | 2.34 | 0.62 |
| 23:DA:956:G:OP2 | 34:DQ:14:ARG:NH2 | 2.33 | 0.62 |
| 13:AM:87:TYR:HB2 | 19:AS:76:PRO:HG3 | 1.81 | 0.62 |
| 1:AA:1306:A:H1' | 1:AA:1332:A:C6 | 2.33 | 0.62 |
| 23:DA:2119:A:C2 | 23:DA:2170:A:H2' | 2.35 | 0.62 |
| 23:DA:2318:G:N2 | 36:DS:3:ARG:HD3 | 2.14 | 0.62 |
| 1:CA:166:G:H2' | 1:CA:167:G:C8 | 2.34 | 0.62 |
| 1:CA:1103:C:H2' | 1:CA:1104:G:O4' | 1.99 | 0.62 |
| 2:CB:167:PRO:HG3 | 2:CB:188:ALA:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:138:TYR:HD2 | 4:CD:139:ARG:N | 1.98 | 0.62 |
| 23:DA:2306:C:H5' | 23:DA:2307:G:H2' | 1.80 | 0.62 |
| 23:BA:2567:G:H2' | 23:BA:2568:C:C6 | 2.34 | 0.62 |
| 1:AA:1135:U:H2' | 1:AA:1137:C:O4' | 1.99 | 0.62 |
| 23:BA:1405:U:H2' | 23:BA:1406:U:C6 | 2.35 | 0.62 |
| 1:CA:1356:G:H2' | 1:CA:1357:A:H8 | 1.61 | 0.62 |
| 1:CA:1155:G:H2' | 1:CA:1156:G:C8 | 2.34 | 0.62 |
| 1:AA:191:G:H1' | 56:AA:1977:HOH:O | 2.00 | 0.62 |
| 33:BP:59:LEU:HD11 | 52:B8:10:ALA:HB2 | 1.81 | 0.62 |
| 23:BA:2327:A:H2' | 23:BA:2328:A:C8 | 2.34 | 0.62 |
| 26:BE:175:VAL:HG23 | 26:BE:177:PRO:HD3 | 1.80 | 0.62 |
| 23:BA:83:G:OP1 | 42:BY:95:LYS:NZ | 2.32 | 0.62 |
| 7:CG:149:ARG:HB2 | 11:CK:59:TYR:CD1 | 2.35 | 0.62 |
| 26:DE:135:HIS:CD2 | 26:DE:135:HIS:H | 2.18 | 0.62 |
| 23:BA:1763:G:OP1 | 23:BA:1763:G:H4' | 1.99 | 0.62 |
| 23:BA:1858:G:O6 | 56:BA:4008:HOH:O | 2.13 | 0.62 |
| 1:AA:1315:U:H2' | 1:AA:1316:G:O4' | 1.99 | 0.62 |
| 1:CA:1347:G:N1 | 1:CA:1374:A:OP2 | 2.28 | 0.62 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:N6 | 1.97 | 0.62 |
| 1:CA:1157:A:H4' | 1:CA:1158:C:O5' | 2.00 | 0.62 |
| 23:BA:1914:C:H2' | 23:BA:1915:U:H6 | 1.65 | 0.62 |
| 37:BT:11:GLU:OE1 | 37:BT:57:PHE:HB3 | 2.00 | 0.62 |
| 1:CA:918:A:H2' | 1:CA:919:A:C8 | 2.33 | 0.62 |
| 1:CA:1005:A:H1' | 1:CA:1036:G:N2 | 2.13 | 0.62 |
| 23:BA:2127:G:H21 | 23:BA:2173:A:H1' | 1.64 | 0.62 |
| 23:BA:1049:C:H4' | 23:BA:1050:A:OP1 | 1.99 | 0.62 |
| 1:CA:1323:G:O2' | 1:CA:1362:C:O2' | 2.18 | 0.62 |
| 9:AI:65:VAL:HG22 | 9:AI:73:GLN:HG2 | 1.81 | 0.62 |
| 1:CA:735:C:H2' | 1:CA:736:C:C6 | 2.33 | 0.62 |
| 34:BQ:27:VAL:N | 34:BQ:138:ASP:OD1 | 2.33 | 0.62 |
| 27:DF:185:ASP:HA | 27:DF:188:ARG:CD | 2.30 | 0.62 |
| 23:BA:1560:G:H3' | 56:BA:4361:HOH:O | 1.99 | 0.62 |
| 1:AA:745:C:OP1 | 1:AA:851:G:O2' | 2.18 | 0.62 |
| 1:AA:828:A:H2' | 1:AA:829:G:O4' | 2.00 | 0.62 |
| 1:CA:158:G:N2 | 1:CA:163:C:O2 | 2.32 | 0.62 |
| 23:BA:2760:C:H2' | 23:BA:2761:G:H5'' | 1.81 | 0.62 |
| 1:CA:662:G:O2' | 1:CA:836:G:OP1 | 2.17 | 0.62 |
| 25:DD:148:GLU:OE1 | 25:DD:151:LYS:NZ | 2.22 | 0.62 |
| 23:BA:2104:G:N7 | 23:BA:2186:G:N2 | 2.48 | 0.62 |
| 2:AB:15:VAL:HG23 | 2:AB:209:ARG:HG2 | 1.82 | 0.62 |
| 38:BU:92:ARG:HA | 38:BU:95:LEU:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1113:C:N3 | 1:CA:1187:G:N2 | 2.45 | 0.62 |
| 23:BA:580:C:H2' | 23:BA:581:C:C6 | 2.35 | 0.62 |
| 23:BA:2318:G:O2' | 23:BA:2319:G:OP1 | 2.15 | 0.62 |
| 1:CA:1239:A:H62 | 1:CA:1299:A:H61 | 1.48 | 0.62 |
| 23:BA:2206:G:H5' | 23:BA:2207:G:C5 | 2.35 | 0.62 |
| 14:CN:24:CYS:HB2 | 14:CN:40:CYS:H | 1.65 | 0.62 |
| 36:DS:96:GLY:HA2 | 36:DS:97:ARG:C | 2.20 | 0.62 |
| 1:AA:1347:G:H5'' | 9:AI:107:ARG:HG2 | 1.80 | 0.62 |
| 2:CB:78:GLN:O | 2:CB:94:ASN:ND2 | 2.32 | 0.62 |
| 23:DA:184:C:H2' | 23:DA:185:U:C6 | 2.35 | 0.62 |
| 14:AN:12:ARG:O | 14:AN:14:PRO:HD3 | 1.99 | 0.62 |
| 1:CA:664:G:P | 18:CR:64:ARG:HH21 | 2.21 | 0.62 |
| 1:AA:1026:G:H21 | 1:AA:1027:C:H5' | 1.65 | 0.62 |
| 1:AA:1065:U:H1' | 1:AA:1066:C:OP2 | 1.99 | 0.62 |
| 23:DA:271(I):G:N2 | 23:DA:271(O):C:N3 | 2.43 | 0.62 |
| 21:CU:3:LYS:HG2 | 21:CU:10:ARG:HG3 | 1.82 | 0.62 |
| 1:CA:1238:A:OP2 | 1:CA:1335:C:H1' | 1.99 | 0.62 |
| 23:BA:1721:G:H2' | 23:BA:1740:G:O6 | 2.00 | 0.62 |
| 23:DA:1495:A:H2' | 23:DA:1496:A:C8 | 2.35 | 0.62 |
| 2:AB:167:PRO:HG3 | 2:AB:188:ALA:HB2 | 1.80 | 0.62 |
| 41:DX:36:LYS:HG2 | 41:DX:54:VAL:HB | 1.81 | 0.62 |
| 1:CA:745:C:H2' | 1:CA:746:A:H8 | 1.63 | 0.62 |
| 27:BF:65:TRP:HH2 | 27:BF:72:ARG:HH21 | 1.48 | 0.62 |
| 1:AA:194:C:H2' | 1:AA:195:A:H5'' | 1.82 | 0.62 |
| 1:CA:542:G:H2' | 1:CA:543:C:C6 | 2.35 | 0.62 |
| 23:DA:203:C:H3' | 23:DA:204:A:H5'' | 1.81 | 0.62 |
| 1:CA:1135:U:H2' | 1:CA:1137:C:O4' | 1.99 | 0.62 |
| 1:CA:971:G:OP1 | 1:CA:972:C:H5'' | 2.00 | 0.62 |
| 23:BA:188:G:H1 | 23:BA:208:C:H42 | 1.48 | 0.62 |
| 27:BF:185:ASP:HA | 27:BF:188:ARG:CD | 2.30 | 0.62 |
| 2:AB:136:VAL:HA | 2:AB:139:LYS:HB3 | 1.82 | 0.62 |
| 5:AE:76:ILE:HG12 | 5:AE:77:PRO:HD2 | 1.81 | 0.62 |
| 23:BA:1153:C:OP1 | 38:BU:92:ARG:NH1 | 2.33 | 0.62 |
| 23:BA:2602:A:H4' | 23:BA:2603:G:OP1 | 2.00 | 0.62 |
| 3:CC:181:ASN:ND2 | 3:CC:181:ASN:O | 2.33 | 0.62 |
| 1:CA:1165:C:N3 | 1:CA:1171:G:N2 | 2.48 | 0.61 |
| 2:AB:28:PHE:HD2 | 2:AB:194:PRO:HG3 | 1.63 | 0.61 |
| 23:BA:307:G:N2 | 23:BA:309:G:H3' | 2.15 | 0.61 |
| 1:CA:957:U:O2' | 1:CA:959:A:N7 | 2.32 | 0.61 |
| 1:AA:353:A:H5' | 1:AA:353:A:H8 | 1.65 | 0.61 |
| 23:DA:1494:A:H2' | 23:DA:1495:A:C8 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:131:ARG:NH2 | 3:CC:166:GLU:OE2 | 2.32 | 0.61 |
| 23:DA:2377:A:H2' | 23:DA:2378:A:C8 | 2.34 | 0.61 |
| 24:BB:49:C:OP1 | 36:BS:97:ARG:N | 2.33 | 0.61 |
| 1:AA:1048:G:OP1 | 14:AN:3:ARG:HB3 | 1.99 | 0.61 |
| 23:BA:1165:U:H2' | 23:BA:1166:C:C6 | 2.35 | 0.61 |
| 1:CA:971:G:O2' | 1:CA:1365:G:H4' | 2.00 | 0.61 |
| 23:DA:2161:C:H2' | 23:DA:2162:G:C8 | 2.35 | 0.61 |
| 4:CD:155:LEU:HB3 | 4:CD:158:ILE:HB | 1.82 | 0.61 |
| 23:BA:2119:A:C2 | 23:BA:2170:A:H2' | 2.35 | 0.61 |
| 1:AA:142:G:H2' | 1:AA:143:A:C8 | 2.34 | 0.61 |
| 23:BA:250:G:OP2 | 52:B8:13:ARG:NH2 | 2.33 | 0.61 |
| 23:BA:2394:C:OP1 | 52:B8:30:ARG:NH1 | 2.33 | 0.61 |
| 1:CA:1452:C:O2' | 1:CA:1456:G:OP2 | 2.18 | 0.61 |
| 32:DO:64:ARG:HG2 | 32:DO:79:PHE:CG | 2.35 | 0.61 |
| 3:CC:184:TYR:HE1 | 3:CC:199:LYS:HB3 | 1.65 | 0.61 |
| 23:DA:2302:G:O2' | 28:DG:126:ASP:O | 2.16 | 0.61 |
| 13:AM:33:ALA:HB2 | 13:AM:64:TRP:CH2 | 2.35 | 0.61 |
| 5:AE:102:ALA:HB1 | 5:AE:106:PRO:HG2 | 1.81 | 0.61 |
| 1:AA:1109:C:H2' | 1:AA:1110:A:O4' | 2.00 | 0.61 |
| 1:AA:984:C:N3 | 1:AA:1221:G:N2 | 2.43 | 0.61 |
| 1:CA:1379:G:H21 | 1:CA:1381:U:H5 | 1.47 | 0.61 |
| 23:DA:2036:C:C6 | 23:DA:2036:C:H5' | 2.29 | 0.61 |
| 1:CA:1055:A:N1 | 1:CA:1056:U:H1' | 2.14 | 0.61 |
| 23:DA:1351:C:H3' | 56:DA:3935:HOH:O | 1.99 | 0.61 |
| 23:DA:2127:G:H21 | 23:DA:2173:A:H1' | 1.64 | 0.61 |
| 3:CC:18:TRP:CD1 | 14:CN:54:PRO:HA | 2.35 | 0.61 |
| 37:BT:53:ARG:NH1 | 37:BT:60:THR:OG1 | 2.33 | 0.61 |
| 1:CA:663:A:O3' | 18:CR:64:ARG:NH2 | 2.33 | 0.61 |
| 25:BD:222:ARG:NH1 | 56:BD:420:HOH:O | 2.32 | 0.61 |
| 11:CK:13:GLN:N | 11:CK:75:TYR:O | 2.32 | 0.61 |
| 10:CJ:63:PHE:HD1 | 14:CN:58:LYS:HA | 1.65 | 0.61 |
| 10:CJ:47:PHE:O | 10:CJ:63:PHE:N | 2.31 | 0.61 |
| 38:DU:58:ARG:HA | 38:DU:61:TRP:CE3 | 2.36 | 0.61 |
| 31:BN:15:LEU:HB2 | 31:BN:135:PRO:HB2 | 1.82 | 0.61 |
| 7:CG:47:CYS:SG | 7:CG:58:PRO:HB3 | 2.41 | 0.61 |
| 23:BA:467:G:OP1 | 51:B7:33:ARG:NH1 | 2.32 | 0.61 |
| 23:DA:559:G:H22 | 38:DU:49:HIS:CD2 | 2.19 | 0.61 |
| 17:AQ:22:LEU:HD11 | 17:AQ:39:SER:HB3 | 1.82 | 0.61 |
| 6:AF:62:TRP:CH2 | 6:AF:64:GLN:HB2 | 2.36 | 0.61 |
| 1:AA:1442:G:N7 | 1:AA:1442(A):G:C5 | 2.68 | 0.61 |
| 1:CA:1441:G:N2 | 1:CA:1459:C:H5 | 1.98 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2162:G:H1' | 23:BA:2173:A:H1' | 1.82 | 0.61 |
| 5:CE:102:ALA:HB1 | 5:CE:106:PRO:HG2 | 1.82 | 0.61 |
| 10:CJ:45:ARG:O | 10:CJ:65:LEU:N | 2.33 | 0.61 |
| 23:DA:2591:C:OP2 | 25:DD:239:ARG:HB3 | 1.99 | 0.61 |
| 23:BA:1972:A:OP2 | 56:BA:4868:HOH:O | 2.16 | 0.61 |
| 6:AF:97:PHE:HD2 | 18:AR:31:LEU:HD21 | 1.65 | 0.61 |
| 23:DA:2162:G:H1' | 23:DA:2173:A:H1' | 1.81 | 0.61 |
| 23:DA:2318:G:O2' | 23:DA:2319:G:OP1 | 2.15 | 0.61 |
| 23:DA:15:G:H5'' | 56:DA:4619:HOH:O | 2.00 | 0.61 |
| 1:CA:1217:C:H2' | 1:CA:1218:C:C6 | 2.36 | 0.61 |
| 1:CA:376:G:H1 | 1:CA:387:U:H3 | 1.47 | 0.61 |
| 23:BA:668:G:H5'' | 23:BA:669:G:OP2 | 2.01 | 0.61 |
| 23:DA:1815:A:OP2 | 25:DD:54:ARG:NH2 | 2.33 | 0.61 |
| 37:BT:56:GLY:O | 37:BT:59:THR:HG22 | 2.00 | 0.61 |
| 1:AA:376:G:H1 | 1:AA:387:U:H3 | 1.47 | 0.61 |
| 1:CA:1442(A):G:N3 | 1:CA:1442(B):A:H2' | 2.15 | 0.61 |
| 1:AA:977:A:H8 | 1:AA:1223:C:C4 | 2.19 | 0.61 |
| 1:AA:1322:C:OP1 | 19:AS:78:ARG:NH2 | 2.34 | 0.61 |
| 1:CA:955:U:H1' | 1:CA:1227:A:N6 | 2.13 | 0.61 |
| 1:CA:1238:A:N6 | 1:CA:1296:C:O2 | 2.33 | 0.61 |
| 19:AS:46:GLY:HA2 | 19:AS:61:TYR:CE1 | 2.34 | 0.61 |
| 23:DA:1048:A:H4' | 23:DA:1049:C:OP1 | 2.01 | 0.61 |
| 23:DA:143(A):C:H2' | 23:DA:144:C:H6 | 1.65 | 0.61 |
| 10:AJ:42:THR:HG23 | 10:AJ:68:HIS:HA | 1.81 | 0.61 |
| 12:AL:102:ARG:HA | 12:AL:107:ALA:HB1 | 1.82 | 0.61 |
| 45:B1:50:ARG:HG2 | 45:B1:59:THR:HG22 | 1.83 | 0.61 |
| 1:CA:1007:C:O2 | 1:CA:1023:G:N2 | 2.34 | 0.61 |
| 1:CA:1306:A:H3' | 1:CA:1307:U:C6 | 2.36 | 0.61 |
| 23:BA:1534:U:H3' | 23:BA:1535:A:C2 | 2.36 | 0.61 |
| 23:BA:910:A:C5 | 34:BQ:13:GLN:HG3 | 2.35 | 0.61 |
| 23:BA:1030:G:OP2 | 34:BQ:128:LYS:NZ | 2.32 | 0.61 |
| 23:BA:2306:C:H5' | 23:BA:2307:G:H2' | 1.81 | 0.61 |
| 1:CA:1016:A:C5 | 1:CA:1017:G:H1' | 2.35 | 0.61 |
| 1:CA:243:A:H4' | 1:CA:244:U:O5' | 2.00 | 0.61 |
| 23:DA:1327:C:OP2 | 56:DA:4452:HOH:O | 2.16 | 0.61 |
| 1:CA:833:U:H2' | 1:CA:834:C:C6 | 2.36 | 0.61 |
| 1:CA:532:A:N1 | 3:CC:193:TYR:HB3 | 2.16 | 0.61 |
| 23:DA:1584:C:H2' | 23:DA:1586:A:H5' | 1.83 | 0.61 |
| 7:CG:12:LEU:HD21 | 7:CG:24:THR:HB | 1.82 | 0.61 |
| 1:CA:142:G:H2' | 1:CA:143:A:H8 | 1.64 | 0.61 |
| 1:CA:1128:C:H1' | 1:CA:1146:A:H61 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1245:A:H2' | 1:AA:1246:C:H5' | 1.82 | 0.61 |
| 1:AA:765:G:H5'' | 1:AA:766:A:OP1 | 2.00 | 0.61 |
| 19:AS:63:THR:HB | 19:AS:65:ASN:H | 1.65 | 0.61 |
| 2:CB:178:ARG:HH22 | 8:CH:68:ARG:HH22 | 1.48 | 0.61 |
| 38:DU:76:TYR:CE2 | 38:DU:80:ILE:HG13 | 2.35 | 0.61 |
| 23:BA:271(E):U:H2' | 23:BA:271(F):C:C6 | 2.36 | 0.61 |
| 36:BS:14:VAL:O | 36:BS:18:ILE:HG12 | 2.01 | 0.61 |
| 27:DF:126:VAL:HG21 | 27:DF:129:PHE:CE1 | 2.36 | 0.61 |
| 18:CR:44:LEU:HD21 | 18:CR:70:ILE:HD13 | 1.82 | 0.61 |
| 12:AL:79:GLU:O | 12:AL:80:HIS:HB2 | 2.01 | 0.61 |
| 17:CQ:13:ASP:CG | 17:CQ:14:LYS:H | 2.04 | 0.61 |
| 1:AA:1442(A):G:C6 | 1:AA:1442(B):A:C2 | 2.89 | 0.61 |
| 1:AA:1190:G:H4' | 3:AC:176:HIS:CE1 | 2.35 | 0.61 |
| 19:AS:36:ARG:HB2 | 19:AS:72:GLY:CA | 2.31 | 0.61 |
| 1:CA:1131:G:H1 | 1:CA:1143:G:N2 | 1.98 | 0.61 |
| 2:CB:54:THR:O | 2:CB:58:ILE:HG13 | 2.00 | 0.61 |
| 1:CA:1242:C:H4' | 1:CA:1303:C:O3' | 2.01 | 0.61 |
| 1:AA:345:C:OP2 | 37:BT:39:ARG:NH2 | 2.32 | 0.61 |
| 1:AA:1377:A:C8 | 7:AG:7:ALA:HB1 | 2.36 | 0.61 |
| 1:CA:407:G:H4' | 4:CD:116:GLN:HA | 1.83 | 0.61 |
| 23:BA:1584:C:H2' | 23:BA:1586:A:H5' | 1.82 | 0.61 |
| 1:CA:542:G:H2' | 1:CA:543:C:H6 | 1.66 | 0.61 |
| 2:CB:15:VAL:HG23 | 2:CB:209:ARG:HG2 | 1.82 | 0.61 |
| 23:DA:2567:G:H2' | 23:DA:2568:C:C6 | 2.36 | 0.61 |
| 23:DA:1278:A:OP1 | 35:DR:36:THR:HG23 | 2.01 | 0.61 |
| 23:DA:606:U:H4' | 23:DA:658:C:H4' | 1.83 | 0.61 |
| 28:DG:145:THR:OG1 | 28:DG:146:TYR:N | 2.34 | 0.61 |
| 23:DA:492:A:H2' | 23:DA:493:G:O4' | 2.01 | 0.61 |
| 1:AA:1206:G:H2' | 1:AA:1207:G:O4' | 2.01 | 0.60 |
| 2:AB:82:ARG:HG2 | 2:AB:92:TYR:OH | 2.01 | 0.60 |
| 2:CB:77:ALA:HB2 | 2:CB:211:ILE:HG12 | 1.81 | 0.60 |
| 23:BA:1047:G:H2' | 23:BA:1110:G:N2 | 2.16 | 0.60 |
| 1:CA:994:A:H2 | 14:CN:4:LYS:HD3 | 1.66 | 0.60 |
| 25:DD:206:LEU:HD22 | 25:DD:211:ARG:HG2 | 1.83 | 0.60 |
| 1:AA:1347:G:O2' | 1:AA:1373:G:O6 | 2.13 | 0.60 |
| 23:BA:1187:G:O6 | 56:BA:4432:HOH:O | 2.13 | 0.60 |
| 1:AA:123:C:O2' | 1:AA:290:C:O2 | 2.17 | 0.60 |
| 23:DA:1816:G:OP2 | 56:DA:3705:HOH:O | 2.16 | 0.60 |
| 30:BI:139:GLN:HE21 | 30:BI:139:GLN:HA | 1.65 | 0.60 |
| 16:AP:20:VAL:HG23 | 16:AP:34:GLU:O | 2.01 | 0.60 |
| 23:DA:2327:A:H2' | 23:DA:2328:A:C8 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1459:C:H2' | 1:AA:1460:A:C5 | 2.35 | 0.60 |
| 1:AA:983:A:H2 | 1:AA:984:C:C6 | 2.19 | 0.60 |
| 23:DA:1014:U:H2' | 23:DA:1015:G:C8 | 2.35 | 0.60 |
| 23:BA:1784:A:OP1 | 56:BA:4606:HOH:O | 2.16 | 0.60 |
| 1:CA:745:C:OP1 | 1:CA:851:G:O2' | 2.18 | 0.60 |
| 1:CA:376:G:OP2 | 16:CP:67:THR:HG21 | 2.00 | 0.60 |
| 2:AB:24:TRP:HZ3 | 2:AB:29:ALA:HB2 | 1.65 | 0.60 |
| 43:BZ:48:PHE:HE2 | 43:BZ:71:VAL:HG11 | 1.65 | 0.60 |
| 25:BD:108:PRO:HG2 | 25:BD:111:LEU:HG | 1.83 | 0.60 |
| 4:CD:89:THR:HB | 4:CD:204:ILE:HD11 | 1.83 | 0.60 |
| 23:BA:387:U:OP1 | 56:BA:3957:HOH:O | 2.16 | 0.60 |
| 12:CL:27:LEU:O | 12:CL:29:GLY:N | 2.34 | 0.60 |
| 43:BZ:158:PRO:O | 43:BZ:161:VAL:HB | 2.02 | 0.60 |
| 1:AA:501:C:OP1 | 12:AL:117:ARG:NH2 | 2.34 | 0.60 |
| 30:DI:102:SER:HA | 30:DI:106:GLY:HA3 | 1.83 | 0.60 |
| 51:D7:23:ARG:HB3 | 51:D7:23:ARG:HH11 | 1.65 | 0.60 |
| 22:AX:69:ASP:HB2 | 22:AX:72:ALA:HB2 | 1.83 | 0.60 |
| 1:CA:1442(A):G:C6 | 1:CA:1442(B):A:C2 | 2.89 | 0.60 |
| 1:CA:878:G:H5' | 8:CH:89:PRO:HG2 | 1.81 | 0.60 |
| 41:DX:32:PRO:HA | 41:DX:77:LYS:HB2 | 1.84 | 0.60 |
| 6:CF:61:LEU:HB3 | 6:CF:63:TYR:CE2 | 2.33 | 0.60 |
| 1:AA:1251:A:N3 | 1:AA:1369:C:O2' | 2.29 | 0.60 |
| 23:DA:143:G:H2' | 23:DA:143(A):C:C6 | 2.36 | 0.60 |
| 23:BA:644:A:H4' | 23:BA:645:C:C5 | 2.36 | 0.60 |
| 23:DA:2835:A:N3 | 56:DA:4320:HOH:O | 2.30 | 0.60 |
| 42:DY:102:CYS:O | 42:DY:104:GLY:N | 2.34 | 0.60 |
| 6:AF:69:GLU:O | 6:AF:72:VAL:HG13 | 2.00 | 0.60 |
| 1:AA:532:A:H61 | 3:AC:193:TYR:HB3 | 1.65 | 0.60 |
| 24:DB:110:G:H2' | 24:DB:111:G:H8 | 1.66 | 0.60 |
| 1:AA:1220:G:H1' | 19:AS:52:TYR:CD2 | 2.36 | 0.60 |
| 1:AA:1186:G:H4' | 9:AI:110:GLU:OE1 | 2.02 | 0.60 |
| 23:DA:1047:G:H21 | 23:DA:1111:A:N6 | 1.99 | 0.60 |
| 23:DA:1153:C:OP1 | 38:DU:92:ARG:NH1 | 2.33 | 0.60 |
| 37:BT:53:ARG:HH11 | 37:BT:53:ARG:HB3 | 1.66 | 0.60 |
| 1:CA:59:A:H1' | 1:CA:354:G:N2 | 2.17 | 0.60 |
| 24:DB:110:G:H2' | 24:DB:111:G:C8 | 2.35 | 0.60 |
| 16:CP:49:LEU:HD11 | 16:CP:51:VAL:HG23 | 1.83 | 0.60 |
| 27:DF:46:ARG:HG2 | 27:DF:46:ARG:HH11 | 1.66 | 0.60 |
| 1:CA:509:A:H3' | 56:CA:1939:HOH:O | 2.00 | 0.60 |
| 23:BA:527:C:OP1 | 56:BA:4556:HOH:O | 2.15 | 0.60 |
| 23:BA:1131:G:H21 | 31:BN:73:THR:HG21 | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1051:C:N4 | 1:AA:1207:G:C6 | 2.69 | 0.60 |
| 19:AS:51:VAL:HB | 19:AS:75:ALA:HB3 | 1.84 | 0.60 |
| 1:AA:1300:G:O2' | 1:AA:1303:C:N4 | 2.34 | 0.60 |
| 23:BA:2318:G:H22 | 36:BS:3:ARG:HH11 | 1.48 | 0.60 |
| 1:AA:102:G:H2' | 1:AA:103:C:C6 | 2.36 | 0.60 |
| 23:DA:528:A:N1 | 23:DA:2042:A:H2' | 2.17 | 0.60 |
| 49:D5:20:ARG:HG2 | 49:D5:23:HIS:CD2 | 2.36 | 0.60 |
| 23:BA:1819:A:H4' | 23:BA:1820:U:O5' | 2.01 | 0.60 |
| 28:BG:106:LEU:HD12 | 28:BG:110:ALA:HB3 | 1.81 | 0.60 |
| 17:CQ:48:GLU:HB2 | 17:CQ:50:LYS:HG2 | 1.83 | 0.60 |
| 1:AA:100:C:H2' | 1:AA:101:A:C8 | 2.36 | 0.60 |
| 23:BA:9:U:H3 | 23:BA:2629:A:H2 | 1.48 | 0.60 |
| 1:CA:41:G:H2' | 1:CA:42:G:C8 | 2.36 | 0.60 |
| 15:AO:8:LYS:HG2 | 15:AO:12:ILE:HD11 | 1.84 | 0.60 |
| 7:AG:41:ARG:O | 7:AG:45:ASP:N | 2.29 | 0.60 |
| 1:AA:627:G:H2' | 1:AA:628:G:H8 | 1.66 | 0.60 |
| 23:BA:430:G:OP1 | 56:BA:4251:HOH:O | 2.16 | 0.60 |
| 1:CA:1401:G:OP1 | 22:CX:80:LYS:HE2 | 2.02 | 0.60 |
| 23:DA:2228:G:O6 | 56:DA:4148:HOH:O | 2.11 | 0.60 |
| 28:DG:11:TYR:CZ | 28:DG:16:ARG:HD3 | 2.36 | 0.60 |
| 1:AA:171:A:H2' | 1:AA:172:A:H8 | 1.65 | 0.60 |
| 19:AS:45:VAL:HA | 19:AS:62:ILE:HB | 1.81 | 0.60 |
| 14:CN:25:VAL:H | 14:CN:39:LEU:HD23 | 1.65 | 0.60 |
| 1:AA:735:C:H2' | 1:AA:736:C:C6 | 2.34 | 0.60 |
| 1:CA:745:C:H2' | 1:CA:746:A:C8 | 2.37 | 0.60 |
| 23:DA:1587:A:H2' | 23:DA:1588:C:C6 | 2.36 | 0.60 |
| 12:CL:79:GLU:O | 12:CL:80:HIS:HB2 | 2.01 | 0.60 |
| 23:BA:747:U:O2 | 23:BA:2014:A:H1' | 2.01 | 0.60 |
| 3:AC:36:ASP:HA | 3:AC:39:ILE:HB | 1.83 | 0.60 |
| 23:DA:1165:U:H2' | 23:DA:1166:C:C6 | 2.37 | 0.60 |
| 1:AA:303:A:H2' | 1:AA:304:U:O4' | 2.01 | 0.60 |
| 23:DA:2572:A:N7 | 26:DE:145:LYS:HB2 | 2.16 | 0.60 |
| 23:DA:1470:G:N7 | 56:DA:4123:HOH:O | 2.32 | 0.60 |
| 1:AA:510:A:OP2 | 56:AA:1890:HOH:O | 2.17 | 0.60 |
| 23:DA:760:G:OP1 | 56:DA:3635:HOH:O | 2.17 | 0.60 |
| 1:AA:1014:A:H4' | 19:AS:14:HIS:CE1 | 2.37 | 0.60 |
| 1:CA:1128:C:H5' | 9:CI:16:ARG:HH12 | 1.66 | 0.60 |
| 1:CA:1236:A:H4' | 1:CA:1304:G:H5' | 1.84 | 0.60 |
| 1:AA:1256:A:OP2 | 1:AA:1279:A:N6 | 2.34 | 0.60 |
| 33:DP:127:ALA:O | 33:DP:148:LEU:HD23 | 2.02 | 0.60 |
| 1:CA:1027:C:C4 | 1:CA:1034:G:N1 | 2.70 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:DZ:48:PHE:HE2 | 43:DZ:71:VAL:HG11 | 1.66 | 0.60 |
| 23:DA:1430:C:H2' | 23:DA:1431:U:C6 | 2.36 | 0.60 |
| 25:BD:108:PRO:HB3 | 25:BD:143:HIS:CE1 | 2.37 | 0.60 |
| 22:AX:69:ASP:HB3 | 22:AX:71:TYR:H | 1.66 | 0.60 |
| 1:CA:41:G:H2' | 1:CA:42:G:H8 | 1.67 | 0.60 |
| 1:CA:1063:C:H2' | 1:CA:1064:G:C8 | 2.36 | 0.60 |
| 23:BA:2845:G:O2' | 23:BA:2846:G:H5' | 2.02 | 0.60 |
| 30:BI:145:VAL:HG12 | 30:BI:146:ALA:H | 1.67 | 0.60 |
| 28:BG:77:ILE:N | 28:BG:82:LEU:O | 2.30 | 0.60 |
| 24:BB:110:G:H2' | 24:BB:111:G:C8 | 2.36 | 0.60 |
| 23:DA:620:G:N3 | 23:DA:620:G:H5'' | 2.16 | 0.60 |
| 24:DB:14:U:O3' | 24:DB:108:U:O2' | 2.19 | 0.60 |
| 5:CE:6:PHE:HB2 | 5:CE:34:VAL:HG22 | 1.82 | 0.60 |
| 1:CA:1046:A:H3' | 1:CA:1047:G:C8 | 2.37 | 0.60 |
| 23:BA:887:A:H5' | 23:BA:889:C:H41 | 1.67 | 0.60 |
| 2:AB:87:ARG:HD2 | 2:AB:219:VAL:HG11 | 1.83 | 0.60 |
| 1:CA:677:U:H3 | 1:CA:713:G:H22 | 1.48 | 0.60 |
| 23:DA:1021:A:H62 | 23:DA:1141:U:H3 | 1.48 | 0.60 |
| 1:CA:981:U:H2' | 1:CA:982:U:C5 | 2.36 | 0.60 |
| 23:BA:2136:C:N4 | 23:BA:2155:G:H1 | 2.00 | 0.60 |
| 36:DS:10:ARG:NH2 | 36:DS:91:PRO:HB2 | 2.16 | 0.60 |
| 24:DB:49:C:OP1 | 36:DS:97:ARG:N | 2.33 | 0.60 |
| 27:BF:184:TYR:O | 27:BF:188:ARG:HG3 | 2.02 | 0.60 |
| 25:DD:108:PRO:HB3 | 25:DD:143:HIS:HE1 | 1.66 | 0.60 |
| 24:BB:110:G:H2' | 24:BB:111:G:H8 | 1.67 | 0.60 |
| 1:AA:937:A:H3' | 1:AA:938:A:H8 | 1.65 | 0.60 |
| 42:BY:76:CYS:HB3 | 42:BY:79:CYS:HB2 | 1.82 | 0.60 |
| 40:DW:80:PRO:O | 40:DW:100:THR:HB | 2.01 | 0.60 |
| 51:D7:34:ARG:NH1 | 51:D7:41:ARG:O | 2.34 | 0.60 |
| 23:BA:1796:U:H2' | 23:BA:1797:C:C6 | 2.37 | 0.60 |
| 26:DE:32:PRO:HA | 26:DE:90:THR:HG22 | 1.84 | 0.60 |
| 23:DA:226:G:H21 | 23:DA:228:A:H62 | 1.49 | 0.60 |
| 1:CA:1441:G:N2 | 1:CA:1459:C:C5 | 2.70 | 0.60 |
| 23:DA:2335:A:N7 | 23:DA:2337:G:C5 | 2.70 | 0.60 |
| 1:AA:1121:U:H2' | 1:AA:1122:U:C6 | 2.37 | 0.60 |
| 23:BA:1177:A:H3' | 23:BA:1177:A:OP1 | 2.02 | 0.60 |
| 1:CA:1179:A:H2' | 1:CA:1180:A:O4' | 2.02 | 0.60 |
| 23:BA:1607:C:H4' | 23:BA:1608:A:O5' | 2.02 | 0.60 |
| 30:BI:83:ALA:HA | 30:BI:89:TYR:CD2 | 2.36 | 0.60 |
| 1:CA:174:C:H2' | 1:CA:175:C:H6 | 1.65 | 0.60 |
| 24:DB:52:A:N6 | 36:DS:33:LYS:HG2 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|--------------------|--------------------------|-------------------|
| 23:DA:2199:A:H3' | 23:DA:2200:C:C6 | 2.37 | 0.60 |
| 37:BT:53:ARG:NH1 | 37:BT:53:ARG:HB3 | 2.16 | 0.60 |
| 1:CA:450:G:OP1 | 16:CP:43:LYS:NZ | 2.35 | 0.60 |
| 1:AA:158:G:N2 | 1:AA:163:C:O2 | 2.34 | 0.60 |
| 23:BA:2199:A:H3' | 23:BA:2200:C:H6 | 1.65 | 0.60 |
| 41:BX:36:LYS:HG2 | 41:BX:54:VAL:HB | 1.83 | 0.60 |
| 3:AC:35:GLU:O | 3:AC:38:ARG:N | 2.34 | 0.60 |
| 30:BI:115:ALA:HB2 | 30:BI:129:THR:OG1 | 2.01 | 0.60 |
| 34:DQ:122:GLY:HA2 | 34:DQ:125:LEU:HD12 | 1.83 | 0.60 |
| 1:CA:1442(A):G:C2 | 1:CA:1442(B):A:H2' | 2.37 | 0.60 |
| 23:DA:2712(A):A:H5'' | 23:DA:2713:A:OP2 | 2.01 | 0.60 |
| 1:CA:1305:G:H1' | 1:CA:1306:A:C8 | 2.36 | 0.60 |
| 3:CC:137:ALA:O | 3:CC:141:VAL:HG23 | 2.02 | 0.60 |
| 23:BA:71:A:H2 | 41:BX:31:HIS:HE1 | 1.47 | 0.60 |
| 23:BA:1048:A:H4' | 23:BA:1049:C:OP1 | 2.00 | 0.60 |
| 23:DA:1721:G:H2' | 23:DA:1740:G:O6 | 2.01 | 0.60 |
| 38:DU:76:TYR:OH | 38:DU:92:ARG:NH1 | 2.35 | 0.60 |
| 1:AA:1125:U:H5' | 1:AA:1126:U:H5 | 1.67 | 0.60 |
| 1:AA:323:U:O3' | 20:AT:22:ARG:HD3 | 2.02 | 0.60 |
| 23:BA:1277:G:OP1 | 56:BA:3727:HOH:O | 2.17 | 0.60 |
| 1:CA:552:U:H4' | 12:CL:86:ARG:HG2 | 1.84 | 0.60 |
| 9:CI:46:ALA:HB1 | 9:CI:77:ILE:HB | 1.84 | 0.60 |
| 9:CI:49:PRO:HG2 | 9:CI:78:LYS:HA | 1.84 | 0.60 |
| 48:D4:14:ILE:HG22 | 48:D4:33:VAL:HG23 | 1.84 | 0.60 |
| 1:CA:972:C:H2' | 10:CJ:55:LYS:HB2 | 1.84 | 0.59 |
| 10:CJ:49:VAL:HG21 | 14:CN:41:ARG:HB2 | 1.83 | 0.59 |
| 1:AA:1305:G:H5'' | 21:AU:5:ASP:HA | 1.84 | 0.59 |
| 1:AA:1100:C:O2' | 1:AA:1102:A:OP1 | 2.13 | 0.59 |
| 23:DA:2808:U:H5' | 23:DA:2891:G:O6 | 2.02 | 0.59 |
| 3:CC:35:GLU:O | 3:CC:39:ILE:HG13 | 2.02 | 0.59 |
| 1:CA:438:G:OP1 | 4:CD:125:HIS:HE1 | 1.85 | 0.59 |
| 44:D0:53:MET:HG3 | 44:D0:59:LEU:CD2 | 2.32 | 0.59 |
| 9:AI:28:VAL:HG21 | 9:AI:37:PHE:CE2 | 2.37 | 0.59 |
| 50:B6:9:LEU:HD13 | 50:B6:51:GLU:HG3 | 1.84 | 0.59 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:HE2 | 1.67 | 0.59 |
| 27:BF:129:PHE:CD2 | 27:BF:163:VAL:HG21 | 2.37 | 0.59 |
| 4:AD:89:THR:HB | 4:AD:204:ILE:HD11 | 1.82 | 0.59 |
| 25:DD:33:LEU:O | 25:DD:64:ILE:HG13 | 2.02 | 0.59 |
| 1:AA:535:A:OP1 | 56:AA:1882:HOH:O | 2.17 | 0.59 |
| 23:DA:994:C:H3' | 38:DU:54:LYS:HE3 | 1.83 | 0.59 |
| 1:AA:904:C:OP2 | 56:AA:1900:HOH:O | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:986:A:H2' | 1:AA:987:G:C8 | 2.37 | 0.59 |
| 1:AA:1130:A:N6 | 1:AA:1144:G:H1' | 2.17 | 0.59 |
| 10:CJ:20:ALA:O | 10:CJ:24:VAL:N | 2.35 | 0.59 |
| 1:AA:1162:C:N4 | 1:AA:1174:G:H1 | 1.98 | 0.59 |
| 1:AA:1309:G:O6 | 1:AA:1328:C:N3 | 2.35 | 0.59 |
| 1:CA:1014:A:H2' | 1:CA:1015:A:C8 | 2.37 | 0.59 |
| 5:CE:76:ILE:HG12 | 5:CE:77:PRO:HD2 | 1.83 | 0.59 |
| 23:DA:94:C:H5' | 23:DA:94(A):G:OP2 | 2.01 | 0.59 |
| 23:DA:1796:U:H2' | 23:DA:1797:C:C6 | 2.37 | 0.59 |
| 23:DA:2104:G:N7 | 23:DA:2186:G:N2 | 2.49 | 0.59 |
| 2:AB:195:ASP:O | 8:AH:74:PRO:HG3 | 2.01 | 0.59 |
| 1:CA:683:G:H2' | 1:CA:684:A:C8 | 2.37 | 0.59 |
| 48:B4:42:PHE:CB | 48:B4:43:TYR:HB2 | 2.27 | 0.59 |
| 1:AA:1131:G:H2' | 1:AA:1132:C:C6 | 2.38 | 0.59 |
| 1:CA:1306:A:H1' | 1:CA:1332:A:C2 | 2.37 | 0.59 |
| 19:AS:62:ILE:HA | 19:AS:66:MET:SD | 2.42 | 0.59 |
| 1:CA:1072:G:H2' | 1:CA:1073:U:C6 | 2.37 | 0.59 |
| 3:CC:11:ARG:HD3 | 3:CC:178:LEU:O | 2.02 | 0.59 |
| 1:CA:542:G:P | 4:CD:10:ARG:HH22 | 2.26 | 0.59 |
| 23:BA:2612:C:O5' | 49:B5:2:ALA:HB3 | 2.02 | 0.59 |
| 41:BX:27:THR:HG23 | 41:BX:80:ILE:HG13 | 1.84 | 0.59 |
| 10:CJ:37:PRO:HA | 10:CJ:72:VAL:HG12 | 1.83 | 0.59 |
| 1:AA:495:A:O2' | 56:AA:1993:HOH:O | 2.17 | 0.59 |
| 1:CA:927:G:O2' | 1:CA:1503:A:N7 | 2.35 | 0.59 |
| 1:CA:316:G:OP2 | 1:CA:351:G:O2' | 2.20 | 0.59 |
| 23:DA:580:C:H2' | 23:DA:581:C:H6 | 1.66 | 0.59 |
| 4:AD:9:CYS:HA | 4:AD:12:CYS:HB2 | 1.84 | 0.59 |
| 1:CA:973:G:H4' | 14:CN:41:ARG:HH22 | 1.68 | 0.59 |
| 23:DA:330:A:C2 | 23:DA:1210:A:H2' | 2.27 | 0.59 |
| 7:CG:16:LEU:HD22 | 9:CI:45:ALA:N | 2.16 | 0.59 |
| 1:CA:169:C:H2' | 1:CA:170:U:H6 | 1.68 | 0.59 |
| 44:B0:27:GLU:HG3 | 44:B0:68:GLU:HA | 1.84 | 0.59 |
| 4:CD:26:CYS:HA | 4:CD:31:CYS:HB2 | 1.83 | 0.59 |
| 1:CA:509:A:H5'' | 4:CD:55:ALA:HB2 | 1.83 | 0.59 |
| 4:CD:72:GLU:OE1 | 4:CD:207:TYR:OH | 2.13 | 0.59 |
| 23:BA:1449:A:H5' | 23:BA:1450:G:OP2 | 2.03 | 0.59 |
| 26:DE:128:SER:OG | 26:DE:129:HIS:N | 2.35 | 0.59 |
| 23:BA:2773:C:H5'' | 26:BE:164:ARG:HG2 | 1.84 | 0.59 |
| 1:CA:583:A:H2' | 1:CA:584:G:O4' | 2.02 | 0.59 |
| 23:DA:192:C:OP1 | 56:DA:3825:HOH:O | 2.16 | 0.59 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:H6 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CI:9:ARG:HB2 | 9:CI:14:VAL:HG13 | 1.83 | 0.59 |
| 7:AG:30:ILE:HA | 7:AG:105:VAL:HG21 | 1.83 | 0.59 |
| 23:BA:2406:U:H2' | 23:BA:2406:U:OP2 | 2.02 | 0.59 |
| 1:CA:1117:G:H1' | 1:CA:1184:G:H22 | 1.66 | 0.59 |
| 23:DA:1639:U:C2' | 23:DA:1640:C:H5'' | 2.33 | 0.59 |
| 1:AA:484:G:HO2' | 1:AA:485:G:P | 2.25 | 0.59 |
| 1:CA:1015:A:H2' | 1:CA:1016:A:O4' | 2.02 | 0.59 |
| 23:DA:1049:C:H4' | 23:DA:1050:A:OP1 | 2.02 | 0.59 |
| 23:DA:873:G:N2 | 23:DA:905:U:O2 | 2.36 | 0.59 |
| 1:CA:765:G:H5'' | 1:CA:766:A:OP1 | 2.03 | 0.59 |
| 40:BW:84:ARG:HG3 | 40:BW:98:LYS:HD2 | 1.84 | 0.59 |
| 23:BA:652(B):A:H2' | 23:BA:652(B):A:N3 | 2.18 | 0.59 |
| 23:DA:2294:C:P | 36:DS:89:ARG:HH22 | 2.26 | 0.59 |
| 1:AA:1422:G:H5' | 32:BO:48:PRO:HB3 | 1.84 | 0.59 |
| 1:CA:1442(B):A:N7 | 37:DT:118:ARG:NH2 | 2.50 | 0.59 |
| 23:BA:2820:A:OP1 | 35:BR:4:LEU:HD23 | 2.01 | 0.59 |
| 1:AA:958:A:N6 | 19:AS:77:THR:O | 2.35 | 0.59 |
| 1:CA:1371:G:H5'' | 9:CI:69:GLY:N | 2.13 | 0.59 |
| 1:CA:1373:G:H4' | 7:CG:31:MET:HE3 | 1.84 | 0.59 |
| 1:AA:975:A:H4' | 1:AA:976:G:H5'' | 1.84 | 0.59 |
| 1:AA:1157:A:H1' | 1:AA:1181:G:N2 | 2.17 | 0.59 |
| 1:CA:1158:C:O2' | 1:CA:1160:G:OP1 | 2.12 | 0.59 |
| 1:CA:166:G:N7 | 56:CA:1921:HOH:O | 2.32 | 0.59 |
| 3:CC:115:LEU:HA | 3:CC:118:GLN:HG2 | 1.85 | 0.59 |
| 38:DU:76:TYR:HH | 38:DU:92:ARG:NH1 | 2.00 | 0.59 |
| 23:BA:61:G:H1 | 23:BA:94:C:H42 | 1.49 | 0.59 |
| 1:AA:501:C:H1' | 1:AA:549:C:H1' | 1.85 | 0.59 |
| 40:DW:79:GLY:HA3 | 40:DW:100:THR:HG22 | 1.85 | 0.59 |
| 1:AA:833:U:H2' | 1:AA:834:C:C6 | 2.37 | 0.59 |
| 1:CA:627:G:H2' | 1:CA:628:G:H8 | 1.68 | 0.59 |
| 18:AR:44:LEU:HD21 | 18:AR:70:ILE:HD13 | 1.85 | 0.59 |
| 1:CA:737:A:H2' | 1:CA:738:C:C6 | 2.37 | 0.59 |
| 13:CM:24:GLY:HA3 | 13:CM:66:LEU:HD22 | 1.84 | 0.59 |
| 1:AA:1321:C:C5' | 1:AA:1322:C:H5'' | 2.32 | 0.59 |
| 1:CA:1249:C:N4 | 1:CA:1287:A:H5' | 2.18 | 0.59 |
| 16:CP:28:ARG:HH11 | 16:CP:28:ARG:HG2 | 1.66 | 0.59 |
| 1:AA:186:C:H2' | 1:AA:187:C:H6 | 1.68 | 0.59 |
| 23:DA:911:A:OP1 | 56:DA:4345:HOH:O | 2.17 | 0.59 |
| 38:BU:76:TYR:CE2 | 38:BU:80:ILE:HG13 | 2.37 | 0.59 |
| 36:BS:96:GLY:HA2 | 36:BS:97:ARG:C | 2.22 | 0.59 |
| 1:CA:615:C:H2' | 1:CA:616:G:H8 | 1.68 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:753:A:OP1 | 15:CO:69:TYR:OH | 2.19 | 0.59 |
| 2:AB:115:LEU:HD13 | 2:AB:145:LEU:HB3 | 1.83 | 0.59 |
| 1:CA:1203:C:OP1 | 14:CN:3:ARG:NH1 | 2.33 | 0.59 |
| 36:DS:67:ARG:HG2 | 36:DS:71:ARG:NH2 | 2.18 | 0.59 |
| 23:BA:196:A:O4' | 33:BP:46:LYS:HE2 | 2.03 | 0.59 |
| 1:CA:1442(B):A:N7 | 37:DT:118:ARG:CZ | 2.66 | 0.59 |
| 9:CI:31:GLN:CD | 9:CI:36:TYR:HD1 | 2.05 | 0.59 |
| 1:AA:1325:C:H5' | 21:AU:17:THR:HG21 | 1.85 | 0.59 |
| 23:BA:1049:C:H2' | 23:BA:1050:A:H8 | 1.68 | 0.59 |
| 1:CA:833:U:H2' | 1:CA:834:C:H6 | 1.67 | 0.59 |
| 1:AA:652:U:C2 | 1:AA:752:G:N2 | 2.71 | 0.59 |
| 27:BF:85:GLY:O | 56:BF:403:HOH:O | 2.15 | 0.59 |
| 14:AN:24:CYS:HB2 | 14:AN:40:CYS:HB3 | 1.85 | 0.59 |
| 28:BG:124:SER:HB2 | 28:BG:131:TYR:CE1 | 2.37 | 0.59 |
| 29:BH:117:PRO:HB3 | 29:BH:123:PHE:CE2 | 2.37 | 0.59 |
| 23:BA:2867:G:OP2 | 37:BT:119:LYS:NZ | 2.31 | 0.59 |
| 1:CA:913:A:H4' | 1:CA:914:A:O5' | 2.03 | 0.59 |
| 23:DA:928:G:N1 | 56:DA:4230:HOH:O | 2.32 | 0.59 |
| 6:CF:70:ASP:OD1 | 6:CF:70:ASP:N | 2.36 | 0.59 |
| 1:CA:408:A:OP1 | 4:CD:113:SER:OG | 2.17 | 0.59 |
| 1:AA:1516:G:H2' | 1:AA:1518:A:OP2 | 2.03 | 0.59 |
| 23:BA:253:C:OP2 | 52:B8:5:LYS:NZ | 2.30 | 0.59 |
| 1:AA:983:A:H3' | 1:AA:984:C:C5' | 2.33 | 0.59 |
| 19:AS:10:PHE:HZ | 19:AS:37:ARG:HD3 | 1.68 | 0.59 |
| 1:AA:266:G:H5'' | 1:AA:267:C:C5 | 2.38 | 0.59 |
| 5:AE:80:ILE:HD12 | 5:AE:138:ALA:HB1 | 1.84 | 0.59 |
| 1:AA:1328:C:OP1 | 13:AM:28:ALA:HB1 | 2.03 | 0.59 |
| 42:DY:23:ARG:HG2 | 42:DY:42:VAL:HG22 | 1.83 | 0.59 |
| 1:CA:382:A:H2' | 1:CA:383:A:H8 | 1.68 | 0.59 |
| 1:CA:1189:C:OP1 | 14:CN:58:LYS:NZ | 2.29 | 0.59 |
| 23:DA:1050:A:H2' | 23:DA:1051:G:H8 | 1.68 | 0.59 |
| 1:AA:15:G:H8 | 1:AA:1396:A:HO2' | 1.51 | 0.59 |
| 23:DA:1509(A):A:H3' | 23:DA:1509(B):A:H8 | 1.67 | 0.59 |
| 18:CR:31:LEU:HD23 | 18:CR:31:LEU:H | 1.67 | 0.59 |
| 27:BF:50:SER:HB2 | 27:BF:94:PRO:HD3 | 1.84 | 0.59 |
| 22:AX:14:GLU:HA | 22:AX:17:ARG:HD3 | 1.83 | 0.59 |
| 1:AA:858:G:O6 | 1:AA:869:G:H3' | 2.02 | 0.59 |
| 23:BA:203:C:H3' | 23:BA:204:A:H5'' | 1.85 | 0.59 |
| 41:BX:8:ILE:O | 46:B2:36:ARG:NH2 | 2.35 | 0.59 |
| 23:BA:2272:U:H5'' | 23:BA:2273:A:OP1 | 2.02 | 0.59 |
| 3:CC:70:VAL:O | 3:CC:105:GLU:HA | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1459:C:C6 | 1:AA:1460:A:C5 | 2.91 | 0.59 |
| 1:CA:857:C:H2' | 1:CA:858:G:O4' | 2.03 | 0.59 |
| 23:BA:784:A:H5' | 23:BA:785:G:OP1 | 2.02 | 0.59 |
| 23:BA:1047:G:H21 | 23:BA:1111:A:N6 | 2.01 | 0.59 |
| 3:CC:138:VAL:HG22 | 3:CC:151:VAL:HG23 | 1.85 | 0.59 |
| 1:CA:944:G:H2' | 1:CA:1338:G:O6 | 2.02 | 0.59 |
| 1:CA:1246:C:N3 | 1:CA:1291:G:O6 | 2.36 | 0.59 |
| 23:BA:546:C:H2' | 23:BA:547:A:H5' | 1.83 | 0.59 |
| 6:CF:62:TRP:CH2 | 6:CF:64:GLN:HB2 | 2.37 | 0.59 |
| 1:CA:377:G:H2' | 1:CA:378:G:C8 | 2.37 | 0.59 |
| 3:AC:27:LYS:O | 3:AC:31:HIS:CE1 | 2.55 | 0.59 |
| 7:CG:64:GLN:HG3 | 7:CG:128:ALA:HB1 | 1.85 | 0.59 |
| 1:CA:1131:G:H2' | 1:CA:1132:C:C6 | 2.38 | 0.58 |
| 9:CI:29:ASN:HD21 | 9:CI:65:VAL:H | 1.51 | 0.58 |
| 23:BA:2406:U:OP1 | 56:BA:4496:HOH:O | 2.17 | 0.58 |
| 23:BA:1790:C:H5'' | 23:BA:1791:A:OP1 | 2.02 | 0.58 |
| 14:CN:24:CYS:HA | 14:CN:39:LEU:HA | 1.85 | 0.58 |
| 45:B1:3:LYS:HB2 | 45:B1:61:ARG:HH11 | 1.68 | 0.58 |
| 1:CA:1269:A:OP1 | 21:CU:24:ARG:HB2 | 2.03 | 0.58 |
| 1:AA:626:U:H2' | 1:AA:627:G:C8 | 2.37 | 0.58 |
| 23:DA:1156:A:C8 | 38:DU:51:LYS:HD2 | 2.38 | 0.58 |
| 41:DX:8:ILE:O | 46:D2:36:ARG:NH2 | 2.36 | 0.58 |
| 2:CB:69:LEU:HD22 | 2:CB:91:PRO:HB2 | 1.85 | 0.58 |
| 4:AD:18:LYS:HA | 4:AD:33:MET:HG3 | 1.84 | 0.58 |
| 23:BA:1865:G:H5' | 23:BA:1866:C:OP2 | 2.03 | 0.58 |
| 23:DA:2321:G:N3 | 23:DA:2321:G:H2' | 2.17 | 0.58 |
| 23:DA:2150:U:H2' | 23:DA:2151:G:H8 | 1.68 | 0.58 |
| 1:AA:1236:A:H2' | 1:AA:1237:C:C6 | 2.38 | 0.58 |
| 28:DG:60:LEU:HD23 | 28:DG:63:ILE:HD12 | 1.85 | 0.58 |
| 1:AA:1309:G:N1 | 1:AA:1328:C:O2 | 2.27 | 0.58 |
| 9:AI:27:THR:HB | 9:AI:62:TYR:CD1 | 2.38 | 0.58 |
| 3:AC:127:ARG:HB3 | 3:AC:127:ARG:NH1 | 2.17 | 0.58 |
| 31:BN:120:LEU:HD22 | 31:BN:122:VAL:HG23 | 1.83 | 0.58 |
| 23:DA:1882:C:H5' | 23:DA:1883:G:OP2 | 2.02 | 0.58 |
| 24:DB:43:C:H5'' | 48:D4:1:MET:HG2 | 1.86 | 0.58 |
| 23:DA:1997:G:OP2 | 56:DA:4358:HOH:O | 2.17 | 0.58 |
| 25:DD:142:VAL:HG23 | 25:DD:193:VAL:HA | 1.85 | 0.58 |
| 23:DA:908:C:OP1 | 34:DQ:22:LYS:HB3 | 2.03 | 0.58 |
| 28:DG:72:ARG:HH12 | 28:DG:87:PRO:HG3 | 1.68 | 0.58 |
| 23:DA:2406:U:C2 | 33:DP:72:PRO:HG2 | 2.38 | 0.58 |
| 23:DA:1899:G:H2' | 23:DA:1899:G:N3 | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:2196:C:OP2 | 56:BA:4415:HOH:O | 2.17 | 0.58 |
| 23:DA:2612:C:O5' | 49:D5:2:ALA:HB3 | 2.03 | 0.58 |
| 23:DA:1833:U:H2' | 23:DA:1834:U:H6 | 1.68 | 0.58 |
| 1:CA:1442:G:N7 | 1:CA:1442(A):G:C5 | 2.71 | 0.58 |
| 1:AA:988:G:H4' | 1:AA:1014:A:H61 | 1.69 | 0.58 |
| 1:CA:1124:G:O2' | 10:CJ:38:ILE:HG21 | 2.03 | 0.58 |
| 1:AA:1131:G:H1 | 1:AA:1143:G:N2 | 2.00 | 0.58 |
| 1:AA:1156:G:N2 | 1:AA:1179:A:H61 | 2.01 | 0.58 |
| 23:DA:2298:A:N6 | 23:DA:2318:G:H8 | 1.98 | 0.58 |
| 7:CG:14:PRO:HA | 7:CG:21:VAL:HA | 1.84 | 0.58 |
| 1:AA:1251:A:H2' | 1:AA:1252:A:O4' | 2.03 | 0.58 |
| 7:AG:99:LEU:HD23 | 7:AG:102:ARG:HH22 | 1.67 | 0.58 |
| 1:CA:1121:U:H2' | 1:CA:1122:U:H5' | 1.85 | 0.58 |
| 29:DH:124:GLU:HB2 | 29:DH:132:ARG:HB3 | 1.85 | 0.58 |
| 1:CA:102:G:H2' | 1:CA:103:C:C6 | 2.38 | 0.58 |
| 8:CH:31:PHE:CE2 | 8:CH:35:ILE:HD11 | 2.38 | 0.58 |
| 23:BA:8:A:OP1 | 31:BN:121:LYS:NZ | 2.36 | 0.58 |
| 23:BA:588:U:H2' | 23:BA:589:C:C6 | 2.38 | 0.58 |
| 2:CB:195:ASP:O | 8:CH:74:PRO:HG3 | 2.02 | 0.58 |
| 23:BA:226:G:H21 | 23:BA:228:A:H62 | 1.50 | 0.58 |
| 23:BA:1426:G:N7 | 25:BD:31:LYS:NZ | 2.51 | 0.58 |
| 23:DA:314:A:C2' | 23:DA:315:G:H5' | 2.32 | 0.58 |
| 23:BA:581:C:H2' | 23:BA:582:G:H8 | 1.69 | 0.58 |
| 33:DP:39:LYS:CB | 33:DP:45:LEU:HG | 2.32 | 0.58 |
| 3:CC:137:ALA:HA | 3:CC:140:ARG:HB2 | 1.84 | 0.58 |
| 1:AA:1172:C:H2' | 1:AA:1173:G:H8 | 1.69 | 0.58 |
| 17:CQ:67:LYS:HA | 17:CQ:70:ARG:HH12 | 1.69 | 0.58 |
| 1:CA:979:C:H42 | 14:CN:18:VAL:HG12 | 1.66 | 0.58 |
| 9:AI:13:ALA:HB2 | 9:AI:68:GLY:HA3 | 1.85 | 0.58 |
| 1:CA:606:G:H5'' | 1:CA:607:A:H5' | 1.85 | 0.58 |
| 23:DA:2023:G:H5' | 23:DA:2617:C:H4' | 1.85 | 0.58 |
| 1:CA:100:C:H2' | 1:CA:101:A:C8 | 2.38 | 0.58 |
| 23:BA:184:C:H2' | 23:BA:185:U:C6 | 2.38 | 0.58 |
| 4:CD:193:ASP:OD1 | 4:CD:193:ASP:N | 2.35 | 0.58 |
| 1:AA:279:A:C5 | 17:AQ:98:LEU:HD23 | 2.39 | 0.58 |
| 1:AA:1095:U:H2' | 1:AA:1096:C:C6 | 2.38 | 0.58 |
| 28:DG:56:ALA:HA | 28:DG:153:ARG:HH21 | 1.67 | 0.58 |
| 23:DA:1045:A:H4' | 23:DA:1047:G:C4 | 2.38 | 0.58 |
| 2:CB:136:VAL:HA | 2:CB:139:LYS:HB3 | 1.85 | 0.58 |
| 1:CA:542:G:OP1 | 4:CD:10:ARG:NH2 | 2.35 | 0.58 |
| 23:DA:2406:U:H2' | 23:DA:2406:U:OP2 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BD:148:GLU:HB2 | 25:BD:151:LYS:HD2 | 1.86 | 0.58 |
| 23:DA:1991:U:H2' | 23:DA:1992:G:H5'' | 1.86 | 0.58 |
| 28:BG:150:ASP:CG | 28:BG:151:ALA:H | 2.07 | 0.58 |
| 1:AA:414:A:H2' | 1:AA:415:A:C8 | 2.39 | 0.58 |
| 45:D1:23:LYS:HB3 | 45:D1:29:GLY:HA3 | 1.85 | 0.58 |
| 1:CA:353:A:H8 | 1:CA:353:A:H5' | 1.69 | 0.58 |
| 1:AA:615:C:H2' | 1:AA:616:G:H8 | 1.68 | 0.58 |
| 3:AC:148:GLY:HA3 | 3:AC:172:ARG:O | 2.03 | 0.58 |
| 1:AA:31:G:N7 | 56:AA:1893:HOH:O | 2.32 | 0.58 |
| 4:AD:26:CYS:HA | 4:AD:31:CYS:HB2 | 1.84 | 0.58 |
| 1:CA:951:G:N2 | 1:CA:952:U:H1' | 2.19 | 0.58 |
| 1:AA:76:C:H3' | 1:AA:77:G:H5'' | 1.85 | 0.58 |
| 23:BA:581:C:H2' | 23:BA:582:G:C8 | 2.39 | 0.58 |
| 10:AJ:38:ILE:HG12 | 10:AJ:71:LEU:O | 2.03 | 0.58 |
| 23:DA:2115:G:C2 | 23:DA:2117:A:N7 | 2.71 | 0.58 |
| 28:BG:11:TYR:CZ | 28:BG:16:ARG:HD3 | 2.38 | 0.58 |
| 1:AA:148:G:H2' | 1:AA:149:A:C8 | 2.34 | 0.58 |
| 13:AM:19:LEU:O | 13:AM:22:ILE:HB | 2.04 | 0.58 |
| 13:AM:3:ARG:HB3 | 13:AM:8:GLU:O | 2.04 | 0.58 |
| 1:CA:174:C:H2' | 1:CA:175:C:C6 | 2.37 | 0.58 |
| 1:AA:1356:G:H2' | 1:AA:1357:A:H8 | 1.67 | 0.58 |
| 19:AS:44:MET:O | 19:AS:47:HIS:ND1 | 2.37 | 0.58 |
| 29:DH:46:GLU:HB2 | 29:DH:49:VAL:HG12 | 1.83 | 0.58 |
| 37:DT:11:GLU:OE1 | 37:DT:57:PHE:HB3 | 2.03 | 0.58 |
| 30:BI:77:LEU:HB3 | 30:BI:142:VAL:HG12 | 1.85 | 0.58 |
| 51:D7:47:ARG:HG3 | 51:D7:47:ARG:HH11 | 1.69 | 0.58 |
| 23:BA:2610:C:H4' | 23:BA:2611:U:OP2 | 2.04 | 0.58 |
| 19:CS:51:VAL:O | 19:CS:57:HIS:HA | 2.04 | 0.58 |
| 23:BA:1021:A:H62 | 23:BA:1141:U:H3 | 1.52 | 0.58 |
| 1:AA:223:U:H2' | 1:AA:224:C:H6 | 1.68 | 0.58 |
| 23:DA:1047:G:H2' | 23:DA:1110:G:H1 | 1.67 | 0.58 |
| 23:BA:1351:C:H3' | 56:BA:3914:HOH:O | 2.03 | 0.58 |
| 23:BA:1352:U:P | 56:BA:3914:HOH:O | 2.60 | 0.58 |
| 11:CK:27:ASN:OD1 | 11:CK:28:THR:N | 2.36 | 0.58 |
| 34:DQ:43:THR:OG1 | 34:DQ:45:GLN:HG2 | 2.04 | 0.58 |
| 23:BA:662:G:OP1 | 56:BA:4541:HOH:O | 2.17 | 0.58 |
| 47:B3:10:LYS:NZ | 47:B3:15:TYR:OH | 2.37 | 0.58 |
| 20:AT:61:SER:O | 20:AT:65:LYS:HG2 | 2.03 | 0.58 |
| 1:CA:300:A:H1' | 1:CA:565:U:O2 | 2.04 | 0.58 |
| 12:AL:83:VAL:HG13 | 12:AL:100:ILE:HG23 | 1.86 | 0.58 |
| 30:DI:104:GLN:HG2 | 30:DI:105:HIS:CD2 | 2.38 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:AC:3:ASN:OD1 | 3:AC:3:ASN:N | 2.37 | 0.58 |
| 1:AA:17:U:H2' | 1:AA:18:C:C6 | 2.38 | 0.58 |
| 2:CB:28:PHE:HD2 | 2:CB:194:PRO:HG3 | 1.68 | 0.58 |
| 19:CS:36:ARG:HB3 | 19:CS:72:GLY:CA | 2.34 | 0.58 |
| 23:BA:2892:A:H2' | 23:BA:2893:G:H5' | 1.84 | 0.58 |
| 18:AR:35:ARG:HB3 | 18:AR:35:ARG:HH11 | 1.66 | 0.58 |
| 23:DA:546:C:H6 | 23:DA:547:A:H5' | 1.68 | 0.58 |
| 1:AA:1253:G:C6 | 1:AA:1254:C:C4 | 2.91 | 0.58 |
| 24:BB:14:U:O3' | 24:BB:108:U:O2' | 2.20 | 0.58 |
| 23:DA:19:C:H2' | 23:DA:20:C:H6 | 1.69 | 0.58 |
| 23:DA:1188:U:H4' | 39:DV:79:VAL:HG22 | 1.84 | 0.58 |
| 7:CG:92:SER:HB2 | 7:CG:93:PRO:HD2 | 1.85 | 0.58 |
| 23:DA:548:A:N6 | 39:DV:19:LYS:H | 2.02 | 0.58 |
| 23:DA:2235:G:O6 | 56:DA:4468:HOH:O | 2.17 | 0.58 |
| 1:CA:1097:C:O2' | 1:CA:1170:A:H1' | 2.04 | 0.58 |
| 8:CH:10:LEU:HD22 | 8:CH:83:ILE:HD11 | 1.85 | 0.58 |
| 1:AA:1231:G:H2' | 1:AA:1232:U:C6 | 2.39 | 0.58 |
| 1:AA:1230:C:H2' | 1:AA:1231:G:H8 | 1.69 | 0.58 |
| 1:AA:972:C:O2 | 10:AJ:55:LYS:HG3 | 2.03 | 0.58 |
| 1:AA:1141:C:H2' | 1:AA:1142:G:C8 | 2.29 | 0.58 |
| 23:DA:2136:C:N4 | 23:DA:2155:G:H1 | 1.98 | 0.58 |
| 23:BA:1429:G:H2' | 23:BA:1430:C:H6 | 1.67 | 0.58 |
| 3:CC:18:TRP:HD1 | 14:CN:54:PRO:HA | 1.69 | 0.58 |
| 16:AP:29:ASP:OD2 | 16:AP:29:ASP:N | 2.35 | 0.58 |
| 3:CC:160:ALA:HB3 | 3:CC:164:ARG:NH2 | 2.19 | 0.58 |
| 1:AA:857:C:H2' | 1:AA:858:G:O4' | 2.04 | 0.58 |
| 23:DA:1602:U:O4 | 56:DA:3941:HOH:O | 2.14 | 0.58 |
| 23:DA:661:C:O3' | 56:DA:4438:HOH:O | 2.17 | 0.58 |
| 23:BA:2002:G:OP2 | 35:BR:9:LYS:NZ | 2.37 | 0.58 |
| 1:CA:814:A:H2' | 1:CA:816:A:H5'' | 1.85 | 0.58 |
| 23:DA:536:A:H2' | 23:DA:537:C:C6 | 2.39 | 0.58 |
| 1:CA:194:C:H2' | 1:CA:195:A:H5'' | 1.85 | 0.58 |
| 23:DA:543:C:H3' | 23:DA:545:G:O4' | 2.04 | 0.58 |
| 1:CA:652:U:C2 | 1:CA:752:G:N2 | 2.71 | 0.58 |
| 1:CA:56:U:H2' | 1:CA:57:G:C8 | 2.38 | 0.58 |
| 23:BA:1899:G:H2' | 23:BA:1899:G:N3 | 2.18 | 0.58 |
| 22:AX:56:VAL:H | 22:AX:59:GLY:HA2 | 1.69 | 0.58 |
| 1:CA:785:G:C2' | 1:CA:786:G:H5' | 2.34 | 0.58 |
| 10:AJ:25:GLU:O | 10:AJ:29:ARG:N | 2.35 | 0.58 |
| 19:CS:36:ARG:HB3 | 19:CS:72:GLY:N | 2.18 | 0.58 |
| 23:DA:1047:G:H2' | 23:DA:1110:G:N2 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:298:G:H5'' | 23:DA:299:A:OP1 | 2.04 | 0.58 |
| 41:BX:32:PRO:HA | 41:BX:77:LYS:HB2 | 1.84 | 0.58 |
| 23:BA:2593:U:H2' | 23:BA:2594:C:C6 | 2.39 | 0.58 |
| 23:DA:1628:G:H2' | 23:DA:1629:U:C6 | 2.39 | 0.58 |
| 5:AE:6:PHE:HB2 | 5:AE:34:VAL:HG22 | 1.84 | 0.58 |
| 20:CT:63:ILE:HD12 | 20:CT:81:LYS:HG2 | 1.85 | 0.58 |
| 23:BA:883:G:H1 | 23:BA:893:C:N4 | 2.02 | 0.57 |
| 23:BA:885:C:N3 | 23:BA:886:C:H1' | 2.19 | 0.57 |
| 1:AA:1095:U:H5'' | 1:AA:1109:C:O2 | 2.04 | 0.57 |
| 23:BA:1689:A:N6 | 23:BA:1698:A:H2 | 1.93 | 0.57 |
| 24:BB:52:A:O2' | 24:BB:53:A:H5'' | 2.03 | 0.57 |
| 9:AI:13:ALA:HA | 9:AI:67:GLY:HA3 | 1.86 | 0.57 |
| 1:CA:1161:C:O2' | 1:CA:1162:C:H5' | 2.04 | 0.57 |
| 23:BA:83:G:N2 | 23:BA:102:G:H2' | 2.19 | 0.57 |
| 1:CA:709:G:H2' | 1:CA:710:G:H8 | 1.69 | 0.57 |
| 1:AA:601:C:H2' | 1:AA:602:A:H8 | 1.68 | 0.57 |
| 1:AA:664:G:P | 18:AR:64:ARG:HH21 | 2.27 | 0.57 |
| 5:AE:12:LEU:HB3 | 5:AE:31:LEU:HB3 | 1.86 | 0.57 |
| 1:CA:303:A:H2' | 1:CA:304:U:O4' | 2.04 | 0.57 |
| 1:CA:1441:G:C2 | 1:CA:1459:C:H5 | 2.21 | 0.57 |
| 3:AC:11:ARG:NH2 | 3:AC:177:THR:O | 2.36 | 0.57 |
| 8:CH:6:ILE:O | 8:CH:10:LEU:HG | 2.04 | 0.57 |
| 1:AA:1318:A:H1' | 19:AS:37:ARG:NH2 | 2.19 | 0.57 |
| 2:AB:69:LEU:HD22 | 2:AB:91:PRO:HB2 | 1.85 | 0.57 |
| 2:AB:71:VAL:O | 2:AB:165:VAL:HG23 | 2.05 | 0.57 |
| 1:AA:1306:A:N6 | 1:AA:1331:G:H1' | 2.18 | 0.57 |
| 28:DG:77:ILE:N | 28:DG:82:LEU:O | 2.37 | 0.57 |
| 21:CU:12:LYS:HB3 | 21:CU:22:ARG:HH11 | 1.69 | 0.57 |
| 23:BA:2161:C:H2' | 23:BA:2162:G:C8 | 2.38 | 0.57 |
| 27:DF:101:LEU:HD12 | 27:DF:102:PRO:HD2 | 1.85 | 0.57 |
| 1:AA:448:A:OP2 | 1:AA:485:G:N1 | 2.35 | 0.57 |
| 4:AD:138:TYR:HD2 | 4:AD:139:ARG:N | 2.02 | 0.57 |
| 1:CA:626:U:H2' | 1:CA:627:G:C8 | 2.39 | 0.57 |
| 23:BA:2294:C:P | 36:BS:89:ARG:HH22 | 2.27 | 0.57 |
| 23:BA:647:G:N7 | 56:BA:5356:HOH:O | 2.32 | 0.57 |
| 24:BB:103:G:OP2 | 56:BB:314:HOH:O | 2.18 | 0.57 |
| 2:CB:17:PHE:H | 2:CB:17:PHE:HD2 | 1.50 | 0.57 |
| 23:BA:2377:A:H2' | 23:BA:2378:A:C8 | 2.39 | 0.57 |
| 1:AA:1459:C:C2' | 1:AA:1460:A:C8 | 2.87 | 0.57 |
| 1:CA:1130:A:H61 | 1:CA:1144:G:Cl' | 2.15 | 0.57 |
| 1:CA:1007:C:H2' | 1:CA:1008:C:C5 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1030(D):A:H62 | 1:CA:1031:G:H21 | 1.53 | 0.57 |
| 23:BA:2318:G:N2 | 36:BS:3:ARG:HH11 | 2.02 | 0.57 |
| 3:CC:132:ARG:O | 3:CC:136:GLN:N | 2.32 | 0.57 |
| 13:AM:15:VAL:HG12 | 13:AM:45:VAL:HG23 | 1.87 | 0.57 |
| 1:CA:448:A:OP2 | 1:CA:485:G:N1 | 2.31 | 0.57 |
| 9:AI:29:ASN:HB2 | 9:AI:36:TYR:CZ | 2.38 | 0.57 |
| 23:BA:769:G:O6 | 56:BA:4262:HOH:O | 2.13 | 0.57 |
| 1:AA:745:C:H2' | 1:AA:746:A:H8 | 1.69 | 0.57 |
| 2:AB:97:TRP:HH2 | 2:AB:176:GLU:CD | 2.07 | 0.57 |
| 23:BA:1014:U:H2' | 23:BA:1015:G:H8 | 1.69 | 0.57 |
| 42:DY:92:ASN:N | 42:DY:93:GLY:HA2 | 2.19 | 0.57 |
| 50:D6:9:LEU:HD13 | 50:D6:51:GLU:HG3 | 1.85 | 0.57 |
| 2:AB:80:ILE:HD11 | 2:AB:215:LEU:HB2 | 1.86 | 0.57 |
| 15:AO:3:ILE:H | 15:AO:3:ILE:HD13 | 1.69 | 0.57 |
| 23:DA:2562:U:H1' | 32:DO:23:ARG:HH11 | 1.69 | 0.57 |
| 1:AA:1320:C:H1' | 19:AS:73:GLU:HB3 | 1.85 | 0.57 |
| 1:CA:940:C:H1' | 1:CA:1374:A:H2 | 1.68 | 0.57 |
| 7:AG:35:LYS:HD2 | 7:AG:38:LEU:HB3 | 1.86 | 0.57 |
| 4:CD:174:LEU:HD23 | 4:CD:185:PHE:HA | 1.87 | 0.57 |
| 1:AA:606:G:H5'' | 1:AA:607:A:H5' | 1.86 | 0.57 |
| 23:BA:2184:G:H2' | 23:BA:2185:C:O4' | 2.03 | 0.57 |
| 23:BA:2853:C:H2' | 23:BA:2854:G:H8 | 1.69 | 0.57 |
| 1:CA:359:U:H2' | 1:CA:360:A:H8 | 1.69 | 0.57 |
| 34:BQ:122:GLY:HA2 | 34:BQ:125:LEU:HD12 | 1.86 | 0.57 |
| 23:DA:271(M):G:O2' | 23:DA:271(N):U:OP1 | 2.18 | 0.57 |
| 1:CA:38:G:C2 | 1:CA:397:A:C2 | 2.92 | 0.57 |
| 1:AA:1492:A:H2' | 1:AA:1492:A:N3 | 2.19 | 0.57 |
| 1:AA:1458:G:N3 | 1:AA:1458:G:H2' | 2.19 | 0.57 |
| 1:CA:1457:G:C6 | 1:CA:1458:G:C5 | 2.92 | 0.57 |
| 1:AA:1095:U:OP2 | 1:AA:1108:G:N1 | 2.31 | 0.57 |
| 1:AA:677:U:H3 | 1:AA:713:G:H22 | 1.50 | 0.57 |
| 1:AA:1015:A:H2' | 1:AA:1016:A:O4' | 2.03 | 0.57 |
| 23:DA:1406:U:H2' | 23:DA:1407:C:C6 | 2.39 | 0.57 |
| 29:DH:3:ARG:CZ | 29:DH:4:ILE:H | 2.17 | 0.57 |
| 39:BV:56:SER:H | 39:BV:100:ARG:HB2 | 1.67 | 0.57 |
| 23:DA:1935:G:H1' | 23:DA:1964:G:N2 | 2.19 | 0.57 |
| 33:DP:46:LYS:HE3 | 33:DP:51:PHE:CD1 | 2.40 | 0.57 |
| 43:BZ:125:LEU:HG | 43:BZ:164:ALA:HB3 | 1.87 | 0.57 |
| 23:BA:2275:C:H6 | 23:BA:2275:C:H5' | 1.69 | 0.57 |
| 25:DD:274:ARG:HA | 25:DD:275:LYS:HB3 | 1.85 | 0.57 |
| 2:CB:87:ARG:HH11 | 2:CB:219:VAL:HG12 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:54:THR:HG21 | 2:CB:201:ILE:HD11 | 1.87 | 0.57 |
| 23:BA:2299:G:O6 | 56:BA:5003:HOH:O | 2.14 | 0.57 |
| 7:CG:41:ARG:O | 7:CG:45:ASP:N | 2.37 | 0.57 |
| 23:BA:1833:U:H2' | 23:BA:1834:U:C6 | 2.39 | 0.57 |
| 35:DR:36:THR:HG22 | 35:DR:37:THR:H | 1.70 | 0.57 |
| 3:AC:36:ASP:O | 3:AC:40:ARG:HG2 | 2.04 | 0.57 |
| 1:AA:414:A:H2' | 1:AA:415:A:H8 | 1.68 | 0.57 |
| 23:BA:530:G:N3 | 23:BA:530:G:O4' | 2.32 | 0.57 |
| 3:AC:17:ASP:O | 3:AC:54:ARG:NH2 | 2.37 | 0.57 |
| 37:BT:26:ASP:OD2 | 37:BT:91:ARG:NH1 | 2.38 | 0.57 |
| 8:AH:63:LEU:HB2 | 8:AH:65:TYR:HE1 | 1.70 | 0.57 |
| 23:BA:543:C:H3' | 23:BA:545:G:O4' | 2.05 | 0.57 |
| 7:CG:62:PHE:HA | 7:CG:124:LEU:HD22 | 1.86 | 0.57 |
| 23:BA:1495:A:H2' | 23:BA:1496:A:C8 | 2.39 | 0.57 |
| 8:AH:36:LEU:HA | 8:AH:39:LEU:HD23 | 1.86 | 0.57 |
| 23:BA:1669:A:H5'' | 23:BA:2550:G:OP1 | 2.04 | 0.57 |
| 23:BA:2335:A:N7 | 23:BA:2337:G:C5 | 2.72 | 0.57 |
| 1:AA:1002:G:H2' | 1:AA:1003:G:H5' | 1.85 | 0.57 |
| 1:AA:1109:C:OP2 | 3:AC:176:HIS:ND1 | 2.36 | 0.57 |
| 1:AA:1305:G:H2' | 21:AU:6:ARG:H | 1.69 | 0.57 |
| 23:BA:1045:A:H4' | 23:BA:1047:G:C4 | 2.40 | 0.57 |
| 13:AM:64:TRP:HB3 | 13:AM:66:LEU:HD23 | 1.87 | 0.57 |
| 23:BA:1014:U:H2' | 23:BA:1015:G:C8 | 2.40 | 0.57 |
| 17:CQ:65:ILE:HD13 | 17:CQ:69:LYS:HE2 | 1.86 | 0.57 |
| 34:DQ:37:LEU:HD21 | 34:DQ:130:LYS:HB2 | 1.87 | 0.57 |
| 23:DA:2853:C:H2' | 23:DA:2854:G:H8 | 1.67 | 0.57 |
| 1:CA:763:G:H2' | 1:CA:764:C:H6 | 1.70 | 0.57 |
| 8:AH:121:ASP:OD1 | 8:AH:121:ASP:N | 2.38 | 0.57 |
| 1:AA:359:U:H2' | 1:AA:360:A:H8 | 1.70 | 0.57 |
| 7:AG:88:PRO:HG2 | 7:AG:152:ALA:HB2 | 1.87 | 0.57 |
| 1:AA:1321:C:H5'' | 1:AA:1322:C:H2' | 1.86 | 0.57 |
| 2:AB:54:THR:O | 2:AB:58:ILE:HG13 | 2.05 | 0.57 |
| 28:DG:19:LEU:HD22 | 28:DG:23:PHE:HE1 | 1.70 | 0.57 |
| 14:CN:22:THR:HG21 | 14:CN:35:ARG:HG2 | 1.86 | 0.57 |
| 1:AA:169:C:H2' | 1:AA:170:U:C6 | 2.39 | 0.57 |
| 1:AA:943:U:H2' | 1:AA:944:G:O4' | 2.03 | 0.57 |
| 1:CA:76:C:H3' | 1:CA:77:G:H5'' | 1.87 | 0.57 |
| 6:CF:7:ASN:OD1 | 6:CF:7:ASN:N | 2.37 | 0.57 |
| 1:AA:814:A:OP2 | 56:AA:2008:HOH:O | 2.17 | 0.57 |
| 23:DA:1963:U:H4' | 23:DA:1964:G:OP1 | 2.05 | 0.57 |
| 28:DG:32:PRO:HB2 | 28:DG:172:LEU:HD22 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 49:D5:45:VAL:HG11 | 49:D5:58:LEU:HD13 | 1.87 | 0.57 |
| 44:B0:40:GLN:OE1 | 44:B0:44:ARG:N | 2.31 | 0.57 |
| 23:DA:1627:G:OP2 | 56:DA:3954:HOH:O | 2.17 | 0.57 |
| 1:AA:785:G:C2' | 1:AA:786:G:H5' | 2.35 | 0.57 |
| 51:B7:23:ARG:HH11 | 51:B7:23:ARG:HB3 | 1.70 | 0.57 |
| 23:BA:2790:A:N3 | 23:BA:2790:A:H3' | 2.19 | 0.57 |
| 23:BA:602:G:O2' | 23:BA:655:A:N6 | 2.37 | 0.57 |
| 13:CM:37:THR:HG21 | 13:CM:56:LEU:HA | 1.87 | 0.57 |
| 20:AT:90:GLN:O | 20:AT:93:GLU:HB3 | 2.04 | 0.57 |
| 1:CA:932:C:H5' | 7:CG:3:ARG:HD3 | 1.86 | 0.57 |
| 3:AC:29:TYR:HE1 | 10:AJ:65:LEU:HD21 | 1.69 | 0.57 |
| 1:CA:1078:U:H2' | 1:CA:1079:G:O4' | 2.05 | 0.57 |
| 10:CJ:40:LEU:HD11 | 10:CJ:69:ASN:HB3 | 1.86 | 0.57 |
| 16:AP:28:ARG:NH1 | 16:AP:29:ASP:OD2 | 2.38 | 0.57 |
| 23:DA:1434:A:H61 | 23:DA:1558:A:H62 | 1.52 | 0.57 |
| 1:CA:186:C:H2' | 1:CA:187:C:H6 | 1.69 | 0.57 |
| 23:DA:1049:C:H2' | 23:DA:1050:A:H8 | 1.70 | 0.57 |
| 49:D5:45:VAL:HA | 49:D5:52:TYR:HB2 | 1.87 | 0.57 |
| 50:D6:16:CYS:HB3 | 50:D6:43:CYS:SG | 2.44 | 0.57 |
| 23:DA:971:C:OP2 | 56:DA:4254:HOH:O | 2.18 | 0.57 |
| 23:DA:1329:U:H5'' | 23:DA:1330:C:H5 | 1.69 | 0.57 |
| 25:DD:2:ALA:HB3 | 25:DD:20:ASP:HB3 | 1.86 | 0.57 |
| 33:BP:84:ASN:HB2 | 33:BP:86:LYS:HD3 | 1.85 | 0.57 |
| 6:AF:22:GLU:O | 6:AF:26:ILE:HG13 | 2.05 | 0.57 |
| 42:DY:76:CYS:HB3 | 42:DY:79:CYS:HB2 | 1.87 | 0.57 |
| 43:DZ:108:PRO:HB2 | 43:DZ:111:VAL:HG23 | 1.85 | 0.57 |
| 30:DI:123:LEU:H | 30:DI:123:LEU:HD23 | 1.69 | 0.57 |
| 43:BZ:33:LEU:HD23 | 43:BZ:90:VAL:HG21 | 1.87 | 0.57 |
| 1:AA:840:C:H4' | 1:AA:841:U:OP1 | 2.05 | 0.57 |
| 1:AA:1296:C:H4' | 1:AA:1302:U:C4 | 2.40 | 0.57 |
| 1:CA:1305:G:H1' | 1:CA:1306:A:H8 | 1.70 | 0.57 |
| 3:AC:23:TYR:OH | 10:AJ:9:ARG:HD2 | 2.04 | 0.57 |
| 23:BA:1174:A:H1' | 23:BA:1175:U:H5'' | 1.87 | 0.57 |
| 1:AA:1179:A:N6 | 1:AA:1180:A:C6 | 2.73 | 0.57 |
| 1:CA:1297:C:C4' | 1:CA:1298:C:H5' | 2.34 | 0.57 |
| 1:CA:437:U:OP1 | 4:CD:155:LEU:HG | 2.04 | 0.57 |
| 23:DA:2184:G:H2' | 23:DA:2185:C:O4' | 2.05 | 0.57 |
| 1:CA:683:G:H2' | 1:CA:684:A:H8 | 1.70 | 0.57 |
| 1:CA:359:U:H2' | 1:CA:360:A:C8 | 2.39 | 0.57 |
| 19:CS:22:LEU:HA | 19:CS:26:GLY:O | 2.05 | 0.57 |
| 23:DA:821:A:H2' | 23:DA:946:G:H5'' | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:642:G:O6 | 56:DA:3715:HOH:O | 2.16 | 0.57 |
| 23:DA:1657:C:H2' | 23:DA:1658:C:C6 | 2.39 | 0.57 |
| 23:BA:2321:G:H2' | 23:BA:2321:G:N3 | 2.20 | 0.57 |
| 35:BR:11:ASN:ND2 | 56:BR:304:HOH:O | 2.38 | 0.57 |
| 11:AK:84:VAL:HG11 | 11:AK:91:ARG:HD2 | 1.87 | 0.57 |
| 6:AF:96:PRO:HB3 | 18:AR:30:ASP:CG | 2.25 | 0.57 |
| 23:DA:848:G:OP1 | 56:DA:4235:HOH:O | 2.18 | 0.56 |
| 1:CA:1166:G:O2' | 1:CA:1169:A:N7 | 2.28 | 0.56 |
| 1:CA:1343:G:H4' | 9:CI:122:ALA:HB3 | 1.86 | 0.56 |
| 1:AA:1072:G:C5 | 1:AA:1073:U:C4 | 2.93 | 0.56 |
| 13:AM:70:LEU:H | 13:AM:73:GLU:CB | 2.17 | 0.56 |
| 24:BB:52:A:N6 | 36:BS:33:LYS:HG2 | 2.20 | 0.56 |
| 23:BA:1329:U:H5'' | 23:BA:1330:C:H5 | 1.69 | 0.56 |
| 27:DF:184:TYR:O | 27:DF:188:ARG:HG3 | 2.05 | 0.56 |
| 1:AA:359:U:H2' | 1:AA:360:A:C8 | 2.40 | 0.56 |
| 23:DA:495:G:H21 | 40:DW:61:ASN:HD21 | 1.53 | 0.56 |
| 53:D9:10:ILE:N | 53:D9:14:CYS:SG | 2.77 | 0.56 |
| 23:BA:2461:C:H2' | 23:BA:2462:U:C6 | 2.39 | 0.56 |
| 43:BZ:179:ASP:HB2 | 43:BZ:182:LYS:HD3 | 1.87 | 0.56 |
| 1:AA:1245:A:C2' | 1:AA:1246:C:H5' | 2.35 | 0.56 |
| 23:BA:558:G:C5 | 56:BA:4943:HOH:O | 2.57 | 0.56 |
| 33:DP:52:GLU:OE2 | 52:D8:57:ARG:NH1 | 2.37 | 0.56 |
| 1:AA:1249:C:N4 | 1:AA:1288:A:OP2 | 2.37 | 0.56 |
| 25:BD:5:LYS:HA | 25:BD:17:THR:HG22 | 1.88 | 0.56 |
| 23:DA:2591:C:OP1 | 25:DD:239:ARG:HG2 | 2.05 | 0.56 |
| 23:DA:580:C:H2' | 23:DA:581:C:C6 | 2.40 | 0.56 |
| 5:AE:12:LEU:HD22 | 5:AE:13:ILE:N | 2.20 | 0.56 |
| 23:DA:422:A:OP2 | 56:DA:4080:HOH:O | 2.18 | 0.56 |
| 6:CF:96:PRO:HB3 | 18:CR:30:ASP:CG | 2.26 | 0.56 |
| 24:BB:40:U:H1' | 24:BB:45:A:H61 | 1.70 | 0.56 |
| 1:CA:555:C:H2' | 1:CA:556:C:C6 | 2.40 | 0.56 |
| 37:DT:93:ARG:HH11 | 37:DT:93:ARG:HG2 | 1.69 | 0.56 |
| 23:BA:1882:C:H5' | 23:BA:1883:G:OP2 | 2.06 | 0.56 |
| 20:CT:73:HIS:HB3 | 20:CT:74:LYS:HG2 | 1.87 | 0.56 |
| 23:DA:1030:G:OP2 | 34:DQ:128:LYS:NZ | 2.35 | 0.56 |
| 23:BA:1991:U:H2' | 23:BA:1992:G:H5'' | 1.87 | 0.56 |
| 1:CA:1443:G:O6 | 1:CA:1459:C:H1' | 2.05 | 0.56 |
| 23:BA:2322:A:H2' | 23:BA:2323:G:O4' | 2.05 | 0.56 |
| 1:AA:1005:A:N6 | 1:AA:1024:G:O2' | 2.39 | 0.56 |
| 1:AA:878:G:H5' | 8:AH:89:PRO:HG2 | 1.88 | 0.56 |
| 1:AA:978:A:O2' | 1:AA:1322:C:N3 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:AB:54:THR:HG21 | 2:AB:201:ILE:HD11 | 1.85 | 0.56 |
| 1:AA:1290:G:H3' | 1:AA:1291:G:H8 | 1.70 | 0.56 |
| 23:DA:1403:C:C5' | 23:DA:1471:A:H1' | 2.35 | 0.56 |
| 23:DA:1607:C:H4' | 23:DA:1608:A:O5' | 2.04 | 0.56 |
| 4:AD:159:ARG:O | 4:AD:162:LEU:N | 2.38 | 0.56 |
| 23:BA:71:A:C8 | 23:BA:71:A:H5' | 2.40 | 0.56 |
| 23:DA:271(E):U:H2' | 23:DA:271(F):C:C6 | 2.39 | 0.56 |
| 1:AA:1148:U:O3' | 9:AI:14:VAL:HG21 | 2.04 | 0.56 |
| 1:AA:263:A:OP2 | 20:AT:79:ARG:NH1 | 2.39 | 0.56 |
| 36:DS:96:GLY:N | 36:DS:99:LYS:H | 2.03 | 0.56 |
| 43:DZ:82:ARG:HB3 | 43:DZ:82:ARG:NH2 | 2.19 | 0.56 |
| 40:DW:18:ARG:NH1 | 40:DW:76:VAL:O | 2.38 | 0.56 |
| 5:CE:80:ILE:HD12 | 5:CE:138:ALA:HB1 | 1.86 | 0.56 |
| 18:CR:35:ARG:HB3 | 18:CR:35:ARG:HH11 | 1.68 | 0.56 |
| 1:AA:21:G:H2' | 1:AA:22:G:C8 | 2.41 | 0.56 |
| 23:DA:1050:A:C4 | 23:DA:1051:G:C8 | 2.93 | 0.56 |
| 1:AA:616:G:C2 | 1:AA:617:G:C8 | 2.93 | 0.56 |
| 1:AA:663:A:O3' | 18:AR:64:ARG:NH2 | 2.38 | 0.56 |
| 23:BA:2023:G:H5' | 23:BA:2617:C:H4' | 1.87 | 0.56 |
| 17:CQ:45:HIS:CD2 | 17:CQ:65:ILE:HG12 | 2.40 | 0.56 |
| 27:BF:28:ILE:HD13 | 27:BF:119:ARG:HE | 1.69 | 0.56 |
| 23:BA:908:C:OP1 | 34:BQ:22:LYS:HB3 | 2.06 | 0.56 |
| 23:DA:2273:A:H2' | 23:DA:2274:A:C8 | 2.40 | 0.56 |
| 40:DW:60:ASN:HD22 | 40:DW:60:ASN:N | 2.02 | 0.56 |
| 28:BG:72:ARG:HH12 | 28:BG:87:PRO:HG3 | 1.69 | 0.56 |
| 26:BE:11:MET:HG2 | 26:BE:24:THR:HB | 1.87 | 0.56 |
| 1:AA:683:G:H2' | 1:AA:684:A:C8 | 2.40 | 0.56 |
| 23:DA:2110:G:H8 | 23:DA:2110:G:OP2 | 1.88 | 0.56 |
| 23:DA:747:U:O2 | 23:DA:2014:A:H1' | 2.04 | 0.56 |
| 23:BA:1762:A:H8 | 23:BA:1762:A:O5' | 1.88 | 0.56 |
| 31:DN:24:GLY:HA2 | 31:DN:27:ALA:HB3 | 1.85 | 0.56 |
| 46:D2:50:ILE:C | 46:D2:52:ASP:H | 2.07 | 0.56 |
| 1:CA:601:C:H2' | 1:CA:602:A:H8 | 1.69 | 0.56 |
| 23:BA:2350:C:O2 | 23:BA:2367:G:N2 | 2.29 | 0.56 |
| 23:DA:2661:G:H2' | 23:DA:2662:A:C8 | 2.41 | 0.56 |
| 23:DA:2322:A:H2' | 23:DA:2323:G:O4' | 2.05 | 0.56 |
| 1:CA:858:G:O6 | 1:CA:869:G:H3' | 2.05 | 0.56 |
| 1:CA:1237:C:N3 | 1:CA:1337:G:N2 | 2.53 | 0.56 |
| 1:CA:1160:G:C6 | 1:CA:1181:G:N1 | 2.74 | 0.56 |
| 1:CA:192:U:H2' | 1:CA:193:C:C6 | 2.35 | 0.56 |
| 1:AA:1249:C:H2' | 1:AA:1250:A:H5'' | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:CE:19:MET:SD | 5:CE:24:ARG:HB3 | 2.46 | 0.56 |
| 23:BA:2615:U:C2 | 49:B5:7:PRO:HA | 2.40 | 0.56 |
| 1:AA:738:C:H2' | 1:AA:739:C:H6 | 1.70 | 0.56 |
| 37:DT:24:PRO:HA | 37:DT:49:VAL:HG22 | 1.87 | 0.56 |
| 29:BH:7:LEU:HD12 | 29:BH:8:PRO:HD2 | 1.87 | 0.56 |
| 51:B7:47:ARG:HH11 | 51:B7:47:ARG:HG3 | 1.70 | 0.56 |
| 26:DE:201:THR:OG1 | 26:DE:202:LYS:N | 2.38 | 0.56 |
| 23:BA:1963:U:H4' | 23:BA:1964:G:OP1 | 2.06 | 0.56 |
| 23:BA:1935:G:H1' | 23:BA:1964:G:N2 | 2.20 | 0.56 |
| 23:DA:1131:G:H21 | 31:DN:73:THR:HG21 | 1.71 | 0.56 |
| 23:DA:1812:A:O2' | 25:DD:45:ASN:N | 2.38 | 0.56 |
| 37:DT:60:THR:HG22 | 37:DT:77:PRO:HA | 1.87 | 0.56 |
| 23:DA:1858:G:H1' | 23:DA:1884:A:N6 | 2.21 | 0.56 |
| 23:BA:690:G:O6 | 56:BA:5170:HOH:O | 2.15 | 0.56 |
| 1:CA:1442(B):A:H62 | 37:DT:118:ARG:NH2 | 2.04 | 0.56 |
| 2:CB:88:ALA:HB1 | 2:CB:222:ILE:HG21 | 1.88 | 0.56 |
| 23:DA:631:A:OP2 | 52:D8:47:LYS:NZ | 2.25 | 0.56 |
| 33:BP:39:LYS:CB | 33:BP:45:LEU:HG | 2.32 | 0.56 |
| 23:BA:1049:C:O2' | 23:BA:1050:A:O5' | 2.22 | 0.56 |
| 6:AF:7:ASN:OD1 | 6:AF:7:ASN:N | 2.38 | 0.56 |
| 7:AG:28:ASN:HD21 | 7:AG:36:LYS:HE2 | 1.69 | 0.56 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:C8 | 2.40 | 0.56 |
| 2:CB:74:LYS:O | 2:CB:78:GLN:HB2 | 2.05 | 0.56 |
| 1:CA:828:A:H2' | 1:CA:829:G:O4' | 2.05 | 0.56 |
| 35:DR:20:LEU:HD21 | 35:DR:40:LYS:HD3 | 1.87 | 0.56 |
| 35:BR:28:LEU:HD12 | 35:BR:48:VAL:HG21 | 1.87 | 0.56 |
| 38:DU:36:ARG:HD2 | 38:DU:40:PHE:CZ | 2.41 | 0.56 |
| 6:CF:67:MET:HE1 | 6:CF:75:LEU:HD13 | 1.86 | 0.56 |
| 23:BA:1786:A:H1' | 23:BA:1938:A:N6 | 2.19 | 0.56 |
| 25:BD:175:LEU:HD12 | 25:BD:185:VAL:HG21 | 1.87 | 0.56 |
| 7:CG:10:ARG:O | 7:CG:94:ARG:NH2 | 2.38 | 0.56 |
| 26:BE:9:VAL:HG22 | 26:BE:25:VAL:HB | 1.88 | 0.56 |
| 17:AQ:4:LYS:HD2 | 17:AQ:5:VAL:H | 1.71 | 0.56 |
| 1:CA:1142:G:C5 | 1:CA:1143:G:H1' | 2.40 | 0.56 |
| 1:CA:1392:G:H21 | 1:CA:1502:A:H8 | 1.52 | 0.56 |
| 28:DG:86:MET:O | 28:DG:88:ILE:HG13 | 2.06 | 0.56 |
| 48:D4:35:VAL:HA | 48:D4:39:CYS:SG | 2.44 | 0.56 |
| 23:BA:1430:C:H2' | 23:BA:1431:U:C6 | 2.39 | 0.56 |
| 3:CC:18:TRP:HE1 | 14:CN:56:VAL:N | 2.02 | 0.56 |
| 44:B0:53:MET:HG3 | 44:B0:59:LEU:CD2 | 2.35 | 0.56 |
| 26:BE:174:ASP:OD2 | 26:BE:175:VAL:N | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:AA:375:U:C2 | 1:AA:376:G:C8 | 2.94 | 0.56 |
| 23:DA:2835:A:N7 | 56:DA:4350:HOH:O | 2.33 | 0.56 |
| 1:AA:1396:A:C2 | 5:AE:19:MET:HG3 | 2.41 | 0.56 |
| 23:BA:185:U:H4' | 23:BA:218:A:H4' | 1.88 | 0.56 |
| 23:BA:252:G:OP2 | 33:BP:50:ARG:NH1 | 2.39 | 0.56 |
| 23:BA:559:G:H22 | 38:BU:49:HIS:CD2 | 2.23 | 0.56 |
| 1:AA:277:C:H5'' | 17:AQ:68:ARG:NH2 | 2.21 | 0.56 |
| 6:CF:69:GLU:O | 6:CF:72:VAL:HG13 | 2.06 | 0.56 |
| 35:BR:50:HIS:CE1 | 35:BR:54:LEU:HD21 | 2.41 | 0.56 |
| 42:BY:86:ARG:HD2 | 42:BY:100:ALA:HA | 1.88 | 0.56 |
| 28:BG:133:LEU:HG | 28:BG:157:ILE:HB | 1.86 | 0.56 |
| 23:DA:1762:A:H8 | 23:DA:1762:A:O5' | 1.87 | 0.56 |
| 12:CL:102:ARG:HA | 12:CL:107:ALA:HB1 | 1.86 | 0.56 |
| 1:CA:991:U:H3' | 1:CA:1212:U:N3 | 2.20 | 0.56 |
| 1:CA:1124:G:H2' | 1:CA:1126:U:O4 | 2.05 | 0.56 |
| 23:BA:1173:G:H1' | 23:BA:1177:A:H61 | 1.70 | 0.56 |
| 23:BA:1140:C:O3' | 31:BN:25:ARG:NH1 | 2.38 | 0.56 |
| 3:CC:6:HIS:CD2 | 3:CC:7:PRO:HD2 | 2.38 | 0.56 |
| 28:DG:5:VAL:HG12 | 48:D4:25:TYR:CE1 | 2.41 | 0.56 |
| 10:CJ:51:ARG:HB2 | 10:CJ:59:SER:OG | 2.05 | 0.56 |
| 18:AR:31:LEU:H | 18:AR:31:LEU:HD23 | 1.69 | 0.56 |
| 1:CA:142:G:H2' | 1:CA:143:A:C8 | 2.40 | 0.56 |
| 23:BA:2199:A:H3' | 23:BA:2200:C:C6 | 2.41 | 0.56 |
| 1:CA:377:G:OP1 | 16:CP:3:LYS:HD2 | 2.06 | 0.56 |
| 23:BA:1494:A:H2' | 23:BA:1495:A:C8 | 2.41 | 0.56 |
| 1:CA:335:C:H2' | 1:CA:336:C:C6 | 2.41 | 0.56 |
| 1:AA:1371:G:H4' | 9:AI:69:GLY:HA3 | 1.87 | 0.56 |
| 32:BO:64:ARG:NH1 | 32:BO:81:ASP:OD2 | 2.38 | 0.56 |
| 23:DA:2477:C:O2 | 53:D9:4:ARG:NH2 | 2.35 | 0.56 |
| 23:BA:1488:G:N2 | 23:BA:1502:C:C2 | 2.73 | 0.56 |
| 34:DQ:24:GLY:O | 34:DQ:102:VAL:HG23 | 2.05 | 0.56 |
| 23:BA:1510:G:H2' | 23:BA:1511:C:C6 | 2.41 | 0.56 |
| 1:CA:1458:G:H2' | 1:CA:1458:G:N3 | 2.20 | 0.56 |
| 23:DA:2335:A:O2' | 23:DA:2336:A:OP2 | 2.21 | 0.56 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:C6 | 2.41 | 0.56 |
| 1:CA:1342:C:H2' | 1:CA:1343:G:H8 | 1.70 | 0.56 |
| 23:DA:1375:C:H3' | 56:DA:3934:HOH:O | 2.05 | 0.56 |
| 1:AA:1276:G:H1' | 1:AA:1282:C:O2' | 2.05 | 0.56 |
| 1:CA:559:A:OP1 | 5:CE:126:ARG:NH2 | 2.32 | 0.56 |
| 1:CA:1072:G:C5 | 1:CA:1073:U:C4 | 2.94 | 0.56 |
| 1:CA:148:G:H2' | 1:CA:149:A:C8 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1587:A:H2' | 23:BA:1588:C:H6 | 1.68 | 0.56 |
| 17:AQ:45:HIS:CD2 | 17:AQ:65:ILE:HG12 | 2.41 | 0.56 |
| 23:DA:1601:G:N7 | 56:DA:3941:HOH:O | 2.33 | 0.56 |
| 23:BA:1268:A:H2' | 23:BA:1269:A:O4' | 2.06 | 0.56 |
| 43:DZ:158:PRO:O | 43:DZ:161:VAL:HB | 2.06 | 0.56 |
| 1:CA:1521:G:H2' | 1:CA:1522:U:C6 | 2.41 | 0.56 |
| 13:CM:94:ARG:HH11 | 13:CM:96:LEU:HD12 | 1.70 | 0.56 |
| 23:DA:1449:A:H5' | 23:DA:1450:G:OP2 | 2.05 | 0.56 |
| 40:BW:80:PRO:O | 40:BW:100:THR:HB | 2.06 | 0.56 |
| 11:CK:23:ALA:O | 11:CK:86:GLY:HA3 | 2.06 | 0.56 |
| 7:AG:116:ALA:HA | 7:AG:119:ARG:HB3 | 1.88 | 0.56 |
| 1:CA:966:G:H8 | 1:CA:966:G:OP2 | 1.88 | 0.56 |
| 23:DA:1865:G:H5' | 23:DA:1866:C:OP2 | 2.06 | 0.56 |
| 1:CA:1222:G:H5'' | 19:CS:78:ARG:HE | 1.70 | 0.56 |
| 1:CA:1084:G:H21 | 1:CA:1102:A:H62 | 1.54 | 0.56 |
| 36:DS:15:ARG:O | 36:DS:19:LYS:HG2 | 2.06 | 0.56 |
| 3:AC:50:ALA:HB1 | 3:AC:70:VAL:HG11 | 1.88 | 0.56 |
| 36:DS:99:LYS:HE2 | 36:DS:103:GLU:OE2 | 2.06 | 0.56 |
| 1:CA:540:G:H2' | 1:CA:541:G:O4' | 2.06 | 0.56 |
| 23:DA:751:A:H5' | 40:DW:90:ARG:HA | 1.86 | 0.56 |
| 23:DA:2492:U:H2' | 23:DA:2493:U:C6 | 2.40 | 0.56 |
| 3:CC:125:GLU:HG3 | 3:CC:189:ALA:HB1 | 1.88 | 0.56 |
| 1:AA:160:A:H2' | 1:AA:161:A:O4' | 2.05 | 0.56 |
| 29:DH:144:VAL:O | 29:DH:148:ILE:HG12 | 2.05 | 0.56 |
| 15:AO:69:TYR:HA | 15:AO:72:ARG:HD3 | 1.86 | 0.56 |
| 3:AC:11:ARG:NE | 3:AC:180:ALA:HB3 | 2.20 | 0.56 |
| 19:AS:36:ARG:HB2 | 19:AS:72:GLY:HA3 | 1.87 | 0.56 |
| 2:AB:51:LEU:O | 2:AB:55:PHE:HD2 | 1.89 | 0.56 |
| 25:BD:118:VAL:N | 25:BD:129:ASN:ND2 | 2.53 | 0.56 |
| 26:DE:174:ASP:OD2 | 26:DE:175:VAL:N | 2.37 | 0.56 |
| 1:CA:1388:C:H2' | 1:CA:1389:C:C6 | 2.40 | 0.56 |
| 7:AG:139:GLU:HB3 | 7:AG:143:ARG:CZ | 2.34 | 0.56 |
| 23:BA:546:C:H6 | 23:BA:547:A:H5' | 1.70 | 0.56 |
| 1:CA:1516:G:H2' | 1:CA:1518:A:OP2 | 2.06 | 0.56 |
| 1:CA:631:G:H2' | 1:CA:632:A:C8 | 2.41 | 0.56 |
| 23:DA:1635:G:OP1 | 56:DA:3959:HOH:O | 2.18 | 0.56 |
| 24:BB:8:U:O3' | 36:BS:25:ARG:NH2 | 2.39 | 0.56 |
| 23:DA:275:G:C2' | 23:DA:276:A:H5' | 2.36 | 0.56 |
| 46:D2:13:ALA:HA | 46:D2:16:LEU:HD12 | 1.88 | 0.56 |
| 1:CA:1492:A:H2' | 1:CA:1492:A:N3 | 2.21 | 0.56 |
| 2:CB:82:ARG:HG2 | 2:CB:92:TYR:OH | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DZ:151:HIS:HD2 | 43:DZ:168:GLU:O | 1.89 | 0.56 |
| 1:AA:1441:G:N2 | 1:AA:1459:C:H5 | 2.02 | 0.55 |
| 22:CX:76:GLY:O | 22:CX:80:LYS:HG2 | 2.05 | 0.55 |
| 23:BA:2298:A:N6 | 23:BA:2318:G:H8 | 2.02 | 0.55 |
| 1:CA:1254:C:N3 | 1:CA:1283:G:N2 | 2.54 | 0.55 |
| 1:CA:1033:G:C8 | 1:CA:1034:G:C8 | 2.94 | 0.55 |
| 23:BA:2591:C:OP2 | 25:BD:239:ARG:HB3 | 2.06 | 0.55 |
| 1:CA:434:U:H2' | 1:CA:435:C:H6 | 1.69 | 0.55 |
| 7:CG:113:GLU:HG3 | 7:CG:119:ARG:HG3 | 1.88 | 0.55 |
| 1:AA:684:A:H2' | 1:AA:685:G:C8 | 2.41 | 0.55 |
| 2:CB:97:TRP:HH2 | 2:CB:176:GLU:CD | 2.10 | 0.55 |
| 1:CA:189(F):U:O2 | 17:CQ:63:ARG:NH2 | 2.38 | 0.55 |
| 32:DO:73:ASP:OD1 | 37:DT:32:TYR:OH | 2.07 | 0.55 |
| 1:AA:999:C:H2' | 1:AA:1000:U:H6 | 1.70 | 0.55 |
| 23:BA:2690:C:OP2 | 35:BR:14:SER:HB3 | 2.06 | 0.55 |
| 1:AA:1459:C:C5' | 1:AA:1460:A:OP2 | 2.54 | 0.55 |
| 1:AA:1037:C:H2' | 1:AA:1038:C:H6 | 1.70 | 0.55 |
| 23:BA:1357:U:OP2 | 56:BA:4686:HOH:O | 2.18 | 0.55 |
| 3:AC:23:TYR:CG | 10:AJ:10:GLY:HA2 | 2.42 | 0.55 |
| 24:DB:66:A:N6 | 24:DB:109:C:H5' | 2.19 | 0.55 |
| 7:CG:71:PRO:HG3 | 7:CG:103:TRP:CZ3 | 2.42 | 0.55 |
| 24:BB:20:C:C2' | 24:BB:21:G:H5' | 2.36 | 0.55 |
| 23:BA:1050:A:C4 | 23:BA:1051:G:C8 | 2.95 | 0.55 |
| 3:CC:154:SER:O | 3:CC:196:LEU:HD13 | 2.07 | 0.55 |
| 23:DA:1364:G:C8 | 45:D1:3:LYS:HD3 | 2.41 | 0.55 |
| 43:DZ:52:SER:OG | 43:DZ:53:ILE:N | 2.39 | 0.55 |
| 5:CE:12:LEU:HD22 | 5:CE:13:ILE:N | 2.21 | 0.55 |
| 6:AF:69:GLU:OE1 | 6:AF:69:GLU:N | 2.39 | 0.55 |
| 1:AA:626:U:H2' | 1:AA:627:G:H8 | 1.72 | 0.55 |
| 1:AA:833:U:H2' | 1:AA:834:C:H6 | 1.70 | 0.55 |
| 26:DE:52:LEU:HB3 | 26:DE:76:ARG:HG2 | 1.89 | 0.55 |
| 28:BG:86:MET:O | 28:BG:88:ILE:HG13 | 2.06 | 0.55 |
| 23:DA:2845:G:O2' | 23:DA:2846:G:H5' | 2.06 | 0.55 |
| 5:AE:110:LEU:HD13 | 5:AE:118:ILE:HG21 | 1.88 | 0.55 |
| 1:AA:1442(A):G:C5 | 1:AA:1442(B):A:C2 | 2.94 | 0.55 |
| 1:AA:1206:G:O4' | 3:AC:194:GLY:HA2 | 2.06 | 0.55 |
| 23:DA:1019:U:H3 | 23:DA:1142(A):A:N6 | 1.99 | 0.55 |
| 19:AS:63:THR:H | 19:AS:66:MET:CG | 2.20 | 0.55 |
| 1:CA:266:G:H5'' | 1:CA:267:C:C5 | 2.41 | 0.55 |
| 1:AA:344:A:H4' | 1:AA:345:C:OP2 | 2.06 | 0.55 |
| 23:DA:1366:A:OP1 | 45:D1:3:LYS:NZ | 2.38 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:428:G:H4' | 1:CA:429:U:O5' | 2.06 | 0.55 |
| 1:AA:1149:C:O2' | 1:AA:1280:A:N1 | 2.35 | 0.55 |
| 1:AA:434:U:H2' | 1:AA:435:C:H6 | 1.70 | 0.55 |
| 23:DA:364:C:OP2 | 56:DA:4247:HOH:O | 2.18 | 0.55 |
| 1:CA:997:U:O4 | 1:CA:1044:A:N1 | 2.39 | 0.55 |
| 1:CA:1060:C:O3' | 10:CJ:59:SER:OG | 2.15 | 0.55 |
| 1:AA:68:G:H22 | 1:AA:101:A:H2 | 1.54 | 0.55 |
| 2:AB:97:TRP:CZ3 | 2:AB:99:GLY:HA2 | 2.40 | 0.55 |
| 23:DA:2014:A:OP1 | 56:DA:3657:HOH:O | 2.18 | 0.55 |
| 20:CT:90:GLN:O | 20:CT:93:GLU:HB3 | 2.06 | 0.55 |
| 8:CH:36:LEU:HA | 8:CH:39:LEU:HD23 | 1.87 | 0.55 |
| 1:CA:553:A:H2' | 1:CA:554:C:C6 | 2.41 | 0.55 |
| 37:BT:106:SER:O | 37:BT:110:ILE:HG12 | 2.06 | 0.55 |
| 35:BR:117:VAL:HG12 | 35:BR:118:GLU:H | 1.71 | 0.55 |
| 1:AA:1305:G:N1 | 1:AA:1331:G:O2' | 2.32 | 0.55 |
| 1:CA:97:G:O2' | 1:CA:98:G:H8 | 1.90 | 0.55 |
| 42:BY:15:VAL:HG21 | 42:BY:42:VAL:HG11 | 1.89 | 0.55 |
| 13:AM:91:ARG:HB2 | 13:AM:98:VAL:HG22 | 1.87 | 0.55 |
| 1:AA:745:C:H2' | 1:AA:746:A:C8 | 2.40 | 0.55 |
| 23:BA:2562:U:H1' | 32:BO:23:ARG:HD3 | 1.87 | 0.55 |
| 1:CA:615:C:H2' | 1:CA:616:G:C8 | 2.42 | 0.55 |
| 1:CA:616:G:C2 | 1:CA:617:G:C8 | 2.95 | 0.55 |
| 1:CA:626:U:H2' | 1:CA:627:G:H8 | 1.72 | 0.55 |
| 33:BP:50:ARG:HD3 | 52:B8:7:HIS:CD2 | 2.41 | 0.55 |
| 6:CF:55:ASP:HB3 | 6:CF:86:ARG:HH12 | 1.72 | 0.55 |
| 10:AJ:43:ARG:O | 10:AJ:67:THR:HG23 | 2.06 | 0.55 |
| 37:BT:20:PRO:HG2 | 37:BT:86:ILE:O | 2.05 | 0.55 |
| 23:BA:652(S):C:H2' | 23:BA:652(T):C:O4' | 2.06 | 0.55 |
| 1:AA:583:A:H2' | 1:AA:584:G:O4' | 2.06 | 0.55 |
| 23:DA:1632:A:N6 | 56:DA:3946:HOH:O | 2.40 | 0.55 |
| 1:AA:806:C:H2' | 1:AA:807:A:H8 | 1.70 | 0.55 |
| 6:AF:67:MET:HE1 | 6:AF:75:LEU:HD13 | 1.87 | 0.55 |
| 45:B1:94:LEU:O | 45:B1:97:LEU:HB2 | 2.06 | 0.55 |
| 23:BA:2096:U:H3 | 23:BA:2193:G:H1 | 1.54 | 0.55 |
| 1:CA:946:A:N6 | 1:CA:1235:U:H3 | 2.03 | 0.55 |
| 1:CA:17:U:H2' | 1:CA:18:C:C6 | 2.41 | 0.55 |
| 1:AA:1016:A:H2' | 1:AA:1017:G:O4' | 2.06 | 0.55 |
| 23:BA:1018:C:O2' | 23:BA:1019:U:H5' | 2.07 | 0.55 |
| 2:AB:178:ARG:HH22 | 8:AH:68:ARG:HH22 | 1.54 | 0.55 |
| 3:CC:172:ARG:HH21 | 3:CC:174:PRO:HG3 | 1.71 | 0.55 |
| 23:DA:27:G:HO2' | 23:DA:28:A:P | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 3:CC:11:ARG:HB3 | 3:CC:15:THR:HB | 1.88 | 0.55 |
| 2:CB:137:ARG:NH1 | 2:CB:137:ARG:HB2 | 2.20 | 0.55 |
| 1:AA:1250:A:H2' | 1:AA:1251:A:O4' | 2.07 | 0.55 |
| 3:CC:118:GLN:HA | 3:CC:121:ALA:HB3 | 1.87 | 0.55 |
| 1:AA:957:U:N3 | 1:AA:960:U:OP2 | 2.39 | 0.55 |
| 5:CE:51:VAL:O | 5:CE:55:VAL:HG23 | 2.07 | 0.55 |
| 1:CA:1060:C:H4' | 10:CJ:51:ARG:HB3 | 1.87 | 0.55 |
| 23:DA:1833:U:H2' | 23:DA:1834:U:C6 | 2.41 | 0.55 |
| 23:BA:1509(A):A:H3' | 23:BA:1509(B):A:H8 | 1.71 | 0.55 |
| 23:BA:536:A:H2' | 23:BA:537:C:C6 | 2.40 | 0.55 |
| 1:CA:575:G:OP1 | 1:CA:575:G:H4' | 2.06 | 0.55 |
| 23:DA:652(S):C:H2' | 23:DA:652(T):C:O4' | 2.05 | 0.55 |
| 23:BA:511:U:C5 | 23:BA:512:G:C5 | 2.94 | 0.55 |
| 1:AA:1452:C:O2' | 1:AA:1456:G:OP2 | 2.20 | 0.55 |
| 2:AB:55:PHE:CD1 | 2:AB:58:ILE:HD12 | 2.41 | 0.55 |
| 28:DG:59:GLU:O | 28:DG:63:ILE:N | 2.40 | 0.55 |
| 2:CB:187:LEU:HD23 | 2:CB:201:ILE:HB | 1.87 | 0.55 |
| 1:AA:1276:G:N2 | 1:AA:1283:G:O4' | 2.39 | 0.55 |
| 23:BA:674:G:C1' | 27:BF:74:ARG:HD3 | 2.37 | 0.55 |
| 48:D4:14:ILE:HD11 | 48:D4:24:THR:OG1 | 2.06 | 0.55 |
| 23:DA:1509(B):A:H3' | 23:DA:1510:G:H8 | 1.72 | 0.55 |
| 2:AB:80:ILE:HG13 | 2:AB:215:LEU:HD12 | 1.89 | 0.55 |
| 1:AA:865:A:H2' | 1:AA:866:C:C6 | 2.42 | 0.55 |
| 23:BA:443:A:N7 | 27:BF:45:ARG:HG2 | 2.21 | 0.55 |
| 23:DA:922:U:O4 | 56:DA:4224:HOH:O | 2.16 | 0.55 |
| 23:BA:1889:A:H2' | 23:BA:1890:A:C8 | 2.41 | 0.55 |
| 23:BA:1419:A:O2' | 23:BA:1421:G:N7 | 2.32 | 0.55 |
| 6:CF:11:ASN:HB3 | 6:CF:14:LEU:HG | 1.89 | 0.55 |
| 1:AA:1002:G:C2' | 1:AA:1003:G:H5' | 2.35 | 0.55 |
| 1:AA:1486:G:H2' | 1:AA:1487:G:O4' | 2.07 | 0.55 |
| 1:CA:1504:G:OP1 | 1:CA:1507:A:H4' | 2.06 | 0.55 |
| 1:CA:223:U:H2' | 1:CA:224:C:C6 | 2.41 | 0.55 |
| 24:DB:52:A:O2' | 24:DB:53:A:H5'' | 2.06 | 0.55 |
| 23:BA:2732:G:H3' | 23:BA:2733:A:O4' | 2.07 | 0.55 |
| 37:DT:23:ARG:HG3 | 37:DT:120:ARG:NH1 | 2.22 | 0.55 |
| 31:DN:99:LEU:HD22 | 31:DN:103:VAL:HG23 | 1.89 | 0.55 |
| 1:AA:55:A:C5 | 1:AA:56:U:C5 | 2.95 | 0.55 |
| 1:AA:575:G:OP1 | 1:AA:575:G:H4' | 2.07 | 0.55 |
| 23:DA:2463:C:C2' | 23:DA:2464:C:H5' | 2.37 | 0.55 |
| 1:CA:277:C:H5'' | 17:CQ:68:ARG:NH2 | 2.22 | 0.55 |
| 30:BI:74:ASN:HD22 | 30:BI:75:LEU:HD13 | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:B2:50:ILE:C | 46:B2:52:ASP:H | 2.07 | 0.55 |
| 34:DQ:42:ILE:HD13 | 34:DQ:97:VAL:HG21 | 1.89 | 0.55 |
| 20:AT:16:HIS:O | 20:AT:19:SER:OG | 2.21 | 0.55 |
| 23:DA:2319:G:H22 | 36:DS:3:ARG:HD2 | 1.71 | 0.55 |
| 13:AM:3:ARG:NH2 | 13:AM:10:PRO:O | 2.29 | 0.55 |
| 23:BA:71:A:H2 | 41:BX:31:HIS:CE1 | 2.24 | 0.55 |
| 1:CA:920:U:C2 | 1:CA:921:U:C5 | 2.95 | 0.55 |
| 3:CC:2:GLY:N | 56:CC:301:HOH:O | 2.40 | 0.55 |
| 30:BI:81:VAL:O | 30:BI:146:ALA:HA | 2.06 | 0.55 |
| 23:DA:196:A:O4' | 33:DP:46:LYS:HE2 | 2.07 | 0.55 |
| 27:DF:123:LEU:HD13 | 27:DF:192:LEU:HD13 | 1.88 | 0.55 |
| 25:DD:175:LEU:HD12 | 25:DD:185:VAL:HG21 | 1.89 | 0.55 |
| 35:DR:12:ARG:HG2 | 35:DR:16:HIS:CG | 2.42 | 0.55 |
| 3:AC:42:LEU:O | 3:AC:46:GLU:HB2 | 2.06 | 0.55 |
| 23:BA:548:A:N6 | 39:BV:19:LYS:H | 2.04 | 0.55 |
| 27:DF:65:TRP:HH2 | 27:DF:72:ARG:HH21 | 1.55 | 0.55 |
| 1:CA:999:C:H2' | 1:CA:1000:U:C6 | 2.41 | 0.55 |
| 33:DP:112:LEU:HD22 | 33:DP:113:LYS:N | 2.22 | 0.55 |
| 24:DB:55:U:O3' | 28:DG:27:ASN:ND2 | 2.40 | 0.55 |
| 38:DU:59:ARG:O | 38:DU:63:VAL:HG23 | 2.07 | 0.55 |
| 1:AA:1065:U:H6 | 1:AA:1190:G:N2 | 2.01 | 0.55 |
| 1:CA:932:C:C5' | 7:CG:3:ARG:HD3 | 2.37 | 0.55 |
| 33:BP:38:GLN:O | 33:BP:40:SER:N | 2.40 | 0.55 |
| 14:AN:37:PHE:CE1 | 14:AN:53:LEU:HD13 | 2.41 | 0.55 |
| 1:CA:978:A:H5'' | 1:CA:979:C:OP2 | 2.06 | 0.55 |
| 40:BW:18:ARG:NH1 | 40:BW:76:VAL:O | 2.39 | 0.55 |
| 3:CC:152:ILE:HD12 | 3:CC:199:LYS:HB2 | 1.88 | 0.55 |
| 1:CA:1189:C:P | 10:CJ:51:ARG:HH22 | 2.30 | 0.55 |
| 23:BA:2629:A:O2' | 23:BA:2630:G:OP2 | 2.17 | 0.55 |
| 23:DA:1419:A:O2' | 23:DA:1421:G:N7 | 2.29 | 0.55 |
| 17:CQ:40:LYS:HD3 | 17:CQ:42:TYR:CZ | 2.42 | 0.55 |
| 7:AG:9:VAL:HG21 | 7:AG:94:ARG:HE | 1.71 | 0.55 |
| 42:DY:43:ASN:OD1 | 42:DY:65:ALA:HB3 | 2.07 | 0.55 |
| 17:CQ:4:LYS:HD2 | 17:CQ:5:VAL:H | 1.71 | 0.55 |
| 7:CG:75:VAL:HA | 7:CG:87:VAL:O | 2.07 | 0.55 |
| 36:BS:49:VAL:HG13 | 36:BS:76:LYS:HD2 | 1.89 | 0.55 |
| 23:BA:272:G:N7 | 23:BA:421:U:H2' | 2.22 | 0.55 |
| 37:DT:109:GLU:O | 37:DT:113:LYS:N | 2.35 | 0.55 |
| 23:BA:885:C:N4 | 23:BA:890:A:C5 | 2.71 | 0.55 |
| 3:AC:191:THR:O | 3:AC:194:GLY:N | 2.36 | 0.55 |
| 28:BG:60:LEU:HD23 | 28:BG:63:ILE:HD12 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:678:U:H2' | 1:CA:679:C:C6 | 2.41 | 0.55 |
| 23:DA:517:C:OP1 | 49:D5:16:ARG:NH2 | 2.40 | 0.55 |
| 23:DA:1494:A:H2' | 23:DA:1495:A:H8 | 1.70 | 0.55 |
| 5:CE:76:ILE:HG22 | 5:CE:93:PRO:HB3 | 1.89 | 0.55 |
| 17:AQ:48:GLU:HB2 | 17:AQ:50:LYS:HG2 | 1.88 | 0.55 |
| 23:BA:1406:U:H2' | 23:BA:1407:C:C6 | 2.42 | 0.55 |
| 23:BA:1858:G:H1' | 23:BA:1884:A:N6 | 2.22 | 0.55 |
| 11:AK:21:ILE:HB | 11:AK:84:VAL:HG22 | 1.88 | 0.55 |
| 1:AA:737:A:H2' | 1:AA:738:C:C6 | 2.41 | 0.55 |
| 23:DA:2463:C:O2' | 23:DA:2464:C:H5' | 2.07 | 0.55 |
| 23:DA:2699:C:H2' | 23:DA:2700:C:O4' | 2.06 | 0.55 |
| 23:BA:1279:G:H4' | 35:BR:31:HIS:CD2 | 2.42 | 0.55 |
| 23:BA:2753:A:N3 | 53:B9:15:LYS:NZ | 2.54 | 0.55 |
| 25:BD:274:ARG:HA | 25:BD:275:LYS:HB3 | 1.88 | 0.55 |
| 1:CA:1486:G:H2' | 1:CA:1487:G:O4' | 2.07 | 0.55 |
| 10:CJ:48:THR:HA | 10:CJ:62:HIS:HA | 1.89 | 0.55 |
| 1:CA:537:G:H5'' | 12:CL:113:ARG:NH1 | 2.21 | 0.55 |
| 23:DA:1300:U:H4' | 23:DA:1301:A:C5' | 2.36 | 0.55 |
| 26:BE:52:LEU:HB3 | 26:BE:76:ARG:HG2 | 1.88 | 0.55 |
| 1:CA:840:C:H4' | 1:CA:841:U:OP1 | 2.06 | 0.54 |
| 2:AB:218:ALA:O | 2:AB:222:ILE:HG13 | 2.07 | 0.54 |
| 7:AG:35:LYS:HD2 | 7:AG:38:LEU:HD22 | 1.88 | 0.54 |
| 23:DA:1019:U:O2' | 23:DA:1021:A:H2 | 1.90 | 0.54 |
| 23:DA:271(D):G:H2' | 23:DA:271(E):U:O4' | 2.07 | 0.54 |
| 6:AF:61:LEU:HB3 | 6:AF:63:TYR:CE2 | 2.41 | 0.54 |
| 30:BI:21:VAL:HG23 | 30:BI:22:LYS:O | 2.07 | 0.54 |
| 1:CA:1002:G:N2 | 1:CA:1039:C:H1' | 2.19 | 0.54 |
| 23:DA:530:G:O4' | 23:DA:530:G:N3 | 2.40 | 0.54 |
| 1:AA:542:G:H2' | 1:AA:543:C:C6 | 2.42 | 0.54 |
| 23:BA:530:G:N1 | 56:BA:4475:HOH:O | 2.16 | 0.54 |
| 1:AA:598:U:H2' | 1:AA:599:C:C6 | 2.42 | 0.54 |
| 1:AA:918:A:H2' | 1:AA:919:A:C8 | 2.42 | 0.54 |
| 48:B4:18:CYS:SG | 48:B4:39:CYS:HB3 | 2.47 | 0.54 |
| 23:BA:2577:A:OP1 | 56:BA:4599:HOH:O | 2.18 | 0.54 |
| 17:CQ:22:LEU:HD11 | 17:CQ:39:SER:HB3 | 1.89 | 0.54 |
| 23:BA:275:G:C2' | 23:BA:276:A:H5' | 2.37 | 0.54 |
| 18:CR:36:ASN:HD22 | 18:CR:36:ASN:C | 2.10 | 0.54 |
| 45:B1:23:LYS:HB3 | 45:B1:29:GLY:HA3 | 1.89 | 0.54 |
| 23:BA:2110:G:H8 | 23:BA:2110:G:OP2 | 1.89 | 0.54 |
| 1:CA:668:G:O2' | 15:CO:46:HIS:HB3 | 2.07 | 0.54 |
| 23:DA:2867:G:OP2 | 37:DT:119:LYS:NZ | 2.35 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 27:BF:46:ARG:HH11 | 27:BF:46:ARG:HG2 | 1.72 | 0.54 |
| 1:CA:1459:C:C4 | 1:CA:1460:A:N6 | 2.75 | 0.54 |
| 8:AH:6:ILE:HB | 8:AH:85:ARG:NH1 | 2.11 | 0.54 |
| 1:AA:1142:G:C5 | 1:AA:1143:G:H1' | 2.42 | 0.54 |
| 1:CA:1320:C:H2' | 1:CA:1321:C:O4' | 2.08 | 0.54 |
| 23:DA:1912:A:O2' | 23:DA:1913:A:OP2 | 2.25 | 0.54 |
| 28:DG:178:PHE:HB3 | 28:DG:180:PHE:CE1 | 2.43 | 0.54 |
| 27:DF:28:ILE:HD13 | 27:DF:119:ARG:HE | 1.71 | 0.54 |
| 2:CB:95:GLN:HG3 | 2:CB:147:LYS:HD3 | 1.89 | 0.54 |
| 31:BN:15:LEU:HD12 | 31:BN:137:LYS:HG2 | 1.90 | 0.54 |
| 37:DT:53:ARG:HH11 | 37:DT:53:ARG:HB3 | 1.71 | 0.54 |
| 34:BQ:43:THR:N | 34:BQ:46:GLN:OE1 | 2.40 | 0.54 |
| 28:DG:38:VAL:HG22 | 28:DG:93:THR:HG23 | 1.89 | 0.54 |
| 1:CA:21:G:H2' | 1:CA:22:G:C8 | 2.42 | 0.54 |
| 30:DI:12:LEU:HD22 | 30:DI:19:VAL:HG21 | 1.89 | 0.54 |
| 23:DA:652(B):A:H2' | 23:DA:652(B):A:N3 | 2.22 | 0.54 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:HE2 | 1.71 | 0.54 |
| 1:AA:1090:U:H3 | 1:AA:1095:U:H3 | 1.56 | 0.54 |
| 1:CA:1127:G:H5' | 9:CI:66:ARG:HH22 | 1.72 | 0.54 |
| 1:AA:951:G:C6 | 1:AA:1231:G:C6 | 2.96 | 0.54 |
| 33:DP:38:GLN:O | 33:DP:40:SER:N | 2.40 | 0.54 |
| 23:BA:2319:G:C2 | 36:BS:3:ARG:HA | 2.42 | 0.54 |
| 1:AA:192:U:H2' | 1:AA:193:C:C6 | 2.39 | 0.54 |
| 1:CA:148:G:O2' | 1:CA:149:A:H5' | 2.08 | 0.54 |
| 1:CA:429:U:H3' | 4:CD:22:LYS:NZ | 2.22 | 0.54 |
| 9:CI:17:VAL:HG21 | 9:CI:80:GLY:HA3 | 1.89 | 0.54 |
| 6:AF:97:PHE:O | 18:AR:31:LEU:HD23 | 2.07 | 0.54 |
| 1:AA:615:C:H2' | 1:AA:616:G:C8 | 2.42 | 0.54 |
| 2:AB:77:ALA:HB2 | 2:AB:211:ILE:HG12 | 1.88 | 0.54 |
| 3:CC:122:GLU:HA | 3:CC:125:GLU:HB2 | 1.88 | 0.54 |
| 44:B0:55:ARG:HB3 | 44:B0:55:ARG:CZ | 2.37 | 0.54 |
| 6:AF:91:VAL:HG12 | 6:AF:92:LYS:O | 2.07 | 0.54 |
| 28:DG:37:VAL:HG23 | 28:DG:99:MET:HG3 | 1.88 | 0.54 |
| 23:DA:2884:U:O2 | 49:D5:53:ALA:HB2 | 2.08 | 0.54 |
| 23:DA:2753:A:N3 | 53:D9:15:LYS:NZ | 2.55 | 0.54 |
| 38:BU:58:ARG:HA | 38:BU:61:TRP:CE3 | 2.43 | 0.54 |
| 26:BE:32:PRO:HA | 26:BE:90:THR:HG22 | 1.89 | 0.54 |
| 23:BA:2880:C:O3' | 35:BR:90:ARG:NH1 | 2.40 | 0.54 |
| 41:DX:5:TYR:CZ | 46:D2:30:ARG:HB2 | 2.42 | 0.54 |
| 1:AA:977:A:H2' | 1:AA:978:A:H5' | 1.89 | 0.54 |
| 2:AB:51:LEU:HD23 | 2:AB:55:PHE:HE2 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2526:G:H5' | 23:DA:2742:C:O2' | 2.08 | 0.54 |
| 1:AA:944:G:N2 | 1:AA:1338:G:C8 | 2.75 | 0.54 |
| 23:DA:997:G:OP1 | 38:DU:92:ARG:HG2 | 2.07 | 0.54 |
| 23:BA:271(M):G:O2' | 23:BA:271(N):U:OP1 | 2.16 | 0.54 |
| 14:AN:24:CYS:SG | 14:AN:25:VAL:N | 2.80 | 0.54 |
| 1:AA:753:A:OP1 | 15:AO:69:TYR:OH | 2.24 | 0.54 |
| 13:AM:20:THR:HG23 | 13:AM:26:GLY:HA2 | 1.89 | 0.54 |
| 26:DE:72:VAL:HA | 26:DE:73:GLU:OE2 | 2.08 | 0.54 |
| 37:BT:51:ARG:HG3 | 37:BT:98:LYS:HE3 | 1.89 | 0.54 |
| 36:BS:67:ARG:HG2 | 36:BS:71:ARG:NH2 | 2.23 | 0.54 |
| 23:DA:2836:U:C4 | 23:DA:2883:A:N6 | 2.76 | 0.54 |
| 1:AA:1025:U:O2 | 1:AA:1036:G:C6 | 2.61 | 0.54 |
| 1:AA:1333:A:H3' | 1:AA:1334:G:C8 | 2.40 | 0.54 |
| 1:AA:1239:A:O2' | 7:AG:114:ARG:HB2 | 2.07 | 0.54 |
| 2:CB:71:VAL:O | 2:CB:165:VAL:HG23 | 2.07 | 0.54 |
| 2:CB:80:ILE:HD11 | 2:CB:215:LEU:HB2 | 1.88 | 0.54 |
| 1:CA:1030(A):G:H2' | 1:CA:1030(C):G:OP2 | 2.08 | 0.54 |
| 1:CA:1242:C:O2' | 1:CA:1303:C:H5'' | 2.08 | 0.54 |
| 1:AA:749:C:H2' | 1:AA:750:G:H8 | 1.72 | 0.54 |
| 7:CG:23:VAL:HG22 | 7:CG:43:PHE:HE2 | 1.71 | 0.54 |
| 23:BA:2307:G:H5' | 23:BA:2308:G:N2 | 2.21 | 0.54 |
| 1:AA:407:G:H1 | 1:AA:435:C:H42 | 1.55 | 0.54 |
| 23:BA:2492:U:H2' | 23:BA:2493:U:H6 | 1.73 | 0.54 |
| 23:DA:185:U:H4' | 23:DA:218:A:H4' | 1.90 | 0.54 |
| 1:CA:160:A:H2' | 1:CA:161:A:O4' | 2.07 | 0.54 |
| 23:BA:630:G:N2 | 23:BA:633:A:OP2 | 2.38 | 0.54 |
| 31:DN:56:ASN:H | 31:DN:125:GLY:HA3 | 1.72 | 0.54 |
| 28:BG:116:ASP:H | 28:BG:136:ARG:HH22 | 1.54 | 0.54 |
| 23:DA:446:G:OP2 | 56:DA:4028:HOH:O | 2.19 | 0.54 |
| 23:DA:1028:A:N6 | 23:DA:1125:G:H2' | 2.22 | 0.54 |
| 1:CA:1490:C:H2' | 1:CA:1491:G:O4' | 2.07 | 0.54 |
| 1:AA:1261:A:H61 | 1:AA:1274:G:C2' | 2.21 | 0.54 |
| 1:CA:1298:C:H5'' | 1:CA:1299:A:C8 | 2.43 | 0.54 |
| 1:CA:392:G:H5' | 16:CP:13:HIS:CE1 | 2.42 | 0.54 |
| 23:BA:1019:U:O2' | 23:BA:1021:A:H2 | 1.91 | 0.54 |
| 1:AA:154:C:H42 | 1:AA:167:G:H1 | 1.55 | 0.54 |
| 2:AB:137:ARG:HB2 | 2:AB:137:ARG:NH1 | 2.21 | 0.54 |
| 4:AD:174:LEU:HD23 | 4:AD:185:PHE:HA | 1.89 | 0.54 |
| 3:CC:186:PHE:HE1 | 3:CC:197:GLY:HA2 | 1.71 | 0.54 |
| 44:D0:27:GLU:HG3 | 44:D0:68:GLU:HA | 1.90 | 0.54 |
| 23:BA:1833:U:O2' | 23:BA:1969:A:N1 | 2.29 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:18:LYS:HA | 4:CD:33:MET:HG3 | 1.90 | 0.54 |
| 17:AQ:65:ILE:HD12 | 17:AQ:65:ILE:H | 1.73 | 0.54 |
| 1:CA:826:C:H2' | 1:CA:827:U:C6 | 2.42 | 0.54 |
| 23:DA:315:G:H2' | 23:DA:316:C:C6 | 2.43 | 0.54 |
| 23:DA:2357:U:O2 | 56:DA:4163:HOH:O | 2.18 | 0.54 |
| 1:AA:1469:G:H2' | 1:AA:1470:G:C8 | 2.43 | 0.54 |
| 23:DA:2850:A:C2 | 23:DA:2851:A:C4 | 2.96 | 0.54 |
| 1:CA:7:G:H21 | 5:CE:121:LYS:HG2 | 1.73 | 0.54 |
| 1:AA:509:A:H5'' | 4:AD:55:ALA:HB2 | 1.88 | 0.54 |
| 30:BI:92:VAL:HG13 | 30:BI:120:ILE:HB | 1.90 | 0.54 |
| 47:D3:18:ASP:N | 47:D3:18:ASP:OD1 | 2.35 | 0.54 |
| 24:DB:61:G:C6 | 24:DB:62:C:C4 | 2.95 | 0.54 |
| 17:CQ:92:ARG:O | 17:CQ:95:TYR:HB2 | 2.07 | 0.54 |
| 23:BA:2463:C:C2' | 23:BA:2464:C:H5' | 2.37 | 0.54 |
| 3:AC:23:TYR:CD2 | 10:AJ:95:GLU:HB2 | 2.43 | 0.54 |
| 23:BA:1912:A:O2' | 23:BA:1913:A:OP2 | 2.25 | 0.54 |
| 23:DA:1507:A:O2' | 23:DA:1508:A:O5' | 2.17 | 0.54 |
| 9:AI:9:ARG:HG2 | 9:AI:104:ARG:HE | 1.72 | 0.54 |
| 23:BA:493:G:O6 | 56:BA:4858:HOH:O | 2.18 | 0.54 |
| 29:DH:69:ARG:HG3 | 29:DH:70:THR:N | 2.23 | 0.54 |
| 3:CC:181:ASN:ND2 | 3:CC:204:LEU:O | 2.41 | 0.54 |
| 7:CG:18:TYR:CE1 | 7:CG:58:PRO:HB2 | 2.43 | 0.54 |
| 46:B2:51:ARG:O | 46:B2:55:ARG:HB2 | 2.06 | 0.54 |
| 26:BE:112:GLY:O | 26:BE:159:HIS:HA | 2.08 | 0.54 |
| 35:BR:103:ARG:HH12 | 35:BR:110:PRO:HD3 | 1.72 | 0.54 |
| 1:CA:65:U:H2' | 1:CA:381:C:H5 | 1.73 | 0.54 |
| 1:AA:945:G:H2' | 1:AA:945:G:N3 | 2.22 | 0.54 |
| 1:AA:539:A:H2' | 1:AA:540:G:C8 | 2.43 | 0.54 |
| 1:AA:37:U:O2' | 1:AA:547:A:N1 | 2.30 | 0.54 |
| 24:DB:105:A:OP1 | 43:DZ:72:ARG:NH1 | 2.38 | 0.54 |
| 1:CA:1443:G:H1 | 1:CA:1459:C:C2' | 2.20 | 0.54 |
| 1:AA:1255:G:H5'' | 3:AC:26:LYS:NZ | 2.22 | 0.54 |
| 23:DA:2116:G:H4' | 23:DA:2117:A:OP1 | 2.08 | 0.54 |
| 1:CA:1250:A:H2 | 1:CA:1370:G:H1' | 1.73 | 0.54 |
| 1:AA:157:G:H1 | 1:AA:164:U:H3 | 1.56 | 0.54 |
| 23:BA:1534:U:H3' | 23:BA:1535:A:N1 | 2.23 | 0.54 |
| 1:CA:605:U:H2' | 1:CA:606:G:H8 | 1.72 | 0.54 |
| 1:AA:407:G:O6 | 1:AA:435:C:N4 | 2.41 | 0.54 |
| 5:AE:76:ILE:HG22 | 5:AE:93:PRO:HB3 | 1.90 | 0.54 |
| 15:CO:75:PRO:O | 15:CO:78:TYR:HB3 | 2.07 | 0.54 |
| 27:BF:126:VAL:HG21 | 27:BF:129:PHE:CE1 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 16:AP:72:ARG:HG2 | 16:AP:73:LEU:HD23 | 1.90 | 0.54 |
| 42:BY:92:ASN:N | 42:BY:93:GLY:HA2 | 2.22 | 0.54 |
| 23:DA:2849:U:H4' | 23:DA:2868:A:C2 | 2.43 | 0.54 |
| 23:DA:903:C:H2' | 23:DA:904:C:C6 | 2.43 | 0.54 |
| 47:B3:7:LYS:HG3 | 47:B3:34:GLU:HG2 | 1.90 | 0.54 |
| 23:BA:141:A:H8 | 23:BA:1408:C:HO2' | 1.48 | 0.54 |
| 23:BA:1774:C:H6 | 23:BA:1774:C:O5' | 1.91 | 0.54 |
| 27:DF:11:VAL:O | 27:DF:17:ARG:HA | 2.08 | 0.54 |
| 18:AR:36:ASN:C | 18:AR:36:ASN:HD22 | 2.10 | 0.54 |
| 23:BA:1693:U:O2' | 25:BD:14:ARG:NH2 | 2.40 | 0.54 |
| 1:CA:769:G:H4' | 1:CA:1513:A:H4' | 1.90 | 0.54 |
| 1:AA:631:G:H2' | 1:AA:632:A:C8 | 2.42 | 0.54 |
| 2:AB:87:ARG:HH11 | 2:AB:219:VAL:HG12 | 1.72 | 0.54 |
| 1:CA:1260:C:OP1 | 1:CA:1284:C:H4' | 2.08 | 0.54 |
| 1:CA:1181:G:N2 | 1:CA:1182:G:H22 | 2.06 | 0.54 |
| 1:AA:1368:G:OP2 | 9:AI:112:LYS:HG2 | 2.07 | 0.54 |
| 1:AA:390:C:H2' | 1:AA:391:G:C8 | 2.43 | 0.54 |
| 4:CD:173:TRP:CD2 | 4:CD:189:PRO:HG3 | 2.43 | 0.54 |
| 45:D1:2:SER:HB3 | 45:D1:46:LEU:HD11 | 1.90 | 0.54 |
| 1:CA:922:G:N3 | 1:CA:1398:A:H2 | 2.06 | 0.54 |
| 43:BZ:52:SER:OG | 43:BZ:53:ILE:N | 2.41 | 0.54 |
| 3:AC:34:LEU:HD13 | 14:AN:25:VAL:HG11 | 1.89 | 0.54 |
| 51:D7:9:ARG:HH21 | 51:D7:47:ARG:HD3 | 1.73 | 0.54 |
| 23:DA:2562:U:H1' | 32:DO:23:ARG:HD3 | 1.90 | 0.54 |
| 23:DA:1321:A:H2' | 23:DA:1322:A:O4' | 2.08 | 0.54 |
| 23:DA:603:A:H4' | 23:DA:604:G:H5' | 1.89 | 0.54 |
| 1:AA:380:G:N2 | 1:AA:384:G:C5 | 2.76 | 0.54 |
| 1:CA:1266:G:H8 | 1:CA:1266:G:OP2 | 1.90 | 0.54 |
| 39:DV:78:LYS:O | 56:DV:202:HOH:O | 2.18 | 0.54 |
| 23:BA:1485:G:H1 | 23:BA:1504:C:H42 | 1.56 | 0.54 |
| 23:DA:878:A:H2' | 23:DA:879:G:H5' | 1.90 | 0.54 |
| 20:AT:73:HIS:HB3 | 20:AT:74:LYS:HG2 | 1.89 | 0.54 |
| 37:BT:109:GLU:O | 37:BT:113:LYS:N | 2.36 | 0.54 |
| 1:AA:1003:G:C2' | 1:AA:1004:A:H4' | 2.27 | 0.54 |
| 1:AA:877:C:H5'' | 8:AH:88:LYS:HD3 | 1.90 | 0.54 |
| 9:CI:70:LYS:HA | 9:CI:73:GLN:HB2 | 1.90 | 0.54 |
| 5:AE:127:ASN:O | 5:AE:131:ILE:HG12 | 2.08 | 0.54 |
| 1:AA:964:A:H5'' | 1:AA:1198:G:O3' | 2.08 | 0.54 |
| 23:BA:1173:G:O2' | 23:BA:1174:A:O5' | 2.26 | 0.54 |
| 1:AA:1118:C:O4' | 1:AA:1179:A:C4 | 2.60 | 0.54 |
| 1:CA:1507:A:O3' | 56:CA:2020:HOH:O | 2.18 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1157:A:C2 | 1:CA:1180:A:H2' | 2.43 | 0.54 |
| 3:CC:43:LEU:O | 3:CC:47:LEU:HB2 | 2.08 | 0.54 |
| 23:BA:975(A):G:H1' | 23:BA:990:A:C2 | 2.43 | 0.54 |
| 23:BA:1050:A:H2' | 23:BA:1051:G:H8 | 1.72 | 0.54 |
| 23:BA:1586:A:H8 | 23:BA:1586:A:O5' | 1.90 | 0.54 |
| 1:CA:60:A:H4' | 1:CA:61:G:O5' | 2.08 | 0.54 |
| 27:BF:64:ILE:HD12 | 27:BF:65:TRP:CE3 | 2.42 | 0.54 |
| 28:BG:44:GLY:HA2 | 28:BG:88:ILE:HG22 | 1.90 | 0.54 |
| 48:B4:36:CYS:N | 48:B4:39:CYS:SG | 2.76 | 0.54 |
| 15:AO:87:ILE:HG22 | 15:AO:88:ARG:H | 1.72 | 0.54 |
| 1:CA:1076:C:H42 | 1:CA:1081:G:H1 | 1.56 | 0.54 |
| 23:DA:2461:C:H2' | 23:DA:2462:U:C6 | 2.43 | 0.54 |
| 2:CB:24:TRP:HZ3 | 2:CB:29:ALA:HB2 | 1.73 | 0.54 |
| 23:BA:322:A:OP1 | 27:BF:168:ARG:NH1 | 2.41 | 0.54 |
| 27:BF:11:VAL:O | 27:BF:17:ARG:HA | 2.08 | 0.54 |
| 23:DA:828:U:H4' | 23:DA:831:G:N1 | 2.23 | 0.54 |
| 1:CA:393:A:OP2 | 16:CP:12:LYS:HD2 | 2.08 | 0.54 |
| 23:BA:1815:A:OP2 | 25:BD:54:ARG:NH2 | 2.41 | 0.54 |
| 23:DA:307:G:N2 | 23:DA:309:G:H3' | 2.23 | 0.54 |
| 9:CI:29:ASN:H | 9:CI:63:ILE:HG22 | 1.73 | 0.53 |
| 13:CM:19:LEU:HA | 13:CM:22:ILE:HD12 | 1.89 | 0.53 |
| 23:BA:1364:G:C8 | 45:B1:3:LYS:HD3 | 2.43 | 0.53 |
| 28:DG:124:SER:HB2 | 28:DG:131:TYR:CZ | 2.43 | 0.53 |
| 36:BS:10:ARG:NH2 | 36:BS:91:PRO:HB2 | 2.23 | 0.53 |
| 23:DA:911:A:H2' | 34:DQ:9:TYR:OH | 2.08 | 0.53 |
| 15:AO:75:PRO:O | 15:AO:78:TYR:HB3 | 2.08 | 0.53 |
| 25:DD:148:GLU:HB2 | 25:DD:151:LYS:HD2 | 1.90 | 0.53 |
| 3:CC:30:ARG:HG3 | 3:CC:31:HIS:CD2 | 2.43 | 0.53 |
| 35:DR:36:THR:HG22 | 35:DR:37:THR:N | 2.23 | 0.53 |
| 30:DI:101:LEU:HD21 | 30:DI:107:VAL:HG12 | 1.90 | 0.53 |
| 20:AT:26:ASN:OD1 | 20:AT:71:THR:HG23 | 2.08 | 0.53 |
| 23:DA:9:U:H3 | 23:DA:2629:A:H2 | 1.52 | 0.53 |
| 23:BA:1812:A:O2' | 25:BD:45:ASN:N | 2.40 | 0.53 |
| 3:AC:7:PRO:HB3 | 3:AC:175:LEU:HD21 | 1.90 | 0.53 |
| 1:CA:15:G:H8 | 1:CA:1396:A:HO2' | 1.56 | 0.53 |
| 14:AN:22:THR:HB | 14:AN:33:VAL:HG21 | 1.91 | 0.53 |
| 23:BA:2513:G:N2 | 26:BE:143:ASN:HD21 | 2.06 | 0.53 |
| 23:BA:1948:G:O6 | 56:BA:4989:HOH:O | 2.18 | 0.53 |
| 31:BN:56:ASN:H | 31:BN:125:GLY:HA3 | 1.73 | 0.53 |
| 23:BA:1427:A:H4' | 23:BA:1428:C:O5' | 2.06 | 0.53 |
| 1:CA:279:A:C5 | 17:CQ:98:LEU:HD23 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:950:U:O4 | 1:CA:1231:G:O6 | 2.26 | 0.53 |
| 8:CH:85:ARG:NE | 8:CH:87:SER:O | 2.41 | 0.53 |
| 1:AA:1320:C:H2' | 1:AA:1321:C:O4' | 2.08 | 0.53 |
| 7:CG:26:PHE:HZ | 7:CG:105:VAL:HB | 1.73 | 0.53 |
| 1:CA:1305:G:H2' | 21:CU:4:GLY:O | 2.08 | 0.53 |
| 1:CA:1304:G:N2 | 1:CA:1332:A:OP2 | 2.38 | 0.53 |
| 5:CE:127:ASN:O | 5:CE:131:ILE:HG12 | 2.09 | 0.53 |
| 1:CA:1394:A:N1 | 1:CA:1500:A:O2' | 2.36 | 0.53 |
| 1:AA:1269:A:C8 | 1:AA:1270:C:H1' | 2.43 | 0.53 |
| 19:CS:46:GLY:HA2 | 19:CS:61:TYR:HE1 | 1.73 | 0.53 |
| 7:CG:114:ARG:O | 7:CG:119:ARG:NH1 | 2.36 | 0.53 |
| 7:CG:113:GLU:HB2 | 7:CG:118:VAL:HB | 1.90 | 0.53 |
| 3:AC:40:ARG:HE | 3:AC:55:VAL:HB | 1.73 | 0.53 |
| 15:CO:69:TYR:HA | 15:CO:72:ARG:HD3 | 1.89 | 0.53 |
| 12:AL:70:ILE:HG12 | 12:AL:100:ILE:HD13 | 1.90 | 0.53 |
| 1:CA:35:G:H2' | 1:CA:36:C:C6 | 2.43 | 0.53 |
| 31:DN:120:LEU:HD22 | 31:DN:122:VAL:HG23 | 1.90 | 0.53 |
| 23:BA:445:C:OP1 | 38:BU:2:PRO:HA | 2.08 | 0.53 |
| 23:BA:603:A:H4' | 23:BA:604:G:H5' | 1.90 | 0.53 |
| 23:DA:1140:C:OP1 | 31:DN:23:LEU:O | 2.25 | 0.53 |
| 1:AA:1249:C:OP1 | 9:AI:36:TYR:OH | 2.24 | 0.53 |
| 34:BQ:27:VAL:HG11 | 34:BQ:134:ARG:HG2 | 1.89 | 0.53 |
| 36:DS:99:LYS:O | 36:DS:103:GLU:HG3 | 2.08 | 0.53 |
| 23:DA:674:G:C1' | 27:DF:74:ARG:HD3 | 2.38 | 0.53 |
| 1:CA:1189:C:OP1 | 10:CJ:51:ARG:NH2 | 2.35 | 0.53 |
| 23:DA:19:C:H2' | 23:DA:20:C:C6 | 2.43 | 0.53 |
| 1:CA:598:U:H2' | 1:CA:599:C:C6 | 2.43 | 0.53 |
| 32:DO:73:ASP:OD2 | 32:DO:73:ASP:N | 2.39 | 0.53 |
| 30:DI:5:LEU:HD11 | 30:DI:19:VAL:HG22 | 1.90 | 0.53 |
| 1:CA:35:G:N2 | 1:CA:550:G:H1' | 2.23 | 0.53 |
| 12:AL:32:PHE:HE1 | 12:AL:86:ARG:HG3 | 1.74 | 0.53 |
| 1:CA:262:A:H2' | 1:CA:263:A:C8 | 2.43 | 0.53 |
| 23:DA:649:G:H2' | 23:DA:650:C:C6 | 2.43 | 0.53 |
| 1:AA:1504:G:OP1 | 1:AA:1507:A:H4' | 2.09 | 0.53 |
| 32:DO:10:VAL:HG13 | 32:DO:17:ARG:O | 2.09 | 0.53 |
| 7:AG:30:ILE:O | 7:AG:32:ARG:NH1 | 2.41 | 0.53 |
| 23:DA:330:A:HO2' | 23:DA:331:A:H8 | 1.55 | 0.53 |
| 23:DA:2741:A:H2' | 23:DA:2742:C:O4' | 2.08 | 0.53 |
| 23:DA:71:A:C8 | 23:DA:71:A:H5' | 2.44 | 0.53 |
| 6:CF:7:ASN:ND2 | 18:CR:34:TYR:HE1 | 2.05 | 0.53 |
| 1:CA:157:G:H1 | 1:CA:164:U:H3 | 1.55 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:447:G:H2' | 1:CA:485:G:N2 | 2.22 | 0.53 |
| 3:CC:148:GLY:HA3 | 3:CC:172:ARG:H | 1.73 | 0.53 |
| 1:AA:447:G:H2' | 1:AA:485:G:N2 | 2.23 | 0.53 |
| 37:DT:64:ARG:HB2 | 37:DT:73:GLU:HG2 | 1.89 | 0.53 |
| 23:DA:2732:G:H3' | 23:DA:2733:A:O4' | 2.07 | 0.53 |
| 1:AA:262:A:C6 | 1:AA:263:A:C6 | 2.97 | 0.53 |
| 23:DA:769:G:H5' | 23:DA:1379:A:N6 | 2.23 | 0.53 |
| 23:DA:1026:U:H5'' | 23:DA:1026:U:O2 | 2.09 | 0.53 |
| 1:CA:407:G:O2' | 4:CD:116:GLN:HG3 | 2.09 | 0.53 |
| 23:BA:271(E):U:H3 | 23:BA:271(S):G:H1 | 1.57 | 0.53 |
| 23:DA:2602:A:H1' | 23:DA:2603:G:C5' | 2.39 | 0.53 |
| 26:DE:9:VAL:HG13 | 26:DE:25:VAL:O | 2.09 | 0.53 |
| 27:BF:68:LYS:HB3 | 27:BF:69:HIS:ND1 | 2.23 | 0.53 |
| 31:DN:36:GLY:HA2 | 31:DN:38:HIS:CE1 | 2.43 | 0.53 |
| 23:DA:1252:G:C2 | 23:DA:1253:A:C2 | 2.96 | 0.53 |
| 23:BA:1929:G:OP1 | 56:BA:3707:HOH:O | 2.18 | 0.53 |
| 23:DA:1279:G:H4' | 35:DR:31:HIS:CD2 | 2.43 | 0.53 |
| 1:CA:1192:C:H3' | 1:CA:1192:C:H6 | 1.74 | 0.53 |
| 23:DA:729:G:OP2 | 25:DD:13:ARG:NH1 | 2.40 | 0.53 |
| 23:BA:2884:U:O2 | 49:B5:53:ALA:HB2 | 2.08 | 0.53 |
| 33:DP:84:ASN:HB2 | 33:DP:86:LYS:HD3 | 1.90 | 0.53 |
| 23:DA:413:C:H6 | 23:DA:413:C:O5' | 1.92 | 0.53 |
| 26:BE:201:THR:OG1 | 26:BE:202:LYS:N | 2.41 | 0.53 |
| 23:DA:1138:G:O2' | 31:DN:105:GLY:HA3 | 2.08 | 0.53 |
| 23:BA:2296:U:N3 | 23:BA:2333:A:N3 | 2.56 | 0.53 |
| 1:AA:77:G:O6 | 1:AA:78:G:C2 | 2.62 | 0.53 |
| 1:AA:951:G:N1 | 1:AA:1231:G:C5 | 2.77 | 0.53 |
| 23:DA:1352:U:P | 56:DA:3932:HOH:O | 2.67 | 0.53 |
| 23:DA:2318:G:H22 | 36:DS:3:ARG:HH11 | 1.56 | 0.53 |
| 13:AM:67:GLU:HB3 | 13:AM:71:ARG:HH21 | 1.73 | 0.53 |
| 13:AM:23:TYR:CE1 | 13:AM:70:LEU:HB3 | 2.44 | 0.53 |
| 1:CA:407:G:H1 | 1:CA:435:C:H42 | 1.55 | 0.53 |
| 1:AA:350:G:O2' | 1:AA:351:G:H5' | 2.08 | 0.53 |
| 23:BA:459:U:H4' | 51:B7:40:TRP:CZ3 | 2.44 | 0.53 |
| 23:BA:994:C:OP2 | 38:BU:54:LYS:NZ | 2.34 | 0.53 |
| 10:CJ:45:ARG:HB3 | 10:CJ:65:LEU:HB3 | 1.91 | 0.53 |
| 15:AO:4:THR:O | 15:AO:8:LYS:N | 2.35 | 0.53 |
| 12:CL:24:VAL:HG13 | 12:CL:98:TYR:CE2 | 2.43 | 0.53 |
| 42:DY:79:CYS:HB3 | 42:DY:81:LYS:H | 1.73 | 0.53 |
| 1:AA:1469:G:H2' | 1:AA:1470:G:H8 | 1.73 | 0.53 |
| 23:DA:2097:C:H2' | 23:DA:2098:U:O4' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1510:U:H2' | 1:AA:1511:G:C8 | 2.44 | 0.53 |
| 8:CH:120:THR:H | 8:CH:123:GLU:HB2 | 1.73 | 0.53 |
| 24:DB:2:C:H2' | 24:DB:3:C:C6 | 2.42 | 0.53 |
| 1:AA:1441:G:C2 | 1:AA:1459:C:C5 | 2.97 | 0.53 |
| 1:CA:1457:G:C6 | 1:CA:1458:G:N7 | 2.76 | 0.53 |
| 1:AA:1097:C:H2' | 1:AA:1098:C:H6 | 1.74 | 0.53 |
| 1:CA:1349:A:H5' | 9:CI:120:ARG:HB3 | 1.90 | 0.53 |
| 48:B4:40:HIS:CE1 | 48:B4:42:PHE:HB2 | 2.44 | 0.53 |
| 1:AA:969:A:H2' | 1:AA:970:C:H5' | 1.90 | 0.53 |
| 3:CC:23:TYR:CE2 | 10:CJ:95:GLU:HB2 | 2.44 | 0.53 |
| 23:DA:2133:G:H21 | 23:DA:2158:A:H62 | 1.55 | 0.53 |
| 23:DA:2638:G:P | 26:DE:82:ARG:HH22 | 2.31 | 0.53 |
| 25:BD:101:GLU:OE1 | 25:BD:103:ARG:NH1 | 2.40 | 0.53 |
| 1:AA:826:C:H4' | 8:AH:12:ARG:HD3 | 1.91 | 0.53 |
| 17:CQ:50:LYS:HD3 | 17:CQ:51:TYR:CE1 | 2.44 | 0.53 |
| 1:AA:542:G:H2' | 1:AA:543:C:H6 | 1.73 | 0.53 |
| 1:AA:683:G:H2' | 1:AA:684:A:H8 | 1.73 | 0.53 |
| 41:DX:35:THR:O | 41:DX:39:ILE:HG13 | 2.08 | 0.53 |
| 49:D5:41:PRO:O | 49:D5:44:THR:OG1 | 2.27 | 0.53 |
| 25:DD:131:LEU:HD22 | 25:DD:136:ILE:HG12 | 1.91 | 0.53 |
| 1:AA:1490:C:H2' | 1:AA:1491:G:O4' | 2.09 | 0.53 |
| 28:BG:145:THR:OG1 | 28:BG:146:TYR:N | 2.40 | 0.53 |
| 3:AC:56:ASP:HB3 | 3:AC:69:HIS:HE1 | 1.73 | 0.53 |
| 1:AA:14:U:O4 | 56:AA:2012:HOH:O | 2.18 | 0.53 |
| 23:DA:2513:G:N2 | 26:DE:143:ASN:HD21 | 2.07 | 0.53 |
| 1:AA:176:C:H2' | 1:AA:177:C:C6 | 2.44 | 0.53 |
| 1:CA:414:A:H2' | 1:CA:415:A:C8 | 2.44 | 0.53 |
| 1:AA:1206:G:C6 | 1:AA:1207:G:C6 | 2.96 | 0.53 |
| 1:AA:1095:U:P | 1:AA:1108:G:H1 | 2.32 | 0.53 |
| 8:CH:6:ILE:HB | 8:CH:85:ARG:NH1 | 2.12 | 0.53 |
| 1:CA:581:G:N2 | 1:CA:760:G:N7 | 2.57 | 0.53 |
| 13:CM:87:TYR:HB2 | 19:CS:73:GLU:HA | 1.90 | 0.53 |
| 10:AJ:8:LEU:HA | 10:AJ:95:GLU:O | 2.09 | 0.53 |
| 23:DA:71:A:OP2 | 23:DA:71:A:H3' | 2.09 | 0.53 |
| 28:DG:105:LYS:NZ | 48:D4:26:SER:HB2 | 2.24 | 0.53 |
| 3:AC:68:VAL:HG12 | 3:AC:70:VAL:HG22 | 1.90 | 0.53 |
| 23:BA:1914:C:OP2 | 23:BA:1914:C:H6 | 1.91 | 0.53 |
| 5:CE:69:VAL:O | 5:CE:71:LEU:N | 2.41 | 0.53 |
| 23:DA:1587:A:H2' | 23:DA:1588:C:H6 | 1.74 | 0.53 |
| 1:CA:611:A:H61 | 1:CA:629:G:H1 | 1.55 | 0.53 |
| 1:CA:738:C:H2' | 1:CA:739:C:H6 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BF:116:ASP:OD1 | 27:BF:119:ARG:NH2 | 2.42 | 0.53 |
| 23:DA:1858:G:H1' | 23:DA:1884:A:H61 | 1.72 | 0.53 |
| 3:CC:112:SER:O | 3:CC:112:SER:OG | 2.25 | 0.53 |
| 1:CA:323:U:O3' | 20:CT:22:ARG:HD3 | 2.09 | 0.53 |
| 1:CA:646:U:H2' | 1:CA:647:C:H6 | 1.74 | 0.53 |
| 1:CA:380:G:N2 | 1:CA:384:G:C5 | 2.77 | 0.53 |
| 30:BI:98:ALA:O | 30:BI:101:LEU:N | 2.38 | 0.53 |
| 23:DA:566:U:H5'' | 33:DP:29:LYS:HE3 | 1.89 | 0.53 |
| 23:BA:1040:C:H2' | 23:BA:1041:C:C1' | 2.39 | 0.53 |
| 35:DR:55:ALA:HB2 | 35:DR:79:LEU:HD13 | 1.90 | 0.53 |
| 43:DZ:152:ALA:HA | 43:DZ:155:LEU:HD13 | 1.89 | 0.53 |
| 1:AA:1457:G:C6 | 1:AA:1458:G:C5 | 2.96 | 0.53 |
| 1:CA:951:G:C6 | 1:CA:1231:G:C6 | 2.97 | 0.53 |
| 2:CB:51:LEU:O | 2:CB:55:PHE:HD2 | 1.92 | 0.53 |
| 1:CA:1030:C:N4 | 1:CA:1031:G:C5 | 2.71 | 0.53 |
| 23:BA:2320:A:H2' | 23:BA:2320:A:N3 | 2.23 | 0.53 |
| 1:CA:1208:C:H2' | 1:CA:1209:C:C6 | 2.43 | 0.53 |
| 13:AM:23:TYR:CD1 | 13:AM:67:GLU:HG2 | 2.39 | 0.53 |
| 1:AA:345:C:H4' | 1:AA:346:G:C4 | 2.44 | 0.53 |
| 7:CG:140:ASP:O | 7:CG:143:ARG:HD2 | 2.08 | 0.53 |
| 24:BB:87:G:N2 | 24:BB:90:A:OP2 | 2.36 | 0.53 |
| 30:BI:110:ASP:N | 30:BI:130:TYR:OH | 2.35 | 0.53 |
| 23:BA:528:A:N1 | 23:BA:2042:A:H2' | 2.23 | 0.53 |
| 29:BH:124:GLU:HB2 | 29:BH:132:ARG:HB3 | 1.90 | 0.53 |
| 34:DQ:27:VAL:N | 34:DQ:138:ASP:OD1 | 2.41 | 0.53 |
| 7:CG:111:ARG:HH22 | 7:CG:122:HIS:HB3 | 1.74 | 0.53 |
| 23:BA:2104:G:O6 | 23:BA:2185:C:N3 | 2.41 | 0.53 |
| 23:DA:1288:U:C2 | 23:DA:1327:C:O2 | 2.61 | 0.53 |
| 6:AF:96:PRO:HB3 | 18:AR:30:ASP:OD2 | 2.09 | 0.53 |
| 25:BD:130:ALA:HB2 | 25:BD:192:THR:HB | 1.90 | 0.53 |
| 23:BA:2849:U:H4' | 23:BA:2868:A:C2 | 2.43 | 0.53 |
| 40:DW:71:VAL:HA | 40:DW:107:LEU:HD12 | 1.91 | 0.53 |
| 28:BG:19:LEU:HD22 | 28:BG:23:PHE:HE1 | 1.74 | 0.53 |
| 47:D3:7:LYS:HG3 | 47:D3:34:GLU:HG2 | 1.91 | 0.53 |
| 1:AA:946:A:O2' | 1:AA:1333:A:N3 | 2.39 | 0.53 |
| 45:B1:82:LEU:O | 45:B1:83:GLU:HG3 | 2.08 | 0.53 |
| 23:DA:826:U:OP1 | 23:DA:2428:G:H3' | 2.09 | 0.53 |
| 23:BA:303:U:O4 | 56:BA:4551:HOH:O | 2.19 | 0.53 |
| 1:AA:1267:C:O2 | 1:AA:1327:C:O2' | 2.23 | 0.53 |
| 10:AJ:49:VAL:HG23 | 14:AN:41:ARG:HB2 | 1.89 | 0.53 |
| 35:BR:36:THR:HG22 | 35:BR:37:THR:H | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 6:CF:97:PHE:HD2 | 18:CR:31:LEU:HD21 | 1.74 | 0.53 |
| 1:CA:943:U:H2' | 1:CA:944:G:C8 | 2.44 | 0.53 |
| 37:DT:53:ARG:HB3 | 37:DT:53:ARG:NH1 | 2.24 | 0.53 |
| 23:DA:2629:A:O2' | 23:DA:2630:G:OP2 | 2.21 | 0.53 |
| 1:AA:1063:C:H2' | 1:AA:1064:G:N7 | 2.24 | 0.53 |
| 23:BA:2661:G:H2' | 23:BA:2662:A:C8 | 2.44 | 0.53 |
| 23:BA:1297:C:OP1 | 23:BA:2710:C:H4' | 2.08 | 0.53 |
| 2:CB:162:ILE:HD11 | 2:CB:184:VAL:HG22 | 1.89 | 0.53 |
| 38:BU:82:GLY:HA3 | 38:BU:113:ALA:HB1 | 1.90 | 0.53 |
| 22:AX:2:GLN:HA | 22:AX:2:GLN:HE21 | 1.72 | 0.53 |
| 23:DA:2324:C:H5'' | 23:DA:2325:G:H5' | 1.90 | 0.53 |
| 1:AA:1078:U:O2 | 5:AE:130:ASN:ND2 | 2.42 | 0.53 |
| 1:AA:189(A):C:H42 | 1:AA:189(J):G:H1 | 1.56 | 0.53 |
| 1:AA:1442(A):G:H3' | 1:AA:1442(B):A:H5'' | 1.91 | 0.53 |
| 48:D4:40:HIS:CE1 | 48:D4:42:PHE:HB2 | 2.44 | 0.53 |
| 8:AH:6:ILE:O | 8:AH:10:LEU:HG | 2.09 | 0.53 |
| 1:AA:1220:G:H1' | 19:AS:52:TYR:HD2 | 1.74 | 0.53 |
| 23:BA:1358:G:OP2 | 56:BA:4687:HOH:O | 2.19 | 0.53 |
| 1:CA:932:C:N4 | 1:CA:1385:G:C6 | 2.77 | 0.53 |
| 1:AA:78:G:H1 | 1:AA:91:C:H42 | 1.54 | 0.53 |
| 2:AB:187:LEU:HD13 | 2:AB:205:ASP:HA | 1.90 | 0.53 |
| 23:DA:2312:U:O2' | 28:DG:40:ASN:ND2 | 2.37 | 0.53 |
| 33:BP:38:GLN:HA | 33:BP:41:ARG:HG2 | 1.91 | 0.53 |
| 23:DA:2126:A:H4' | 23:DA:2127:G:O5' | 2.09 | 0.53 |
| 23:BA:2126:A:H4' | 23:BA:2127:G:O5' | 2.09 | 0.53 |
| 1:CA:1316:G:H4' | 14:CN:18:VAL:HG21 | 1.90 | 0.53 |
| 1:CA:169:C:H2' | 1:CA:170:U:C6 | 2.43 | 0.53 |
| 42:BY:9:LYS:NZ | 42:BY:28:LYS:O | 2.41 | 0.53 |
| 28:DG:111:LEU:HB2 | 28:DG:112:PRO:HD3 | 1.91 | 0.53 |
| 1:AA:59:A:H5'' | 1:AA:60:A:C5' | 2.39 | 0.53 |
| 42:DY:23:ARG:HH11 | 42:DY:23:ARG:HB2 | 1.74 | 0.53 |
| 1:CA:59:A:H3' | 1:CA:331:G:H22 | 1.73 | 0.53 |
| 30:BI:5:LEU:HD12 | 30:BI:5:LEU:H | 1.74 | 0.53 |
| 24:BB:15:A:H1' | 24:BB:110:G:C5 | 2.44 | 0.53 |
| 1:CA:1265:G:H2' | 1:CA:1266:G:C8 | 2.44 | 0.53 |
| 1:AA:553:A:H2' | 1:AA:554:C:C6 | 2.44 | 0.53 |
| 50:D6:13:CYS:SG | 50:D6:47:THR:HG21 | 2.49 | 0.53 |
| 5:CE:68:GLU:CD | 5:CE:70:PRO:HG3 | 2.30 | 0.53 |
| 23:BA:2865:U:O4 | 56:BA:4115:HOH:O | 2.14 | 0.53 |
| 17:AQ:92:ARG:O | 17:AQ:95:TYR:HB2 | 2.09 | 0.53 |
| 11:CK:32:ILE:HD11 | 11:CK:68:ALA:HB1 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:742:G:OP2 | 15:CO:35:ARG:NH2 | 2.42 | 0.53 |
| 27:BF:164:ARG:HD2 | 27:BF:175:THR:HG23 | 1.90 | 0.53 |
| 23:DA:917:A:H5' | 23:DA:918:A:OP2 | 2.08 | 0.53 |
| 23:BA:2516:G:O6 | 23:BA:2517:C:N4 | 2.42 | 0.53 |
| 23:DA:896:A:N1 | 34:DQ:60:ARG:NH2 | 2.56 | 0.53 |
| 1:CA:493:G:HO2' | 1:CA:494:U:H6 | 1.55 | 0.53 |
| 1:AA:1442(A):G:H2' | 1:AA:1442(B):A:O4' | 2.09 | 0.52 |
| 1:AA:1004:A:H2 | 1:AA:1037:C:H42 | 1.58 | 0.52 |
| 1:AA:1059:C:O2' | 10:AJ:53:PRO:HD3 | 2.09 | 0.52 |
| 4:CD:13:ARG:HD2 | 4:CD:38:TYR:O | 2.09 | 0.52 |
| 1:CA:91:C:H2' | 1:CA:92:C:C6 | 2.44 | 0.52 |
| 1:CA:1324:A:C5' | 1:CA:1363:C:H5'' | 2.39 | 0.52 |
| 23:BA:821:A:H2' | 23:BA:946:G:H5'' | 1.90 | 0.52 |
| 4:AD:13:ARG:HD2 | 4:AD:38:TYR:O | 2.09 | 0.52 |
| 1:CA:1244:C:H2' | 1:CA:1245:A:C8 | 2.44 | 0.52 |
| 23:BA:2741:A:H2' | 23:BA:2742:C:O4' | 2.09 | 0.52 |
| 23:BA:83:G:N2 | 23:BA:103:A:OP2 | 2.38 | 0.52 |
| 23:DA:61:G:H1 | 23:DA:94:C:H42 | 1.58 | 0.52 |
| 1:CA:1247:U:H1' | 1:CA:1291:G:N2 | 2.23 | 0.52 |
| 12:AL:32:PHE:O | 12:AL:33:ARG:HD2 | 2.09 | 0.52 |
| 26:DE:195:LEU:HG | 26:DE:196:VAL:N | 2.24 | 0.52 |
| 23:DA:2364:C:H2' | 23:DA:2365:G:O4' | 2.09 | 0.52 |
| 34:BQ:24:GLY:O | 34:BQ:102:VAL:HG23 | 2.08 | 0.52 |
| 50:D6:14:THR:HB | 50:D6:48:VAL:O | 2.09 | 0.52 |
| 1:CA:292:G:N7 | 1:CA:293:G:H1' | 2.24 | 0.52 |
| 23:BA:1301:A:C8 | 23:BA:1303:G:C8 | 2.96 | 0.52 |
| 23:BA:2250:G:C5 | 34:BQ:83:MET:HB2 | 2.44 | 0.52 |
| 6:CF:22:GLU:O | 6:CF:26:ILE:HG13 | 2.08 | 0.52 |
| 30:DI:135:GLU:C | 30:DI:137:PRO:HD3 | 2.30 | 0.52 |
| 7:CG:26:PHE:CZ | 7:CG:105:VAL:HB | 2.45 | 0.52 |
| 1:CA:1298:C:H4' | 1:CA:1299:A:C4 | 2.44 | 0.52 |
| 1:CA:1300:G:N1 | 1:CA:1334:G:H2' | 2.19 | 0.52 |
| 1:CA:1252:A:H2 | 1:CA:1355:G:H1' | 1.72 | 0.52 |
| 1:CA:79:G:N2 | 1:CA:91:C:O2 | 2.43 | 0.52 |
| 2:AB:134:GLU:O | 2:AB:137:ARG:HG3 | 2.10 | 0.52 |
| 1:AA:194:C:C2' | 1:AA:195:A:H5'' | 2.40 | 0.52 |
| 1:AA:709:G:H2' | 1:AA:710:G:H8 | 1.74 | 0.52 |
| 1:AA:742:G:OP2 | 15:AO:35:ARG:NH2 | 2.41 | 0.52 |
| 24:BB:40:U:H1' | 24:BB:45:A:N6 | 2.25 | 0.52 |
| 1:CA:336:C:H2' | 1:CA:337:C:H6 | 1.73 | 0.52 |
| 1:CA:609:A:H5' | 16:CP:18:ARG:HH22 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AI:24:GLY:HA2 | 9:AI:59:PHE:C | 2.29 | 0.52 |
| 50:B6:8:LYS:HD3 | 52:B8:34:TRP:CD2 | 2.44 | 0.52 |
| 23:DA:243:U:OP1 | 52:D8:6:THR:OG1 | 2.14 | 0.52 |
| 3:AC:131:ARG:HH12 | 3:AC:135:LYS:HE3 | 1.73 | 0.52 |
| 10:CJ:10:GLY:HA3 | 10:CJ:94:VAL:HG22 | 1.91 | 0.52 |
| 2:AB:21:ARG:H | 2:AB:21:ARG:NE | 2.07 | 0.52 |
| 23:BA:2564:A:C2 | 23:BA:2647:U:H4' | 2.44 | 0.52 |
| 23:BA:2469:A:H5' | 23:BA:2470:G:OP2 | 2.09 | 0.52 |
| 1:AA:1443:G:H1 | 1:AA:1459:C:C2' | 2.22 | 0.52 |
| 23:DA:2173:A:OP2 | 23:DA:2174:C:H5 | 1.93 | 0.52 |
| 9:CI:28:VAL:HB | 9:CI:36:TYR:CB | 2.34 | 0.52 |
| 4:CD:32:ALA:O | 4:CD:36:ARG:N | 2.42 | 0.52 |
| 1:AA:1323:G:H2' | 1:AA:1324:A:C8 | 2.45 | 0.52 |
| 25:DD:85:ASP:OD2 | 25:DD:88:ARG:NH1 | 2.40 | 0.52 |
| 1:AA:184:G:C4' | 1:AA:224:C:H4' | 2.39 | 0.52 |
| 1:CA:1162:C:H2' | 1:CA:1163:C:H6 | 1.75 | 0.52 |
| 42:BY:23:ARG:HB2 | 42:BY:23:ARG:NH1 | 2.25 | 0.52 |
| 23:BA:975:C:H6 | 56:BA:4752:HOH:O | 1.89 | 0.52 |
| 11:CK:73:MET:HE2 | 11:CK:103:LEU:HD13 | 1.92 | 0.52 |
| 12:CL:32:PHE:HE1 | 12:CL:86:ARG:HG3 | 1.74 | 0.52 |
| 23:DA:819:A:C4 | 23:DA:1189:A:C2 | 2.97 | 0.52 |
| 43:BZ:43:GLU:O | 43:BZ:47:VAL:HG23 | 2.09 | 0.52 |
| 23:BA:2699:C:H2' | 23:BA:2700:C:O4' | 2.09 | 0.52 |
| 23:BA:2580:U:O4 | 56:BA:4292:HOH:O | 2.14 | 0.52 |
| 1:AA:105:G:H2' | 1:AA:106:C:C6 | 2.44 | 0.52 |
| 23:DA:2282:G:H4' | 23:DA:2389:G:O2' | 2.08 | 0.52 |
| 23:BA:2572:A:N7 | 26:BE:144:ARG:HD2 | 2.24 | 0.52 |
| 1:CA:1191:A:OP2 | 3:CC:3:ASN:ND2 | 2.42 | 0.52 |
| 23:BA:1156:A:C8 | 38:BU:51:LYS:HD2 | 2.44 | 0.52 |
| 8:AH:14:ARG:O | 8:AH:18:ARG:HD3 | 2.08 | 0.52 |
| 1:AA:50:A:OP1 | 1:AA:50:A:H8 | 1.92 | 0.52 |
| 28:BG:32:PRO:HB2 | 28:BG:172:LEU:HD22 | 1.91 | 0.52 |
| 28:DG:150:ASP:CG | 28:DG:151:ALA:H | 2.11 | 0.52 |
| 1:CA:1412:C:H2' | 1:CA:1413:A:C8 | 2.45 | 0.52 |
| 1:CA:1442(A):G:C5 | 1:CA:1442(B):A:C2 | 2.96 | 0.52 |
| 23:BA:2296:U:H4' | 23:BA:2297:C:OP1 | 2.09 | 0.52 |
| 1:AA:1003:G:H1 | 1:AA:1037:C:N4 | 2.07 | 0.52 |
| 1:AA:1316:G:H22 | 1:AA:1319:A:C5' | 2.21 | 0.52 |
| 23:BA:911:A:H2' | 34:BQ:9:TYR:OH | 2.08 | 0.52 |
| 1:CA:437:U:O3' | 4:CD:125:HIS:NE2 | 2.39 | 0.52 |
| 23:DA:2180:U:H2' | 23:DA:2181:G:C8 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:485:C:H2' | 23:DA:486:C:H6 | 1.74 | 0.52 |
| 23:BA:315:G:H2' | 23:BA:316:C:C6 | 2.44 | 0.52 |
| 2:AB:213:LEU:HD22 | 2:AB:214:ILE:HD13 | 1.91 | 0.52 |
| 38:BU:76:TYR:OH | 38:BU:92:ARG:NH1 | 2.41 | 0.52 |
| 40:BW:82:LEU:HD22 | 40:BW:84:ARG:NH2 | 2.23 | 0.52 |
| 23:DA:1628:G:H2' | 23:DA:1629:U:H6 | 1.74 | 0.52 |
| 46:D2:51:ARG:O | 46:D2:55:ARG:HB2 | 2.09 | 0.52 |
| 25:DD:130:ALA:HB2 | 25:DD:192:THR:HB | 1.91 | 0.52 |
| 1:AA:913:A:H4' | 1:AA:914:A:O5' | 2.09 | 0.52 |
| 23:DA:443:A:N7 | 27:DF:45:ARG:HG2 | 2.24 | 0.52 |
| 12:AL:110:VAL:HG23 | 12:AL:120:TYR:HB3 | 1.90 | 0.52 |
| 43:BZ:152:ALA:HA | 43:BZ:155:LEU:HD13 | 1.92 | 0.52 |
| 1:CA:501:C:H1' | 1:CA:549:C:H1' | 1.92 | 0.52 |
| 1:AA:1442(B):A:H62 | 37:BT:118:ARG:NH2 | 2.07 | 0.52 |
| 1:CA:1441:G:C3' | 1:CA:1459:C:N4 | 2.73 | 0.52 |
| 1:AA:1238:A:H2 | 1:AA:1241:G:H21 | 1.56 | 0.52 |
| 3:AC:29:TYR:OH | 14:AN:54:PRO:O | 2.28 | 0.52 |
| 1:CA:1030(C):G:N7 | 1:CA:1031:G:N2 | 2.58 | 0.52 |
| 21:CU:12:LYS:O | 21:CU:16:GLY:N | 2.37 | 0.52 |
| 21:CU:12:LYS:HB3 | 21:CU:22:ARG:NH1 | 2.24 | 0.52 |
| 17:AQ:79:SER:OG | 17:AQ:80:GLY:N | 2.41 | 0.52 |
| 23:DA:853:G:H1 | 23:DA:924:C:H42 | 1.56 | 0.52 |
| 23:DA:528:A:C2 | 23:DA:2042:A:H2' | 2.44 | 0.52 |
| 36:DS:11:LYS:O | 36:DS:15:ARG:HG3 | 2.10 | 0.52 |
| 1:AA:6:G:O2' | 1:AA:7:G:H5'' | 2.09 | 0.52 |
| 23:DA:1914:C:H6 | 23:DA:1914:C:OP2 | 1.91 | 0.52 |
| 25:BD:206:LEU:HD22 | 25:BD:211:ARG:HG2 | 1.91 | 0.52 |
| 23:DA:7:G:H2' | 23:DA:8:A:C8 | 2.44 | 0.52 |
| 1:CA:1060:C:N4 | 56:CC:301:HOH:O | 2.42 | 0.52 |
| 23:BA:511:U:O4 | 23:BA:512:G:N1 | 2.43 | 0.52 |
| 25:BD:131:LEU:HD22 | 25:BD:136:ILE:HG12 | 1.91 | 0.52 |
| 1:AA:659:U:H2' | 1:AA:660:G:O4' | 2.10 | 0.52 |
| 23:BA:2850:A:C2 | 23:BA:2851:A:C4 | 2.97 | 0.52 |
| 2:AB:42:ILE:HD12 | 2:AB:203:GLY:HA2 | 1.92 | 0.52 |
| 30:BI:125:GLU:OE1 | 30:BI:143:SER:HB3 | 2.09 | 0.52 |
| 31:BN:24:GLY:HA2 | 31:BN:27:ALA:HB3 | 1.91 | 0.52 |
| 8:AH:111:ILE:HD12 | 8:AH:111:ILE:H | 1.74 | 0.52 |
| 1:AA:990:C:H2' | 1:AA:991:U:C6 | 2.45 | 0.52 |
| 27:DF:164:ARG:HD2 | 27:DF:175:THR:HG23 | 1.90 | 0.52 |
| 1:CA:1459:C:C2' | 1:CA:1460:A:C8 | 2.93 | 0.52 |
| 1:CA:1098:C:H5' | 1:CA:1169:A:H1' | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:AH:85:ARG:NE | 8:AH:87:SER:O | 2.42 | 0.52 |
| 1:CA:586:C:H2' | 1:CA:587:G:H5' | 1.92 | 0.52 |
| 1:CA:1125:U:H5' | 1:CA:1126:U:C5 | 2.44 | 0.52 |
| 1:AA:969:A:OP1 | 10:AJ:55:LYS:NZ | 2.38 | 0.52 |
| 1:CA:18:C:H5'' | 5:CE:127:ASN:HD21 | 1.74 | 0.52 |
| 1:CA:1369:C:H2' | 1:CA:1370:G:C8 | 2.45 | 0.52 |
| 1:AA:66:G:O4' | 1:AA:173:U:C4 | 2.63 | 0.52 |
| 23:BA:2180:U:H2' | 23:BA:2181:G:C8 | 2.45 | 0.52 |
| 36:BS:15:ARG:O | 36:BS:19:LYS:HG2 | 2.09 | 0.52 |
| 9:CI:20:ARG:HB3 | 9:CI:60:ASP:O | 2.10 | 0.52 |
| 23:DA:1049:C:O2' | 23:DA:1050:A:O5' | 2.25 | 0.52 |
| 43:BZ:160:GLY:HA2 | 43:BZ:161:VAL:HB | 1.91 | 0.52 |
| 1:CA:785:G:H2' | 1:CA:786:G:H5' | 1.92 | 0.52 |
| 6:CF:96:PRO:HB3 | 18:CR:30:ASP:OD2 | 2.09 | 0.52 |
| 23:BA:1971:A:C4 | 25:BD:241:PRO:HD3 | 2.44 | 0.52 |
| 34:DQ:26:TYR:CE1 | 34:DQ:28:ALA:HB2 | 2.44 | 0.52 |
| 43:DZ:182:LYS:O | 43:DZ:186:GLU:HG2 | 2.09 | 0.52 |
| 2:CB:21:ARG:NE | 2:CB:21:ARG:H | 2.08 | 0.52 |
| 3:CC:55:VAL:HG12 | 3:CC:57:ILE:HG13 | 1.91 | 0.52 |
| 24:DB:20:C:C2' | 24:DB:21:G:H5' | 2.39 | 0.52 |
| 23:DA:1546:C:H5' | 23:DA:1547:C:H5' | 1.92 | 0.52 |
| 6:AF:70:ASP:OD1 | 6:AF:70:ASP:N | 2.42 | 0.52 |
| 1:CA:1048:G:C6 | 1:CA:1210:C:N4 | 2.77 | 0.52 |
| 2:AB:88:ALA:HB1 | 2:AB:222:ILE:HG21 | 1.92 | 0.52 |
| 1:CA:1053:G:N7 | 1:CA:1199:U:H2' | 2.25 | 0.52 |
| 1:CA:1305:G:C8 | 1:CA:1305:G:OP2 | 2.63 | 0.52 |
| 1:CA:860:A:N6 | 1:CA:861:G:C2 | 2.78 | 0.52 |
| 23:BA:2319:G:N2 | 36:BS:3:ARG:HA | 2.25 | 0.52 |
| 24:BB:61:G:C6 | 24:BB:62:C:C4 | 2.98 | 0.52 |
| 23:BA:1818:U:O4 | 25:BD:154:LYS:HE3 | 2.10 | 0.52 |
| 3:CC:153:VAL:HA | 3:CC:197:GLY:O | 2.10 | 0.52 |
| 23:DA:2200:C:H5' | 23:DA:2201:C:OP2 | 2.07 | 0.52 |
| 7:CG:113:GLU:OE2 | 7:CG:119:ARG:HA | 2.09 | 0.52 |
| 2:CB:97:TRP:CZ2 | 2:CB:101:MET:HB2 | 2.44 | 0.52 |
| 1:AA:999:C:H2' | 1:AA:1000:U:C6 | 2.45 | 0.52 |
| 43:BZ:40:ASP:OD1 | 43:BZ:42:VAL:HG13 | 2.09 | 0.52 |
| 23:DA:1790:C:H5'' | 23:DA:1791:A:OP1 | 2.09 | 0.52 |
| 23:DA:2690:C:OP2 | 35:DR:14:SER:HB3 | 2.10 | 0.52 |
| 35:BR:55:ALA:HB2 | 35:BR:79:LEU:HD13 | 1.91 | 0.52 |
| 11:CK:26:ASN:O | 56:CK:201:HOH:O | 2.18 | 0.52 |
| 23:DA:652(O):C:H2' | 23:DA:652(P):G:C8 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:602:G:O2' | 23:DA:655:A:N6 | 2.43 | 0.52 |
| 8:CH:121:ASP:OD1 | 8:CH:121:ASP:N | 2.40 | 0.52 |
| 1:CA:1109:C:O5' | 1:CA:1109:C:H6 | 1.93 | 0.52 |
| 23:DA:863:A:H2' | 23:DA:864:G:C8 | 2.44 | 0.52 |
| 1:AA:1130:A:H61 | 1:AA:1144:G:C1' | 2.20 | 0.52 |
| 1:CA:1327:C:H2' | 1:CA:1328:C:O4' | 2.09 | 0.52 |
| 3:CC:134:ILE:HG22 | 3:CC:168:ALA:HB3 | 1.91 | 0.52 |
| 23:BA:1403:C:C5' | 23:BA:1471:A:H1' | 2.38 | 0.52 |
| 42:DY:28:LYS:HG3 | 42:DY:40:GLU:HG2 | 1.92 | 0.52 |
| 23:BA:492:A:H2' | 23:BA:493:G:O4' | 2.10 | 0.52 |
| 23:BA:993:G:OP1 | 38:BU:50:ARG:NH2 | 2.43 | 0.52 |
| 11:CK:21:ILE:HB | 11:CK:84:VAL:HG22 | 1.90 | 0.52 |
| 23:BA:102:G:O2' | 23:BA:103:A:O5' | 2.27 | 0.52 |
| 23:DA:143(A):C:H2' | 23:DA:144:C:C6 | 2.44 | 0.52 |
| 23:BA:218:A:C2 | 23:BA:235:U:H4' | 2.45 | 0.52 |
| 31:DN:96:GLU:H | 31:DN:96:GLU:CD | 2.13 | 0.52 |
| 1:AA:1388:C:H2' | 1:AA:1389:C:H6 | 1.75 | 0.52 |
| 23:DA:2096:U:H3 | 23:DA:2193:G:H1 | 1.57 | 0.52 |
| 23:DA:1669:A:H5'' | 23:DA:2550:G:OP1 | 2.10 | 0.52 |
| 36:DS:26:LEU:HD22 | 36:DS:87:PHE:CD1 | 2.45 | 0.52 |
| 23:BA:498:G:O2' | 23:BA:499:U:H5' | 2.10 | 0.52 |
| 19:CS:49:ILE:O | 19:CS:59:PRO:HA | 2.09 | 0.52 |
| 23:BA:2672:G:H8 | 23:BA:2672:G:H5'' | 1.73 | 0.52 |
| 47:B3:18:ASP:N | 47:B3:18:ASP:OD1 | 2.42 | 0.52 |
| 1:AA:1298:C:N4 | 7:AG:114:ARG:HD2 | 2.24 | 0.52 |
| 1:AA:971:G:O2' | 1:AA:1365:G:O3' | 2.28 | 0.52 |
| 19:CS:16:LEU:CA | 19:CS:20:LEU:HB2 | 2.37 | 0.52 |
| 1:CA:1239:A:H4' | 1:CA:1240:U:OP1 | 2.09 | 0.52 |
| 23:DA:71:A:H8 | 23:DA:71:A:H5' | 1.75 | 0.52 |
| 1:AA:750:G:C2 | 15:AO:23:GLY:HA3 | 2.44 | 0.52 |
| 23:BA:2117:A:N6 | 23:BA:2171:A:C6 | 2.78 | 0.52 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:CE1 | 2.45 | 0.52 |
| 4:AD:173:TRP:HB2 | 4:AD:187:ARG:O | 2.10 | 0.52 |
| 7:AG:71:PRO:HG3 | 7:AG:138:LYS:CG | 2.39 | 0.52 |
| 23:DA:2308:G:H4' | 23:DA:2309:A:OP2 | 2.08 | 0.52 |
| 35:DR:37:THR:OG1 | 35:DR:40:LYS:HG3 | 2.09 | 0.52 |
| 43:BZ:98:MET:O | 43:BZ:125:LEU:HD12 | 2.09 | 0.52 |
| 1:CA:1492:A:H4' | 1:CA:1492:A:OP1 | 2.10 | 0.52 |
| 36:BS:35:ILE:HG12 | 36:BS:101:LEU:HD12 | 1.91 | 0.52 |
| 1:AA:756:C:N4 | 56:AA:2015:HOH:O | 2.32 | 0.52 |
| 23:DA:1819:A:H4' | 23:DA:1820:U:O5' | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:229:A:C8 | 23:BA:229:A:H3' | 2.45 | 0.52 |
| 23:BA:878:A:H2' | 23:BA:879:G:H5' | 1.92 | 0.52 |
| 23:DA:944:G:O3' | 56:DA:3793:HOH:O | 2.19 | 0.52 |
| 23:BA:1335:U:O4 | 56:BA:4449:HOH:O | 2.17 | 0.52 |
| 1:CA:1458:G:H3' | 1:CA:1459:C:H5'' | 1.92 | 0.52 |
| 1:CA:1459:C:C5' | 1:CA:1460:A:OP2 | 2.57 | 0.52 |
| 1:CA:1004:A:H2 | 1:CA:1037:C:N4 | 2.08 | 0.52 |
| 23:BA:582:G:H2' | 23:BA:583:G:C8 | 2.44 | 0.52 |
| 23:BA:2319:G:H22 | 36:BS:3:ARG:HD2 | 1.75 | 0.52 |
| 1:CA:1238:A:N7 | 1:CA:1299:A:N1 | 2.57 | 0.52 |
| 1:AA:93:G:O2' | 1:AA:96:U:H5' | 2.10 | 0.52 |
| 1:CA:977:A:H1' | 1:CA:982:U:H3 | 1.74 | 0.52 |
| 37:DT:95:ARG:HG2 | 37:DT:95:ARG:NH1 | 2.19 | 0.52 |
| 23:BA:2364:C:H2' | 23:BA:2365:G:O4' | 2.10 | 0.52 |
| 7:CG:142:GLU:CB | 7:CG:143:ARG:HH21 | 2.22 | 0.52 |
| 23:BA:2109:U:H1' | 23:BA:2181:G:N2 | 2.24 | 0.52 |
| 1:AA:374:A:N1 | 1:AA:390:C:O2' | 2.36 | 0.52 |
| 1:AA:56:U:H2' | 1:AA:57:G:C8 | 2.45 | 0.52 |
| 4:AD:119:GLN:HG2 | 4:AD:123:HIS:CD2 | 2.45 | 0.52 |
| 23:DA:2537:U:H2' | 23:DA:2538:C:C6 | 2.45 | 0.52 |
| 38:DU:44:ASN:ND2 | 39:DV:75:PHE:O | 2.36 | 0.52 |
| 1:AA:763:G:H2' | 1:AA:764:C:H6 | 1.75 | 0.52 |
| 23:DA:1810:A:H2' | 23:DA:1811:G:O4' | 2.09 | 0.52 |
| 29:DH:7:LEU:HD12 | 29:DH:8:PRO:HD2 | 1.92 | 0.52 |
| 5:CE:14:ARG:HE | 5:CE:16:THR:HG22 | 1.74 | 0.52 |
| 23:BA:335:C:H2' | 23:BA:336:C:H6 | 1.75 | 0.52 |
| 47:B3:40:THR:HG23 | 47:B3:43:ILE:HD12 | 1.92 | 0.52 |
| 1:AA:1169:A:H2' | 1:AA:1170:A:H8 | 1.74 | 0.51 |
| 1:AA:1316:G:N2 | 1:AA:1318:A:H3' | 2.25 | 0.51 |
| 13:AM:87:TYR:HB2 | 19:AS:73:GLU:O | 2.10 | 0.51 |
| 1:CA:1128:C:N3 | 1:CA:1143:G:N2 | 2.47 | 0.51 |
| 1:CA:676:A:O2' | 1:CA:677:U:H5' | 2.10 | 0.51 |
| 1:CA:1029:C:N3 | 1:CA:1032:G:O6 | 2.43 | 0.51 |
| 23:BA:1173:G:H1' | 23:BA:1177:A:N6 | 2.24 | 0.51 |
| 6:AF:7:ASN:ND2 | 18:AR:34:TYR:HE1 | 2.05 | 0.51 |
| 23:DA:2109:U:H1' | 23:DA:2181:G:N2 | 2.25 | 0.51 |
| 23:BA:2308:G:H4' | 23:BA:2309:A:OP2 | 2.10 | 0.51 |
| 7:AG:95:ARG:O | 7:AG:99:LEU:HG | 2.10 | 0.51 |
| 7:AG:140:ASP:HA | 7:AG:143:ARG:HB2 | 1.91 | 0.51 |
| 24:BB:48:A:H4' | 36:BS:95:HIS:HD2 | 1.75 | 0.51 |
| 36:BS:95:HIS:C | 36:BS:99:LYS:HB3 | 2.31 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:CR:66:LEU:O | 18:CR:70:ILE:HG13 | 2.11 | 0.51 |
| 12:CL:25:PRO:C | 12:CL:27:LEU:H | 2.11 | 0.51 |
| 22:AX:56:VAL:N | 22:AX:59:GLY:HA2 | 2.24 | 0.51 |
| 1:AA:189:G:H2' | 1:AA:189(A):C:H6 | 1.73 | 0.51 |
| 23:BA:2755:C:HO2' | 23:BA:2756:U:H6 | 1.58 | 0.51 |
| 23:DA:764:A:OP1 | 25:DD:208:LYS:HE2 | 2.10 | 0.51 |
| 23:DA:1688:U:H1' | 23:DA:1701:A:C6 | 2.45 | 0.51 |
| 23:DA:2564:A:C2 | 23:DA:2647:U:H4' | 2.45 | 0.51 |
| 23:DA:706:A:H2' | 23:DA:707:G:O4' | 2.10 | 0.51 |
| 11:AK:73:MET:HG3 | 11:AK:103:LEU:HD21 | 1.91 | 0.51 |
| 24:DB:13:A:N1 | 24:DB:69:G:O2' | 2.38 | 0.51 |
| 1:AA:668:G:O2' | 15:AO:46:HIS:HB3 | 2.10 | 0.51 |
| 23:DA:229:A:C8 | 23:DA:229:A:H3' | 2.45 | 0.51 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:C6 | 2.45 | 0.51 |
| 23:DA:2880:C:O3' | 35:DR:90:ARG:NH1 | 2.43 | 0.51 |
| 28:DG:116:ASP:H | 28:DG:136:ARG:HH22 | 1.57 | 0.51 |
| 7:AG:101:LEU:HA | 7:AG:104:LEU:HD23 | 1.92 | 0.51 |
| 1:CA:971:G:H1 | 1:CA:1363(A):A:H5' | 1.75 | 0.51 |
| 1:AA:1316:G:C6 | 1:AA:1318:A:H5'' | 2.46 | 0.51 |
| 9:CI:10:ARG:CB | 9:CI:75:ASP:HB2 | 2.39 | 0.51 |
| 1:CA:1052:U:H2' | 1:CA:1055:A:OP1 | 2.09 | 0.51 |
| 28:BG:22:ARG:HH21 | 28:BG:175:LEU:HD11 | 1.74 | 0.51 |
| 20:CT:61:SER:O | 20:CT:65:LYS:HG2 | 2.11 | 0.51 |
| 30:BI:83:ALA:HA | 30:BI:89:TYR:HE2 | 1.74 | 0.51 |
| 42:BY:28:LYS:HG3 | 42:BY:40:GLU:HG2 | 1.93 | 0.51 |
| 1:AA:1126:U:H1' | 1:AA:1280:A:C5 | 2.46 | 0.51 |
| 1:AA:428:G:H4' | 1:AA:429:U:O5' | 2.10 | 0.51 |
| 1:CA:826:C:H4' | 8:CH:12:ARG:HD3 | 1.91 | 0.51 |
| 2:CB:16:HIS:CD2 | 2:CB:209:ARG:HG3 | 2.45 | 0.51 |
| 23:DA:581:C:H2' | 23:DA:582:G:C8 | 2.46 | 0.51 |
| 1:CA:666:G:H5' | 1:CA:726:C:H1' | 1.93 | 0.51 |
| 23:BA:1040:C:H2' | 23:BA:1041:C:H1' | 1.91 | 0.51 |
| 7:AG:26:PHE:CG | 7:AG:101:LEU:HD22 | 2.46 | 0.51 |
| 23:DA:2441:C:OP2 | 23:DA:2586:C:O2' | 2.27 | 0.51 |
| 32:BO:77:ILE:HG13 | 37:BT:74:ARG:HG2 | 1.92 | 0.51 |
| 28:BG:111:LEU:HB2 | 28:BG:112:PRO:HD3 | 1.92 | 0.51 |
| 26:DE:111:ARG:HD3 | 26:DE:160:TYR:CE1 | 2.45 | 0.51 |
| 16:CP:72:ARG:HG2 | 16:CP:73:LEU:HD23 | 1.92 | 0.51 |
| 23:DA:2790:A:N3 | 23:DA:2790:A:H3' | 2.25 | 0.51 |
| 23:DA:588:U:H2' | 23:DA:589:C:C6 | 2.45 | 0.51 |
| 1:AA:1022:G:H2' | 1:AA:1023:G:C8 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:D4:40:HIS:O | 48:D4:42:PHE:N | 2.41 | 0.51 |
| 1:AA:1090:U:H2' | 1:AA:1091:U:C6 | 2.44 | 0.51 |
| 1:AA:1222:G:H5'' | 19:AS:78:ARG:CZ | 2.41 | 0.51 |
| 1:CA:1347:G:H1' | 1:CA:1348:U:H5 | 1.75 | 0.51 |
| 28:DG:41:GLN:HG3 | 28:DG:60:LEU:HD11 | 1.93 | 0.51 |
| 1:AA:1277:C:H2' | 1:AA:1279:A:H8 | 1.76 | 0.51 |
| 23:BA:1530:C:O2' | 23:BA:1531:C:P | 2.68 | 0.51 |
| 23:DA:2319:G:C2 | 36:DS:3:ARG:HA | 2.46 | 0.51 |
| 1:CA:958:A:N3 | 1:CA:985:C:O2' | 2.37 | 0.51 |
| 21:AU:15:ARG:HA | 21:AU:15:ARG:HE | 1.76 | 0.51 |
| 1:AA:1372:U:H5'' | 9:AI:71:SER:CB | 2.40 | 0.51 |
| 1:AA:920:U:O4' | 1:AA:1080:A:C2 | 2.64 | 0.51 |
| 4:AD:36:ARG:HB3 | 4:AD:38:TYR:CZ | 2.46 | 0.51 |
| 23:DA:83:G:N2 | 23:DA:102:G:H2' | 2.25 | 0.51 |
| 1:CA:746:A:H2' | 1:CA:747:C:C6 | 2.45 | 0.51 |
| 36:BS:99:LYS:O | 36:BS:103:GLU:HG3 | 2.10 | 0.51 |
| 1:AA:611:A:H61 | 1:AA:629:G:H1 | 1.57 | 0.51 |
| 23:DA:228:A:H2' | 23:DA:230:U:O4' | 2.11 | 0.51 |
| 23:BA:2200:C:H5' | 23:BA:2201:C:OP2 | 2.09 | 0.51 |
| 23:DA:2853:C:H2' | 23:DA:2854:G:C8 | 2.46 | 0.51 |
| 1:AA:277:C:OP1 | 17:AQ:68:ARG:NH2 | 2.41 | 0.51 |
| 1:AA:881:G:P | 12:AL:12:ARG:HH22 | 2.33 | 0.51 |
| 25:BD:130:ALA:C | 25:BD:131:LEU:HD12 | 2.31 | 0.51 |
| 10:CJ:12:ASP:C | 10:CJ:68:HIS:HD2 | 2.13 | 0.51 |
| 10:AJ:33:GLN:O | 10:AJ:34:VAL:HG22 | 2.08 | 0.51 |
| 27:DF:183:VAL:O | 27:DF:187:VAL:HG23 | 2.11 | 0.51 |
| 50:D6:11:LEU:HB2 | 50:D6:21:TYR:HB2 | 1.90 | 0.51 |
| 30:BI:4:ILE:HG21 | 30:BI:47:LEU:HG | 1.92 | 0.51 |
| 32:BO:73:ASP:OD1 | 37:BT:32:TYR:OH | 2.22 | 0.51 |
| 23:DA:1427:A:H4' | 23:DA:1428:C:O5' | 2.11 | 0.51 |
| 23:DA:2208:A:H1' | 23:DA:2219:G:C5 | 2.46 | 0.51 |
| 23:BA:1593:G:H2' | 23:BA:1594:G:C8 | 2.46 | 0.51 |
| 4:AD:193:ASP:N | 4:AD:193:ASP:OD1 | 2.44 | 0.51 |
| 29:DH:154:PRO:HB3 | 29:DH:163:TYR:CZ | 2.44 | 0.51 |
| 1:AA:1460:A:H8 | 1:AA:1460:A:O5' | 1.93 | 0.51 |
| 1:CA:954:G:N2 | 1:CA:1227:A:H62 | 2.08 | 0.51 |
| 2:CB:55:PHE:CD1 | 2:CB:58:ILE:HD12 | 2.45 | 0.51 |
| 23:DA:1530:C:O2' | 23:DA:1531:C:P | 2.68 | 0.51 |
| 1:CA:1157:A:N1 | 1:CA:1180:A:H2' | 2.25 | 0.51 |
| 9:CI:28:VAL:O | 9:CI:36:TYR:HB2 | 2.10 | 0.51 |
| 1:AA:266:G:H5'' | 1:AA:267:C:H5 | 1.73 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:573:G:O2' | 23:DA:574:C:H3' | 2.11 | 0.51 |
| 1:AA:658:G:C2 | 1:AA:749:C:N3 | 2.79 | 0.51 |
| 1:AA:232:G:H1' | 1:AA:262:A:N1 | 2.26 | 0.51 |
| 1:CA:475:G:H2' | 1:CA:476:G:C8 | 2.46 | 0.51 |
| 27:DF:129:PHE:O | 27:DF:132:VAL:HG13 | 2.10 | 0.51 |
| 23:DA:188:G:H1 | 23:DA:208:C:N4 | 2.09 | 0.51 |
| 1:CA:1137:C:H5' | 1:CA:1138:G:C6 | 2.45 | 0.51 |
| 3:CC:30:ARG:HB3 | 14:CN:36:PHE:O | 2.11 | 0.51 |
| 23:DA:1113:U:H2' | 23:DA:1114:G:C8 | 2.46 | 0.51 |
| 17:CQ:66:SER:O | 17:CQ:69:LYS:N | 2.26 | 0.51 |
| 1:AA:540:G:H2' | 1:AA:541:G:O4' | 2.10 | 0.51 |
| 1:CA:806:C:H2' | 1:CA:807:A:H8 | 1.76 | 0.51 |
| 31:BN:99:LEU:HD22 | 31:BN:103:VAL:HG23 | 1.91 | 0.51 |
| 27:BF:34:TRP:HE3 | 27:BF:35:GLU:HG2 | 1.74 | 0.51 |
| 23:BA:1792:G:O2' | 23:BA:1830:C:OP1 | 2.28 | 0.51 |
| 5:AE:68:GLU:CD | 5:AE:70:PRO:HG3 | 2.31 | 0.51 |
| 1:AA:129(A):G:H1' | 1:AA:189(F):U:H2' | 1.91 | 0.51 |
| 23:BA:143(A):C:H2' | 23:BA:144:C:H6 | 1.75 | 0.51 |
| 1:CA:1220:G:H2' | 1:CA:1221:G:C8 | 2.45 | 0.51 |
| 23:BA:2097:C:H2' | 23:BA:2098:U:O4' | 2.10 | 0.51 |
| 1:AA:357:G:N7 | 56:AA:1886:HOH:O | 2.35 | 0.51 |
| 30:DI:134:PRO:C | 30:DI:136:VAL:H | 2.14 | 0.51 |
| 29:BH:24:VAL:HG13 | 29:BH:37:VAL:HG21 | 1.92 | 0.51 |
| 1:CA:939:G:N3 | 1:CA:1375:A:H2 | 2.08 | 0.51 |
| 2:AB:28:PHE:CZ | 2:AB:189:ASP:HA | 2.46 | 0.51 |
| 1:CA:1157:A:H61 | 1:CA:1178:G:H21 | 1.58 | 0.51 |
| 1:AA:149:A:O2' | 1:AA:150:C:C6 | 2.63 | 0.51 |
| 13:AM:23:TYR:HE1 | 13:AM:70:LEU:HB3 | 1.75 | 0.51 |
| 23:BA:2169:A:H3' | 23:BA:2170:A:H8 | 1.75 | 0.51 |
| 28:DG:3:LEU:HD11 | 28:DG:97:ASP:HB3 | 1.92 | 0.51 |
| 1:AA:1080:A:H5' | 5:AE:14:ARG:NH2 | 2.26 | 0.51 |
| 23:BA:2572:A:N7 | 26:BE:145:LYS:HB2 | 2.26 | 0.51 |
| 34:BQ:42:ILE:HD13 | 34:BQ:97:VAL:HG21 | 1.91 | 0.51 |
| 32:DO:31:LYS:HB3 | 32:DO:32:TYR:CE2 | 2.45 | 0.51 |
| 29:DH:40:GLU:OE2 | 29:DH:60:ARG:NH1 | 2.43 | 0.51 |
| 15:CO:87:ILE:HG22 | 15:CO:88:ARG:H | 1.75 | 0.51 |
| 16:CP:75:ARG:HA | 16:CP:80:PHE:HD1 | 1.75 | 0.51 |
| 23:DA:187:G:N3 | 23:DA:1365:A:H2 | 2.08 | 0.51 |
| 1:CA:123:C:O2' | 1:CA:290:C:O2 | 2.20 | 0.51 |
| 1:CA:659:U:H2' | 1:CA:660:G:O4' | 2.11 | 0.51 |
| 23:BA:774:A:H2' | 23:BA:774:A:N3 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2144:U:H2' | 23:DA:2146:C:N4 | 2.26 | 0.51 |
| 23:BA:1782:C:H2' | 23:BA:2608:G:O2' | 2.11 | 0.51 |
| 1:CA:586:C:O2' | 1:CA:878:G:H4' | 2.11 | 0.51 |
| 13:CM:14:ARG:CZ | 13:CM:41:PRO:HB2 | 2.40 | 0.51 |
| 1:CA:757:U:OP1 | 1:CA:822:C:O2' | 2.28 | 0.51 |
| 52:D8:23:VAL:HG12 | 52:D8:47:LYS:HB3 | 1.92 | 0.51 |
| 28:BG:41:GLN:HG3 | 28:BG:60:LEU:HD11 | 1.92 | 0.51 |
| 23:DA:2134:A:N6 | 23:DA:2157:G:H1' | 2.26 | 0.51 |
| 1:CA:1084:G:H5' | 1:CA:1102:A:OP2 | 2.10 | 0.51 |
| 1:AA:939:G:C6 | 1:AA:940:C:N4 | 2.79 | 0.51 |
| 1:AA:390:C:O3' | 16:AP:28:ARG:NH2 | 2.43 | 0.51 |
| 23:BA:271(D):G:H2' | 23:BA:271(E):U:O4' | 2.11 | 0.51 |
| 5:AE:69:VAL:O | 5:AE:71:LEU:N | 2.42 | 0.51 |
| 8:CH:31:PHE:O | 8:CH:35:ILE:HG13 | 2.11 | 0.51 |
| 1:AA:1371:G:H4' | 9:AI:69:GLY:CA | 2.41 | 0.51 |
| 12:AL:24:VAL:HG13 | 12:AL:98:TYR:CE2 | 2.45 | 0.51 |
| 30:BI:16:GLY:O | 30:BI:47:LEU:HD11 | 2.10 | 0.51 |
| 33:DP:95:VAL:HG22 | 33:DP:125:VAL:HB | 1.93 | 0.51 |
| 23:BA:2872:G:O2' | 23:BA:2873:A:H5' | 2.09 | 0.51 |
| 52:B8:61:LEU:O | 52:B8:63:PRO:HD3 | 2.10 | 0.51 |
| 24:BB:2:C:H2' | 24:BB:3:C:C6 | 2.45 | 0.51 |
| 25:DD:67:PHE:HB3 | 25:DD:153:ALA:H | 1.76 | 0.51 |
| 52:D8:61:LEU:C | 52:D8:63:PRO:HD3 | 2.31 | 0.51 |
| 24:DB:7:G:H8 | 24:DB:7:G:H5'' | 1.76 | 0.51 |
| 37:BT:18:ASP:OD1 | 37:BT:18:ASP:N | 2.37 | 0.51 |
| 26:BE:135:HIS:H | 26:BE:135:HIS:CD2 | 2.26 | 0.51 |
| 1:CA:50:A:OP1 | 1:CA:50:A:H8 | 1.93 | 0.51 |
| 28:DG:6:ALA:O | 28:DG:10:LYS:N | 2.38 | 0.51 |
| 12:CL:110:VAL:HG23 | 12:CL:120:TYR:HB3 | 1.92 | 0.51 |
| 23:BA:2036:C:H5' | 23:BA:2036:C:C6 | 2.33 | 0.51 |
| 9:CI:9:ARG:NH1 | 9:CI:104:ARG:HE | 2.09 | 0.51 |
| 23:BA:26:G:H1' | 23:BA:515:A:H61 | 1.76 | 0.51 |
| 1:CA:1305:G:H8 | 21:CU:5:ASP:HA | 1.76 | 0.51 |
| 1:CA:1240:U:O5' | 1:CA:1241:G:H8 | 1.93 | 0.51 |
| 1:CA:1241:G:H5'' | 1:CA:1242:C:OP2 | 2.10 | 0.51 |
| 9:CI:31:GLN:NE2 | 9:CI:36:TYR:HD1 | 2.09 | 0.51 |
| 1:AA:148:G:O2' | 1:AA:149:A:H5' | 2.10 | 0.51 |
| 28:BG:105:LYS:NZ | 48:B4:26:SER:HB2 | 2.26 | 0.51 |
| 3:CC:36:ASP:O | 3:CC:40:ARG:HG2 | 2.11 | 0.51 |
| 13:AM:12:ASN:O | 13:AM:44:ARG:HB3 | 2.10 | 0.51 |
| 7:CG:69:VAL:HA | 7:CG:138:LYS:HB2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:2116:G:H4' | 23:BA:2117:A:OP1 | 2.11 | 0.51 |
| 7:AG:103:TRP:HZ3 | 7:AG:138:LYS:HB2 | 1.75 | 0.51 |
| 23:DA:2199:A:H5'' | 23:DA:2200:C:OP2 | 2.10 | 0.51 |
| 1:CA:1188:A:H2' | 1:CA:1189:C:H5' | 1.93 | 0.51 |
| 12:CL:32:PHE:O | 12:CL:33:ARG:HD2 | 2.10 | 0.51 |
| 18:CR:36:ASN:ND2 | 18:CR:39:VAL:H | 2.09 | 0.51 |
| 5:AE:78:HIS:HA | 8:AH:105:ARG:HG3 | 1.93 | 0.51 |
| 29:BH:46:GLU:HB2 | 29:BH:49:VAL:HG12 | 1.93 | 0.51 |
| 4:CD:128:VAL:HA | 4:CD:145:GLU:O | 2.11 | 0.51 |
| 23:DA:396:G:O3' | 45:D1:44:PRO:HA | 2.11 | 0.51 |
| 24:BB:7:G:H5'' | 24:BB:7:G:H8 | 1.75 | 0.51 |
| 1:CA:990:C:C4 | 1:CA:991:U:C4 | 2.99 | 0.51 |
| 1:CA:838:G:N2 | 1:CA:849:C:C2 | 2.79 | 0.51 |
| 13:CM:18:ALA:HB2 | 13:CM:45:VAL:HG21 | 1.92 | 0.51 |
| 2:CB:84:GLU:HB3 | 2:CB:219:VAL:HG21 | 1.93 | 0.51 |
| 2:CB:20:GLU:HG3 | 2:CB:191:ASP:OD1 | 2.10 | 0.51 |
| 1:CA:1359:C:OP1 | 14:CN:22:THR:OG1 | 2.20 | 0.51 |
| 23:DA:2318:G:N2 | 36:DS:3:ARG:HH11 | 2.09 | 0.51 |
| 20:AT:12:ALA:O | 20:AT:15:ARG:HB2 | 2.10 | 0.51 |
| 14:AN:57:ARG:HG2 | 14:AN:58:LYS:N | 2.26 | 0.51 |
| 7:CG:137:LYS:HA | 7:CG:140:ASP:CG | 2.32 | 0.51 |
| 1:CA:184:G:C4' | 1:CA:224:C:H4' | 2.41 | 0.51 |
| 36:DS:14:VAL:HG11 | 36:DS:90:GLY:O | 2.10 | 0.51 |
| 1:AA:1348:U:C2 | 1:AA:1349:A:C8 | 2.99 | 0.51 |
| 15:CO:39:LEU:HD13 | 15:CO:56:LEU:HD23 | 1.92 | 0.51 |
| 28:DG:133:LEU:HG | 28:DG:157:ILE:HB | 1.92 | 0.51 |
| 10:AJ:13:HIS:HB3 | 10:AJ:68:HIS:ND1 | 2.26 | 0.51 |
| 2:CB:12:GLU:O | 2:CB:16:HIS:ND1 | 2.40 | 0.51 |
| 43:BZ:69:THR:HG22 | 43:BZ:90:VAL:HA | 1.93 | 0.51 |
| 32:BO:64:ARG:HG2 | 32:BO:79:PHE:CG | 2.46 | 0.51 |
| 43:DZ:151:HIS:N | 43:DZ:154:ASP:OD1 | 2.42 | 0.51 |
| 31:DN:55:VAL:HG22 | 31:DN:125:GLY:HA3 | 1.92 | 0.51 |
| 23:DA:627:A:H62 | 33:DP:84:ASN:HD21 | 1.59 | 0.51 |
| 26:DE:111:ARG:HD3 | 26:DE:160:TYR:CD1 | 2.45 | 0.51 |
| 42:BY:102:CYS:O | 42:BY:104:GLY:N | 2.44 | 0.51 |
| 9:AI:20:ARG:O | 9:AI:60:ASP:N | 2.44 | 0.51 |
| 23:BA:288:C:H2' | 23:BA:289:A:H8 | 1.75 | 0.51 |
| 23:DA:340:A:H2' | 23:DA:341:G:O4' | 2.10 | 0.51 |
| 1:AA:300:A:H1' | 1:AA:565:U:O2 | 2.11 | 0.51 |
| 29:BH:137:ASP:HB3 | 29:BH:140:LYS:HE2 | 1.93 | 0.51 |
| 1:CA:865:A:H2' | 1:CA:866:C:C6 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:AF:44:GLY:HA2 | 6:AF:59:TYR:CZ | 2.46 | 0.51 |
| 5:AE:51:VAL:O | 5:AE:55:VAL:HG23 | 2.10 | 0.51 |
| 23:BA:1999:C:H5'' | 23:BA:2723:C:O2' | 2.11 | 0.51 |
| 26:DE:37:ARG:HB2 | 26:DE:46:ALA:N | 2.26 | 0.51 |
| 23:BA:1252:G:C2 | 23:BA:1253:A:C2 | 2.99 | 0.51 |
| 30:BI:25:TYR:CD1 | 30:BI:30:LEU:HD11 | 2.46 | 0.51 |
| 1:AA:1190:G:H5'' | 3:AC:4:LYS:HA | 1.93 | 0.51 |
| 13:CM:10:PRO:HG2 | 13:CM:45:VAL:HG11 | 1.93 | 0.51 |
| 1:CA:1347:G:O2' | 1:CA:1373:G:N1 | 2.38 | 0.51 |
| 23:DA:784:A:C5 | 25:DD:229:VAL:HG21 | 2.46 | 0.51 |
| 23:DA:1018:C:O2' | 23:DA:1019:U:H5' | 2.10 | 0.51 |
| 27:BF:101:LEU:HB3 | 27:BF:106:ARG:HD3 | 1.92 | 0.51 |
| 23:BA:2134:A:N6 | 23:BA:2157:G:H1' | 2.26 | 0.51 |
| 9:AI:14:VAL:HG22 | 9:AI:66:ARG:O | 2.11 | 0.51 |
| 5:CE:135:THR:O | 5:CE:138:ALA:HB3 | 2.11 | 0.51 |
| 19:CS:10:PHE:CE2 | 19:CS:38:SER:HB3 | 2.45 | 0.51 |
| 35:BR:36:THR:HG22 | 35:BR:37:THR:N | 2.25 | 0.51 |
| 1:CA:1063:C:OP2 | 1:CA:1064:G:O2' | 2.27 | 0.51 |
| 23:DA:1510:G:H2' | 23:DA:1511:C:C6 | 2.46 | 0.51 |
| 2:AB:97:TRP:HZ3 | 2:AB:99:GLY:HA2 | 1.76 | 0.51 |
| 43:DZ:160:GLY:HA2 | 43:DZ:161:VAL:HB | 1.92 | 0.51 |
| 20:CT:16:HIS:O | 20:CT:19:SER:N | 2.44 | 0.51 |
| 27:DF:181:LEU:HD11 | 27:DF:186:ILE:HD11 | 1.93 | 0.51 |
| 45:D1:86:SER:HB3 | 45:D1:89:GLU:OE2 | 2.10 | 0.51 |
| 23:DA:1336:A:H2' | 23:DA:1337:G:C8 | 2.46 | 0.51 |
| 23:BA:1654:A:OP1 | 35:BR:1:MET:HA | 2.11 | 0.51 |
| 23:DA:265:A:H1' | 23:DA:266:G:O4' | 2.11 | 0.51 |
| 8:CH:63:LEU:HB2 | 8:CH:65:TYR:CE1 | 2.46 | 0.51 |
| 43:DZ:101:PRO:O | 43:DZ:102:LEU:HD12 | 2.11 | 0.51 |
| 4:AD:121:VAL:HA | 4:AD:126:ILE:HG12 | 1.92 | 0.51 |
| 50:B6:23:THR:OG1 | 50:B6:24:GLU:N | 2.44 | 0.51 |
| 7:AG:58:PRO:HA | 7:AG:61:VAL:HG23 | 1.93 | 0.51 |
| 40:DW:35:ILE:HG23 | 49:D5:28:PRO:HD2 | 1.93 | 0.51 |
| 1:AA:978:A:H61 | 1:AA:1316:G:H1' | 1.75 | 0.51 |
| 1:CA:1345:U:OP1 | 9:CI:120:ARG:HD3 | 2.11 | 0.51 |
| 1:AA:77:G:O6 | 1:AA:78:G:N1 | 2.44 | 0.51 |
| 1:AA:91:C:H2' | 1:AA:92:C:C6 | 2.46 | 0.51 |
| 1:CA:1004:A:H2' | 1:CA:1036:G:O6 | 2.11 | 0.51 |
| 23:DA:2320:A:N3 | 23:DA:2320:A:H2' | 2.25 | 0.51 |
| 1:CA:1284:C:H3' | 1:CA:1285:A:H2' | 1.93 | 0.51 |
| 23:BA:71:A:OP2 | 23:BA:71:A:H3' | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:271(F):C:H2' | 23:DA:271(G):C:C6 | 2.38 | 0.51 |
| 2:AB:12:GLU:O | 2:AB:16:HIS:ND1 | 2.41 | 0.51 |
| 23:DA:1796:U:H2' | 23:DA:1797:C:H6 | 1.74 | 0.51 |
| 1:CA:616:G:C2 | 1:CA:617:G:N7 | 2.79 | 0.51 |
| 23:DA:1342:A:OP2 | 56:DA:3939:HOH:O | 2.19 | 0.51 |
| 20:CT:69:GLY:O | 20:CT:73:HIS:NE2 | 2.43 | 0.51 |
| 1:AA:57:G:H2' | 1:AA:58:C:C6 | 2.46 | 0.51 |
| 23:DA:1297:C:OP1 | 23:DA:2710:C:H4' | 2.11 | 0.51 |
| 1:CA:6:G:O2' | 1:CA:7:G:H5'' | 2.11 | 0.51 |
| 16:CP:11:SER:OG | 16:CP:12:LYS:N | 2.44 | 0.51 |
| 1:AA:189:G:H2' | 1:AA:189(A):C:C6 | 2.46 | 0.51 |
| 23:DA:229:A:H3' | 23:DA:229:A:H8 | 1.76 | 0.51 |
| 1:CA:460:G:O6 | 1:CA:470:C:H5'' | 2.11 | 0.51 |
| 8:CH:63:LEU:HB2 | 8:CH:65:TYR:HE1 | 1.75 | 0.51 |
| 23:BA:187:G:N3 | 23:BA:1365:A:H2 | 2.09 | 0.51 |
| 22:AX:88:HIS:O | 22:AX:92:LEU:HB2 | 2.11 | 0.51 |
| 23:BA:1927:A:H2' | 23:BA:1928:A:C8 | 2.46 | 0.51 |
| 23:DA:2839:G:H5' | 35:DR:46:GLY:HA2 | 1.92 | 0.51 |
| 12:CL:6:THR:OG1 | 12:CL:9:GLN:HG3 | 2.10 | 0.51 |
| 1:AA:667:G:H4' | 15:AO:51:HIS:CE1 | 2.46 | 0.51 |
| 26:BE:7:VAL:HG13 | 26:BE:27:LEU:HB3 | 1.93 | 0.51 |
| 7:AG:22:LEU:O | 7:AG:25:ALA:HB3 | 2.11 | 0.51 |
| 35:DR:72:ASP:O | 35:DR:76:VAL:HG23 | 2.11 | 0.51 |
| 23:DA:2610:C:H4' | 23:DA:2611:U:OP2 | 2.11 | 0.51 |
| 1:CA:838:G:H2' | 1:CA:839:U:H5'' | 1.93 | 0.50 |
| 1:CA:1006:C:O2 | 1:CA:1024:G:H1' | 2.10 | 0.50 |
| 1:CA:966:G:H5'' | 1:CA:969:A:N7 | 2.26 | 0.50 |
| 1:CA:1254:C:N4 | 1:CA:1283:G:H1 | 2.06 | 0.50 |
| 1:AA:1312:G:C2 | 1:AA:1326:C:C2 | 2.99 | 0.50 |
| 1:CA:658:G:C2 | 1:CA:749:C:N3 | 2.79 | 0.50 |
| 1:AA:7:G:H21 | 5:AE:121:LYS:HG2 | 1.76 | 0.50 |
| 24:DB:37:C:C5 | 24:DB:38:C:C5 | 2.99 | 0.50 |
| 13:AM:92:HIS:NE2 | 13:AM:98:VAL:HG11 | 2.25 | 0.50 |
| 23:BA:1858:G:H1' | 23:BA:1884:A:H61 | 1.76 | 0.50 |
| 10:CJ:62:HIS:CD2 | 10:CJ:62:HIS:H | 2.29 | 0.50 |
| 1:CA:1192:C:C5 | 1:CA:1193:G:C8 | 2.99 | 0.50 |
| 27:BF:158:THR:O | 27:BF:164:ARG:NH1 | 2.44 | 0.50 |
| 23:DA:1693:U:O2' | 25:DD:14:ARG:NH2 | 2.44 | 0.50 |
| 23:DA:796:C:H2' | 23:DA:797:C:C6 | 2.47 | 0.50 |
| 24:BB:37:C:C5 | 24:BB:38:C:C5 | 2.98 | 0.50 |
| 1:CA:189:G:H2' | 1:CA:189(A):C:H6 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:581:G:N2 | 1:AA:760:G:N7 | 2.59 | 0.50 |
| 43:DZ:39:VAL:HG21 | 43:DZ:44:PHE:HB2 | 1.93 | 0.50 |
| 29:DH:80:SER:OG | 29:DH:81:GLU:N | 2.44 | 0.50 |
| 1:AA:953:G:C5 | 1:AA:1229:A:C6 | 2.98 | 0.50 |
| 23:DA:2672:G:H5' | 23:DA:2672:G:H8 | 1.76 | 0.50 |
| 41:DX:21:PHE:CZ | 41:DX:92:LEU:HD12 | 2.46 | 0.50 |
| 7:AG:88:PRO:HG3 | 7:AG:149:ARG:CA | 2.30 | 0.50 |
| 23:BA:2173:A:OP2 | 23:BA:2174:C:H5 | 1.93 | 0.50 |
| 31:BN:23:LEU:HB2 | 31:BN:60:ILE:HG12 | 1.92 | 0.50 |
| 3:CC:56:ASP:O | 3:CC:67:THR:HB | 2.11 | 0.50 |
| 23:BA:2782:G:N7 | 56:BA:4087:HOH:O | 2.35 | 0.50 |
| 15:CO:82:ILE:O | 15:CO:86:GLY:N | 2.44 | 0.50 |
| 23:DA:459:U:H4' | 51:D7:40:TRP:CZ3 | 2.46 | 0.50 |
| 38:BU:76:TYR:HH | 38:BU:92:ARG:HH11 | 1.57 | 0.50 |
| 23:DA:2590:A:OP2 | 25:DD:238:GLY:HA2 | 2.12 | 0.50 |
| 23:DA:1586:A:H8 | 23:DA:1586:A:O5' | 1.93 | 0.50 |
| 23:BA:543:C:H42 | 23:BA:549:G:H1 | 1.60 | 0.50 |
| 23:DA:2350:C:H2' | 23:DA:2351:G:O4' | 2.12 | 0.50 |
| 23:DA:2632:A:O2' | 23:DA:2811:G:O2' | 2.23 | 0.50 |
| 23:BA:141:A:C8 | 23:BA:1408:C:O2' | 2.60 | 0.50 |
| 25:BD:137:PRO:O | 25:BD:140:THR:HG23 | 2.12 | 0.50 |
| 27:BF:34:TRP:CE3 | 27:BF:35:GLU:HG2 | 2.45 | 0.50 |
| 1:CA:688:G:O2' | 1:CA:704:A:N1 | 2.36 | 0.50 |
| 23:BA:2839:G:C5' | 35:BR:46:GLY:HA2 | 2.40 | 0.50 |
| 23:BA:2839:G:H5' | 35:BR:46:GLY:HA2 | 1.92 | 0.50 |
| 1:AA:292:G:N7 | 1:AA:293:G:H1' | 2.26 | 0.50 |
| 43:BZ:101:PRO:O | 43:BZ:102:LEU:HD12 | 2.11 | 0.50 |
| 23:DA:662:G:OP1 | 56:DA:4439:HOH:O | 2.19 | 0.50 |
| 23:BA:748:G:C8 | 40:BW:89:ALA:HB1 | 2.46 | 0.50 |
| 12:CL:83:VAL:HG13 | 12:CL:100:ILE:HG23 | 1.93 | 0.50 |
| 37:DT:106:SER:O | 37:DT:110:ILE:HG12 | 2.11 | 0.50 |
| 1:AA:586:C:C2' | 1:AA:587:G:H5' | 2.42 | 0.50 |
| 1:AA:586:C:H2' | 1:AA:587:G:H5' | 1.94 | 0.50 |
| 1:CA:586:C:C2' | 1:CA:587:G:H5' | 2.41 | 0.50 |
| 1:CA:1055:A:C2 | 1:CA:1056:U:H1' | 2.46 | 0.50 |
| 28:DG:89:GLY:C | 28:DG:90:LEU:HD23 | 2.31 | 0.50 |
| 3:AC:22:TRP:CH2 | 14:AN:54:PRO:HG2 | 2.46 | 0.50 |
| 1:CA:1029:C:O2 | 1:CA:1032:G:N1 | 2.44 | 0.50 |
| 23:DA:1641:A:H2' | 23:DA:1642:G:O4' | 2.11 | 0.50 |
| 28:DG:11:TYR:HA | 28:DG:15:VAL:HB | 1.92 | 0.50 |
| 1:CA:1285:A:H4' | 1:CA:1286:A:O5' | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:750:G:C2 | 15:CO:23:GLY:HA3 | 2.46 | 0.50 |
| 1:CA:436:C:O2' | 1:CA:437:U:OP2 | 2.25 | 0.50 |
| 14:CN:23:ARG:HD2 | 14:CN:28:GLY:C | 2.31 | 0.50 |
| 23:BA:314:A:O2' | 23:BA:315:G:H5' | 2.10 | 0.50 |
| 23:DA:207:A:H2' | 23:DA:208:C:O4' | 2.11 | 0.50 |
| 23:DA:2150:U:H2' | 23:DA:2151:G:C8 | 2.47 | 0.50 |
| 1:AA:601:C:H2' | 1:AA:602:A:C8 | 2.45 | 0.50 |
| 17:CQ:45:HIS:HD2 | 17:CQ:65:ILE:HG12 | 1.76 | 0.50 |
| 7:CG:87:VAL:HG22 | 7:CG:151:TYR:HB3 | 1.93 | 0.50 |
| 23:DA:863:A:N7 | 56:DA:4347:HOH:O | 2.35 | 0.50 |
| 23:DA:1799:G:H5' | 23:DA:1819:A:H61 | 1.76 | 0.50 |
| 1:AA:130:A:C8 | 17:AQ:63:ARG:HG3 | 2.46 | 0.50 |
| 1:CA:1058:G:N2 | 10:CJ:53:PRO:HG3 | 2.26 | 0.50 |
| 23:DA:1925:C:O2' | 23:DA:1926:U:H5' | 2.11 | 0.50 |
| 23:BA:80:G:O6 | 56:BA:4435:HOH:O | 2.18 | 0.50 |
| 30:DI:56:LYS:O | 30:DI:60:GLU:HG2 | 2.11 | 0.50 |
| 23:BA:1977:A:OP2 | 56:BA:4902:HOH:O | 2.18 | 0.50 |
| 23:BA:796:C:H2' | 23:BA:797:C:C6 | 2.46 | 0.50 |
| 1:AA:769:G:H4' | 1:AA:1513:A:H4' | 1.93 | 0.50 |
| 48:D4:12:ALA:HA | 48:D4:29:PRO:HA | 1.93 | 0.50 |
| 1:CA:1346:A:H1' | 1:CA:1347:G:H5'' | 1.94 | 0.50 |
| 1:CA:1378:C:H5'' | 1:CA:1379:G:OP2 | 2.11 | 0.50 |
| 23:DA:2114:A:O2' | 23:DA:2168:G:H5' | 2.11 | 0.50 |
| 23:DA:2173:A:H2' | 23:DA:2174:C:H5' | 1.92 | 0.50 |
| 1:AA:1016:A:H3' | 1:AA:1017:G:H8 | 1.76 | 0.50 |
| 23:DA:1364:G:OP1 | 45:D1:2:SER:HA | 2.12 | 0.50 |
| 23:BA:769:G:N7 | 56:BA:4267:HOH:O | 2.35 | 0.50 |
| 1:CA:1016:A:O2' | 1:CA:1217:C:O2' | 2.25 | 0.50 |
| 7:CG:115:ARG:O | 7:CG:119:ARG:HD3 | 2.12 | 0.50 |
| 1:AA:872:A:C8 | 1:AA:874:G:C8 | 3.00 | 0.50 |
| 23:DA:2104:G:O6 | 23:DA:2185:C:N3 | 2.44 | 0.50 |
| 23:BA:530:G:C6 | 23:BA:2022:U:H5'' | 2.46 | 0.50 |
| 1:CA:601:C:H2' | 1:CA:602:A:C8 | 2.46 | 0.50 |
| 6:CF:69:GLU:N | 6:CF:69:GLU:OE1 | 2.45 | 0.50 |
| 23:DA:2465:C:O2 | 23:DA:2486:G:C2 | 2.64 | 0.50 |
| 23:DA:1638:C:O2 | 23:DA:2698:U:O2' | 2.25 | 0.50 |
| 24:BB:17:C:H2' | 24:BB:18:G:O4' | 2.11 | 0.50 |
| 23:DA:1794:U:H2' | 23:DA:1795:C:C6 | 2.47 | 0.50 |
| 29:DH:24:VAL:HG13 | 29:DH:37:VAL:HG21 | 1.92 | 0.50 |
| 23:DA:979:G:H3' | 23:DA:980:A:C5' | 2.41 | 0.50 |
| 10:CJ:28:ARG:CB | 10:CJ:34:VAL:HG21 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:375:C:H5'' | 56:DA:4596:HOH:O | 2.10 | 0.50 |
| 23:BA:2523:G:O6 | 56:BA:5195:HOH:O | 2.19 | 0.50 |
| 1:CA:1510:U:H2' | 1:CA:1511:G:C8 | 2.46 | 0.50 |
| 1:CA:1457:G:N1 | 1:CA:1458:G:C5 | 2.79 | 0.50 |
| 1:CA:1141:C:H2' | 1:CA:1142:G:C8 | 2.34 | 0.50 |
| 1:CA:673:G:O3' | 6:CF:87:ARG:NH2 | 2.44 | 0.50 |
| 1:AA:1154:G:C6 | 1:AA:1155:G:C6 | 2.99 | 0.50 |
| 23:BA:2130:U:O2' | 23:BA:2133:G:O2' | 2.11 | 0.50 |
| 9:CI:28:VAL:HG23 | 9:CI:33:PHE:HA | 1.94 | 0.50 |
| 23:BA:2206:G:HO2' | 23:BA:2207:G:P | 2.34 | 0.50 |
| 4:AD:155:LEU:HD23 | 4:AD:156:GLU:N | 2.26 | 0.50 |
| 1:CA:1173:G:C5 | 1:CA:1174:G:N7 | 2.79 | 0.50 |
| 2:CB:167:PRO:CG | 2:CB:188:ALA:HB2 | 2.42 | 0.50 |
| 23:BA:2638:G:P | 26:BE:82:ARG:HH22 | 2.34 | 0.50 |
| 1:AA:1374:A:O2' | 7:AG:28:ASN:HB3 | 2.12 | 0.50 |
| 7:AG:103:TRP:CZ3 | 7:AG:138:LYS:HB2 | 2.47 | 0.50 |
| 23:BA:1558:A:N3 | 23:BA:1558:A:O4' | 2.45 | 0.50 |
| 24:DB:90:A:N7 | 24:DB:91:C:H1' | 2.27 | 0.50 |
| 1:CA:187:C:H5'' | 20:CT:86:ARG:HG3 | 1.93 | 0.50 |
| 10:CJ:63:PHE:HA | 14:CN:58:LYS:HA | 1.94 | 0.50 |
| 23:DA:2272:U:H5'' | 23:DA:2273:A:OP1 | 2.11 | 0.50 |
| 48:B4:35:VAL:HA | 48:B4:39:CYS:SG | 2.52 | 0.50 |
| 1:AA:1070:U:H2' | 1:AA:1071:C:H6 | 1.76 | 0.50 |
| 6:AF:19:LEU:HD11 | 6:AF:59:TYR:CZ | 2.47 | 0.50 |
| 26:DE:37:ARG:HB2 | 26:DE:46:ALA:H | 1.77 | 0.50 |
| 23:DA:1766:U:H2' | 23:DA:1767:C:H6 | 1.76 | 0.50 |
| 14:AN:34:TYR:O | 14:AN:38:GLY:N | 2.40 | 0.50 |
| 23:BA:649:G:H2' | 23:BA:650:C:C6 | 2.46 | 0.50 |
| 36:DS:49:VAL:HG13 | 36:DS:76:LYS:HD2 | 1.92 | 0.50 |
| 23:BA:2286:A:OP1 | 50:B6:29:ASN:ND2 | 2.44 | 0.50 |
| 26:DE:38:THR:O | 26:DE:42:ASP:N | 2.43 | 0.50 |
| 1:AA:1459:C:P | 1:AA:1460:A:OP2 | 2.69 | 0.50 |
| 1:CA:1459:C:O5' | 1:CA:1460:A:OP2 | 2.30 | 0.50 |
| 1:AA:1237:C:HO2' | 1:AA:1300:G:H22 | 1.53 | 0.50 |
| 2:CB:187:LEU:HD13 | 2:CB:205:ASP:HA | 1.93 | 0.50 |
| 23:BA:1177:A:P | 23:BA:1177:A:H3' | 2.51 | 0.50 |
| 1:CA:1328:C:H5'' | 13:CM:28:ALA:HB3 | 1.94 | 0.50 |
| 9:CI:114:TYR:CD2 | 9:CI:114:TYR:N | 2.80 | 0.50 |
| 1:CA:1117:G:H1' | 1:CA:1184:G:N2 | 2.26 | 0.50 |
| 41:DX:31:HIS:CD2 | 41:DX:33:LYS:H | 2.29 | 0.50 |
| 1:AA:148:G:C2 | 1:AA:149:A:N7 | 2.80 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:749:C:H2' | 1:CA:750:G:H8 | 1.77 | 0.50 |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:HB2 | 1.93 | 0.50 |
| 1:AA:1288:A:H2' | 1:AA:1289:A:O4' | 2.12 | 0.50 |
| 34:BQ:134:ARG:O | 34:BQ:138:ASP:HB2 | 2.11 | 0.50 |
| 1:AA:1079:G:H2' | 1:AA:1080:A:C8 | 2.47 | 0.50 |
| 23:BA:279:C:H42 | 23:BA:361:G:H1 | 1.59 | 0.50 |
| 1:CA:407:G:O6 | 1:CA:435:C:N4 | 2.45 | 0.50 |
| 27:DF:22:ALA:HB1 | 27:DF:24:LEU:HD22 | 1.92 | 0.50 |
| 36:BS:11:LYS:O | 36:BS:15:ARG:HG3 | 2.12 | 0.50 |
| 1:AA:142:G:N3 | 1:AA:143:A:C8 | 2.80 | 0.50 |
| 23:BA:1026:U:HO2' | 23:BA:1027:A:P | 2.33 | 0.50 |
| 23:DA:1430:C:H2' | 23:DA:1431:U:H6 | 1.77 | 0.50 |
| 7:CG:24:THR:HG22 | 7:CG:27:ILE:HD11 | 1.93 | 0.50 |
| 1:AA:616:G:C2 | 1:AA:617:G:N7 | 2.79 | 0.50 |
| 23:DA:1328:G:H8 | 23:DA:1328:G:O5' | 1.94 | 0.50 |
| 31:DN:34:LEU:O | 31:DN:49:GLY:HA3 | 2.11 | 0.50 |
| 23:BA:1651:G:H2' | 23:BA:1652:A:O4' | 2.12 | 0.50 |
| 28:BG:98:ARG:HB2 | 28:BG:98:ARG:NH1 | 2.26 | 0.50 |
| 27:DF:71:GLY:N | 56:DF:402:HOH:O | 2.21 | 0.50 |
| 23:BA:2144:U:H2' | 23:BA:2146:C:N4 | 2.26 | 0.50 |
| 23:BA:481:G:H1' | 23:BA:507:A:N1 | 2.27 | 0.50 |
| 24:DB:77:U:H4' | 43:DZ:84:GLU:OE1 | 2.12 | 0.50 |
| 1:AA:544:G:C2 | 1:AA:545:C:C2 | 3.00 | 0.50 |
| 1:AA:269:C:H2' | 1:AA:270:A:C8 | 2.47 | 0.50 |
| 30:BI:29:TYR:O | 30:BI:32:PRO:HD2 | 2.11 | 0.50 |
| 1:AA:1459:C:O5' | 1:AA:1460:A:OP2 | 2.30 | 0.50 |
| 23:DA:2296:U:N3 | 23:DA:2333:A:N3 | 2.60 | 0.50 |
| 1:CA:1088:G:N2 | 1:CA:1089:G:H1' | 2.27 | 0.50 |
| 1:CA:976:G:OP2 | 14:CN:32:SER:N | 2.43 | 0.50 |
| 1:AA:1111:A:N6 | 3:AC:177:THR:HA | 2.19 | 0.50 |
| 1:AA:1316:G:N1 | 1:AA:1318:A:H5'' | 2.27 | 0.50 |
| 9:CI:71:SER:HA | 9:CI:74:ILE:HB | 1.94 | 0.50 |
| 1:CA:1352:C:H1' | 1:CA:1371:G:N2 | 2.26 | 0.50 |
| 23:BA:1178:C:H2' | 23:BA:1179:C:C6 | 2.46 | 0.50 |
| 23:BA:1021:A:H3' | 23:BA:1021:A:C8 | 2.47 | 0.50 |
| 50:D6:4:GLU:HG3 | 50:D6:5:VAL:N | 2.27 | 0.50 |
| 1:AA:1287:A:C2 | 1:AA:1353:G:H1' | 2.47 | 0.50 |
| 3:CC:186:PHE:HA | 3:CC:198:VAL:O | 2.11 | 0.50 |
| 1:CA:1151:A:N3 | 10:CJ:70:ARG:NH2 | 2.60 | 0.50 |
| 34:DQ:27:VAL:HG11 | 34:DQ:134:ARG:HG2 | 1.94 | 0.50 |
| 15:AO:82:ILE:O | 15:AO:86:GLY:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:485:C:H2' | 23:BA:486:C:H6 | 1.76 | 0.50 |
| 1:CA:918:A:H2' | 1:CA:919:A:H8 | 1.74 | 0.50 |
| 8:AH:63:LEU:HB2 | 8:AH:65:TYR:CE1 | 2.45 | 0.50 |
| 1:AA:1388:C:H2' | 1:AA:1389:C:C6 | 2.46 | 0.50 |
| 23:BA:187:G:N7 | 56:BA:4299:HOH:O | 2.35 | 0.50 |
| 1:AA:646:U:H2' | 1:AA:647:C:H6 | 1.75 | 0.50 |
| 37:DT:51:ARG:HG3 | 37:DT:98:LYS:HE3 | 1.94 | 0.50 |
| 1:CA:811:C:H4' | 1:CA:900:A:N6 | 2.27 | 0.50 |
| 23:BA:576:U:O5' | 23:BA:576:U:H6 | 1.95 | 0.50 |
| 31:DN:67:LEU:HA | 31:DN:87:LEU:HD12 | 1.93 | 0.50 |
| 23:BA:95:G:O2' | 46:B2:46:GLN:HA | 2.12 | 0.50 |
| 29:BH:171:LEU:HD23 | 29:BH:171:LEU:H | 1.76 | 0.50 |
| 45:D1:51:VAL:HG11 | 45:D1:74:VAL:HG21 | 1.92 | 0.50 |
| 14:CN:2:ALA:HB1 | 14:CN:6:LEU:HD13 | 1.92 | 0.50 |
| 23:DA:2345:G:O6 | 56:DA:4167:HOH:O | 2.19 | 0.50 |
| 16:CP:20:VAL:HG23 | 16:CP:34:GLU:O | 2.12 | 0.50 |
| 33:BP:38:GLN:C | 33:BP:40:SER:H | 2.14 | 0.50 |
| 1:CA:1391:U:H2' | 1:CA:1392:G:C8 | 2.46 | 0.50 |
| 28:DG:81:LYS:CB | 28:DG:82:LEU:HD12 | 2.41 | 0.50 |
| 2:CB:80:ILE:HG13 | 2:CB:215:LEU:HD12 | 1.93 | 0.50 |
| 1:AA:1279:A:H61 | 3:AC:26:LYS:NZ | 2.09 | 0.50 |
| 23:DA:2126:A:H1' | 23:DA:2127:G:OP2 | 2.12 | 0.50 |
| 31:BN:132:ALA:HB3 | 31:BN:133:GLN:NE2 | 2.27 | 0.50 |
| 13:AM:15:VAL:O | 13:AM:19:LEU:HD13 | 2.12 | 0.50 |
| 23:DA:996:A:C2 | 23:DA:997:G:C8 | 3.00 | 0.50 |
| 23:DA:2773:C:O2' | 23:DA:2774:C:H5' | 2.12 | 0.50 |
| 23:BA:1026:U:H5'' | 23:BA:1026:U:O2 | 2.12 | 0.50 |
| 1:AA:1521:G:H2' | 1:AA:1522:U:H6 | 1.76 | 0.50 |
| 23:DA:69:C:N4 | 56:DA:4046:HOH:O | 2.45 | 0.50 |
| 1:AA:1357:A:H5'' | 1:AA:1358:U:OP2 | 2.11 | 0.50 |
| 1:AA:1396:A:H2 | 5:AE:19:MET:HG3 | 1.77 | 0.50 |
| 1:CA:1339:A:N6 | 1:CA:1340:A:N3 | 2.59 | 0.50 |
| 1:CA:544:G:C2 | 1:CA:545:C:C2 | 3.00 | 0.50 |
| 50:D6:14:THR:HG21 | 50:D6:48:VAL:HG13 | 1.93 | 0.50 |
| 23:BA:1300:U:H4' | 23:BA:1301:A:C5' | 2.41 | 0.50 |
| 4:AD:101:LEU:HD23 | 4:AD:102:ASP:N | 2.27 | 0.50 |
| 23:BA:286:C:H42 | 23:BA:355:G:H1 | 1.60 | 0.50 |
| 23:BA:860:U:C2 | 23:BA:2268:A:C8 | 3.00 | 0.50 |
| 32:BO:35:VAL:HG21 | 32:BO:103:ALA:HB3 | 1.93 | 0.50 |
| 43:DZ:180:VAL:O | 43:DZ:183:LEU:HB2 | 2.12 | 0.50 |
| 1:AA:65:U:H2' | 1:AA:381:C:C5 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:CU:6:ARG:HA | 21:CU:11:GLY:HA3 | 1.92 | 0.50 |
| 23:DA:2755:C:HO2' | 23:DA:2756:U:H6 | 1.60 | 0.50 |
| 1:AA:688:G:O2' | 1:AA:704:A:N1 | 2.41 | 0.50 |
| 23:BA:2251:G:C6 | 23:BA:2252:G:C5 | 3.00 | 0.50 |
| 23:BA:413:C:O5' | 23:BA:413:C:H6 | 1.95 | 0.50 |
| 23:BA:980:A:N3 | 23:BA:2037:G:O2' | 2.36 | 0.50 |
| 1:AA:425:G:O3' | 4:AD:45:GLN:NE2 | 2.44 | 0.50 |
| 1:AA:1360:A:H3' | 1:AA:1361:G:H8 | 1.77 | 0.50 |
| 13:CM:3:ARG:HB3 | 13:CM:8:GLU:O | 2.12 | 0.50 |
| 1:CA:1309:G:C6 | 1:CA:1329:A:C6 | 3.00 | 0.50 |
| 28:DG:44:GLY:HA2 | 28:DG:88:ILE:HG22 | 1.94 | 0.50 |
| 23:DA:784:A:H5' | 23:DA:785:G:OP1 | 2.11 | 0.50 |
| 1:AA:954:G:N2 | 1:AA:1227:A:H62 | 2.09 | 0.50 |
| 23:DA:2125:G:N2 | 23:DA:2126:A:H62 | 2.10 | 0.50 |
| 1:AA:1178:G:N2 | 1:AA:1180:A:H3' | 2.26 | 0.50 |
| 23:BA:2158:A:H1' | 23:BA:2159:G:C8 | 2.47 | 0.50 |
| 7:CG:143:ARG:O | 7:CG:147:ALA:N | 2.37 | 0.50 |
| 13:CM:69:GLU:C | 13:CM:71:ARG:H | 2.15 | 0.50 |
| 2:AB:167:PRO:CG | 2:AB:188:ALA:HB2 | 2.42 | 0.50 |
| 25:DD:101:GLU:OE1 | 25:DD:103:ARG:HD3 | 2.12 | 0.50 |
| 7:CG:113:GLU:HB2 | 7:CG:119:ARG:HG3 | 1.92 | 0.50 |
| 36:BS:96:GLY:N | 36:BS:99:LYS:H | 2.10 | 0.50 |
| 5:CE:104:ALA:O | 5:CE:107:ARG:HG2 | 2.12 | 0.50 |
| 24:DB:111:G:H2' | 24:DB:112:U:H6 | 1.77 | 0.50 |
| 1:AA:652:U:O4 | 1:AA:752:G:O2' | 2.27 | 0.50 |
| 30:DI:76:THR:O | 30:DI:105:HIS:HE1 | 1.94 | 0.50 |
| 23:BA:2275:C:C6 | 23:BA:2275:C:H5' | 2.47 | 0.50 |
| 23:BA:534:U:H5' | 38:BU:42:ALA:HB1 | 1.93 | 0.50 |
| 23:BA:979:G:H3' | 23:BA:980:A:C5' | 2.42 | 0.50 |
| 41:BX:61:GLY:HA3 | 41:BX:73:ARG:O | 2.11 | 0.50 |
| 7:AG:43:PHE:HA | 7:AG:46:ALA:HB3 | 1.93 | 0.50 |
| 30:BI:123:LEU:H | 30:BI:123:LEU:HD23 | 1.76 | 0.50 |
| 25:DD:254:THR:O | 25:DD:254:THR:OG1 | 2.28 | 0.50 |
| 17:AQ:31:LEU:HD23 | 17:AQ:32:TYR:CZ | 2.47 | 0.50 |
| 23:BA:1339:G:H5'' | 41:BX:16:LYS:HD3 | 1.94 | 0.50 |
| 14:CN:26:ARG:HH11 | 14:CN:47:LEU:HD21 | 1.76 | 0.50 |
| 1:CA:1025:U:O2 | 1:CA:1036:G:O6 | 2.30 | 0.49 |
| 1:AA:975:A:H8 | 1:AA:975:A:H5' | 1.76 | 0.49 |
| 1:CA:966:G:H5'' | 1:CA:969:A:C8 | 2.46 | 0.49 |
| 23:BA:330:A:C2 | 23:BA:1210:A:H2' | 2.34 | 0.49 |
| 10:AJ:40:LEU:HD12 | 10:AJ:69:ASN:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:AJ:8:LEU:HD22 | 10:AJ:96:ILE:HA | 1.94 | 0.49 |
| 23:DA:1689:A:N6 | 23:DA:1698:A:H2 | 1.98 | 0.49 |
| 45:D1:82:LEU:O | 45:D1:83:GLU:HG3 | 2.11 | 0.49 |
| 1:AA:1016:A:H3' | 1:AA:1017:G:C8 | 2.47 | 0.49 |
| 23:DA:2472:G:H5' | 23:DA:2473:U:C5' | 2.39 | 0.49 |
| 1:CA:438:G:H4' | 4:CD:123:HIS:ND1 | 2.27 | 0.49 |
| 1:AA:369:C:O2' | 1:AA:370:C:H5' | 2.12 | 0.49 |
| 2:AB:132:LYS:O | 2:AB:135:GLN:HG2 | 2.11 | 0.49 |
| 27:BF:22:ALA:HB1 | 27:BF:24:LEU:HD22 | 1.94 | 0.49 |
| 1:CA:1111:A:H8 | 1:CA:1111:A:O5' | 1.94 | 0.49 |
| 23:DA:1328:G:H2' | 23:DA:1330:C:C5 | 2.47 | 0.49 |
| 23:BA:1419:A:C8 | 23:BA:1421:G:C6 | 3.00 | 0.49 |
| 1:CA:414:A:H2' | 1:CA:415:A:H8 | 1.77 | 0.49 |
| 23:BA:725:G:C6 | 23:BA:726:G:N1 | 2.80 | 0.49 |
| 1:AA:757:U:H2' | 1:AA:758:G:O4' | 2.12 | 0.49 |
| 1:CA:1278:U:H5' | 1:CA:1279:A:O4' | 2.12 | 0.49 |
| 24:DB:17:C:H2' | 24:DB:18:G:O4' | 2.12 | 0.49 |
| 23:BA:960:A:C8 | 23:BA:962:G:C8 | 3.00 | 0.49 |
| 23:BA:216:A:C4 | 23:BA:432:A:C2 | 3.00 | 0.49 |
| 51:D7:8:ASN:OD1 | 51:D7:8:ASN:C | 2.50 | 0.49 |
| 1:AA:587:G:O2' | 1:AA:588:G:OP2 | 2.26 | 0.49 |
| 2:CB:84:GLU:OE1 | 2:CB:216:SER:HA | 2.12 | 0.49 |
| 9:AI:16:ARG:HB2 | 9:AI:64:THR:HG22 | 1.93 | 0.49 |
| 23:BA:30:G:H2' | 23:BA:31:C:C6 | 2.47 | 0.49 |
| 2:CB:28:PHE:CZ | 2:CB:189:ASP:HA | 2.47 | 0.49 |
| 1:AA:1255:G:H5'' | 3:AC:26:LYS:HZ1 | 1.77 | 0.49 |
| 23:BA:1174:A:H5' | 23:BA:1177:A:N6 | 2.25 | 0.49 |
| 1:CA:1370:G:H5'' | 9:CI:12:GLU:OE2 | 2.12 | 0.49 |
| 23:BA:2033:A:P | 56:BA:4596:HOH:O | 2.69 | 0.49 |
| 41:BX:31:HIS:CD2 | 41:BX:33:LYS:H | 2.30 | 0.49 |
| 2:AB:179:LYS:HA | 8:AH:72:PRO:HG3 | 1.93 | 0.49 |
| 1:AA:1379:G:O6 | 7:AG:2:ALA:N | 2.45 | 0.49 |
| 23:DA:1506:C:H2' | 23:DA:1507:A:H5' | 1.95 | 0.49 |
| 23:BA:2165:G:H2' | 23:BA:2166:G:C8 | 2.47 | 0.49 |
| 9:AI:8:GLY:CA | 9:AI:76:ALA:HB1 | 2.41 | 0.49 |
| 23:BA:2782:G:OP2 | 56:BA:4090:HOH:O | 2.18 | 0.49 |
| 4:CD:9:CYS:SG | 4:CD:22:LYS:NZ | 2.70 | 0.49 |
| 23:DA:184:C:H2' | 23:DA:185:U:H6 | 1.77 | 0.49 |
| 25:BD:108:PRO:HB3 | 25:BD:143:HIS:HE1 | 1.75 | 0.49 |
| 1:CA:55:A:C5 | 1:CA:56:U:C5 | 3.00 | 0.49 |
| 23:BA:2853:C:H2' | 23:BA:2854:G:C8 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2350:C:H2' | 23:BA:2351:G:O4' | 2.12 | 0.49 |
| 43:DZ:179:ASP:HB2 | 43:DZ:182:LYS:HD3 | 1.94 | 0.49 |
| 15:CO:15:PHE:CE2 | 15:CO:84:LYS:HD2 | 2.48 | 0.49 |
| 40:BW:86:LEU:HD22 | 40:BW:96:ILE:HD11 | 1.94 | 0.49 |
| 1:CA:191:G:N2 | 20:CT:103:GLY:HA2 | 2.26 | 0.49 |
| 23:DA:2496:C:OP1 | 34:DQ:82:ARG:HB3 | 2.12 | 0.49 |
| 23:BA:686:G:OP1 | 51:B7:11:LYS:NZ | 2.30 | 0.49 |
| 13:CM:33:ALA:HA | 13:CM:36:LYS:CB | 2.43 | 0.49 |
| 32:BO:10:VAL:HG13 | 32:BO:17:ARG:O | 2.12 | 0.49 |
| 1:CA:502:G:C2 | 1:CA:503:C:C2 | 3.00 | 0.49 |
| 41:BX:50:LYS:HB3 | 41:BX:84:ALA:HB2 | 1.93 | 0.49 |
| 1:AA:1027:C:H2' | 1:AA:1028:C:C4 | 2.47 | 0.49 |
| 2:CB:218:ALA:O | 2:CB:222:ILE:HG13 | 2.12 | 0.49 |
| 21:AU:5:ASP:O | 21:AU:11:GLY:HA3 | 2.11 | 0.49 |
| 33:DP:38:GLN:C | 33:DP:40:SER:H | 2.13 | 0.49 |
| 1:CA:448:A:P | 1:CA:485:G:H22 | 2.35 | 0.49 |
| 1:AA:250:A:H4' | 1:AA:251:G:O5' | 2.12 | 0.49 |
| 3:CC:175:LEU:H | 3:CC:175:LEU:HD12 | 1.77 | 0.49 |
| 23:BA:1506:C:H2' | 23:BA:1507:A:H5' | 1.94 | 0.49 |
| 23:DA:1513:C:H2' | 23:DA:1514:U:H6 | 1.77 | 0.49 |
| 1:AA:1123:A:N6 | 1:AA:1150:U:H3 | 2.08 | 0.49 |
| 1:CA:1001(A):G:H2' | 1:CA:1002:G:H8 | 1.77 | 0.49 |
| 23:BA:1434:A:H61 | 23:BA:1558:A:H62 | 1.59 | 0.49 |
| 1:CA:103:C:P | 20:CT:17:ARG:HH21 | 2.36 | 0.49 |
| 23:DA:102:G:HO2' | 23:DA:103:A:P | 2.34 | 0.49 |
| 17:AQ:45:HIS:HD2 | 17:AQ:65:ILE:HG12 | 1.76 | 0.49 |
| 25:DD:238:GLY:O | 25:DD:239:ARG:HB3 | 2.13 | 0.49 |
| 41:DX:9:LEU:HA | 46:D2:36:ARG:HH21 | 1.77 | 0.49 |
| 23:BA:2516:G:C6 | 23:BA:2517:C:N4 | 2.80 | 0.49 |
| 6:AF:42:GLU:OE1 | 6:AF:59:TYR:OH | 2.26 | 0.49 |
| 3:CC:139:GLN:O | 3:CC:143:GLU:HB2 | 2.13 | 0.49 |
| 23:DA:2010:G:O6 | 56:DA:4669:HOH:O | 2.19 | 0.49 |
| 23:BA:1028:A:N6 | 23:BA:1125:G:H2' | 2.28 | 0.49 |
| 31:BN:58:ASP:N | 31:BN:58:ASP:OD1 | 2.43 | 0.49 |
| 29:DH:171:LEU:H | 29:DH:171:LEU:HD23 | 1.77 | 0.49 |
| 1:AA:618:C:H5' | 1:AA:619:U:H5'' | 1.94 | 0.49 |
| 43:DZ:138:GLU:HG2 | 43:DZ:156:LYS:NZ | 2.28 | 0.49 |
| 1:AA:1517:G:H1' | 23:BA:1919:A:O3' | 2.12 | 0.49 |
| 4:AD:31:CYS:O | 4:AD:31:CYS:SG | 2.70 | 0.49 |
| 2:CB:219:VAL:O | 2:CB:222:ILE:HB | 2.12 | 0.49 |
| 1:CA:1371:G:H2' | 1:CA:1372:U:O4' | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:226:ARG:HG3 | 2:AB:227:GLY:H | 1.78 | 0.49 |
| 1:AA:1053:G:O6 | 1:AA:1199:U:H2' | 2.12 | 0.49 |
| 1:CA:757:U:H2' | 1:CA:758:G:O4' | 2.11 | 0.49 |
| 23:BA:2406:U:C2 | 33:BP:72:PRO:HG2 | 2.48 | 0.49 |
| 21:CU:12:LYS:HZ1 | 21:CU:19:GLY:HA3 | 1.76 | 0.49 |
| 23:BA:2133:G:C2' | 23:BA:2158:A:H61 | 2.26 | 0.49 |
| 1:CA:77:G:O6 | 1:CA:78:G:N1 | 2.45 | 0.49 |
| 23:DA:1268:A:H2' | 23:DA:1269:A:O4' | 2.12 | 0.49 |
| 7:CG:103:TRP:CE2 | 7:CG:137:LYS:HD2 | 2.47 | 0.49 |
| 1:CA:1094:G:H22 | 1:CA:1105:A:H62 | 1.61 | 0.49 |
| 23:DA:1512:U:H2' | 23:DA:1513:C:C6 | 2.46 | 0.49 |
| 42:DY:40:GLU:O | 42:DY:42:VAL:HG23 | 2.11 | 0.49 |
| 23:BA:2602:A:H1' | 23:BA:2603:G:C5' | 2.41 | 0.49 |
| 37:BT:91:ARG:HH11 | 37:BT:120:ARG:NH1 | 2.09 | 0.49 |
| 13:CM:50:GLU:O | 13:CM:53:VAL:HG12 | 2.12 | 0.49 |
| 1:CA:1513:A:H2' | 1:CA:1514:C:C6 | 2.47 | 0.49 |
| 23:DA:443:A:H1' | 23:DA:1201:C:O4' | 2.12 | 0.49 |
| 23:DA:1889:A:H2' | 23:DA:1890:A:C8 | 2.47 | 0.49 |
| 23:DA:105:C:H2' | 23:DA:106:C:C6 | 2.47 | 0.49 |
| 8:CH:51:VAL:HG11 | 8:CH:60:ARG:HG3 | 1.94 | 0.49 |
| 46:B2:13:ALA:HA | 46:B2:16:LEU:HD12 | 1.93 | 0.49 |
| 23:DA:1489:U:H6 | 23:DA:1489:U:H3' | 1.78 | 0.49 |
| 23:DA:557:U:H2' | 23:DA:558:G:H8 | 1.77 | 0.49 |
| 4:CD:25:ARG:O | 4:CD:27:TYR:N | 2.43 | 0.49 |
| 2:CB:213:LEU:HD22 | 2:CB:214:ILE:HD13 | 1.95 | 0.49 |
| 1:AA:1446:U:H4' | 1:AA:1447:A:C2 | 2.48 | 0.49 |
| 23:DA:2250:G:C5 | 34:DQ:83:MET:HB2 | 2.47 | 0.49 |
| 6:CF:49:ALA:HB2 | 18:CR:78:LEU:O | 2.12 | 0.49 |
| 2:AB:187:LEU:HD23 | 2:AB:201:ILE:HB | 1.94 | 0.49 |
| 23:BA:1171:G:OP2 | 23:BA:1171:G:H8 | 1.96 | 0.49 |
| 1:AA:1345:U:C6 | 1:AA:1377:A:H2 | 2.30 | 0.49 |
| 23:BA:2892:A:H2' | 23:BA:2893:G:C5' | 2.42 | 0.49 |
| 47:D3:46:ASN:O | 47:D3:50:VAL:HG22 | 2.13 | 0.49 |
| 5:CE:91:LEU:HD12 | 5:CE:120:THR:HG22 | 1.94 | 0.49 |
| 1:AA:826:C:H2' | 1:AA:827:U:C6 | 2.48 | 0.49 |
| 2:AB:24:TRP:CZ3 | 2:AB:29:ALA:HB2 | 2.47 | 0.49 |
| 24:DB:15:A:H1' | 24:DB:110:G:C5 | 2.47 | 0.49 |
| 1:CA:35:G:N1 | 1:CA:550:G:C2 | 2.81 | 0.49 |
| 8:AH:48:TYR:HA | 8:AH:60:ARG:O | 2.13 | 0.49 |
| 22:CX:53:THR:HG23 | 22:CX:62:HIS:HB3 | 1.94 | 0.49 |
| 24:BB:106:G:H5' | 43:BZ:31:ARG:HG2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:DA:1774:C:H6 | 23:DA:1774:C:O5' | 1.94 | 0.49 |
| 1:AA:336:C:H2' | 1:AA:337:C:H6 | 1.77 | 0.49 |
| 1:AA:1459:C:H3' | 1:AA:1459:C:H6 | 1.77 | 0.49 |
| 1:CA:1212:U:H5' | 1:CA:1213:A:OP1 | 2.13 | 0.49 |
| 21:AU:10:ARG:HA | 21:AU:13:ILE:HG22 | 1.94 | 0.49 |
| 1:CA:1023:G:H8 | 1:CA:1023:G:OP2 | 1.95 | 0.49 |
| 28:BG:11:TYR:HA | 28:BG:15:VAL:HB | 1.93 | 0.49 |
| 23:BA:784:A:C5 | 25:BD:229:VAL:HG21 | 2.47 | 0.49 |
| 23:BA:1840:G:C6 | 23:BA:1841:U:C4 | 3.01 | 0.49 |
| 1:CA:254:G:OP1 | 17:CQ:67:LYS:O | 2.30 | 0.49 |
| 17:AQ:76:LEU:HD21 | 17:AQ:79:SER:N | 2.27 | 0.49 |
| 7:CG:137:LYS:HD3 | 7:CG:140:ASP:HB2 | 1.95 | 0.49 |
| 24:BB:31:C:N4 | 36:BS:32:LEU:HD13 | 2.28 | 0.49 |
| 9:AI:3:GLN:NE2 | 9:AI:18:PHE:HA | 2.27 | 0.49 |
| 4:AD:108:LEU:HB3 | 4:AD:110:PHE:HE1 | 1.78 | 0.49 |
| 4:AD:108:LEU:CD1 | 4:AD:174:LEU:HD13 | 2.43 | 0.49 |
| 7:CG:51:GLN:HG3 | 7:CG:58:PRO:HD3 | 1.95 | 0.49 |
| 53:D9:10:ILE:HD12 | 53:D9:32:HIS:HA | 1.93 | 0.49 |
| 23:BA:2580:U:C5 | 23:BA:2581:G:C6 | 3.01 | 0.49 |
| 1:AA:130:A:OP2 | 1:AA:189(F):U:C2 | 2.66 | 0.49 |
| 24:BB:43:C:H5'' | 48:B4:1:MET:HG2 | 1.93 | 0.49 |
| 1:AA:1350:A:H2' | 1:AA:1351:U:C6 | 2.47 | 0.49 |
| 10:AJ:56:HIS:O | 10:AJ:58:ASP:N | 2.46 | 0.49 |
| 43:DZ:125:LEU:HG | 43:DZ:164:ALA:HB3 | 1.94 | 0.49 |
| 23:BA:1952:A:C6 | 23:BA:1953:A:N1 | 2.80 | 0.49 |
| 42:BY:6:HIS:H | 42:BY:6:HIS:CD2 | 2.30 | 0.49 |
| 1:AA:436:C:O2' | 1:AA:437:U:OP2 | 2.22 | 0.49 |
| 38:BU:59:ARG:O | 38:BU:63:VAL:HG23 | 2.12 | 0.49 |
| 23:BA:1688:U:H1' | 23:BA:1701:A:C6 | 2.48 | 0.49 |
| 23:BA:2335:A:O2' | 23:BA:2336:A:OP2 | 2.28 | 0.49 |
| 23:BA:885:C:H5' | 23:BA:886:C:OP2 | 2.13 | 0.49 |
| 23:BA:886:C:H2' | 23:BA:887:A:H5' | 1.95 | 0.49 |
| 23:DA:2711:A:OP1 | 23:DA:2712(A):A:OP1 | 2.31 | 0.49 |
| 1:CA:951:G:C5 | 1:CA:1231:G:C6 | 3.01 | 0.49 |
| 1:CA:974:A:H8 | 1:CA:974:A:OP1 | 1.95 | 0.49 |
| 7:CG:29:LYS:HB3 | 7:CG:105:VAL:HG11 | 1.93 | 0.49 |
| 1:CA:674:G:H2' | 1:CA:675:A:C8 | 2.47 | 0.49 |
| 1:AA:1178:G:O2' | 1:AA:1180:A:N7 | 2.33 | 0.49 |
| 1:CA:1251:A:H4' | 9:CI:12:GLU:OE2 | 2.12 | 0.49 |
| 7:CG:71:PRO:HB3 | 7:CG:138:LYS:O | 2.13 | 0.49 |
| 23:BA:826:U:C4' | 33:BP:55:ARG:HB2 | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:2114:A:O2' | 23:BA:2168:G:H5' | 2.12 | 0.49 |
| 1:AA:1353:G:H2' | 1:AA:1354:C:H6 | 1.77 | 0.49 |
| 4:CD:108:LEU:CD1 | 4:CD:174:LEU:HD13 | 2.43 | 0.49 |
| 23:BA:1364:G:OP1 | 45:B1:2:SER:HA | 2.13 | 0.49 |
| 23:BA:528:A:C2 | 23:BA:2043:C:H4' | 2.47 | 0.49 |
| 24:DB:90:A:C5 | 24:DB:91:C:H1' | 2.48 | 0.49 |
| 10:CJ:51:ARG:CZ | 10:CJ:61:GLU:HB3 | 2.43 | 0.49 |
| 43:BZ:48:PHE:O | 43:BZ:52:SER:N | 2.45 | 0.49 |
| 8:AH:20:TYR:HA | 8:AH:65:TYR:CE2 | 2.47 | 0.49 |
| 17:CQ:65:ILE:HD12 | 17:CQ:65:ILE:H | 1.78 | 0.49 |
| 1:AA:460:G:O6 | 1:AA:470:C:H5'' | 2.13 | 0.49 |
| 23:BA:2203:U:O2' | 23:BA:2205:C:H5' | 2.12 | 0.49 |
| 32:DO:115:VAL:HG13 | 32:DO:121:VAL:HG21 | 1.94 | 0.49 |
| 6:AF:55:ASP:HB3 | 6:AF:86:ARG:HH12 | 1.75 | 0.49 |
| 23:BA:2150:U:H2' | 23:BA:2151:G:H8 | 1.77 | 0.49 |
| 20:CT:26:ASN:OD1 | 20:CT:71:THR:HG23 | 2.12 | 0.49 |
| 1:AA:1083:U:C5 | 1:AA:1084:G:C6 | 3.01 | 0.49 |
| 23:DA:1031:G:H1 | 23:DA:1123:C:H42 | 1.59 | 0.49 |
| 23:BA:2648:C:H2' | 23:BA:2649:U:C6 | 2.47 | 0.49 |
| 1:CA:950:U:N3 | 1:CA:1231:G:N1 | 2.42 | 0.49 |
| 1:AA:1320:C:N4 | 19:AS:36:ARG:HG3 | 2.28 | 0.49 |
| 23:BA:1533:G:N2 | 23:BA:1536:C:H5 | 2.00 | 0.49 |
| 2:CB:185:ILE:HA | 2:CB:199:TYR:O | 2.13 | 0.49 |
| 17:CQ:76:LEU:HD21 | 17:CQ:79:SER:N | 2.27 | 0.49 |
| 1:CA:93:G:O2' | 1:CA:96:U:H5' | 2.13 | 0.49 |
| 9:AI:15:ALA:HB1 | 9:AI:63:ILE:HG23 | 1.95 | 0.49 |
| 45:B1:2:SER:HB3 | 45:B1:46:LEU:HD11 | 1.95 | 0.49 |
| 1:AA:22:G:H2' | 1:AA:23:C:C6 | 2.48 | 0.49 |
| 23:DA:1405:U:H2' | 23:DA:1406:U:H6 | 1.74 | 0.49 |
| 1:CA:186:C:O3' | 20:CT:82:SER:HB2 | 2.13 | 0.49 |
| 23:DA:2307:G:H5' | 23:DA:2308:G:N2 | 2.28 | 0.49 |
| 7:AG:139:GLU:HB3 | 7:AG:143:ARG:NH2 | 2.28 | 0.49 |
| 23:DA:143:G:H2' | 23:DA:143(A):C:H6 | 1.77 | 0.49 |
| 23:BA:1799:G:H5' | 23:BA:1819:A:H61 | 1.77 | 0.49 |
| 23:DA:1156:A:OP2 | 56:DA:4263:HOH:O | 2.20 | 0.49 |
| 18:AR:30:ASP:HB3 | 18:AR:33:ASP:HB2 | 1.94 | 0.49 |
| 42:BY:90:LEU:C | 42:BY:92:ASN:H | 2.15 | 0.49 |
| 1:CA:993:G:H2' | 1:CA:995:C:H41 | 1.78 | 0.49 |
| 42:BY:68:HIS:ND1 | 42:BY:70:SER:HB3 | 2.28 | 0.49 |
| 23:BA:96:G:H4' | 46:B2:48:HIS:CD2 | 2.48 | 0.49 |
| 33:BP:138:LEU:HD23 | 33:BP:145:PRO:HG3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1469:G:H2' | 1:CA:1470:G:C8 | 2.48 | 0.49 |
| 40:BW:14:PRO:HG2 | 40:BW:78:GLU:HG2 | 1.94 | 0.49 |
| 24:BB:105:A:OP1 | 43:BZ:72:ARG:NH1 | 2.37 | 0.49 |
| 30:DI:58:LEU:HG | 30:DI:59:ALA:N | 2.28 | 0.49 |
| 1:CA:396:G:O2' | 1:CA:398:C:OP1 | 2.19 | 0.49 |
| 26:BE:2:LYS:HG3 | 26:BE:200:GLU:HB2 | 1.95 | 0.49 |
| 23:BA:2322:A:N6 | 23:BA:2335:A:C6 | 2.72 | 0.49 |
| 1:CA:1210:C:H3' | 1:CA:1211:U:C5' | 2.43 | 0.49 |
| 1:AA:1003:G:N2 | 1:AA:1004:A:O2' | 2.45 | 0.49 |
| 1:CA:952:U:O2 | 1:CA:1229:A:N1 | 2.46 | 0.49 |
| 8:AH:10:LEU:HD22 | 8:AH:83:ILE:HD11 | 1.95 | 0.49 |
| 1:AA:1224:G:C6 | 1:AA:1363:C:N3 | 2.81 | 0.49 |
| 10:AJ:40:LEU:HB2 | 10:AJ:69:ASN:HB2 | 1.94 | 0.49 |
| 1:CA:986:A:H2' | 1:CA:987:G:C8 | 2.47 | 0.49 |
| 23:DA:2125:G:N2 | 23:DA:2126:A:N6 | 2.61 | 0.49 |
| 23:DA:2158:A:H1' | 23:DA:2159:G:C8 | 2.48 | 0.49 |
| 1:CA:1026:G:N3 | 1:CA:1027:C:H5' | 2.28 | 0.49 |
| 1:CA:448:A:OP2 | 1:CA:485:G:N2 | 2.45 | 0.49 |
| 23:BA:2593:U:H2' | 23:BA:2594:C:H6 | 1.76 | 0.49 |
| 23:DA:947:G:N2 | 23:DA:971:C:C2 | 2.81 | 0.49 |
| 7:AG:113:GLU:HG2 | 7:AG:119:ARG:HB2 | 1.95 | 0.49 |
| 1:AA:270:A:H2' | 1:AA:271:C:C6 | 2.47 | 0.49 |
| 17:CQ:86:GLU:HG2 | 17:CQ:90:ILE:HD11 | 1.95 | 0.49 |
| 1:AA:420:U:N3 | 1:AA:422:C:N3 | 2.60 | 0.49 |
| 23:BA:1356:G:C6 | 23:BA:1357:U:C4 | 3.01 | 0.49 |
| 1:AA:946:A:OP2 | 1:AA:946:A:H8 | 1.95 | 0.49 |
| 21:AU:5:ASP:HB3 | 21:AU:8:THR:OG1 | 2.11 | 0.49 |
| 1:AA:1255:G:H2' | 1:AA:1258:G:H21 | 1.77 | 0.49 |
| 1:CA:868:C:H2' | 1:CA:869:G:O4' | 2.13 | 0.49 |
| 1:AA:1057:G:N2 | 1:AA:1204:A:H1' | 2.28 | 0.49 |
| 1:AA:674:G:H2' | 1:AA:675:A:C8 | 2.47 | 0.49 |
| 1:CA:1240:U:H3' | 1:CA:1241:G:O4' | 2.13 | 0.49 |
| 3:CC:32:LEU:HD21 | 3:CC:59:ARG:CZ | 2.43 | 0.49 |
| 3:CC:148:GLY:CA | 3:CC:172:ARG:H | 2.25 | 0.49 |
| 23:DA:271(E):U:H3 | 23:DA:271(S):G:H1 | 1.60 | 0.49 |
| 33:DP:64:LYS:HA | 52:D8:13:ARG:HB3 | 1.94 | 0.49 |
| 19:CS:12:ASP:HB2 | 19:CS:38:SER:OG | 2.13 | 0.49 |
| 23:BA:1796:U:H2' | 23:BA:1797:C:H6 | 1.77 | 0.49 |
| 17:CQ:66:SER:HB3 | 17:CQ:69:LYS:HB2 | 1.95 | 0.49 |
| 23:DA:2854:G:H2' | 23:DA:2855:C:C6 | 2.47 | 0.49 |
| 23:BA:2461:C:H2' | 23:BA:2462:U:H6 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 33:DP:83:VAL:CG1 | 33:DP:112:LEU:HD21 | 2.43 | 0.49 |
| 23:DA:2462:U:H1' | 23:DA:2491:U:O4 | 2.13 | 0.49 |
| 23:BA:2648:C:H2' | 23:BA:2649:U:H6 | 1.78 | 0.49 |
| 31:BN:39:ARG:NH2 | 31:BN:41:ASP:OD2 | 2.44 | 0.49 |
| 23:BA:751:A:H5' | 40:BW:90:ARG:HA | 1.95 | 0.49 |
| 23:BA:1657:C:H2' | 23:BA:1658:C:C6 | 2.48 | 0.49 |
| 23:DA:704:G:H1' | 23:DA:726:G:N2 | 2.27 | 0.49 |
| 1:CA:830:G:H2' | 1:CA:831:U:O4' | 2.13 | 0.49 |
| 2:AB:78:GLN:O | 2:AB:94:ASN:ND2 | 2.43 | 0.49 |
| 2:CB:47:THR:HG23 | 2:CB:202:PRO:HG2 | 1.95 | 0.49 |
| 3:AC:59:ARG:HG2 | 3:AC:64:VAL:CB | 2.43 | 0.49 |
| 1:AA:692:U:O2' | 1:AA:694:A:N7 | 2.39 | 0.49 |
| 23:DA:774:A:N3 | 23:DA:774:A:H2' | 2.28 | 0.49 |
| 1:AA:417:C:H6 | 1:AA:417:C:O5' | 1.96 | 0.49 |
| 24:BB:96:U:H2' | 24:BB:97:G:H8 | 1.78 | 0.49 |
| 23:DA:1593:G:H2' | 23:DA:1594:G:C8 | 2.48 | 0.49 |
| 1:AA:1458:G:H3' | 1:AA:1459:C:H5'' | 1.94 | 0.48 |
| 23:DA:848:G:H2' | 23:DA:849:A:C8 | 2.48 | 0.48 |
| 1:AA:959:A:O2' | 1:AA:961:U:H5' | 2.13 | 0.48 |
| 1:AA:986:A:H1' | 19:AS:54:GLY:O | 2.13 | 0.48 |
| 1:CA:1144:G:H21 | 1:CA:1146:A:H61 | 1.60 | 0.48 |
| 1:AA:971:G:H1' | 1:AA:1365:G:O2' | 2.13 | 0.48 |
| 31:DN:132:ALA:HB3 | 31:DN:133:GLN:NE2 | 2.28 | 0.48 |
| 1:CA:1320:C:H42 | 19:CS:36:ARG:HE | 1.61 | 0.48 |
| 23:BA:1140:C:OP1 | 31:BN:23:LEU:O | 2.30 | 0.48 |
| 1:CA:266:G:H5'' | 1:CA:267:C:H5 | 1.77 | 0.48 |
| 7:CG:66:VAL:HA | 7:CG:69:VAL:HG23 | 1.93 | 0.48 |
| 23:BA:826:U:H4' | 33:BP:55:ARG:HB2 | 1.95 | 0.48 |
| 5:AE:91:LEU:HD12 | 5:AE:120:THR:HG22 | 1.94 | 0.48 |
| 13:CM:23:TYR:CD1 | 13:CM:67:GLU:HA | 2.48 | 0.48 |
| 20:CT:56:MET:HE2 | 20:CT:88:VAL:HG21 | 1.95 | 0.48 |
| 1:CA:766:A:H2' | 1:CA:767:A:O4' | 2.12 | 0.48 |
| 23:DA:2293:C:H2' | 23:DA:2294:C:C6 | 2.48 | 0.48 |
| 23:BA:1866:C:H2' | 23:BA:1876:A:O4' | 2.13 | 0.48 |
| 23:BA:226:G:H21 | 23:BA:228:A:N6 | 2.10 | 0.48 |
| 23:BA:1509(B):A:H3' | 23:BA:1510:G:H8 | 1.77 | 0.48 |
| 23:BA:1419:A:O2' | 23:BA:1420:U:H5'' | 2.13 | 0.48 |
| 23:BA:1638:C:O2 | 23:BA:2698:U:O2' | 2.28 | 0.48 |
| 12:CL:70:ILE:HG12 | 12:CL:100:ILE:HD13 | 1.95 | 0.48 |
| 3:CC:139:GLN:HA | 3:CC:142:MET:HB2 | 1.93 | 0.48 |
| 8:AH:51:VAL:HG11 | 8:AH:60:ARG:HG3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:1632:A:C6 | 23:BA:1633:G:C6 | 3.01 | 0.48 |
| 4:AD:177:ASP:CG | 4:AD:180:GLY:HA3 | 2.33 | 0.48 |
| 1:CA:881:G:P | 12:CL:12:ARG:HH22 | 2.35 | 0.48 |
| 1:AA:859:A:H2' | 1:AA:860:A:O4' | 2.13 | 0.48 |
| 23:BA:127:A:H5'' | 23:BA:128:C:C6 | 2.48 | 0.48 |
| 42:DY:6:HIS:CD2 | 42:DY:6:HIS:H | 2.31 | 0.48 |
| 23:BA:1794:U:H2' | 23:BA:1795:C:H6 | 1.78 | 0.48 |
| 23:DA:955:C:OP1 | 34:DQ:87:LYS:HE2 | 2.13 | 0.48 |
| 43:BZ:180:VAL:O | 43:BZ:183:LEU:HB2 | 2.12 | 0.48 |
| 1:AA:1360:A:H3' | 1:AA:1361:G:C8 | 2.48 | 0.48 |
| 1:AA:978:A:N6 | 1:AA:1316:G:H1' | 2.28 | 0.48 |
| 1:CA:1124:G:H1' | 10:CJ:38:ILE:HG21 | 1.95 | 0.48 |
| 1:CA:1373:G:OP1 | 7:CG:36:LYS:HB2 | 2.13 | 0.48 |
| 2:AB:84:GLU:HB3 | 2:AB:219:VAL:HG21 | 1.96 | 0.48 |
| 1:AA:1234:C:H2' | 1:AA:1235:U:C6 | 2.48 | 0.48 |
| 1:AA:963:G:N2 | 1:AA:972:C:N3 | 2.50 | 0.48 |
| 1:AA:1202:G:N2 | 14:AN:43:CYS:SG | 2.85 | 0.48 |
| 23:BA:2130:U:H2' | 23:BA:2131:G:N7 | 2.27 | 0.48 |
| 23:BA:784:A:C8 | 23:BA:792:G:C5 | 3.01 | 0.48 |
| 17:AQ:55:ASP:HA | 17:AQ:79:SER:HA | 1.95 | 0.48 |
| 23:DA:2154:G:H2' | 23:DA:2155:G:C8 | 2.48 | 0.48 |
| 5:AE:71:LEU:HD23 | 5:AE:115:VAL:HG22 | 1.95 | 0.48 |
| 9:CI:20:ARG:HG2 | 9:CI:21:PRO:O | 2.13 | 0.48 |
| 36:BS:96:GLY:N | 36:BS:99:LYS:HB3 | 2.28 | 0.48 |
| 23:DA:870:A:C2 | 23:DA:908:C:C2 | 3.01 | 0.48 |
| 18:AR:36:ASN:ND2 | 18:AR:39:VAL:H | 2.11 | 0.48 |
| 1:CA:1069:C:H4' | 1:CA:1192:C:O2 | 2.13 | 0.48 |
| 23:DA:2648:C:H2' | 23:DA:2649:U:C6 | 2.48 | 0.48 |
| 1:CA:420:U:N3 | 1:CA:422:C:N3 | 2.61 | 0.48 |
| 32:DO:35:VAL:HG21 | 32:DO:103:ALA:HB3 | 1.95 | 0.48 |
| 1:AA:1067:A:H8 | 1:AA:1067:A:O5' | 1.96 | 0.48 |
| 1:CA:346:G:H2' | 1:CA:347:G:O4' | 2.14 | 0.48 |
| 31:DN:62:VAL:CG1 | 31:DN:66:LYS:HB2 | 2.44 | 0.48 |
| 2:AB:149:LEU:HD23 | 2:AB:149:LEU:HA | 1.62 | 0.48 |
| 12:CL:42:THR:HB | 12:CL:52:LEU:HD12 | 1.94 | 0.48 |
| 1:AA:775:G:O2' | 1:AA:776:G:H5' | 2.13 | 0.48 |
| 23:DA:1654:A:OP1 | 35:DR:1:MET:HA | 2.13 | 0.48 |
| 41:DX:11:PRO:HG2 | 41:DX:13:LEU:HD21 | 1.95 | 0.48 |
| 1:AA:1457:G:C6 | 1:AA:1458:G:N7 | 2.82 | 0.48 |
| 1:CA:1165:C:C2 | 1:CA:1171:G:N2 | 2.81 | 0.48 |
| 1:AA:838:G:H2' | 1:AA:839:U:H5'' | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1314:C:H2' | 1:AA:1315:U:C6 | 2.47 | 0.48 |
| 3:AC:153:VAL:HG22 | 3:AC:198:VAL:HG13 | 1.95 | 0.48 |
| 1:CA:1004:A:C2 | 1:CA:1037:C:N4 | 2.82 | 0.48 |
| 1:AA:1231:G:H2' | 1:AA:1232:U:H6 | 1.76 | 0.48 |
| 2:CB:77:ALA:HB1 | 2:CB:211:ILE:HG21 | 1.94 | 0.48 |
| 1:CA:9:G:H2' | 1:CA:10:A:C8 | 2.48 | 0.48 |
| 1:AA:1058:G:C6 | 1:AA:1059:C:N3 | 2.80 | 0.48 |
| 1:AA:1059:C:P | 3:AC:199:LYS:HZ1 | 2.35 | 0.48 |
| 3:CC:132:ARG:O | 3:CC:136:GLN:HB2 | 2.13 | 0.48 |
| 23:BA:1664:A:OP1 | 56:BA:4773:HOH:O | 2.19 | 0.48 |
| 1:AA:1293:G:O2' | 1:AA:1294:G:OP2 | 2.25 | 0.48 |
| 23:BA:1047:G:H2' | 23:BA:1110:G:N1 | 2.26 | 0.48 |
| 23:DA:171:G:H2' | 23:DA:172:C:O4' | 2.14 | 0.48 |
| 23:DA:1505:C:H2' | 23:DA:1506:C:H6 | 1.78 | 0.48 |
| 1:AA:1309:G:C6 | 1:AA:1329:A:C5 | 3.00 | 0.48 |
| 27:BF:197:ASP:O | 27:BF:201:VAL:HG12 | 2.12 | 0.48 |
| 9:AI:9:ARG:HG2 | 9:AI:104:ARG:HH21 | 1.78 | 0.48 |
| 1:CA:1013:G:HO2' | 1:CA:1014:A:H8 | 1.58 | 0.48 |
| 23:DA:102:G:O2' | 23:DA:103:A:O5' | 2.26 | 0.48 |
| 48:D4:22:ILE:HG22 | 48:D4:24:THR:HG23 | 1.95 | 0.48 |
| 41:BX:9:LEU:HA | 46:B2:36:ARG:HH21 | 1.79 | 0.48 |
| 12:AL:86:ARG:HB2 | 12:AL:101:VAL:HG22 | 1.94 | 0.48 |
| 1:CA:189(A):C:H42 | 1:CA:189(J):G:H1 | 1.60 | 0.48 |
| 1:AA:335:C:H2' | 1:AA:336:C:C6 | 2.48 | 0.48 |
| 23:BA:2205:C:O2 | 23:BA:2220:G:C2 | 2.66 | 0.48 |
| 24:BB:96:U:H2' | 24:BB:97:G:C8 | 2.47 | 0.48 |
| 4:CD:120:LEU:HB3 | 4:CD:126:ILE:HD11 | 1.94 | 0.48 |
| 23:DA:975:C:H5 | 56:DA:4455:HOH:O | 1.95 | 0.48 |
| 1:AA:933:G:O6 | 7:AG:3:ARG:NH2 | 2.46 | 0.48 |
| 23:DA:333:G:H5'' | 23:DA:334:C:OP2 | 2.12 | 0.48 |
| 49:B5:20:ARG:HG2 | 49:B5:23:HIS:CD2 | 2.48 | 0.48 |
| 23:BA:729:G:OP2 | 25:BD:13:ARG:NH1 | 2.45 | 0.48 |
| 29:BH:67:LEU:O | 29:BH:71:LEU:HB2 | 2.13 | 0.48 |
| 23:DA:444:C:H4' | 27:DF:49:ALA:HB2 | 1.94 | 0.48 |
| 23:BA:573:G:O2' | 23:BA:574:C:H3' | 2.13 | 0.48 |
| 22:AX:22:ALA:O | 22:AX:25:ALA:HB3 | 2.13 | 0.48 |
| 23:BA:955:C:OP1 | 34:BQ:87:LYS:HE2 | 2.13 | 0.48 |
| 35:DR:103:ARG:HH12 | 35:DR:110:PRO:HD3 | 1.77 | 0.48 |
| 26:BE:119:ARG:HG2 | 26:BE:160:TYR:HB2 | 1.94 | 0.48 |
| 43:DZ:150:LEU:O | 43:DZ:171:ILE:HG13 | 2.13 | 0.48 |
| 23:DA:1316:U:H2' | 23:DA:1317:A:C8 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:512:U:H2' | 1:CA:513:C:H6 | 1.79 | 0.48 |
| 1:AA:1443:G:O6 | 1:AA:1459:C:O2 | 2.31 | 0.48 |
| 1:AA:1443:G:O6 | 1:AA:1444:C:C4 | 2.66 | 0.48 |
| 1:AA:1459:C:C2' | 1:AA:1460:A:N7 | 2.77 | 0.48 |
| 23:DA:2713:A:N3 | 23:DA:2713:A:H2' | 2.29 | 0.48 |
| 1:AA:838:G:N2 | 1:AA:849:C:C2 | 2.81 | 0.48 |
| 1:AA:1301:U:H4' | 13:AM:21:TYR:OH | 2.14 | 0.48 |
| 28:BG:59:GLU:O | 28:BG:63:ILE:HG13 | 2.13 | 0.48 |
| 23:BA:2318:G:N3 | 23:BA:2318:G:H2' | 2.28 | 0.48 |
| 1:AA:954:G:H21 | 1:AA:1227:A:H62 | 1.61 | 0.48 |
| 23:DA:2165:G:H2' | 23:DA:2166:G:C8 | 2.48 | 0.48 |
| 23:DA:2318:G:N3 | 23:DA:2318:G:H2' | 2.29 | 0.48 |
| 1:CA:390:C:H2' | 1:CA:391:G:C8 | 2.49 | 0.48 |
| 1:AA:97:G:O2' | 1:AA:98:G:H8 | 1.91 | 0.48 |
| 1:AA:1268:A:H1' | 1:AA:1327:C:H5' | 1.94 | 0.48 |
| 33:BP:52:GLU:OE1 | 33:BP:55:ARG:NH1 | 2.47 | 0.48 |
| 1:CA:1071:C:H5'' | 5:CE:49:PRO:HG2 | 1.94 | 0.48 |
| 37:BT:95:ARG:HG2 | 37:BT:95:ARG:NH1 | 2.26 | 0.48 |
| 1:AA:223:U:H2' | 1:AA:224:C:C6 | 2.49 | 0.48 |
| 23:BA:1366:A:OP1 | 45:B1:3:LYS:NZ | 2.46 | 0.48 |
| 50:B6:14:THR:HG21 | 50:B6:48:VAL:HG13 | 1.95 | 0.48 |
| 42:DY:15:VAL:HG21 | 42:DY:42:VAL:HG11 | 1.94 | 0.48 |
| 1:CA:1086:U:H4' | 1:CA:1389:C:H5'' | 1.94 | 0.48 |
| 23:BA:83:G:H22 | 23:BA:102:G:H2' | 1.77 | 0.48 |
| 42:BY:79:CYS:HB3 | 42:BY:81:LYS:H | 1.77 | 0.48 |
| 1:CA:684:A:H2' | 1:CA:685:G:C8 | 2.47 | 0.48 |
| 1:CA:625:G:C6 | 1:CA:626:U:C4 | 3.01 | 0.48 |
| 1:AA:806:C:H2' | 1:AA:807:A:C8 | 2.48 | 0.48 |
| 1:AA:230:G:H1' | 16:AP:25:ARG:HH22 | 1.78 | 0.48 |
| 3:AC:59:ARG:HA | 3:AC:64:VAL:HA | 1.93 | 0.48 |
| 23:DA:968:G:H2' | 23:DA:969:U:O4' | 2.13 | 0.48 |
| 48:B4:14:ILE:HG22 | 48:B4:33:VAL:HG23 | 1.95 | 0.48 |
| 23:DA:223:A:O2' | 23:DA:420:C:O2 | 2.32 | 0.48 |
| 3:AC:114:PRO:HD3 | 3:AC:183:ASP:OD1 | 2.13 | 0.48 |
| 27:DF:50:SER:OG | 27:DF:51:THR:N | 2.45 | 0.48 |
| 23:BA:848:G:H2' | 23:BA:849:A:C8 | 2.49 | 0.48 |
| 32:DO:77:ILE:HG13 | 37:DT:74:ARG:HG2 | 1.95 | 0.48 |
| 2:CB:37:ASN:O | 2:CB:39:ILE:HD12 | 2.13 | 0.48 |
| 37:DT:28:VAL:HG13 | 37:DT:86:ILE:HG23 | 1.95 | 0.48 |
| 1:AA:1412:C:H2' | 1:AA:1413:A:C8 | 2.49 | 0.48 |
| 23:BA:535:C:O3' | 38:BU:53:ARG:NH1 | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:659:C:H4' | 27:DF:100:THR:O | 2.12 | 0.48 |
| 8:CH:37:ARG:HE | 8:CH:37:ARG:HB3 | 1.50 | 0.48 |
| 23:DA:2275:C:H5' | 23:DA:2275:C:H6 | 1.78 | 0.48 |
| 20:AT:86:ARG:CZ | 20:AT:86:ARG:HB3 | 2.42 | 0.48 |
| 2:AB:95:GLN:HG3 | 2:AB:147:LYS:HD3 | 1.95 | 0.48 |
| 26:BE:72:VAL:HA | 26:BE:73:GLU:OE2 | 2.13 | 0.48 |
| 23:BA:271(I):G:H2' | 23:BA:271(J):C:C6 | 2.48 | 0.48 |
| 23:BA:2069:G:OP2 | 56:BA:3862:HOH:O | 2.20 | 0.48 |
| 1:CA:859:A:H2' | 1:CA:860:A:O4' | 2.13 | 0.48 |
| 1:CA:560:U:OP2 | 56:CA:1914:HOH:O | 2.20 | 0.48 |
| 1:CA:1508:G:P | 56:CA:2020:HOH:O | 2.71 | 0.48 |
| 3:CC:111:LEU:HD23 | 3:CC:141:VAL:HG13 | 1.94 | 0.48 |
| 1:AA:1338:G:H5' | 1:AA:1339:A:OP2 | 2.13 | 0.48 |
| 17:CQ:76:LEU:HD21 | 17:CQ:79:SER:H | 1.79 | 0.48 |
| 2:AB:178:ARG:NH1 | 2:AB:196:LEU:O | 2.46 | 0.48 |
| 23:BA:71:A:H8 | 23:BA:71:A:H5' | 1.75 | 0.48 |
| 23:BA:2807:G:N1 | 23:BA:2808:U:C2 | 2.82 | 0.48 |
| 1:CA:1256:A:H5' | 1:CA:1258:G:O4' | 2.13 | 0.48 |
| 23:DA:2748:A:H5' | 29:DH:4:ILE:HD12 | 1.94 | 0.48 |
| 23:DA:493:G:H2' | 23:DA:494:G:O4' | 2.14 | 0.48 |
| 1:CA:626:U:C2 | 1:CA:627:G:C8 | 3.02 | 0.48 |
| 31:DN:30:ILE:HG22 | 31:DN:34:LEU:HD22 | 1.94 | 0.48 |
| 6:CF:19:LEU:HD11 | 6:CF:59:TYR:CZ | 2.49 | 0.48 |
| 23:DA:335:C:H2' | 23:DA:336:C:H6 | 1.79 | 0.48 |
| 1:CA:1446:U:H4' | 1:CA:1447:A:C2 | 2.49 | 0.48 |
| 23:BA:828:U:H4' | 23:BA:831:G:N1 | 2.28 | 0.48 |
| 34:BQ:63:LYS:HD2 | 34:BQ:65:PHE:CZ | 2.49 | 0.48 |
| 33:BP:95:VAL:HG22 | 33:BP:125:VAL:HB | 1.96 | 0.48 |
| 23:DA:2469:A:H5' | 23:DA:2470:G:OP2 | 2.13 | 0.48 |
| 2:CB:42:ILE:HD12 | 2:CB:203:GLY:HA2 | 1.96 | 0.48 |
| 31:DN:39:ARG:NH2 | 31:DN:41:ASP:OD2 | 2.46 | 0.48 |
| 1:AA:1441:G:N2 | 1:AA:1459:C:C6 | 2.82 | 0.48 |
| 1:CA:1460:A:O5' | 1:CA:1460:A:H8 | 1.95 | 0.48 |
| 1:CA:990:C:N4 | 1:CA:991:U:O4 | 2.47 | 0.48 |
| 1:AA:1206:G:C6 | 1:AA:1207:G:C5 | 3.00 | 0.48 |
| 1:CA:1023:G:C2' | 1:CA:1024:G:H5' | 2.43 | 0.48 |
| 7:CG:88:PRO:O | 7:CG:89:MET:HG3 | 2.13 | 0.48 |
| 39:DV:60:GLU:HB2 | 39:DV:97:LYS:HE2 | 1.95 | 0.48 |
| 36:DS:96:GLY:H | 36:DS:99:LYS:H | 1.60 | 0.48 |
| 1:AA:60:A:H4' | 1:AA:61:G:O5' | 2.14 | 0.48 |
| 23:DA:910:A:C6 | 23:DA:911:A:C6 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1245:A:N6 | 1:CA:1292:U:H3 | 2.10 | 0.48 |
| 23:DA:485:C:H2' | 23:DA:486:C:C6 | 2.48 | 0.48 |
| 30:BI:5:LEU:HD12 | 30:BI:17:GLN:O | 2.13 | 0.48 |
| 35:BR:37:THR:OG1 | 35:BR:40:LYS:HG3 | 2.13 | 0.48 |
| 22:AX:69:ASP:HB3 | 22:AX:71:TYR:N | 2.29 | 0.48 |
| 15:AO:4:THR:H | 15:AO:7:GLU:HB2 | 1.79 | 0.48 |
| 23:BA:7:G:H2' | 23:BA:8:A:C8 | 2.48 | 0.48 |
| 1:AA:1084:G:H5'' | 1:AA:1085:U:OP2 | 2.13 | 0.48 |
| 28:BG:104:GLU:O | 28:BG:108:ASN:ND2 | 2.47 | 0.48 |
| 17:CQ:31:LEU:HD23 | 17:CQ:32:TYR:CZ | 2.48 | 0.48 |
| 20:AT:38:LYS:O | 20:AT:41:ILE:HG13 | 2.14 | 0.48 |
| 1:AA:830:G:H2' | 1:AA:831:U:O4' | 2.14 | 0.48 |
| 23:DA:1999:C:H5'' | 23:DA:2723:C:O2' | 2.14 | 0.48 |
| 26:BE:92:THR:O | 26:BE:95:ILE:HG23 | 2.12 | 0.48 |
| 32:DO:4:PRO:O | 32:DO:5:GLN:HB2 | 2.13 | 0.48 |
| 1:AA:393:A:C2 | 1:AA:394:G:C8 | 3.02 | 0.48 |
| 28:BG:132:ASN:OD1 | 28:BG:158:ALA:HA | 2.13 | 0.48 |
| 28:DG:104:GLU:O | 28:DG:108:ASN:ND2 | 2.47 | 0.48 |
| 23:BA:2324:C:H5'' | 23:BA:2325:G:H5' | 1.95 | 0.48 |
| 29:DH:67:LEU:O | 29:DH:71:LEU:HB2 | 2.14 | 0.48 |
| 23:BA:12:U:O2 | 23:BA:12:U:H2' | 2.14 | 0.48 |
| 8:CH:111:ILE:HD12 | 8:CH:111:ILE:H | 1.78 | 0.48 |
| 5:AE:137:GLU:O | 5:AE:141:GLN:HB2 | 2.14 | 0.48 |
| 23:DA:1040:C:H2' | 23:DA:1041:C:H1' | 1.95 | 0.48 |
| 40:BW:71:VAL:HA | 40:BW:107:LEU:HD12 | 1.94 | 0.48 |
| 1:CA:1210:C:H1' | 1:CA:1214:C:C2 | 2.49 | 0.48 |
| 23:BA:2175:C:H2' | 23:BA:2176:A:O4' | 2.14 | 0.48 |
| 9:CI:65:VAL:HG13 | 9:CI:73:GLN:NE2 | 2.28 | 0.48 |
| 1:CA:1003:G:H1 | 1:CA:1037:C:N4 | 2.12 | 0.48 |
| 28:DG:59:GLU:O | 28:DG:63:ILE:HG13 | 2.14 | 0.48 |
| 1:AA:1099:G:H3' | 1:AA:1100:C:H6 | 1.77 | 0.48 |
| 1:AA:677:U:H2' | 1:AA:678:U:C6 | 2.48 | 0.48 |
| 10:CJ:9:ARG:O | 10:CJ:95:GLU:N | 2.28 | 0.48 |
| 1:AA:766:A:H2' | 1:AA:767:A:O4' | 2.13 | 0.48 |
| 23:BA:2127:G:N2 | 23:BA:2173:A:H1' | 2.28 | 0.48 |
| 1:AA:1326:C:H5'' | 21:AU:19:GLY:HA2 | 1.95 | 0.48 |
| 1:AA:391:G:C6 | 1:AA:392:G:C5 | 3.02 | 0.48 |
| 23:DA:2001:A:H2' | 23:DA:2002:G:C8 | 2.49 | 0.48 |
| 1:AA:1262:C:N4 | 1:AA:1273:G:H1 | 2.07 | 0.48 |
| 23:DA:300:A:P | 42:DY:86:ARG:HH22 | 2.36 | 0.48 |
| 25:BD:101:GLU:OE1 | 25:BD:103:ARG:HD3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AL:102:ARG:NH2 | 12:AL:109:GLY:O | 2.47 | 0.48 |
| 23:BA:1494:A:H2' | 23:BA:1495:A:H8 | 1.78 | 0.48 |
| 51:B7:9:ARG:HB3 | 51:B7:46:VAL:HG23 | 1.96 | 0.48 |
| 7:AG:108:ALA:CB | 7:AG:120:ILE:HG12 | 2.43 | 0.48 |
| 2:CB:97:TRP:CZ3 | 2:CB:99:GLY:HA2 | 2.49 | 0.48 |
| 23:DA:2464:C:H1' | 56:DA:3666:HOH:O | 2.13 | 0.48 |
| 46:B2:50:ILE:O | 46:B2:51:ARG:HB3 | 2.13 | 0.48 |
| 31:DN:67:LEU:HA | 31:DN:67:LEU:HD22 | 1.71 | 0.48 |
| 44:B0:23:VAL:HG13 | 44:B0:38:VAL:HG23 | 1.95 | 0.48 |
| 23:DA:1488:G:N2 | 23:DA:1502:C:C2 | 2.82 | 0.48 |
| 1:CA:1427:U:H2' | 1:CA:1428:A:C8 | 2.49 | 0.48 |
| 22:AX:27:LEU:HD21 | 22:AX:85:LEU:HD13 | 1.95 | 0.48 |
| 27:DF:39:TRP:O | 27:DF:43:LYS:HG2 | 2.13 | 0.48 |
| 23:BA:2751:G:C4 | 29:BH:2:SER:N | 2.82 | 0.48 |
| 37:DT:26:ASP:OD2 | 37:DT:91:ARG:NH1 | 2.47 | 0.48 |
| 34:DQ:38:GLU:HB2 | 34:DQ:127:ILE:HG22 | 1.95 | 0.48 |
| 30:BI:102:SER:HA | 30:BI:106:GLY:HA3 | 1.95 | 0.48 |
| 1:CA:636:U:H2' | 1:CA:637:G:H8 | 1.78 | 0.48 |
| 32:BO:107:ARG:CZ | 37:BT:36:GLU:HG3 | 2.43 | 0.48 |
| 23:BA:652(J):G:H21 | 47:D3:5:LYS:NZ | 2.12 | 0.48 |
| 23:DA:1651:G:N2 | 23:DA:2007:C:C2 | 2.82 | 0.48 |
| 23:DA:709:U:H2' | 23:DA:710:G:C8 | 2.49 | 0.48 |
| 23:BA:2315:G:H2' | 23:BA:2316:C:C6 | 2.49 | 0.48 |
| 2:CB:102:LEU:HB3 | 2:CB:180:LEU:HD12 | 1.96 | 0.48 |
| 11:CK:33:THR:HA | 11:CK:40:ILE:HG12 | 1.95 | 0.48 |
| 23:DA:1001:A:H2' | 23:DA:1002:G:O4' | 2.13 | 0.48 |
| 23:DA:498:G:O2' | 23:DA:499:U:H5' | 2.14 | 0.48 |
| 29:DH:117:PRO:HB3 | 29:DH:123:PHE:CE2 | 2.48 | 0.48 |
| 1:CA:1251:A:H61 | 1:CA:1354:C:HO2' | 1.55 | 0.48 |
| 1:CA:1508:G:H2' | 1:CA:1509:C:C6 | 2.49 | 0.48 |
| 16:CP:28:ARG:HG2 | 16:CP:29:ASP:OD2 | 2.13 | 0.48 |
| 1:AA:767:A:H2' | 1:AA:768:A:O4' | 2.14 | 0.48 |
| 13:AM:13:LYS:HA | 13:AM:44:ARG:HB3 | 1.96 | 0.48 |
| 23:BA:171:G:H2' | 23:BA:172:C:O4' | 2.13 | 0.48 |
| 1:CA:1085:U:C2 | 1:CA:1094:G:O6 | 2.67 | 0.48 |
| 23:BA:1113:U:H2' | 23:BA:1114:G:C8 | 2.49 | 0.48 |
| 1:AA:1377:A:C8 | 1:AA:1377:A:C3' | 2.96 | 0.48 |
| 4:AD:108:LEU:HD12 | 4:AD:174:LEU:HD13 | 1.94 | 0.48 |
| 26:DE:175:VAL:CG2 | 26:DE:177:PRO:HD3 | 2.43 | 0.48 |
| 36:DS:62:LYS:HB3 | 36:DS:97:ARG:HD2 | 1.96 | 0.48 |
| 23:DA:1159:U:H2' | 23:DA:1160:G:H8 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 36:BS:14:VAL:HG11 | 36:BS:90:GLY:O | 2.14 | 0.48 |
| 1:CA:921:U:O2 | 5:CE:19:MET:HB2 | 2.14 | 0.48 |
| 23:DA:645:C:O2 | 23:DA:645:C:H2' | 2.13 | 0.48 |
| 36:BS:62:LYS:HB3 | 36:BS:97:ARG:HD2 | 1.95 | 0.48 |
| 13:AM:5:ALA:HA | 13:AM:61:GLU:HG2 | 1.96 | 0.48 |
| 1:AA:375:U:C4 | 1:AA:376:G:N7 | 2.82 | 0.48 |
| 24:DB:110:G:C2 | 24:DB:111:G:C5 | 3.01 | 0.48 |
| 23:BA:2001:A:H2' | 23:BA:2002:G:C8 | 2.49 | 0.48 |
| 23:BA:646:A:H2' | 23:BA:647:G:O4' | 2.14 | 0.48 |
| 1:CA:38:G:H22 | 1:CA:397:A:H5'' | 1.78 | 0.48 |
| 30:DI:5:LEU:H | 30:DI:5:LEU:HD12 | 1.79 | 0.48 |
| 1:AA:1271:G:C6 | 1:AA:1272:G:C6 | 3.01 | 0.48 |
| 1:AA:1351:U:H1' | 7:AG:33:ASP:HB3 | 1.94 | 0.48 |
| 23:DA:1652:A:OP1 | 35:DR:8:ARG:NH1 | 2.44 | 0.48 |
| 27:DF:34:TRP:HE3 | 27:DF:35:GLU:HG2 | 1.79 | 0.48 |
| 31:BN:36:GLY:HA2 | 31:BN:38:HIS:CE1 | 2.49 | 0.48 |
| 23:BA:363(A):A:H2' | 23:BA:363(B):G:H8 | 1.78 | 0.48 |
| 16:AP:75:ARG:HA | 16:AP:80:PHE:HD1 | 1.79 | 0.48 |
| 2:AB:44:LEU:HA | 2:AB:47:THR:OG1 | 2.13 | 0.48 |
| 30:DI:29:TYR:O | 30:DI:32:PRO:HD2 | 2.14 | 0.48 |
| 23:BA:1001:A:H2' | 23:BA:1002:G:O4' | 2.13 | 0.48 |
| 26:DE:120:TRP:CE3 | 26:DE:155:LYS:HD3 | 2.49 | 0.48 |
| 43:DZ:43:GLU:O | 43:DZ:47:VAL:HG23 | 2.14 | 0.48 |
| 26:BE:21:VAL:HG23 | 26:BE:185:LYS:HG3 | 1.96 | 0.48 |
| 23:DA:1464:C:H2' | 23:DA:1465:G:C8 | 2.48 | 0.48 |
| 24:DB:33:G:C6 | 24:DB:34:U:N3 | 2.82 | 0.48 |
| 16:AP:65:GLN:HE21 | 16:AP:65:GLN:HB3 | 1.42 | 0.48 |
| 1:CA:962:C:H2' | 1:CA:963:G:O4' | 2.13 | 0.48 |
| 1:CA:968:A:OP1 | 1:CA:968:A:H8 | 1.97 | 0.48 |
| 30:DI:79:ILE:HA | 30:DI:80:PRO:HD2 | 1.66 | 0.48 |
| 4:CD:101:LEU:HD23 | 4:CD:102:ASP:N | 2.29 | 0.48 |
| 23:DA:2722:G:H5' | 35:DR:4:LEU:HD12 | 1.96 | 0.48 |
| 23:BA:1359:A:N6 | 23:BA:1372:U:C5 | 2.82 | 0.48 |
| 7:CG:32:ARG:HA | 7:CG:32:ARG:HD3 | 1.50 | 0.48 |
| 1:AA:1303:C:H2' | 1:AA:1304:G:H5' | 1.95 | 0.48 |
| 23:DA:784:A:O4' | 25:DD:227:ASN:ND2 | 2.46 | 0.48 |
| 23:BA:2312:U:O2' | 28:BG:40:ASN:ND2 | 2.41 | 0.48 |
| 1:AA:1279:A:H61 | 3:AC:26:LYS:HZ3 | 1.61 | 0.48 |
| 23:BA:2173:A:H2' | 23:BA:2174:C:H5' | 1.96 | 0.48 |
| 3:CC:7:PRO:O | 3:CC:11:ARG:NH1 | 2.47 | 0.48 |
| 1:CA:1149:C:H2' | 1:CA:1150:U:C6 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:BW:4:LYS:HE2 | 40:BW:6:ILE:HD11 | 1.96 | 0.48 |
| 23:BA:1433:U:O2 | 23:BA:1561:G:C2 | 2.67 | 0.48 |
| 23:BA:1423:G:H2' | 23:BA:1424:G:C8 | 2.47 | 0.48 |
| 48:D4:14:ILE:HG23 | 48:D4:31:ILE:HB | 1.95 | 0.48 |
| 18:AR:66:LEU:O | 18:AR:70:ILE:HG13 | 2.14 | 0.48 |
| 1:AA:651:C:H2' | 1:AA:652:U:C6 | 2.49 | 0.48 |
| 1:CA:300:A:O2' | 1:CA:564:C:N3 | 2.38 | 0.48 |
| 37:BT:123:GLN:O | 37:BT:126:ALA:HB3 | 2.14 | 0.48 |
| 10:CJ:62:HIS:CD2 | 10:CJ:62:HIS:N | 2.81 | 0.48 |
| 43:DZ:98:MET:HE3 | 43:DZ:100:VAL:HG22 | 1.95 | 0.48 |
| 11:CK:92:GLU:HB3 | 11:CK:96:ARG:HH12 | 1.77 | 0.48 |
| 33:BP:101:VAL:HA | 33:BP:106:LEU:O | 2.13 | 0.48 |
| 45:D1:94:LEU:O | 45:D1:97:LEU:HB2 | 2.13 | 0.48 |
| 23:DA:2196:C:OP2 | 56:DA:4151:HOH:O | 2.20 | 0.48 |
| 1:CA:1276:G:H2' | 1:CA:1277:C:O4' | 2.13 | 0.48 |
| 44:D0:40:GLN:OE1 | 44:D0:44:ARG:N | 2.37 | 0.48 |
| 3:AC:79:ARG:H | 3:AC:82:GLU:HB3 | 1.76 | 0.48 |
| 2:CB:117:GLU:O | 2:CB:120:ALA:HB3 | 2.14 | 0.48 |
| 39:DV:82:ARG:N | 39:DV:82:ARG:HD2 | 2.29 | 0.48 |
| 23:BA:1388:G:H4' | 23:BA:1525:G:O2' | 2.14 | 0.48 |
| 1:CA:989:C:C4 | 1:CA:990:C:C4 | 3.02 | 0.48 |
| 1:CA:1236:A:O2' | 1:CA:1304:G:H4' | 2.13 | 0.48 |
| 23:DA:2319:G:N2 | 36:DS:3:ARG:HA | 2.29 | 0.48 |
| 1:CA:1251:A:N3 | 1:CA:1369:C:O2' | 2.34 | 0.48 |
| 28:BG:3:LEU:HD11 | 28:BG:97:ASP:HB3 | 1.95 | 0.48 |
| 1:AA:156:G:C6 | 1:AA:166:G:C6 | 3.02 | 0.48 |
| 20:CT:25:ARG:O | 20:CT:29:LYS:HG3 | 2.14 | 0.48 |
| 1:CA:1360:A:C6 | 14:CN:18:VAL:HG11 | 2.49 | 0.48 |
| 3:CC:175:LEU:HD23 | 3:CC:201:TYR:HE2 | 1.79 | 0.48 |
| 23:BA:528:A:O2' | 23:BA:529:A:H5' | 2.14 | 0.48 |
| 40:DW:82:LEU:HD22 | 40:DW:84:ARG:NH2 | 2.28 | 0.48 |
| 1:CA:324:G:OP2 | 56:CA:1973:HOH:O | 2.20 | 0.48 |
| 12:CL:32:PHE:HB3 | 12:CL:84:LEU:HD11 | 1.95 | 0.48 |
| 1:AA:1106:G:H5'' | 3:AC:172:ARG:HG2 | 1.94 | 0.48 |
| 23:DA:973:A:O4' | 23:DA:1188:U:C6 | 2.66 | 0.48 |
| 23:DA:1188:U:C4' | 39:DV:79:VAL:HG22 | 2.44 | 0.48 |
| 1:CA:1516:G:N1 | 1:CA:1519:A:OP2 | 2.45 | 0.48 |
| 23:BA:2110:G:O2' | 23:BA:2120:G:H5' | 2.14 | 0.48 |
| 23:DA:1467:C:C5 | 23:DA:1546:C:H2' | 2.49 | 0.48 |
| 7:AG:62:PHE:HZ | 7:AG:101:LEU:HD21 | 1.78 | 0.48 |
| 8:CH:20:TYR:HA | 8:CH:65:TYR:CE2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 29:DH:20:ALA:HB3 | 29:DH:23:ARG:HB2 | 1.96 | 0.48 |
| 32:DO:54:GLU:HB2 | 56:DO:303:HOH:O | 2.14 | 0.48 |
| 23:DA:1996:C:O3' | 56:DA:4359:HOH:O | 2.20 | 0.48 |
| 23:BA:1925:C:O2' | 23:BA:1926:U:H5' | 2.14 | 0.48 |
| 23:DA:2665:A:OP2 | 56:DA:3746:HOH:O | 2.20 | 0.48 |
| 5:AE:36:ASP:OD2 | 5:AE:38:GLN:N | 2.44 | 0.48 |
| 35:DR:50:HIS:CE1 | 35:DR:54:LEU:HD21 | 2.48 | 0.48 |
| 23:DA:1564:C:H2' | 23:DA:1565:C:C6 | 2.48 | 0.48 |
| 1:CA:671:G:H2' | 1:CA:672:U:C6 | 2.48 | 0.48 |
| 1:AA:748:C:H6 | 1:AA:748:C:O5' | 1.97 | 0.48 |
| 5:AE:104:ALA:O | 5:AE:107:ARG:HG2 | 2.14 | 0.48 |
| 1:AA:1459:C:H2' | 1:AA:1460:A:C8 | 2.48 | 0.47 |
| 1:CA:1442(A):G:H3' | 1:CA:1442(B):A:H5'' | 1.96 | 0.47 |
| 1:AA:1300:G:HO2' | 1:AA:1301:U:P | 2.37 | 0.47 |
| 1:CA:673:G:H5'' | 6:CF:87:ARG:CZ | 2.44 | 0.47 |
| 1:CA:1296:C:H5'' | 1:CA:1302:U:C4 | 2.49 | 0.47 |
| 16:CP:28:ARG:NH1 | 16:CP:29:ASP:OD2 | 2.46 | 0.47 |
| 1:CA:176:C:H2' | 1:CA:177:C:C6 | 2.49 | 0.47 |
| 3:CC:134:ILE:HD11 | 3:CC:153:VAL:HG23 | 1.95 | 0.47 |
| 4:CD:108:LEU:HD12 | 4:CD:174:LEU:HD13 | 1.96 | 0.47 |
| 1:AA:1226:C:H5'' | 19:AS:80:TYR:CD1 | 2.50 | 0.47 |
| 25:DD:71:ASP:HB3 | 25:DD:103:ARG:NH2 | 2.27 | 0.47 |
| 5:AE:75:THR:HA | 5:AE:115:VAL:HG13 | 1.96 | 0.47 |
| 36:DS:56:LEU:C | 36:DS:58:LEU:HD22 | 2.34 | 0.47 |
| 19:AS:47:HIS:HB2 | 19:AS:49:ILE:HG13 | 1.95 | 0.47 |
| 1:CA:57:G:H2' | 1:CA:58:C:C6 | 2.49 | 0.47 |
| 7:AG:26:PHE:HA | 7:AG:101:LEU:HD13 | 1.96 | 0.47 |
| 1:CA:458:C:H2' | 1:CA:460:G:C8 | 2.49 | 0.47 |
| 43:DZ:98:MET:CE | 43:DZ:100:VAL:HG22 | 2.43 | 0.47 |
| 11:AK:23:ALA:O | 11:AK:86:GLY:HA3 | 2.13 | 0.47 |
| 50:B6:11:LEU:HB3 | 50:B6:49:HIS:HB3 | 1.96 | 0.47 |
| 44:D0:14:ARG:HH11 | 44:D0:14:ARG:HG3 | 1.78 | 0.47 |
| 23:DA:1388:G:H4' | 23:DA:1525:G:O2' | 2.13 | 0.47 |
| 7:AG:75:VAL:CG1 | 7:AG:144:MET:HB3 | 2.44 | 0.47 |
| 23:BA:2208:A:H1' | 23:BA:2219:G:C5 | 2.49 | 0.47 |
| 16:CP:4:ILE:HB | 16:CP:66:PRO:HB3 | 1.94 | 0.47 |
| 20:AT:36:LEU:HA | 20:AT:36:LEU:HD13 | 1.61 | 0.47 |
| 2:AB:102:LEU:HB3 | 2:AB:180:LEU:HD12 | 1.94 | 0.47 |
| 23:BA:1011:G:OP2 | 38:BU:66:ASN:ND2 | 2.44 | 0.47 |
| 36:DS:35:ILE:HG12 | 36:DS:101:LEU:HD12 | 1.96 | 0.47 |
| 25:DD:158:ALA:O | 25:DD:161:THR:OG1 | 2.25 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:BX:24:GLY:O | 41:BX:83:VAL:HG22 | 2.14 | 0.47 |
| 38:BU:109:LEU:HD23 | 38:BU:109:LEU:HA | 1.67 | 0.47 |
| 15:AO:61:GLY:O | 15:AO:65:ARG:HG3 | 2.14 | 0.47 |
| 1:CA:1442(A):G:H2' | 1:CA:1442(B):A:O4' | 2.14 | 0.47 |
| 1:CA:1089:G:N1 | 1:CA:1096:C:N4 | 2.39 | 0.47 |
| 1:AA:983:A:N3 | 1:AA:984:C:H5' | 2.28 | 0.47 |
| 1:AA:1307:U:H6 | 1:AA:1307:U:O5' | 1.97 | 0.47 |
| 1:AA:1128:C:H1' | 1:AA:1146:A:N6 | 2.29 | 0.47 |
| 23:BA:31:C:N4 | 56:BA:5264:HOH:O | 2.46 | 0.47 |
| 13:CM:85:GLY:HA3 | 13:CM:86:CYS:HA | 1.32 | 0.47 |
| 13:CM:92:HIS:CE1 | 13:CM:98:VAL:HG21 | 2.49 | 0.47 |
| 1:AA:165:C:H2' | 1:AA:166:G:H8 | 1.79 | 0.47 |
| 1:CA:149:A:O2' | 1:CA:150:C:C6 | 2.67 | 0.47 |
| 23:DA:1047:G:H2' | 23:DA:1110:G:N1 | 2.29 | 0.47 |
| 10:CJ:44:VAL:HG22 | 10:CJ:66:ARG:HD3 | 1.95 | 0.47 |
| 1:CA:375:U:C2 | 1:CA:376:G:C8 | 3.01 | 0.47 |
| 5:AE:8:GLU:HB2 | 5:AE:34:VAL:HG23 | 1.96 | 0.47 |
| 1:AA:600:C:H2' | 1:AA:601:C:C6 | 2.49 | 0.47 |
| 1:AA:785:G:H2' | 1:AA:786:G:H5' | 1.94 | 0.47 |
| 27:DF:64:ILE:HD11 | 27:DF:75:HIS:HB2 | 1.95 | 0.47 |
| 34:BQ:43:THR:OG1 | 34:BQ:45:GLN:HG2 | 2.13 | 0.47 |
| 1:CA:545:C:OP2 | 4:CD:62:GLN:NE2 | 2.46 | 0.47 |
| 1:CA:401:C:OP1 | 4:CD:73:ARG:NH2 | 2.47 | 0.47 |
| 27:BF:183:VAL:O | 27:BF:187:VAL:HG23 | 2.14 | 0.47 |
| 43:BZ:108:PRO:HB2 | 43:BZ:111:VAL:HG23 | 1.96 | 0.47 |
| 32:BO:98:VAL:HG13 | 32:BO:117:LEU:HB3 | 1.97 | 0.47 |
| 1:CA:309:G:H2' | 1:CA:310:G:H8 | 1.79 | 0.47 |
| 7:CG:133:GLY:HA2 | 7:CG:136:LYS:CB | 2.44 | 0.47 |
| 23:BA:863:A:H2' | 23:BA:864:G:C8 | 2.49 | 0.47 |
| 31:BN:34:LEU:O | 31:BN:49:GLY:HA3 | 2.14 | 0.47 |
| 1:CA:1319:A:H5' | 19:CS:4:SER:HA | 1.96 | 0.47 |
| 8:AH:56:LYS:HA | 8:AH:57:PRO:HD2 | 1.73 | 0.47 |
| 1:AA:977:A:C8 | 1:AA:1223:C:C4 | 3.00 | 0.47 |
| 1:CA:940:C:N3 | 1:CA:1343:G:N2 | 2.60 | 0.47 |
| 1:AA:1246:C:H2' | 1:AA:1247:U:O4' | 2.14 | 0.47 |
| 1:AA:1127:G:O2' | 9:AI:16:ARG:NH2 | 2.48 | 0.47 |
| 23:BA:330:A:HO2' | 23:BA:331:A:H8 | 1.62 | 0.47 |
| 1:AA:1277:C:H2' | 1:AA:1278:U:H5'' | 1.97 | 0.47 |
| 1:CA:1157:A:C5 | 1:CA:1181:G:C2 | 3.03 | 0.47 |
| 3:CC:136:GLN:HB2 | 3:CC:136:GLN:HE21 | 1.50 | 0.47 |
| 1:AA:657:G:H2' | 1:AA:658:G:H8 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:2119:A:H2' | 23:BA:2119:A:OP1 | 2.15 | 0.47 |
| 1:AA:1347:G:H5'' | 9:AI:107:ARG:CG | 2.44 | 0.47 |
| 23:BA:2713:A:N3 | 23:BA:2713:A:H2' | 2.30 | 0.47 |
| 1:CA:1017:G:H2' | 1:CA:1018:C:C6 | 2.49 | 0.47 |
| 23:BA:645:C:H2' | 23:BA:645:C:O2 | 2.14 | 0.47 |
| 1:CA:564:C:O2' | 8:CH:91:ARG:NH2 | 2.34 | 0.47 |
| 34:DQ:39:PRO:HA | 34:DQ:97:VAL:O | 2.14 | 0.47 |
| 23:BA:229:A:H8 | 23:BA:229:A:H3' | 1.77 | 0.47 |
| 1:CA:806:C:H2' | 1:CA:807:A:C8 | 2.50 | 0.47 |
| 39:BV:52:VAL:CG2 | 39:BV:55:ALA:HB3 | 2.44 | 0.47 |
| 5:CE:110:LEU:HD13 | 5:CE:118:ILE:HG21 | 1.95 | 0.47 |
| 1:CA:717:C:H4' | 11:CK:117:ASN:HB3 | 1.95 | 0.47 |
| 34:DQ:2:LEU:HB3 | 34:DQ:70:PRO:HG3 | 1.96 | 0.47 |
| 7:CG:80:VAL:HG23 | 7:CG:83:ALA:O | 2.14 | 0.47 |
| 41:BX:5:TYR:CZ | 46:B2:30:ARG:HB2 | 2.48 | 0.47 |
| 27:DF:117:ARG:HD3 | 27:DF:117:ARG:HA | 1.57 | 0.47 |
| 28:BG:38:VAL:HG22 | 28:BG:93:THR:HG23 | 1.95 | 0.47 |
| 23:BA:2091:U:O2' | 45:B1:47:GLN:HG3 | 2.14 | 0.47 |
| 23:BA:1246:A:OP1 | 27:BF:38:ARG:NH1 | 2.45 | 0.47 |
| 39:BV:76:LYS:HB2 | 39:BV:81:TYR:HB3 | 1.96 | 0.47 |
| 23:BA:789:A:H5'' | 56:BA:4568:HOH:O | 2.14 | 0.47 |
| 33:BP:65:ARG:HD3 | 33:BP:66:GLY:N | 2.29 | 0.47 |
| 7:AG:32:ARG:O | 7:AG:35:LYS:HG3 | 2.15 | 0.47 |
| 1:AA:1128:C:N3 | 1:AA:1143:G:N2 | 2.51 | 0.47 |
| 1:CA:965:A:OP1 | 1:CA:1198:G:H5'' | 2.14 | 0.47 |
| 13:CM:97:PRO:HB2 | 13:CM:103:THR:HG22 | 1.95 | 0.47 |
| 10:AJ:38:ILE:HG13 | 10:AJ:40:LEU:HD21 | 1.96 | 0.47 |
| 1:AA:1203:C:H2' | 1:AA:1204:A:O4' | 2.14 | 0.47 |
| 1:AA:954:G:H2' | 1:AA:955:U:C6 | 2.50 | 0.47 |
| 23:BA:1320:C:P | 56:BA:5012:HOH:O | 2.67 | 0.47 |
| 23:DA:1268:A:P | 56:DA:3880:HOH:O | 2.70 | 0.47 |
| 1:AA:1375:A:O3' | 7:AG:29:LYS:HE2 | 2.14 | 0.47 |
| 1:AA:370:C:H2' | 1:AA:371:G:C8 | 2.49 | 0.47 |
| 1:CA:604:G:C5 | 1:CA:605:U:C5 | 3.02 | 0.47 |
| 1:CA:475:G:H2' | 1:CA:476:G:H8 | 1.78 | 0.47 |
| 50:B6:14:THR:HB | 50:B6:48:VAL:O | 2.13 | 0.47 |
| 20:CT:86:ARG:CZ | 20:CT:86:ARG:HB3 | 2.43 | 0.47 |
| 1:CA:616:G:N2 | 1:CA:624:C:O2 | 2.42 | 0.47 |
| 2:CB:70:PHE:CD2 | 2:CB:163:PHE:HB3 | 2.50 | 0.47 |
| 1:CA:263:A:OP2 | 20:CT:79:ARG:NH1 | 2.47 | 0.47 |
| 23:BA:1513:C:H2' | 23:BA:1514:U:H6 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:CP:71:ARG:O | 16:CP:75:ARG:N | 2.47 | 0.47 |
| 23:BA:2094:G:H5' | 30:BI:25:TYR:CD2 | 2.50 | 0.47 |
| 23:DA:557:U:O2 | 31:DN:45:ASN:HB2 | 2.15 | 0.47 |
| 16:AP:23:ASP:OD1 | 16:AP:25:ARG:HG3 | 2.14 | 0.47 |
| 25:BD:10:THR:OG1 | 25:BD:13:ARG:HB2 | 2.15 | 0.47 |
| 23:BA:1628:G:H2' | 23:BA:1629:U:C6 | 2.49 | 0.47 |
| 4:AD:72:GLU:OE1 | 4:AD:207:TYR:OH | 2.19 | 0.47 |
| 1:AA:1113:C:H2' | 1:AA:1114:C:C6 | 2.48 | 0.47 |
| 23:DA:1540:U:H2' | 23:DA:1541:G:O4' | 2.15 | 0.47 |
| 7:CG:127:ALA:HB1 | 7:CG:135:VAL:HG13 | 1.96 | 0.47 |
| 23:BA:495:G:H21 | 40:BW:61:ASN:HD21 | 1.61 | 0.47 |
| 1:CA:930:C:H2' | 1:CA:931:C:H6 | 1.79 | 0.47 |
| 34:BQ:11:LYS:HE2 | 34:BQ:88:GLY:O | 2.15 | 0.47 |
| 4:CD:14:ARG:HA | 4:CD:39:PRO:HB3 | 1.97 | 0.47 |
| 23:DA:445:C:OP1 | 38:DU:2:PRO:HA | 2.14 | 0.47 |
| 3:AC:153:VAL:HA | 3:AC:197:GLY:O | 2.14 | 0.47 |
| 1:AA:1352:C:OP1 | 21:AU:3:LYS:NZ | 2.47 | 0.47 |
| 23:BA:2133:G:H21 | 23:BA:2158:A:H62 | 1.61 | 0.47 |
| 1:AA:96:U:O2' | 1:AA:97:G:H8 | 1.98 | 0.47 |
| 7:CG:42:ILE:CA | 7:CG:45:ASP:HB2 | 2.41 | 0.47 |
| 28:BG:5:VAL:HG12 | 48:B4:25:TYR:CE1 | 2.49 | 0.47 |
| 25:DD:118:VAL:N | 25:DD:129:ASN:ND2 | 2.60 | 0.47 |
| 1:CA:73:G:C6 | 1:CA:97:G:C6 | 3.02 | 0.47 |
| 30:BI:130:TYR:HD2 | 30:BI:132:PRO:HD3 | 1.79 | 0.47 |
| 23:BA:528:A:C2 | 23:BA:2042:A:H2' | 2.49 | 0.47 |
| 2:CB:61:LEU:HD21 | 2:CB:160:ASP:HB2 | 1.97 | 0.47 |
| 1:AA:142:G:H1 | 1:AA:221:C:H42 | 1.61 | 0.47 |
| 7:CG:108:ALA:O | 7:CG:119:ARG:HB3 | 2.14 | 0.47 |
| 2:AB:16:HIS:CD2 | 2:AB:209:ARG:HG3 | 2.49 | 0.47 |
| 1:CA:767:A:H2' | 1:CA:768:A:O4' | 2.14 | 0.47 |
| 43:DZ:126:VAL:HG21 | 43:DZ:161:VAL:HG13 | 1.96 | 0.47 |
| 23:DA:652(T):C:H2' | 23:DA:652(U):G:C8 | 2.49 | 0.47 |
| 27:DF:158:THR:O | 27:DF:164:ARG:NH1 | 2.44 | 0.47 |
| 1:AA:580:U:H2' | 1:AA:581:G:O4' | 2.15 | 0.47 |
| 23:BA:830:G:H4' | 23:BA:831:G:OP2 | 2.15 | 0.47 |
| 11:AK:33:THR:HA | 11:AK:40:ILE:HG12 | 1.97 | 0.47 |
| 8:AH:97:VAL:HG21 | 8:AH:128:GLY:HA2 | 1.96 | 0.47 |
| 23:BA:1321:A:H2' | 23:BA:1322:A:O4' | 2.14 | 0.47 |
| 18:CR:32:ARG:HA | 18:CR:69:THR:HG21 | 1.96 | 0.47 |
| 45:B1:51:VAL:HG11 | 45:B1:74:VAL:HG21 | 1.95 | 0.47 |
| 2:AB:86:GLU:C | 2:AB:89:GLY:H | 2.17 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:491:G:H2' | 1:CA:492:G:O4' | 2.15 | 0.47 |
| 23:DA:322:A:OP1 | 27:DF:168:ARG:NH1 | 2.48 | 0.47 |
| 23:BA:244:A:C2 | 23:BA:255:A:C4 | 3.02 | 0.47 |
| 23:DA:868:U:H2' | 23:DA:869:G:O4' | 2.14 | 0.47 |
| 1:AA:666:G:H5' | 1:AA:726:C:H1' | 1.97 | 0.47 |
| 16:AP:4:ILE:HB | 16:AP:66:PRO:HB3 | 1.95 | 0.47 |
| 1:CA:1441:G:C2 | 1:CA:1459:C:C5 | 3.02 | 0.47 |
| 1:CA:1458:G:N2 | 1:CA:1459:C:O4' | 2.47 | 0.47 |
| 33:BP:65:ARG:HB3 | 56:BP:311:HOH:O | 2.14 | 0.47 |
| 3:AC:180:ALA:O | 3:AC:203:PHE:HE1 | 1.96 | 0.47 |
| 9:CI:9:ARG:HD2 | 9:CI:104:ARG:HH21 | 1.78 | 0.47 |
| 1:AA:1307:U:C4 | 1:AA:1308:U:C5 | 3.03 | 0.47 |
| 56:CA:1967:HOH:O | 16:CP:13:HIS:CD2 | 2.67 | 0.47 |
| 23:BA:2126:A:H1' | 23:BA:2127:G:OP2 | 2.14 | 0.47 |
| 23:DA:141:A:C8 | 23:DA:1408:C:O2' | 2.55 | 0.47 |
| 24:DB:31:C:N4 | 36:DS:32:LEU:HD13 | 2.30 | 0.47 |
| 23:BA:2243:U:H2' | 23:BA:2244:U:H6 | 1.79 | 0.47 |
| 1:AA:142:G:C4 | 1:AA:143:A:C8 | 3.03 | 0.47 |
| 23:DA:530:G:C6 | 23:DA:2022:U:H5'' | 2.50 | 0.47 |
| 1:CA:59:A:H5'' | 1:CA:60:A:C5' | 2.45 | 0.47 |
| 23:BA:993:G:C6 | 23:BA:994:C:C4 | 3.03 | 0.47 |
| 17:AQ:66:SER:HB3 | 17:AQ:69:LYS:HB2 | 1.97 | 0.47 |
| 1:CA:920:U:H2' | 1:CA:921:U:H6 | 1.78 | 0.47 |
| 50:B6:25:LYS:HE3 | 50:B6:30:THR:O | 2.15 | 0.47 |
| 1:CA:113:G:N3 | 1:CA:353:A:O2' | 2.37 | 0.47 |
| 23:BA:2462:U:H1' | 23:BA:2491:U:O4 | 2.15 | 0.47 |
| 23:BA:322:A:OP2 | 27:BF:169:ASN:HB2 | 2.14 | 0.47 |
| 23:DA:1488:G:N1 | 23:DA:1489:U:O2 | 2.47 | 0.47 |
| 1:AA:458:C:H2' | 1:AA:460:G:C8 | 2.49 | 0.47 |
| 1:AA:460:G:H1' | 1:AA:472:A:H61 | 1.80 | 0.47 |
| 22:CX:3:LEU:HD21 | 22:CX:24:PHE:HB2 | 1.96 | 0.47 |
| 23:BA:2505:G:H2' | 23:BA:2576:G:O6 | 2.13 | 0.47 |
| 23:BA:1545:A:H2' | 23:BA:1546:C:O4' | 2.15 | 0.47 |
| 3:AC:132:ARG:O | 3:AC:136:GLN:N | 2.39 | 0.47 |
| 23:BA:1578:U:H2' | 23:BA:1579:A:H5' | 1.96 | 0.47 |
| 31:BN:96:GLU:CD | 31:BN:96:GLU:H | 2.18 | 0.47 |
| 8:AH:31:PHE:CE2 | 8:AH:35:ILE:HD11 | 2.49 | 0.47 |
| 23:DA:1339:G:H5'' | 41:DX:16:LYS:HD3 | 1.97 | 0.47 |
| 23:DA:212:G:O2' | 23:DA:213:A:H5' | 2.15 | 0.47 |
| 23:DA:684:G:OP1 | 51:D7:16:HIS:ND1 | 2.46 | 0.47 |
| 6:CF:45:LEU:HD11 | 6:CF:57:GLN:OE1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:16:LEU:HD22 | 9:AI:45:ALA:H | 1.79 | 0.47 |
| 23:DA:2336:A:H61 | 44:D0:43:THR:CG2 | 2.28 | 0.47 |
| 23:BA:885:C:H3' | 23:BA:886:C:H6 | 1.79 | 0.47 |
| 1:AA:977:A:C2' | 1:AA:978:A:H5' | 2.45 | 0.47 |
| 23:BA:1358:G:O2' | 23:BA:1359:A:H5' | 2.14 | 0.47 |
| 2:CB:226:ARG:HG3 | 2:CB:227:GLY:H | 1.80 | 0.47 |
| 1:CA:1225:A:H2' | 1:CA:1225:A:N3 | 2.30 | 0.47 |
| 1:AA:1298:C:C4 | 7:AG:114:ARG:HD2 | 2.49 | 0.47 |
| 1:CA:1023:G:H3' | 1:CA:1024:G:C8 | 2.49 | 0.47 |
| 1:AA:971:G:OP1 | 1:AA:972:C:H5'' | 2.15 | 0.47 |
| 1:CA:1053:G:N7 | 1:CA:1200:C:H5'' | 2.30 | 0.47 |
| 1:CA:946:A:C2 | 1:CA:1236:A:C2 | 3.02 | 0.47 |
| 1:AA:676:A:O2' | 1:AA:677:U:H5' | 2.15 | 0.47 |
| 23:DA:2127:G:N2 | 23:DA:2173:A:H1' | 2.29 | 0.47 |
| 23:DA:2117:A:N6 | 23:DA:2166:G:H22 | 2.11 | 0.47 |
| 1:AA:1327:C:H5'' | 21:AU:20:LYS:HB2 | 1.96 | 0.47 |
| 2:CB:179:LYS:HA | 8:CH:72:PRO:HG3 | 1.96 | 0.47 |
| 1:AA:345:C:H4' | 1:AA:346:G:C5 | 2.50 | 0.47 |
| 1:AA:346:G:H2' | 1:AA:347:G:O4' | 2.15 | 0.47 |
| 7:CG:71:PRO:HA | 7:CG:138:LYS:NZ | 2.30 | 0.47 |
| 9:AI:27:THR:HA | 9:AI:31:GLN:O | 2.14 | 0.47 |
| 3:CC:182:ILE:HG23 | 3:CC:202:ILE:C | 2.34 | 0.47 |
| 23:BA:975:C:C6 | 56:BA:4752:HOH:O | 2.56 | 0.47 |
| 1:AA:605:U:H2' | 1:AA:606:G:H8 | 1.76 | 0.47 |
| 1:AA:1133:G:H2' | 1:AA:1134:G:C8 | 2.50 | 0.47 |
| 23:DA:218:A:C2 | 23:DA:235:U:H4' | 2.49 | 0.47 |
| 43:BZ:126:VAL:HG21 | 43:BZ:161:VAL:HG13 | 1.95 | 0.47 |
| 1:CA:709:G:C4 | 1:CA:710:G:C8 | 3.02 | 0.47 |
| 1:AA:626:U:C2 | 1:AA:627:G:C8 | 3.03 | 0.47 |
| 24:BB:110:G:C2 | 24:BB:111:G:C5 | 3.02 | 0.47 |
| 1:CA:1063:C:H3' | 1:CA:1064:G:H2' | 1.96 | 0.47 |
| 28:BG:81:LYS:CB | 28:BG:82:LEU:HD12 | 2.44 | 0.47 |
| 5:CE:8:GLU:HB2 | 5:CE:34:VAL:HG23 | 1.96 | 0.47 |
| 23:DA:226:G:H21 | 23:DA:228:A:N6 | 2.13 | 0.47 |
| 23:DA:192:C:O2' | 23:DA:802:A:N3 | 2.42 | 0.47 |
| 13:CM:60:VAL:HG13 | 13:CM:64:TRP:CZ3 | 2.50 | 0.47 |
| 5:AE:19:MET:SD | 5:AE:24:ARG:HB3 | 2.55 | 0.47 |
| 23:DA:543:C:H42 | 23:DA:549:G:H1 | 1.62 | 0.47 |
| 37:DT:93:ARG:NH1 | 37:DT:93:ARG:HG2 | 2.30 | 0.47 |
| 23:DA:2698:U:H2' | 23:DA:2699:C:C6 | 2.50 | 0.47 |
| 23:BA:1695:G:H2' | 23:BA:1696:G:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:879:G:H2' | 23:DA:880:G:O4' | 2.14 | 0.47 |
| 31:BN:55:VAL:HG22 | 31:BN:125:GLY:HA3 | 1.96 | 0.47 |
| 1:AA:552:U:H4' | 12:AL:86:ARG:HG2 | 1.96 | 0.47 |
| 23:BA:2469:A:C2 | 23:BA:2482:G:C8 | 3.03 | 0.47 |
| 23:DA:1545:A:H2' | 23:DA:1546:C:O4' | 2.14 | 0.47 |
| 23:DA:396:G:H1' | 45:D1:42:GLN:HB3 | 1.97 | 0.47 |
| 29:DH:37:VAL:HG12 | 29:DH:38:SER:O | 2.14 | 0.47 |
| 23:BA:1794:U:H2' | 23:BA:1795:C:C6 | 2.49 | 0.47 |
| 23:BA:2505:G:O6 | 23:BA:2576:G:H2' | 2.14 | 0.47 |
| 23:DA:2011:U:OP1 | 40:DW:42:ARG:NH1 | 2.48 | 0.47 |
| 2:CB:142:LEU:HG | 2:CB:146:GLN:HE21 | 1.80 | 0.47 |
| 23:BA:1810:A:H2' | 23:BA:1811:G:O4' | 2.14 | 0.47 |
| 1:CA:505:G:C6 | 1:CA:535:A:C2 | 3.03 | 0.47 |
| 11:AK:46:GLY:HA2 | 11:AK:50:TYR:O | 2.15 | 0.47 |
| 23:BA:652(O):C:H2' | 23:BA:652(P):G:C8 | 2.50 | 0.47 |
| 1:CA:819:A:H4' | 1:CA:820:U:OP2 | 2.13 | 0.47 |
| 11:AK:32:ILE:HD11 | 11:AK:68:ALA:HB1 | 1.96 | 0.47 |
| 23:DA:1578:U:H2' | 23:DA:1579:A:H5' | 1.97 | 0.47 |
| 25:BD:33:LEU:O | 25:BD:64:ILE:HG13 | 2.14 | 0.47 |
| 1:AA:131:C:OP2 | 1:AA:189(G):G:O2' | 2.32 | 0.47 |
| 43:BZ:151:HIS:HD2 | 43:BZ:168:GLU:O | 1.98 | 0.47 |
| 23:DA:2881:C:H2' | 23:DA:2882:A:O4' | 2.15 | 0.47 |
| 32:BO:4:PRO:O | 32:BO:5:GLN:HB2 | 2.14 | 0.47 |
| 23:BA:2674:G:H2' | 23:BA:2675:A:C8 | 2.49 | 0.47 |
| 32:DO:98:VAL:HG13 | 32:DO:117:LEU:HB3 | 1.96 | 0.47 |
| 39:DV:65:GLY:HA3 | 39:DV:91:TYR:CZ | 2.50 | 0.47 |
| 6:CF:99:ALA:HB3 | 18:CR:29:PHE:CE1 | 2.49 | 0.47 |
| 38:DU:14:HIS:HA | 38:DU:32:PHE:CE2 | 2.50 | 0.47 |
| 27:BF:117:ARG:HA | 27:BF:117:ARG:HD3 | 1.56 | 0.47 |
| 32:BO:70:LYS:HE2 | 32:BO:70:LYS:HB3 | 1.70 | 0.47 |
| 33:DP:138:LEU:HD23 | 33:DP:145:PRO:HG3 | 1.97 | 0.47 |
| 23:DA:1849:G:H2' | 23:DA:1850:G:H8 | 1.79 | 0.47 |
| 2:AB:155:LEU:HD11 | 2:AB:159:PRO:HD3 | 1.95 | 0.47 |
| 18:AR:32:ARG:HA | 18:AR:69:THR:HG21 | 1.96 | 0.47 |
| 1:CA:109:A:C6 | 1:CA:326:G:C6 | 3.03 | 0.47 |
| 26:BE:10:GLY:HA2 | 26:BE:192:ASN:OD1 | 2.14 | 0.47 |
| 23:DA:86:C:H4' | 23:DA:104:U:H1' | 1.97 | 0.47 |
| 1:AA:1460:A:H2' | 1:AA:1461:G:O4' | 2.15 | 0.47 |
| 1:AA:1004:A:H2' | 1:AA:1036:G:O6 | 2.15 | 0.47 |
| 1:AA:1027:C:C1' | 1:AA:1034:G:H22 | 2.27 | 0.47 |
| 1:AA:1002:G:N2 | 1:AA:1039:C:H1' | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:973:G:C3' | 1:CA:974:A:H5'' | 2.37 | 0.47 |
| 9:CI:10:ARG:O | 9:CI:72:GLY:HA2 | 2.15 | 0.47 |
| 1:AA:1053:G:C3' | 1:AA:1054:C:H5' | 2.44 | 0.47 |
| 1:AA:1276:G:H2' | 1:AA:1277:C:O4' | 2.15 | 0.47 |
| 23:DA:1204:A:N1 | 23:DA:1241:A:N7 | 2.63 | 0.47 |
| 23:BA:301:G:C4 | 23:BA:302:C:C5 | 3.03 | 0.47 |
| 1:AA:51:A:C6 | 1:AA:353:A:C2 | 3.02 | 0.47 |
| 10:AJ:49:VAL:CG2 | 14:AN:41:ARG:HB2 | 2.44 | 0.47 |
| 2:CB:171:ALA:HA | 2:CB:174:VAL:HB | 1.96 | 0.47 |
| 1:AA:1125:U:H5' | 1:AA:1126:U:C5 | 2.47 | 0.47 |
| 2:AB:111:ARG:HD3 | 2:AB:111:ARG:HA | 1.54 | 0.47 |
| 1:AA:1399:C:C2 | 1:AA:1401:G:C5 | 3.03 | 0.47 |
| 19:CS:12:ASP:O | 19:CS:14:HIS:N | 2.40 | 0.47 |
| 23:DA:1429:G:H2' | 23:DA:1430:C:H6 | 1.77 | 0.47 |
| 1:CA:1133:G:H2' | 1:CA:1134:G:C8 | 2.50 | 0.47 |
| 23:DA:2262:U:H4' | 23:DA:2328:A:C2 | 2.50 | 0.47 |
| 1:AA:937:A:H3' | 1:AA:938:A:C8 | 2.48 | 0.47 |
| 6:CF:97:PHE:O | 18:CR:31:LEU:HD23 | 2.15 | 0.47 |
| 1:CA:555:C:H2' | 1:CA:556:C:H6 | 1.79 | 0.47 |
| 11:CK:32:ILE:HG12 | 11:CK:32:ILE:H | 1.57 | 0.47 |
| 23:BA:2516:G:C6 | 23:BA:2517:C:C4 | 3.02 | 0.47 |
| 35:DR:50:HIS:O | 35:DR:54:LEU:HD22 | 2.15 | 0.47 |
| 43:BZ:151:HIS:N | 43:BZ:154:ASP:OD1 | 2.46 | 0.47 |
| 47:D3:44:ARG:O | 47:D3:48:GLU:HG3 | 2.15 | 0.47 |
| 39:BV:60:GLU:HB2 | 39:BV:97:LYS:HE2 | 1.96 | 0.47 |
| 23:BA:34:C:H5'' | 23:BA:35:G:OP2 | 2.15 | 0.47 |
| 23:BA:1641:A:H2' | 23:BA:1642:G:O4' | 2.14 | 0.47 |
| 23:DA:614(C):A:C4 | 27:DF:180:GLY:HA2 | 2.50 | 0.47 |
| 5:CE:78:HIS:HA | 8:CH:105:ARG:HG3 | 1.95 | 0.47 |
| 43:DZ:40:ASP:OD1 | 43:DZ:42:VAL:HG13 | 2.15 | 0.47 |
| 23:DA:1039:G:H1' | 23:DA:1117:G:N2 | 2.30 | 0.47 |
| 1:CA:1229:A:H2' | 1:CA:1230:C:C6 | 2.50 | 0.47 |
| 10:CJ:49:VAL:CG2 | 14:CN:41:ARG:HB2 | 2.43 | 0.47 |
| 1:AA:959:A:C2 | 1:AA:1221:G:N3 | 2.83 | 0.47 |
| 19:AS:52:TYR:HD1 | 19:AS:57:HIS:CD2 | 2.32 | 0.47 |
| 1:CA:964:A:H8 | 1:CA:964:A:O5' | 1.98 | 0.47 |
| 10:AJ:9:ARG:HG3 | 10:AJ:95:GLU:HB3 | 1.96 | 0.47 |
| 1:CA:9:G:H2' | 1:CA:10:A:H8 | 1.79 | 0.47 |
| 23:BA:1529:G:O2' | 23:BA:1530:C:H5' | 2.15 | 0.47 |
| 1:AA:673:G:O3' | 6:AF:87:ARG:NH2 | 2.48 | 0.47 |
| 23:DA:2807:G:N1 | 23:DA:2808:U:C2 | 2.83 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1299:A:C4 | 1:CA:1301:U:H1' | 2.50 | 0.47 |
| 1:CA:77:G:O6 | 1:CA:78:G:C2 | 2.68 | 0.47 |
| 4:CD:159:ARG:O | 4:CD:162:LEU:N | 2.47 | 0.47 |
| 5:AE:90:VAL:O | 5:AE:91:LEU:HD13 | 2.15 | 0.47 |
| 28:DG:5:VAL:HG11 | 28:DG:101:ILE:HG12 | 1.96 | 0.47 |
| 1:AA:475:G:H2' | 1:AA:476:G:C8 | 2.49 | 0.47 |
| 38:DU:76:TYR:CZ | 38:DU:80:ILE:HG13 | 2.49 | 0.47 |
| 1:AA:836:G:C6 | 1:AA:851:G:C6 | 3.03 | 0.47 |
| 35:BR:20:LEU:HD21 | 35:BR:40:LYS:HD3 | 1.96 | 0.47 |
| 10:CJ:45:ARG:N | 10:CJ:65:LEU:O | 2.33 | 0.47 |
| 1:AA:1492:A:H4' | 1:AA:1492:A:OP1 | 2.14 | 0.47 |
| 1:CA:130:A:O2' | 1:CA:131:C:O5' | 2.32 | 0.47 |
| 30:BI:72:LEU:C | 30:BI:74:ASN:H | 2.17 | 0.47 |
| 26:DE:67:PHE:HD1 | 26:DE:72:VAL:HG12 | 1.80 | 0.47 |
| 1:AA:539:A:OP2 | 12:AL:115:LYS:HD2 | 2.14 | 0.47 |
| 31:DN:30:ILE:HG23 | 31:DN:52:VAL:HG11 | 1.97 | 0.47 |
| 23:BA:576:U:H2' | 23:BA:577:G:C8 | 2.49 | 0.47 |
| 4:CD:121:VAL:HA | 4:CD:126:ILE:HG12 | 1.95 | 0.47 |
| 15:AO:15:PHE:CE2 | 15:AO:84:LYS:HD2 | 2.49 | 0.47 |
| 25:DD:172:TYR:CD1 | 25:DD:186:HIS:HA | 2.50 | 0.47 |
| 15:CO:74:ASP:OD1 | 15:CO:76:GLU:HB2 | 2.15 | 0.47 |
| 52:B8:54:GLU:O | 52:B8:58:ILE:HG12 | 2.15 | 0.47 |
| 23:BA:2536:G:C6 | 23:BA:2537:U:C4 | 3.03 | 0.47 |
| 9:CI:105:ASP:HB2 | 9:CI:107:ARG:HD3 | 1.97 | 0.47 |
| 7:AG:13:GLN:O | 7:AG:21:VAL:HA | 2.15 | 0.47 |
| 1:AA:403:C:H2' | 1:AA:404:U:H6 | 1.79 | 0.47 |
| 23:DA:2777:G:H5'' | 23:DA:2778:A:H5' | 1.97 | 0.47 |
| 1:AA:1112:C:O5' | 1:AA:1112:C:H6 | 1.98 | 0.47 |
| 30:DI:124:GLY:H | 30:DI:144:VAL:HG13 | 1.80 | 0.47 |
| 30:DI:110:ASP:N | 30:DI:130:TYR:OH | 2.45 | 0.47 |
| 23:DA:2820:A:O2' | 23:DA:2821:A:OP1 | 2.29 | 0.47 |
| 1:CA:949:A:C6 | 1:CA:950:U:C4 | 3.03 | 0.47 |
| 23:BA:2176:A:H5' | 23:BA:2177:C:OP2 | 2.15 | 0.47 |
| 10:CJ:50:ILE:CA | 10:CJ:60:ARG:HG2 | 2.32 | 0.47 |
| 1:AA:1190:G:OP1 | 3:AC:5:ILE:N | 2.48 | 0.47 |
| 23:DA:2311:A:O2' | 23:DA:2312:U:O4' | 2.33 | 0.47 |
| 1:CA:1395:C:O2' | 1:CA:1401:G:O2' | 2.13 | 0.47 |
| 23:BA:819:A:C4 | 23:BA:1189:A:C2 | 3.03 | 0.47 |
| 23:DA:2317:C:N4 | 23:DA:2318:G:C6 | 2.83 | 0.47 |
| 23:DA:2319:G:H1' | 23:DA:2320:A:H5'' | 1.97 | 0.47 |
| 1:AA:943:U:O4 | 1:AA:1340:A:N1 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CN:4:LYS:HA | 14:CN:7:ILE:HG12 | 1.96 | 0.47 |
| 14:CN:18:VAL:HG12 | 14:CN:18:VAL:O | 2.15 | 0.47 |
| 1:AA:939:G:O2' | 1:AA:1375:A:H2' | 2.15 | 0.47 |
| 9:AI:7:THR:HG21 | 9:AI:9:ARG:HH11 | 1.80 | 0.47 |
| 1:AA:627:G:H2' | 1:AA:628:G:C8 | 2.48 | 0.47 |
| 1:AA:627:G:N3 | 1:AA:628:G:C8 | 2.83 | 0.47 |
| 28:DG:66:GLN:HG2 | 48:D4:1:MET:HE3 | 1.97 | 0.47 |
| 23:BA:184:C:H2' | 23:BA:185:U:H6 | 1.79 | 0.47 |
| 1:CA:56:U:H2' | 1:CA:57:G:H8 | 1.80 | 0.47 |
| 23:DA:2846:G:H2' | 23:DA:2847:U:O4' | 2.15 | 0.47 |
| 26:BE:52:LEU:O | 26:BE:76:ARG:HG2 | 2.15 | 0.47 |
| 1:CA:232:G:H1' | 1:CA:262:A:N1 | 2.30 | 0.47 |
| 33:DP:84:ASN:ND2 | 33:DP:117:GLU:HB2 | 2.29 | 0.47 |
| 23:BA:1649:G:N1 | 23:BA:2009:G:C6 | 2.83 | 0.47 |
| 43:DZ:102:LEU:HD13 | 43:DZ:123:ASP:HA | 1.97 | 0.47 |
| 1:AA:1446:U:H4' | 1:AA:1447:A:C6 | 2.50 | 0.47 |
| 23:BA:2008:C:OP2 | 56:BA:4713:HOH:O | 2.20 | 0.47 |
| 23:DA:1695:G:H2' | 23:DA:1696:G:O4' | 2.15 | 0.47 |
| 50:D6:25:LYS:HE3 | 50:D6:30:THR:O | 2.13 | 0.47 |
| 44:B0:24:LYS:O | 44:B0:25:ARG:HD3 | 2.15 | 0.47 |
| 23:DA:272:G:N7 | 23:DA:421:U:H2' | 2.30 | 0.47 |
| 17:AQ:86:GLU:O | 17:AQ:90:ILE:HG13 | 2.15 | 0.47 |
| 28:BG:37:VAL:HG23 | 28:BG:99:MET:HG3 | 1.96 | 0.47 |
| 13:CM:16:ASP:HB3 | 13:CM:34:LEU:HD11 | 1.97 | 0.47 |
| 26:DE:92:THR:O | 26:DE:95:ILE:HG23 | 2.14 | 0.47 |
| 24:DB:24:G:H4' | 24:DB:25:A:C8 | 2.49 | 0.47 |
| 32:DO:107:ARG:CZ | 37:DT:36:GLU:HG3 | 2.44 | 0.47 |
| 23:DA:652(Q):G:H2' | 23:DA:652(R):C:C6 | 2.50 | 0.47 |
| 37:BT:93:ARG:HH11 | 37:BT:93:ARG:HG2 | 1.79 | 0.47 |
| 23:DA:1891:G:O5' | 23:DA:1891:G:H8 | 1.97 | 0.47 |
| 53:D9:17:ILE:HD13 | 53:D9:17:ILE:HA | 1.61 | 0.47 |
| 6:CF:25:ILE:CD1 | 6:CF:82:ARG:HE | 2.28 | 0.47 |
| 1:CA:1441:G:N3 | 1:CA:1459:C:H5 | 2.13 | 0.46 |
| 2:AB:185:ILE:HA | 2:AB:199:TYR:O | 2.15 | 0.46 |
| 1:AA:1362:C:H2' | 1:AA:1363:C:H5" | 1.97 | 0.46 |
| 1:CA:1401:G:C2 | 1:CA:1402:C:H1' | 2.50 | 0.46 |
| 23:DA:1021:A:C8 | 23:DA:1021:A:H3' | 2.50 | 0.46 |
| 28:DG:11:TYR:HB2 | 28:DG:176:LEU:HD21 | 1.97 | 0.46 |
| 23:DA:1530:C:H1' | 23:DA:1531:C:OP1 | 2.14 | 0.46 |
| 3:CC:19:GLU:HA | 3:CC:54:ARG:HH12 | 1.80 | 0.46 |
| 23:DA:2206:G:HO2' | 23:DA:2207:G:P | 2.38 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:CG:69:VAL:HG21 | 7:CG:104:LEU:CD1 | 2.40 | 0.46 |
| 1:CA:1323:G:H4' | 1:CA:1363:C:C2 | 2.50 | 0.46 |
| 1:AA:934:C:H42 | 1:AA:939:G:N2 | 2.13 | 0.46 |
| 29:BH:154:PRO:HB3 | 29:BH:163:TYR:CE2 | 2.51 | 0.46 |
| 1:AA:1347:G:C8 | 9:AI:107:ARG:HB3 | 2.49 | 0.46 |
| 1:AA:309:G:H2' | 1:AA:310:G:H8 | 1.79 | 0.46 |
| 42:DY:86:ARG:HD2 | 42:DY:100:ALA:HA | 1.97 | 0.46 |
| 34:DQ:133:ARG:HG2 | 34:DQ:134:ARG:N | 2.29 | 0.46 |
| 12:AL:25:PRO:C | 12:AL:27:LEU:H | 2.16 | 0.46 |
| 20:AT:30:LYS:HA | 20:AT:33:ILE:HD13 | 1.97 | 0.46 |
| 38:BU:76:TYR:CZ | 38:BU:80:ILE:HG13 | 2.50 | 0.46 |
| 1:CA:350:G:O2' | 1:CA:351:G:H5' | 2.15 | 0.46 |
| 1:AA:921:U:H2' | 1:AA:922:G:O4' | 2.15 | 0.46 |
| 1:CA:600:C:H2' | 1:CA:601:C:C6 | 2.50 | 0.46 |
| 23:BA:879:G:H2' | 23:BA:880:G:O4' | 2.15 | 0.46 |
| 23:DA:2536:G:C6 | 23:DA:2537:U:C4 | 3.03 | 0.46 |
| 43:DZ:121:HIS:HB3 | 43:DZ:123:ASP:O | 2.15 | 0.46 |
| 16:AP:23:ASP:O | 16:AP:26:ARG:HB2 | 2.15 | 0.46 |
| 6:CF:44:GLY:HA2 | 6:CF:59:TYR:CZ | 2.50 | 0.46 |
| 29:BH:40:GLU:OE2 | 29:BH:60:ARG:NH1 | 2.48 | 0.46 |
| 43:DZ:19:ARG:HA | 43:DZ:23:LYS:O | 2.15 | 0.46 |
| 8:CH:25:ASP:HA | 8:CH:59:LEU:O | 2.15 | 0.46 |
| 28:DG:132:ASN:OD1 | 28:DG:158:ALA:HA | 2.15 | 0.46 |
| 42:DY:7:VAL:HG21 | 42:DY:72:VAL:HG12 | 1.96 | 0.46 |
| 1:CA:956:U:H4' | 19:CS:82:GLY:O | 2.15 | 0.46 |
| 30:BI:127:VAL:HA | 30:BI:140:LEU:O | 2.15 | 0.46 |
| 23:BA:414:C:H2' | 23:BA:415:A:C8 | 2.51 | 0.46 |
| 2:CB:59:GLU:O | 2:CB:63:MET:HG2 | 2.15 | 0.46 |
| 34:BQ:26:TYR:CE1 | 34:BQ:28:ALA:HB2 | 2.50 | 0.46 |
| 25:DD:132:PRO:HD3 | 25:DD:190:TYR:CZ | 2.50 | 0.46 |
| 23:DA:527:C:C4 | 23:DA:2779:U:H2' | 2.49 | 0.46 |
| 2:CB:233:SER:OG | 2:CB:234:PRO:HD2 | 2.15 | 0.46 |
| 1:AA:1198:G:C6 | 1:AA:1199:U:C4 | 3.04 | 0.46 |
| 23:DA:2169:A:H3' | 23:DA:2170:A:H8 | 1.81 | 0.46 |
| 23:DA:2298:A:H2' | 23:DA:2299:G:O4' | 2.15 | 0.46 |
| 17:CQ:55:ASP:HA | 17:CQ:79:SER:HA | 1.97 | 0.46 |
| 23:BA:2472:G:H5' | 23:BA:2473:U:C5' | 2.40 | 0.46 |
| 13:AM:10:PRO:O | 13:AM:45:VAL:HG11 | 2.15 | 0.46 |
| 16:AP:28:ARG:HG2 | 16:AP:29:ASP:OD2 | 2.15 | 0.46 |
| 26:BE:47:VAL:CG1 | 26:BE:86:PRO:HD2 | 2.42 | 0.46 |
| 1:AA:746:A:H2' | 1:AA:747:C:C6 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:910:A:N7 | 34:DQ:13:GLN:HG3 | 2.29 | 0.46 |
| 30:BI:9:LEU:HB3 | 30:BI:12:LEU:HB2 | 1.97 | 0.46 |
| 11:CK:84:VAL:CG1 | 11:CK:91:ARG:HD2 | 2.44 | 0.46 |
| 7:CG:119:ARG:HB2 | 7:CG:119:ARG:HE | 1.45 | 0.46 |
| 1:AA:1137:C:H5' | 1:AA:1138:G:C6 | 2.50 | 0.46 |
| 36:BS:96:GLY:H | 36:BS:99:LYS:H | 1.64 | 0.46 |
| 23:DA:1049:C:H1' | 23:DA:1113:U:H4' | 1.97 | 0.46 |
| 30:BI:73:GLU:HG2 | 30:BI:139:GLN:O | 2.15 | 0.46 |
| 23:BA:443:A:H1' | 23:BA:1201:C:O4' | 2.14 | 0.46 |
| 23:BA:143(A):C:H2' | 23:BA:144:C:C6 | 2.50 | 0.46 |
| 27:DF:110:LEU:HD21 | 27:DF:181:LEU:HG | 1.96 | 0.46 |
| 9:AI:43:ALA:O | 9:AI:45:ALA:HA | 2.15 | 0.46 |
| 23:BA:709:U:H2' | 23:BA:710:G:C8 | 2.51 | 0.46 |
| 1:AA:555:C:H2' | 1:AA:556:C:C6 | 2.50 | 0.46 |
| 47:D3:10:LYS:NZ | 47:D3:15:TYR:OH | 2.47 | 0.46 |
| 23:BA:896:A:N1 | 34:BQ:60:ARG:NH2 | 2.63 | 0.46 |
| 41:BX:35:THR:O | 41:BX:39:ILE:HG13 | 2.16 | 0.46 |
| 38:BU:36:ARG:HD2 | 38:BU:40:PHE:CZ | 2.50 | 0.46 |
| 43:BZ:138:GLU:HG2 | 43:BZ:156:LYS:NZ | 2.30 | 0.46 |
| 1:CA:105:G:H2' | 1:CA:106:C:C6 | 2.51 | 0.46 |
| 37:DT:118:ARG:HG3 | 37:DT:118:ARG:HH11 | 1.80 | 0.46 |
| 19:AS:9:VAL:HG12 | 19:AS:10:PHE:H | 1.80 | 0.46 |
| 1:CA:1349:A:H2' | 1:CA:1350:A:C8 | 2.39 | 0.46 |
| 1:CA:1006:C:H42 | 1:CA:1024:G:N2 | 1.93 | 0.46 |
| 33:DP:65:ARG:HD3 | 33:DP:66:GLY:N | 2.30 | 0.46 |
| 1:CA:1307:U:H2' | 1:CA:1308:U:C6 | 2.50 | 0.46 |
| 28:DG:19:LEU:HG | 28:DG:175:LEU:HD22 | 1.97 | 0.46 |
| 1:CA:1240:U:C5' | 1:CA:1241:G:H8 | 2.29 | 0.46 |
| 1:CA:1297:C:C3' | 1:CA:1298:C:H5' | 2.44 | 0.46 |
| 1:CA:1157:A:C6 | 1:CA:1180:A:C5 | 3.03 | 0.46 |
| 1:CA:413:G:N7 | 4:CD:35:ARG:NH2 | 2.63 | 0.46 |
| 4:CD:36:ARG:HB3 | 4:CD:38:TYR:CZ | 2.51 | 0.46 |
| 19:CS:36:ARG:HB3 | 19:CS:72:GLY:HA3 | 1.97 | 0.46 |
| 23:BA:207:A:H2' | 23:BA:208:C:O4' | 2.15 | 0.46 |
| 25:DD:118:VAL:N | 25:DD:129:ASN:HD22 | 2.09 | 0.46 |
| 1:CA:1106:G:H5'' | 3:CC:172:ARG:CD | 2.44 | 0.46 |
| 1:AA:1328:C:H2' | 1:AA:1329:A:H8 | 1.80 | 0.46 |
| 23:DA:2544:G:H1' | 23:DA:2646:C:H4' | 1.97 | 0.46 |
| 1:CA:707:C:O2' | 1:CA:708:C:H5' | 2.16 | 0.46 |
| 3:CC:147:LYS:O | 3:CC:203:PHE:HD2 | 1.97 | 0.46 |
| 23:DA:512:G:C8 | 56:DA:3836:HOH:O | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1016:A:H1' | 1:CA:1218:C:H1' | 1.97 | 0.46 |
| 36:BS:59:LYS:HE2 | 36:BS:60:GLY:HA2 | 1.98 | 0.46 |
| 7:CG:44:TYR:HA | 7:CG:47:CYS:HB2 | 1.97 | 0.46 |
| 23:DA:582:G:H2' | 23:DA:583:G:C8 | 2.50 | 0.46 |
| 23:BA:1450:G:H2' | 23:BA:1450(A):C:H6 | 1.80 | 0.46 |
| 10:AJ:32:ALA:HA | 10:AJ:33:GLN:HA | 1.70 | 0.46 |
| 1:AA:1380:U:C5 | 7:AG:3:ARG:HA | 2.50 | 0.46 |
| 2:AB:47:THR:HG23 | 2:AB:202:PRO:HG2 | 1.97 | 0.46 |
| 23:BA:118:A:C8 | 23:BA:119:A:C8 | 3.03 | 0.46 |
| 11:CK:99:GLN:HG3 | 11:CK:105:VAL:HG11 | 1.97 | 0.46 |
| 23:DA:2870:C:H2' | 23:DA:2871:C:O4' | 2.16 | 0.46 |
| 1:CA:11:G:C6 | 1:CA:12:U:C4 | 3.03 | 0.46 |
| 1:AA:928:G:C2 | 1:AA:1390:U:O2 | 2.68 | 0.46 |
| 34:BQ:2:LEU:HB3 | 34:BQ:70:PRO:HG3 | 1.97 | 0.46 |
| 23:DA:1106:G:O2' | 23:DA:1107:G:OP1 | 2.29 | 0.46 |
| 33:BP:82:GLY:HA2 | 33:BP:113:LYS:O | 2.15 | 0.46 |
| 23:BA:54:G:O6 | 56:BA:3995:HOH:O | 2.20 | 0.46 |
| 24:BB:46:A:C5 | 24:BB:47:C:C5 | 3.03 | 0.46 |
| 23:BA:944:G:H2' | 56:BA:4981:HOH:O | 2.15 | 0.46 |
| 23:DA:1945:G:H2' | 23:DA:1946:U:C6 | 2.51 | 0.46 |
| 29:DH:149:ARG:NH1 | 29:DH:167:GLU:OE1 | 2.49 | 0.46 |
| 29:DH:149:ARG:HG3 | 29:DH:162:ILE:O | 2.15 | 0.46 |
| 1:CA:1441:G:H5' | 1:CA:1442:G:OP1 | 2.15 | 0.46 |
| 1:AA:1027:C:C2 | 1:AA:1034:G:N1 | 2.82 | 0.46 |
| 1:CA:953:G:C6 | 1:CA:1228:C:N3 | 2.82 | 0.46 |
| 23:DA:2175:C:H2' | 23:DA:2176:A:O4' | 2.16 | 0.46 |
| 23:BA:27:G:O2' | 23:BA:28:A:OP2 | 2.26 | 0.46 |
| 23:BA:2319:G:H1' | 23:BA:2320:A:H5'' | 1.98 | 0.46 |
| 1:CA:1501:C:N4 | 1:CA:1504:G:C2 | 2.84 | 0.46 |
| 21:AU:12:LYS:HE2 | 21:AU:21:TYR:HD1 | 1.81 | 0.46 |
| 3:CC:32:LEU:CD1 | 3:CC:59:ARG:HD2 | 2.44 | 0.46 |
| 23:BA:1534:U:O2' | 23:BA:1535:A:P | 2.73 | 0.46 |
| 23:BA:188:G:H1 | 23:BA:208:C:N4 | 2.13 | 0.46 |
| 39:DV:95:LEU:HD13 | 39:DV:97:LYS:HD3 | 1.98 | 0.46 |
| 9:AI:18:PHE:CD1 | 9:AI:62:TYR:HB3 | 2.51 | 0.46 |
| 23:BA:1505:C:H2' | 23:BA:1506:C:H6 | 1.80 | 0.46 |
| 23:DA:2002:G:OP2 | 35:DR:9:LYS:NZ | 2.48 | 0.46 |
| 1:AA:1104:G:C2 | 1:AA:1105:A:C4 | 3.03 | 0.46 |
| 13:AM:102:ARG:NH1 | 13:AM:104:ARG:HD3 | 2.31 | 0.46 |
| 3:AC:36:ASP:HB2 | 3:AC:40:ARG:NH1 | 2.30 | 0.46 |
| 34:DQ:103:MET:CE | 34:DQ:125:LEU:HD13 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:BA:228:A:H2' | 23:BA:230:U:O4' | 2.15 | 0.46 |
| 51:D7:9:ARG:HB3 | 51:D7:46:VAL:HG23 | 1.97 | 0.46 |
| 23:DA:2110:G:O2' | 23:DA:2120:G:H5' | 2.15 | 0.46 |
| 23:BA:2463:C:O2' | 23:BA:2464:C:H5' | 2.16 | 0.46 |
| 1:CA:1264:C:O2' | 1:CA:1265:G:H5' | 2.15 | 0.46 |
| 1:AA:545:C:OP2 | 4:AD:62:GLN:NE2 | 2.49 | 0.46 |
| 1:CA:191:G:H21 | 20:CT:103:GLY:HA2 | 1.81 | 0.46 |
| 25:BD:13:ARG:HD2 | 25:BD:16:MET:HE3 | 1.96 | 0.46 |
| 23:DA:1040:C:H2' | 23:DA:1041:C:C1' | 2.44 | 0.46 |
| 47:D3:10:LYS:HB3 | 47:D3:53:LEU:HA | 1.97 | 0.46 |
| 4:AD:157:LEU:O | 4:AD:161:ASN:ND2 | 2.29 | 0.46 |
| 23:BA:265:A:N6 | 23:BA:427:U:O2' | 2.43 | 0.46 |
| 23:BA:1907:G:C6 | 23:BA:1908:C:C4 | 3.04 | 0.46 |
| 25:DD:112:GLN:HB2 | 25:DD:115:GLN:OE1 | 2.16 | 0.46 |
| 25:DD:77:ALA:HA | 25:DD:97:TYR:HA | 1.97 | 0.46 |
| 23:BA:2774:C:H2' | 23:BA:2775:A:O4' | 2.15 | 0.46 |
| 23:DA:634:C:H2' | 23:DA:635:C:C6 | 2.51 | 0.46 |
| 23:DA:1282:U:H2' | 23:DA:1283:G:O4' | 2.15 | 0.46 |
| 23:DA:39:C:H2' | 23:DA:40:C:H6 | 1.78 | 0.46 |
| 3:AC:123:GLN:O | 3:AC:128:PHE:HB2 | 2.16 | 0.46 |
| 23:BA:2729:G:H2' | 23:BA:2730:C:O4' | 2.16 | 0.46 |
| 23:DA:775:G:C4 | 23:DA:794:G:C8 | 3.03 | 0.46 |
| 23:BA:706:A:H2' | 23:BA:707:G:O4' | 2.16 | 0.46 |
| 43:BZ:39:VAL:HG21 | 43:BZ:44:PHE:HB2 | 1.98 | 0.46 |
| 1:AA:1151:A:O4' | 10:AJ:39:PRO:HB2 | 2.16 | 0.46 |
| 1:AA:986:A:O2' | 19:AS:55:LYS:O | 2.34 | 0.46 |
| 1:CA:1349:A:C2 | 1:CA:1374:A:C5 | 3.02 | 0.46 |
| 1:AA:1330:U:O4 | 1:AA:1331:G:C2 | 2.68 | 0.46 |
| 3:AC:23:TYR:HA | 10:AJ:11:PHE:CE1 | 2.51 | 0.46 |
| 1:CA:1300:G:HO2' | 1:CA:1301:U:P | 2.38 | 0.46 |
| 23:DA:2133:G:C2' | 23:DA:2158:A:H61 | 2.28 | 0.46 |
| 6:CF:61:LEU:HD23 | 6:CF:63:TYR:OH | 2.16 | 0.46 |
| 1:AA:1164:G:C4 | 1:AA:1173:G:C2 | 3.03 | 0.46 |
| 23:BA:2117:A:N6 | 23:BA:2166:G:H22 | 2.10 | 0.46 |
| 9:AI:8:GLY:O | 9:AI:14:VAL:HA | 2.15 | 0.46 |
| 4:AD:173:TRP:CD2 | 4:AD:189:PRO:HG3 | 2.51 | 0.46 |
| 4:CD:173:TRP:HB2 | 4:CD:187:ARG:O | 2.15 | 0.46 |
| 27:DF:185:ASP:OD1 | 27:DF:188:ARG:NH1 | 2.45 | 0.46 |
| 23:BA:1557:C:H5'' | 23:BA:1558:A:OP2 | 2.16 | 0.46 |
| 1:CA:922:G:H1' | 5:CE:19:MET:HB2 | 1.98 | 0.46 |
| 1:CA:324:G:N2 | 1:CA:327:A:C8 | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:CT:77:ALA:O | 20:CT:81:LYS:HG3 | 2.15 | 0.46 |
| 32:DO:23:ARG:HG3 | 32:DO:24:VAL:N | 2.30 | 0.46 |
| 23:BA:534:U:O2' | 38:BU:49:HIS:CD2 | 2.68 | 0.46 |
| 1:AA:914:A:OP1 | 56:AA:1805:HOH:O | 2.21 | 0.46 |
| 23:BA:143:G:H2' | 23:BA:143(A):C:C6 | 2.50 | 0.46 |
| 22:CX:53:THR:HG23 | 22:CX:62:HIS:ND1 | 2.30 | 0.46 |
| 34:DQ:2:LEU:HB3 | 34:DQ:70:PRO:CG | 2.45 | 0.46 |
| 23:DA:2818:G:O2' | 23:DA:2819:G:H5' | 2.16 | 0.46 |
| 1:AA:489:C:C4 | 1:AA:490:G:N7 | 2.84 | 0.46 |
| 1:CA:270:A:H2' | 1:CA:271:C:C6 | 2.51 | 0.46 |
| 23:BA:2223:G:H2' | 23:BA:2224:G:H5' | 1.97 | 0.46 |
| 29:BH:90:LYS:O | 29:BH:160:LYS:HA | 2.16 | 0.46 |
| 16:AP:14:ASN:OD1 | 16:AP:16:HIS:CE1 | 2.69 | 0.46 |
| 23:DA:448:U:H1' | 27:DF:84:VAL:HG11 | 1.97 | 0.46 |
| 32:DO:87:ILE:HG22 | 32:DO:93:PRO:HA | 1.97 | 0.46 |
| 37:DT:18:ASP:OD1 | 37:DT:18:ASP:N | 2.28 | 0.46 |
| 7:CG:96:GLN:HB3 | 7:CG:96:GLN:HE21 | 1.49 | 0.46 |
| 35:BR:12:ARG:HG2 | 35:BR:16:HIS:CG | 2.50 | 0.46 |
| 23:DA:1025:G:C4 | 23:DA:1135:C:H1' | 2.51 | 0.46 |
| 1:CA:949:A:H1' | 1:CA:1364:U:C2 | 2.49 | 0.46 |
| 1:CA:1170:A:H5'' | 1:CA:1171:G:OP2 | 2.16 | 0.46 |
| 19:AS:12:ASP:O | 19:AS:14:HIS:N | 2.42 | 0.46 |
| 1:CA:940:C:H1' | 1:CA:1374:A:C2 | 2.49 | 0.46 |
| 1:AA:963:G:HO2' | 10:AJ:54:PHE:HE2 | 1.62 | 0.46 |
| 1:CA:1206:G:C4 | 1:CA:1207:G:C8 | 3.04 | 0.46 |
| 2:CB:55:PHE:HA | 2:CB:58:ILE:HD12 | 1.98 | 0.46 |
| 23:DA:1866:C:H2' | 23:DA:1876:A:O4' | 2.16 | 0.46 |
| 23:DA:2130:U:OP2 | 23:DA:2132:U:H5 | 1.98 | 0.46 |
| 1:AA:102:G:O2' | 1:AA:151:A:N3 | 2.46 | 0.46 |
| 23:DA:247:G:H4' | 23:DA:386:G:C5 | 2.51 | 0.46 |
| 1:CA:96:U:O2' | 1:CA:97:G:H8 | 1.99 | 0.46 |
| 20:CT:12:ALA:O | 20:CT:15:ARG:HB2 | 2.15 | 0.46 |
| 9:AI:15:ALA:HA | 9:AI:65:VAL:HB | 1.96 | 0.46 |
| 1:CA:1499:A:O2' | 1:CA:1520:G:H5' | 2.15 | 0.46 |
| 23:BA:278:A:HO2' | 23:BA:279:C:P | 2.33 | 0.46 |
| 34:DQ:134:ARG:O | 34:DQ:138:ASP:HB2 | 2.15 | 0.46 |
| 1:AA:1254:C:H5' | 1:AA:1356:G:H4' | 1.97 | 0.46 |
| 23:DA:1797:C:C2' | 23:DA:1798:U:H5' | 2.46 | 0.46 |
| 51:B7:9:ARG:HH21 | 51:B7:47:ARG:HD3 | 1.80 | 0.46 |
| 34:DQ:26:TYR:HE1 | 34:DQ:28:ALA:HB2 | 1.80 | 0.46 |
| 28:DG:10:LYS:O | 28:DG:14:GLU:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:2839:G:C5' | 35:DR:46:GLY:HA2 | 2.46 | 0.46 |
| 2:AB:74:LYS:O | 2:AB:78:GLN:HB2 | 2.15 | 0.46 |
| 1:AA:932:C:H2' | 1:AA:933:G:C8 | 2.51 | 0.46 |
| 23:DA:2279:G:O6 | 44:D0:14:ARG:HD2 | 2.16 | 0.46 |
| 20:AT:36:LEU:HD12 | 20:AT:55:ILE:HG23 | 1.97 | 0.46 |
| 47:D3:40:THR:HG23 | 47:D3:43:ILE:HD12 | 1.98 | 0.46 |
| 23:DA:787:U:OP1 | 56:DA:4090:HOH:O | 2.20 | 0.46 |
| 36:BS:36:TYR:N | 36:BS:36:TYR:CD1 | 2.84 | 0.46 |
| 9:CI:27:THR:HB | 9:CI:61:ALA:O | 2.15 | 0.46 |
| 22:CX:63:ALA:HB3 | 22:CX:81:LEU:HD23 | 1.97 | 0.46 |
| 52:D8:31:HIS:O | 52:D8:32:LEU:HB2 | 2.16 | 0.46 |
| 23:DA:1910:G:O2' | 23:DA:1911:U:H5' | 2.15 | 0.46 |
| 51:B7:8:ASN:OD1 | 51:B7:8:ASN:C | 2.53 | 0.46 |
| 33:DP:6:LEU:HD23 | 33:DP:6:LEU:HA | 1.60 | 0.46 |
| 22:AX:23:LYS:HA | 22:AX:23:LYS:HD3 | 1.72 | 0.46 |
| 24:DB:8:U:H5' | 24:DB:9:G:OP2 | 2.16 | 0.46 |
| 23:DA:2054:A:H5'' | 23:DA:2055:C:O5' | 2.16 | 0.46 |
| 25:BD:112:GLN:HA | 25:BD:112:GLN:NE2 | 2.31 | 0.46 |
| 43:BZ:24:LEU:C | 43:BZ:24:LEU:HD12 | 2.36 | 0.46 |
| 1:CA:1443:G:O6 | 1:CA:1444:C:C4 | 2.69 | 0.46 |
| 23:DA:848:G:N3 | 23:DA:933:A:H1' | 2.30 | 0.46 |
| 1:AA:1206:G:C2 | 1:AA:1207:G:C4 | 3.04 | 0.46 |
| 23:BA:807:U:OP2 | 33:BP:41:ARG:NH2 | 2.49 | 0.46 |
| 1:AA:678:U:H2' | 1:AA:679:C:C6 | 2.50 | 0.46 |
| 3:CC:110:ASN:O | 3:CC:141:VAL:HG22 | 2.15 | 0.46 |
| 23:BA:1142(A):A:C5 | 23:BA:1144:G:C5 | 3.03 | 0.46 |
| 23:BA:2137:C:H42 | 23:BA:2154:G:H1 | 1.64 | 0.46 |
| 1:CA:604:G:H2' | 1:CA:605:U:O4' | 2.16 | 0.46 |
| 23:DA:1003:G:N2 | 23:DA:1153:C:C2 | 2.84 | 0.46 |
| 28:DG:106:LEU:HD12 | 28:DG:110:ALA:CB | 2.43 | 0.46 |
| 45:D1:50:ARG:HG2 | 45:D1:59:THR:CG2 | 2.45 | 0.46 |
| 1:AA:1392:G:N2 | 1:AA:1502:A:H8 | 2.13 | 0.46 |
| 23:DA:1485:G:H1 | 23:DA:1504:C:N4 | 2.13 | 0.46 |
| 1:CA:1246:C:H2' | 1:CA:1247:U:H6 | 1.81 | 0.46 |
| 1:CA:651:C:H2' | 1:CA:652:U:C6 | 2.50 | 0.46 |
| 1:AA:276:G:O3' | 17:AQ:68:ARG:NH1 | 2.49 | 0.46 |
| 37:DT:105:LEU:HB3 | 37:DT:109:GLU:HB2 | 1.98 | 0.46 |
| 1:AA:384:G:H2' | 1:AA:385:C:H6 | 1.80 | 0.46 |
| 1:AA:269:C:H2' | 1:AA:270:A:H8 | 1.79 | 0.46 |
| 23:BA:1259:G:H2' | 23:BA:1260:G:C8 | 2.51 | 0.46 |
| 23:DA:319:C:H2' | 23:DA:320:A:O4' | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DE:2:LYS:HG3 | 26:DE:200:GLU:HB2 | 1.97 | 0.46 |
| 23:BA:1829:A:P | 56:BA:5038:HOH:O | 2.73 | 0.46 |
| 23:BA:1932:A:H2' | 23:BA:1933:G:O4' | 2.16 | 0.46 |
| 23:BA:213:A:H2' | 23:BA:214:G:O4' | 2.15 | 0.46 |
| 20:CT:43:LEU:HA | 20:CT:43:LEU:HD23 | 1.71 | 0.46 |
| 1:CA:403:C:O2' | 4:CD:122:ARG:NH1 | 2.49 | 0.46 |
| 28:DG:129:GLY:HA2 | 28:DG:166:ASP:HA | 1.98 | 0.46 |
| 8:AH:87:SER:HB2 | 8:AH:93:VAL:HB | 1.96 | 0.46 |
| 1:AA:982:U:H5'' | 14:AN:6:LEU:HD23 | 1.98 | 0.46 |
| 10:AJ:7:LYS:HA | 10:AJ:71:LEU:HA | 1.97 | 0.46 |
| 23:DA:1529:G:O2' | 23:DA:1530:C:H5' | 2.15 | 0.46 |
| 3:CC:137:ALA:CA | 3:CC:140:ARG:HD3 | 2.41 | 0.46 |
| 10:AJ:61:GLU:OE2 | 14:AN:49:HIS:NE2 | 2.43 | 0.46 |
| 1:AA:1173:G:C6 | 1:AA:1174:G:C8 | 3.04 | 0.46 |
| 1:CA:192:U:O3' | 20:CT:57:ARG:HD2 | 2.16 | 0.46 |
| 4:CD:119:GLN:HG2 | 4:CD:123:HIS:CD2 | 2.50 | 0.46 |
| 24:BB:91:C:C2' | 24:BB:92:C:H5' | 2.46 | 0.46 |
| 2:CB:134:GLU:O | 2:CB:137:ARG:HG3 | 2.16 | 0.46 |
| 8:CH:113:SER:O | 8:CH:131:GLY:HA3 | 2.16 | 0.46 |
| 10:CJ:11:PHE:HA | 10:CJ:66:ARG:O | 2.15 | 0.46 |
| 1:AA:377:G:H2' | 1:AA:378:G:H8 | 1.76 | 0.46 |
| 30:BI:133:HIS:HD2 | 30:BI:134:PRO:HD2 | 1.80 | 0.46 |
| 23:BA:2186:G:H2' | 23:BA:2186:G:N3 | 2.30 | 0.46 |
| 40:DW:9:TYR:H | 40:DW:102:HIS:CE1 | 2.34 | 0.46 |
| 1:AA:868:C:H2' | 1:AA:869:G:O4' | 2.16 | 0.46 |
| 23:BA:2273:A:H2' | 23:BA:2274:A:C8 | 2.50 | 0.46 |
| 34:DQ:43:THR:N | 34:DQ:46:GLN:OE1 | 2.42 | 0.46 |
| 1:AA:865:A:H2' | 1:AA:866:C:H6 | 1.81 | 0.46 |
| 1:CA:1266:G:C8 | 1:CA:1266:G:OP2 | 2.69 | 0.46 |
| 12:AL:119:LYS:HB2 | 12:AL:120:TYR:CD1 | 2.51 | 0.46 |
| 3:AC:64:VAL:O | 3:AC:99:VAL:HA | 2.15 | 0.46 |
| 1:AA:860:A:N6 | 1:AA:861:G:C2 | 2.84 | 0.46 |
| 23:DA:2440:C:H5' | 56:DA:4295:HOH:O | 2.14 | 0.46 |
| 1:AA:1192:C:C5 | 1:AA:1193:G:C8 | 3.04 | 0.46 |
| 4:CD:88:VAL:HA | 5:CE:97:GLY:HA2 | 1.98 | 0.46 |
| 23:BA:859:G:O2' | 23:BA:916:G:O6 | 2.28 | 0.46 |
| 5:CE:137:GLU:O | 5:CE:141:GLN:HB2 | 2.15 | 0.46 |
| 30:DI:46:ALA:HA | 30:DI:49:ALA:HB3 | 1.97 | 0.46 |
| 25:BD:172:TYR:CD1 | 25:BD:186:HIS:HA | 2.50 | 0.46 |
| 23:DA:1646:C:H3' | 56:DA:3850:HOH:O | 2.15 | 0.46 |
| 43:DZ:75:ASN:HB2 | 43:DZ:85:HIS:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:854:G:H3' | 1:CA:871:U:O4 | 2.16 | 0.46 |
| 23:BA:333:G:H5'' | 23:BA:334:C:OP2 | 2.14 | 0.46 |
| 45:B1:86:SER:HB3 | 45:B1:89:GLU:OE2 | 2.16 | 0.46 |
| 23:BA:470:A:OP1 | 27:BF:59:TYR:HE2 | 1.99 | 0.46 |
| 23:BA:257:A:H2' | 23:BA:258:G:O4' | 2.16 | 0.46 |
| 1:AA:1222:G:OP1 | 1:AA:1321:C:H2' | 2.15 | 0.46 |
| 1:AA:979:C:C4 | 1:AA:1318:A:N6 | 2.84 | 0.46 |
| 19:AS:12:ASP:OD2 | 19:AS:37:ARG:NH1 | 2.44 | 0.46 |
| 9:CI:13:ALA:HB3 | 9:CI:72:GLY:C | 2.37 | 0.46 |
| 2:AB:20:GLU:HG3 | 2:AB:191:ASP:OD1 | 2.16 | 0.46 |
| 2:AB:55:PHE:HA | 2:AB:58:ILE:HD12 | 1.98 | 0.46 |
| 1:CA:1030(D):A:N6 | 1:CA:1031:G:H21 | 2.14 | 0.46 |
| 23:DA:2172:U:H4' | 23:DA:2173:A:OP2 | 2.15 | 0.46 |
| 1:CA:1297:C:H5'' | 1:CA:1299:A:N7 | 2.30 | 0.46 |
| 1:AA:103:C:P | 20:AT:17:ARG:HH21 | 2.39 | 0.46 |
| 1:AA:941:G:C2 | 1:AA:942:G:C8 | 3.03 | 0.46 |
| 17:CQ:79:SER:OG | 17:CQ:80:GLY:N | 2.48 | 0.46 |
| 1:AA:1367:C:C4 | 1:AA:1368:G:N7 | 2.84 | 0.46 |
| 24:DB:66:A:H61 | 24:DB:109:C:C5' | 2.24 | 0.46 |
| 23:DA:1026:U:HO2' | 23:DA:1027:A:P | 2.38 | 0.46 |
| 5:CE:75:THR:HG23 | 5:CE:76:ILE:O | 2.16 | 0.46 |
| 1:CA:1111:A:H61 | 3:CC:177:THR:HA | 1.79 | 0.46 |
| 9:CI:17:VAL:CG2 | 9:CI:80:GLY:HA3 | 2.46 | 0.46 |
| 1:AA:1055:A:H62 | 1:AA:1200:C:H42 | 1.64 | 0.46 |
| 7:CG:111:ARG:HH12 | 7:CG:122:HIS:HB2 | 1.80 | 0.46 |
| 31:BN:13:TRP:O | 31:BN:135:PRO:HA | 2.16 | 0.46 |
| 23:DA:760:G:H2' | 23:DA:761:A:O4' | 2.15 | 0.46 |
| 1:AA:922:G:H1' | 5:AE:19:MET:HB2 | 1.97 | 0.46 |
| 1:CA:539:A:H2' | 1:CA:540:G:C8 | 2.51 | 0.46 |
| 23:BA:2464:C:O2' | 23:BA:2465:C:P | 2.74 | 0.46 |
| 1:AA:105:G:H2' | 1:AA:106:C:H6 | 1.81 | 0.46 |
| 23:DA:2208:A:H1' | 23:DA:2219:G:C4 | 2.51 | 0.46 |
| 48:B4:22:ILE:HG22 | 48:B4:24:THR:HG23 | 1.97 | 0.46 |
| 39:BV:52:VAL:HG21 | 39:BV:55:ALA:HB3 | 1.98 | 0.46 |
| 23:BA:212:G:O2' | 23:BA:213:A:H5' | 2.16 | 0.46 |
| 23:BA:2836:U:H2' | 23:BA:2837:G:C8 | 2.51 | 0.46 |
| 46:D2:22:GLU:HG2 | 46:D2:64:LEU:HD11 | 1.97 | 0.46 |
| 2:CB:155:LEU:HD11 | 2:CB:159:PRO:HD3 | 1.97 | 0.46 |
| 23:DA:2190:G:H2' | 23:DA:2191:G:O4' | 2.16 | 0.46 |
| 44:D0:55:ARG:HB3 | 44:D0:55:ARG:CZ | 2.46 | 0.46 |
| 23:BA:64:A:O3' | 41:BX:71:GLY:HA3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:110:GLN:O | 2:CB:114:ARG:HB2 | 2.16 | 0.46 |
| 41:BX:60:ARG:HB3 | 41:BX:60:ARG:HE | 1.43 | 0.46 |
| 1:AA:512:U:H2' | 1:AA:513:C:H6 | 1.81 | 0.46 |
| 49:B5:41:PRO:O | 49:B5:44:THR:OG1 | 2.34 | 0.46 |
| 15:AO:26:GLU:HG2 | 15:AO:26:GLU:H | 1.44 | 0.46 |
| 1:AA:1441:G:N3 | 1:AA:1459:C:C5 | 2.84 | 0.46 |
| 45:D1:54:ALA:HB1 | 45:D1:83:GLU:HB3 | 1.97 | 0.46 |
| 33:DP:52:GLU:HG3 | 52:D8:57:ARG:HH22 | 1.81 | 0.46 |
| 10:CJ:8:LEU:CD1 | 10:CJ:20:ALA:HB2 | 2.41 | 0.46 |
| 28:DG:76:SER:CA | 28:DG:83:ARG:HA | 2.44 | 0.46 |
| 48:D4:34:GLU:CD | 48:D4:35:VAL:H | 2.20 | 0.46 |
| 15:AO:39:LEU:HD13 | 15:AO:56:LEU:HD23 | 1.98 | 0.46 |
| 9:AI:17:VAL:HG21 | 9:AI:80:GLY:C | 2.36 | 0.46 |
| 2:CB:171:ALA:O | 2:CB:175:ARG:N | 2.39 | 0.46 |
| 23:DA:1423:G:H2' | 23:DA:1424:G:C8 | 2.46 | 0.46 |
| 9:CI:6:GLY:O | 9:CI:17:VAL:HB | 2.16 | 0.46 |
| 23:BA:2846:G:H2' | 23:BA:2847:U:O4' | 2.16 | 0.46 |
| 1:CA:614:A:H2' | 1:CA:615:C:H6 | 1.80 | 0.46 |
| 1:CA:763:G:H2' | 1:CA:764:C:C6 | 2.50 | 0.46 |
| 23:BA:2193:G:H2' | 23:BA:2194:G:C8 | 2.51 | 0.46 |
| 23:BA:2233:U:H2' | 23:BA:2234:G:C8 | 2.50 | 0.46 |
| 37:BT:105:LEU:HB3 | 37:BT:109:GLU:HB2 | 1.98 | 0.46 |
| 1:CA:262:A:C6 | 1:CA:263:A:C6 | 3.04 | 0.46 |
| 23:BA:2850:A:OP2 | 23:BA:2866:U:C5 | 2.69 | 0.46 |
| 52:D8:61:LEU:O | 52:D8:63:PRO:HD3 | 2.16 | 0.46 |
| 1:CA:636:U:H2' | 1:CA:637:G:C8 | 2.51 | 0.46 |
| 27:DF:34:TRP:CE3 | 27:DF:35:GLU:HG2 | 2.51 | 0.46 |
| 27:DF:168:ARG:HH11 | 27:DF:168:ARG:CB | 2.29 | 0.46 |
| 23:DA:213:A:H2' | 23:DA:214:G:O4' | 2.16 | 0.46 |
| 23:BA:2836:U:C4 | 23:BA:2883:A:N6 | 2.84 | 0.46 |
| 23:DA:1699:G:N2 | 56:DA:4405:HOH:O | 2.34 | 0.46 |
| 40:DW:40:ASN:O | 40:DW:41:LYS:HG2 | 2.16 | 0.46 |
| 4:AD:25:ARG:O | 4:AD:27:TYR:N | 2.46 | 0.46 |
| 36:DS:74:ALA:HB2 | 36:DS:105:ALA:HA | 1.97 | 0.46 |
| 23:BA:2685:G:H2' | 23:BA:2686:G:H5'' | 1.97 | 0.46 |
| 23:BA:652(Q):G:H2' | 23:BA:652(R):C:C6 | 2.51 | 0.46 |
| 25:DD:146:GLU:HB2 | 25:DD:189:CYS:HB3 | 1.96 | 0.46 |
| 23:DA:363(D):G:O2' | 23:DA:363(E):U:H5' | 2.16 | 0.46 |
| 25:DD:154:LYS:C | 25:DD:155:LEU:HD12 | 2.36 | 0.46 |
| 36:BS:74:ALA:HB2 | 36:BS:105:ALA:HA | 1.97 | 0.46 |
| 20:CT:59:ALA:O | 20:CT:62:LEU:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:77:C:OP1 | 46:D2:59:ARG:HD3 | 2.16 | 0.46 |
| 1:AA:536:C:H2' | 1:AA:537:G:C8 | 2.51 | 0.46 |
| 23:BA:1188:U:H4' | 39:BV:79:VAL:HG22 | 1.97 | 0.46 |
| 3:CC:37:GLN:NE2 | 14:CN:52:GLN:OE1 | 2.49 | 0.46 |
| 1:CA:1342:C:H1' | 9:CI:124:GLN:OE1 | 2.17 | 0.45 |
| 2:AB:233:SER:OG | 2:AB:234:PRO:HD2 | 2.17 | 0.45 |
| 21:CU:3:LYS:HG2 | 21:CU:10:ARG:CG | 2.45 | 0.45 |
| 23:BA:2304:G:H21 | 28:BG:156:ASP:CG | 2.19 | 0.45 |
| 23:DA:833:U:O2' | 33:DP:52:GLU:HG2 | 2.15 | 0.45 |
| 1:CA:1010:G:N2 | 1:CA:1020:U:H1' | 2.31 | 0.45 |
| 1:AA:173:U:C6 | 1:AA:197:A:C2 | 3.03 | 0.45 |
| 1:AA:154:C:N4 | 1:AA:167:G:H1 | 2.15 | 0.45 |
| 7:CG:73:MET:HG3 | 7:CG:89:MET:O | 2.15 | 0.45 |
| 23:DA:29:U:H2' | 23:DA:30:G:H8 | 1.77 | 0.45 |
| 1:AA:1381:U:H2' | 1:AA:1381:U:O2 | 2.14 | 0.45 |
| 11:CK:67:ASP:OD2 | 11:CK:71:LYS:HE3 | 2.16 | 0.45 |
| 23:DA:1434:A:O2' | 23:DA:1435:G:H5' | 2.16 | 0.45 |
| 1:AA:1104:G:C6 | 1:AA:1105:A:C5 | 3.04 | 0.45 |
| 28:DG:110:ALA:HA | 28:DG:140:ILE:O | 2.16 | 0.45 |
| 13:AM:102:ARG:HH12 | 13:AM:104:ARG:HD3 | 1.80 | 0.45 |
| 9:AI:7:THR:N | 9:AI:83:ARG:HD3 | 2.29 | 0.45 |
| 31:DN:13:TRP:O | 31:DN:135:PRO:HA | 2.15 | 0.45 |
| 23:BA:2526:G:H5' | 23:BA:2742:C:O2' | 2.16 | 0.45 |
| 23:DA:2592:G:H2' | 23:DA:2593:U:O4' | 2.16 | 0.45 |
| 7:CG:61:VAL:O | 7:CG:64:GLN:HB3 | 2.16 | 0.45 |
| 23:BA:2022:U:O2' | 23:BA:2617:C:H5' | 2.16 | 0.45 |
| 1:AA:599:C:H4' | 8:AH:130:GLY:C | 2.36 | 0.45 |
| 33:DP:84:ASN:CG | 33:DP:117:GLU:HB2 | 2.35 | 0.45 |
| 47:D3:7:LYS:HE2 | 47:D3:32:GLN:O | 2.16 | 0.45 |
| 23:BA:2850:A:OP2 | 23:BA:2866:U:H5 | 1.98 | 0.45 |
| 1:AA:189(F):U:O2 | 17:AQ:63:ARG:NH2 | 2.49 | 0.45 |
| 52:B8:61:LEU:C | 52:B8:63:PRO:HD3 | 2.37 | 0.45 |
| 23:DA:2784:C:H1' | 26:DE:37:ARG:HH12 | 1.80 | 0.45 |
| 3:AC:30:ARG:NH2 | 14:AN:38:GLY:HA2 | 2.32 | 0.45 |
| 23:BA:1652:A:OP1 | 35:BR:8:ARG:NH1 | 2.49 | 0.45 |
| 2:AB:74:LYS:HG2 | 2:AB:74:LYS:H | 1.56 | 0.45 |
| 32:DO:117:LEU:HD23 | 32:DO:117:LEU:HA | 1.74 | 0.45 |
| 25:BD:112:GLN:HB2 | 25:BD:115:GLN:OE1 | 2.15 | 0.45 |
| 23:DA:2657:A:O3' | 29:DH:160:LYS:NZ | 2.49 | 0.45 |
| 23:DA:414:C:H2' | 23:DA:415:A:C8 | 2.50 | 0.45 |
| 23:BA:448:U:H1' | 27:BF:84:VAL:HG11 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:AB:143:GLU:O | 2:AB:146:GLN:HB2 | 2.16 | 0.45 |
| 4:CD:91:SER:O | 4:CD:95:GLY:N | 2.38 | 0.45 |
| 27:BF:39:TRP:O | 27:BF:43:LYS:HG2 | 2.15 | 0.45 |
| 6:CF:91:VAL:HG12 | 6:CF:92:LYS:O | 2.16 | 0.45 |
| 56:DA:4218:HOH:O | 51:D7:48:LYS:NZ | 2.47 | 0.45 |
| 8:CH:97:VAL:HG21 | 8:CH:128:GLY:HA2 | 1.99 | 0.45 |
| 1:AA:782:A:O3' | 1:AA:1515:C:H4' | 2.17 | 0.45 |
| 1:AA:516:U:C4 | 1:AA:517:G:C6 | 3.05 | 0.45 |
| 23:BA:2282:G:OP1 | 23:BA:2283:C:H1' | 2.16 | 0.45 |
| 23:DA:2335:A:N6 | 23:DA:2337:G:H1' | 2.31 | 0.45 |
| 9:CI:110:GLU:OE1 | 9:CI:120:ARG:NH2 | 2.49 | 0.45 |
| 2:AB:32:ILE:HD11 | 2:AB:40:HIS:CG | 2.52 | 0.45 |
| 1:AA:1060:C:H2' | 1:AA:1061:G:C8 | 2.40 | 0.45 |
| 23:BA:581:C:OP1 | 38:BU:33:ARG:HG3 | 2.16 | 0.45 |
| 1:CA:560:U:H4' | 1:CA:561:U:H5'' | 1.98 | 0.45 |
| 1:AA:1057:G:H2' | 1:AA:1058:G:C8 | 2.51 | 0.45 |
| 1:CA:1251:A:H1' | 1:CA:1369:C:O2' | 2.17 | 0.45 |
| 1:CA:1283:G:H2' | 1:CA:1284:C:C6 | 2.51 | 0.45 |
| 1:AA:1243:C:N3 | 1:AA:1294:G:N2 | 2.64 | 0.45 |
| 13:AM:14:ARG:HA | 13:AM:44:ARG:HA | 1.99 | 0.45 |
| 1:CA:1106:G:O3' | 3:CC:172:ARG:HD2 | 2.15 | 0.45 |
| 1:AA:1378:C:OP2 | 1:AA:1378:C:H2' | 2.15 | 0.45 |
| 3:CC:18:TRP:HE1 | 14:CN:56:VAL:H | 1.64 | 0.45 |
| 13:CM:23:TYR:HB3 | 13:CM:67:GLU:CD | 2.37 | 0.45 |
| 4:CD:107:ARG:NE | 4:CD:173:TRP:HZ2 | 2.14 | 0.45 |
| 23:DA:997:G:O2' | 23:DA:998:C:H5' | 2.16 | 0.45 |
| 2:CB:135:GLN:O | 2:CB:139:LYS:N | 2.42 | 0.45 |
| 23:DA:535:C:O3' | 38:DU:53:ARG:NH1 | 2.48 | 0.45 |
| 1:CA:624:C:H2' | 1:CA:625:G:C8 | 2.51 | 0.45 |
| 23:BA:2293:C:H2' | 23:BA:2294:C:C6 | 2.51 | 0.45 |
| 40:BW:79:GLY:HA3 | 40:BW:100:THR:HG22 | 1.98 | 0.45 |
| 4:CD:62:GLN:HB3 | 4:CD:66:ARG:HD2 | 1.98 | 0.45 |
| 16:CP:75:ARG:HA | 16:CP:80:PHE:CD1 | 2.52 | 0.45 |
| 1:CA:189:G:H2' | 1:CA:189(A):C:C6 | 2.51 | 0.45 |
| 3:AC:30:ARG:NE | 14:AN:35:ARG:O | 2.46 | 0.45 |
| 1:AA:65:U:H2' | 1:AA:381:C:H5 | 1.79 | 0.45 |
| 23:DA:725:G:C6 | 23:DA:726:G:N1 | 2.84 | 0.45 |
| 1:AA:1067:A:N3 | 1:AA:1068:G:H1' | 2.31 | 0.45 |
| 23:DA:1178:C:H2' | 23:DA:1179:C:C6 | 2.51 | 0.45 |
| 23:DA:2815:C:H5' | 49:D5:29:THR:HG21 | 1.97 | 0.45 |
| 11:AK:34:ASP:OD2 | 11:AK:38:ASN:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 25:BD:166:GLN:HB2 | 25:BD:174:ILE:HG22 | 1.97 | 0.45 |
| 44:B0:51:VAL:N | 44:B0:62:LEU:HD12 | 2.31 | 0.45 |
| 9:AI:96:LEU:HA | 9:AI:101:PHE:HB2 | 1.98 | 0.45 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:CD1 | 2.52 | 0.45 |
| 30:DI:45:LYS:HD2 | 30:DI:45:LYS:HA | 1.73 | 0.45 |
| 13:AM:4:ILE:HD11 | 13:AM:57:ARG:HA | 1.97 | 0.45 |
| 41:BX:11:PRO:HD3 | 46:B2:37:PHE:CE2 | 2.52 | 0.45 |
| 23:DA:288:C:H2' | 23:DA:289:A:H8 | 1.81 | 0.45 |
| 46:B2:9:GLN:HE22 | 46:B2:56:GLN:HG2 | 1.82 | 0.45 |
| 8:AH:37:ARG:HE | 8:AH:37:ARG:HB3 | 1.51 | 0.45 |
| 23:BA:2190:G:H2' | 23:BA:2191:G:O4' | 2.15 | 0.45 |
| 1:AA:721:G:H4' | 1:AA:722:A:O4' | 2.17 | 0.45 |
| 23:DA:2296:U:H4' | 23:DA:2297:C:OP1 | 2.15 | 0.45 |
| 1:AA:1220:G:C2 | 1:AA:1221:G:H1' | 2.52 | 0.45 |
| 1:CA:1124:G:C5 | 1:CA:1127:G:N2 | 2.83 | 0.45 |
| 1:CA:1346:A:C1' | 1:CA:1347:G:H5'' | 2.47 | 0.45 |
| 2:AB:87:ARG:HH21 | 2:AB:233:SER:N | 2.13 | 0.45 |
| 1:CA:1022:G:H2' | 1:CA:1023:G:C1' | 2.47 | 0.45 |
| 1:AA:1146:A:C6 | 1:AA:1147:C:C4 | 3.05 | 0.45 |
| 23:DA:1352:U:O2 | 23:DA:1570:A:H2 | 1.99 | 0.45 |
| 1:CA:1030:C:C5 | 1:CA:1032:G:N2 | 2.84 | 0.45 |
| 23:DA:2318:G:O2' | 23:DA:2319:G:H5'' | 2.15 | 0.45 |
| 1:CA:958:A:N6 | 1:CA:959:A:C6 | 2.84 | 0.45 |
| 23:BA:2287:A:C5 | 23:BA:2289:G:C5 | 3.04 | 0.45 |
| 21:AU:12:LYS:HB3 | 21:AU:17:THR:O | 2.16 | 0.45 |
| 1:AA:1075:C:P | 2:AB:179:LYS:HZ1 | 2.32 | 0.45 |
| 9:AI:31:GLN:HG2 | 9:AI:36:TYR:HD1 | 1.81 | 0.45 |
| 1:CA:1173:G:H2' | 1:CA:1174:G:C8 | 2.44 | 0.45 |
| 23:BA:2711:A:OP1 | 23:BA:2712(A):A:OP1 | 2.34 | 0.45 |
| 23:BA:2833:G:C3' | 23:BA:2834:G:H5' | 2.44 | 0.45 |
| 1:AA:1392:G:H21 | 1:AA:1502:A:H8 | 1.63 | 0.45 |
| 40:DW:4:LYS:HE2 | 40:DW:6:ILE:HD11 | 1.98 | 0.45 |
| 23:BA:2567:G:H2' | 23:BA:2568:C:H6 | 1.81 | 0.45 |
| 1:CA:1134:G:H2' | 1:CA:1135:U:H5' | 1.99 | 0.45 |
| 10:CJ:45:ARG:HD3 | 14:CN:36:PHE:CE1 | 2.51 | 0.45 |
| 23:DA:1050:A:H2' | 23:DA:1051:G:C8 | 2.50 | 0.45 |
| 23:DA:314:A:O2' | 23:DA:315:G:H5' | 2.15 | 0.45 |
| 23:BA:2387:U:OP1 | 44:B0:55:ARG:NH2 | 2.49 | 0.45 |
| 1:AA:509:A:OP2 | 56:AA:1888:HOH:O | 2.21 | 0.45 |
| 23:DA:878:A:C6 | 23:DA:900:A:C8 | 3.03 | 0.45 |
| 10:CJ:10:GLY:O | 10:CJ:68:HIS:N | 2.34 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1512:U:H2' | 23:BA:1513:C:C6 | 2.51 | 0.45 |
| 29:BH:37:VAL:HG12 | 29:BH:38:SER:O | 2.15 | 0.45 |
| 4:AD:62:GLN:HB3 | 4:AD:66:ARG:HD2 | 1.98 | 0.45 |
| 16:AP:75:ARG:HA | 16:AP:80:PHE:CD1 | 2.51 | 0.45 |
| 23:DA:1205:U:H4' | 23:DA:1206:G:OP2 | 2.16 | 0.45 |
| 8:AH:31:PHE:O | 8:AH:35:ILE:HG13 | 2.16 | 0.45 |
| 26:BE:195:LEU:HG | 26:BE:196:VAL:N | 2.30 | 0.45 |
| 39:DV:52:VAL:CG2 | 39:DV:55:ALA:HB3 | 2.45 | 0.45 |
| 3:AC:85:ARG:HA | 3:AC:88:ARG:CB | 2.46 | 0.45 |
| 23:DA:2872:G:O2' | 23:DA:2873:A:H5' | 2.16 | 0.45 |
| 9:AI:55:ALA:HB3 | 9:AI:58:HIS:CB | 2.46 | 0.45 |
| 23:BA:909:A:C6 | 23:BA:912:C:C2 | 3.05 | 0.45 |
| 23:DA:1425:G:H2' | 23:DA:1426:G:C8 | 2.51 | 0.45 |
| 15:CO:61:GLY:O | 15:CO:65:ARG:HG3 | 2.17 | 0.45 |
| 1:AA:1011:G:H2' | 1:AA:1012:U:C6 | 2.52 | 0.45 |
| 25:BD:96:HIS:NE2 | 25:BD:102:LYS:HE2 | 2.31 | 0.45 |
| 42:DY:44:ILE:HA | 42:DY:63:LYS:O | 2.17 | 0.45 |
| 23:BA:1292:U:H2' | 23:BA:1293:C:C6 | 2.51 | 0.45 |
| 23:DA:2505:G:O6 | 23:DA:2576:G:H2' | 2.16 | 0.45 |
| 23:BA:2140:C:H2' | 23:BA:2141:G:H8 | 1.80 | 0.45 |
| 24:DB:28:C:H2' | 24:DB:29:A:C8 | 2.50 | 0.45 |
| 1:CA:1201:A:H1' | 1:CA:1202:G:OP2 | 2.17 | 0.45 |
| 23:DA:614(A):U:O5' | 23:DA:614(A):U:H6 | 2.00 | 0.45 |
| 23:DA:586:A:N1 | 23:DA:809:G:O2' | 2.34 | 0.45 |
| 26:DE:181:LEU:HA | 26:DE:181:LEU:HD13 | 1.66 | 0.45 |
| 49:B5:36:CYS:O | 49:B5:37:LYS:HD3 | 2.16 | 0.45 |
| 1:AA:902:G:H2' | 1:AA:903:G:H8 | 1.82 | 0.45 |
| 1:AA:1190:G:C5' | 3:AC:4:LYS:HA | 2.47 | 0.45 |
| 5:AE:126:ARG:HA | 5:AE:131:ILE:HD11 | 1.98 | 0.45 |
| 1:CA:580:U:H2' | 1:CA:581:G:O4' | 2.15 | 0.45 |
| 1:CA:1308:U:OP1 | 13:CM:110:ARG:HD2 | 2.17 | 0.45 |
| 13:CM:87:TYR:CD1 | 19:CS:76:PRO:HB3 | 2.51 | 0.45 |
| 1:AA:1275:A:H2' | 1:AA:1276:G:C8 | 2.51 | 0.45 |
| 23:DA:2117:A:H61 | 23:DA:2166:G:N2 | 2.10 | 0.45 |
| 23:DA:2173:A:C2' | 23:DA:2174:C:H5' | 2.47 | 0.45 |
| 23:DA:945:A:H2 | 56:DA:3920:HOH:O | 2.00 | 0.45 |
| 15:AO:56:LEU:O | 15:AO:60:VAL:HG23 | 2.17 | 0.45 |
| 23:BA:2115:G:H4' | 23:BA:2167:U:C4' | 2.45 | 0.45 |
| 23:BA:1328:G:H8 | 23:BA:1328:G:O5' | 1.99 | 0.45 |
| 36:DS:32:LEU:O | 36:DS:62:LYS:HE2 | 2.15 | 0.45 |
| 4:CD:173:TRP:CG | 4:CD:189:PRO:HG3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2887:U:H2' | 23:DA:2888:C:H6 | 1.80 | 0.45 |
| 23:DA:1266:G:O2' | 23:DA:2012:G:O6 | 2.28 | 0.45 |
| 23:DA:1154:G:O5' | 23:DA:1154:G:H8 | 1.99 | 0.45 |
| 1:AA:1149:C:H2' | 1:AA:1150:U:O4' | 2.16 | 0.45 |
| 43:DZ:69:THR:HG22 | 43:DZ:90:VAL:HA | 1.98 | 0.45 |
| 13:AM:90:LEU:C | 13:AM:91:ARG:HG2 | 2.36 | 0.45 |
| 25:BD:71:ASP:HB3 | 25:BD:103:ARG:NH2 | 2.28 | 0.45 |
| 23:BA:485:C:H2' | 23:BA:486:C:C6 | 2.51 | 0.45 |
| 2:AB:100:GLY:N | 2:AB:176:GLU:OE2 | 2.46 | 0.45 |
| 34:BQ:103:MET:CE | 34:BQ:125:LEU:HD13 | 2.46 | 0.45 |
| 37:BT:120:ARG:HA | 37:BT:123:GLN:HG2 | 1.97 | 0.45 |
| 23:DA:2271:G:C6 | 23:DA:2272:U:C4 | 3.05 | 0.45 |
| 1:AA:684:A:C6 | 1:AA:685:G:C6 | 3.04 | 0.45 |
| 27:DF:64:ILE:HG13 | 27:DF:65:TRP:N | 2.31 | 0.45 |
| 20:AT:73:HIS:C | 20:AT:74:LYS:HG2 | 2.37 | 0.45 |
| 1:CA:1190:G:H5'' | 3:CC:3:ASN:O | 2.17 | 0.45 |
| 23:BA:1903:G:OP1 | 25:BD:241:PRO:HB2 | 2.16 | 0.45 |
| 2:CB:21:ARG:H | 2:CB:21:ARG:HE | 1.64 | 0.45 |
| 23:DA:863:A:H2' | 23:DA:864:G:H8 | 1.80 | 0.45 |
| 1:AA:763:G:H2' | 1:AA:764:C:C6 | 2.52 | 0.45 |
| 23:DA:1794:U:H2' | 23:DA:1795:C:H6 | 1.80 | 0.45 |
| 43:DZ:144:LEU:HD12 | 43:DZ:144:LEU:HA | 1.77 | 0.45 |
| 27:DF:51:THR:HG23 | 27:DF:92:PRO:HG2 | 1.97 | 0.45 |
| 1:CA:403:C:H2' | 1:CA:404:U:H6 | 1.80 | 0.45 |
| 15:AO:26:GLU:OE1 | 15:AO:77:ARG:HG2 | 2.16 | 0.45 |
| 6:AF:49:ALA:HB2 | 18:AR:78:LEU:O | 2.16 | 0.45 |
| 8:AH:112:LEU:HB3 | 8:AH:133:LEU:HA | 1.97 | 0.45 |
| 23:BA:2777:G:H5'' | 23:BA:2778:A:H5' | 1.98 | 0.45 |
| 20:AT:56:MET:HE2 | 20:AT:88:VAL:HG21 | 1.99 | 0.45 |
| 23:DA:1441:G:H2' | 23:DA:1442:G:C8 | 2.50 | 0.45 |
| 23:DA:2290:G:C2 | 23:DA:2343:C:O2 | 2.69 | 0.45 |
| 28:BG:89:GLY:C | 28:BG:90:LEU:HD23 | 2.36 | 0.45 |
| 23:BA:2054:A:H5'' | 23:BA:2055:C:O5' | 2.16 | 0.45 |
| 11:CK:46:GLY:HA2 | 11:CK:50:TYR:O | 2.16 | 0.45 |
| 1:AA:35:G:O2' | 12:AL:121:GLY:HA2 | 2.17 | 0.45 |
| 13:AM:114:ARG:HG2 | 13:AM:114:ARG:H | 1.28 | 0.45 |
| 44:D0:51:VAL:N | 44:D0:62:LEU:HD12 | 2.31 | 0.45 |
| 43:DZ:61:LEU:HD13 | 43:DZ:61:LEU:HA | 1.72 | 0.45 |
| 1:AA:445:G:N3 | 1:AA:445:G:H2' | 2.31 | 0.45 |
| 31:BN:67:LEU:HA | 31:BN:87:LEU:HD12 | 1.98 | 0.45 |
| 23:DA:2408:U:OP2 | 56:DA:4072:HOH:O | 2.21 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:CA:990:C:H2' | 1:CA:991:U:C6 | 2.51 | 0.45 |
| 1:AA:1097:C:H2' | 1:AA:1098:C:C6 | 2.51 | 0.45 |
| 1:AA:1110:A:H2' | 1:AA:1111:A:O4' | 2.15 | 0.45 |
| 13:CM:40:ASN:HA | 13:CM:41:PRO:HD2 | 1.85 | 0.45 |
| 1:AA:1240:U:H3' | 1:AA:1241:G:H8 | 1.80 | 0.45 |
| 1:AA:1053:G:O2' | 1:AA:1199:U:H5 | 2.00 | 0.45 |
| 1:AA:975:A:H5'' | 1:AA:1363(A):A:N6 | 2.32 | 0.45 |
| 1:CA:1399:C:C2 | 1:CA:1502:A:N6 | 2.85 | 0.45 |
| 21:CU:10:ARG:HE | 21:CU:10:ARG:CA | 2.27 | 0.45 |
| 1:CA:677:U:H2' | 1:CA:678:U:C6 | 2.51 | 0.45 |
| 1:CA:1029:C:N4 | 1:CA:1030(A):G:H22 | 2.15 | 0.45 |
| 1:CA:1287:A:H61 | 1:CA:1370:G:H21 | 1.65 | 0.45 |
| 23:BA:1320:C:O2' | 56:BA:4949:HOH:O | 2.21 | 0.45 |
| 1:CA:957:U:O2 | 1:CA:959:A:C8 | 2.69 | 0.45 |
| 23:DA:1394:U:C4 | 23:DA:1395:A:C5 | 3.04 | 0.45 |
| 10:AJ:48:THR:HA | 10:AJ:62:HIS:CB | 2.43 | 0.45 |
| 1:CA:706:A:N3 | 11:CK:31:THR:HG21 | 2.32 | 0.45 |
| 1:AA:370:C:H2' | 1:AA:371:G:H8 | 1.81 | 0.45 |
| 23:DA:102:G:O2' | 23:DA:103:A:P | 2.75 | 0.45 |
| 1:AA:627:G:O2' | 1:AA:628:G:H5' | 2.17 | 0.45 |
| 16:CP:43:LYS:HD3 | 16:CP:48:TRP:CZ3 | 2.50 | 0.45 |
| 23:DA:581:C:H2' | 23:DA:582:G:H8 | 1.80 | 0.45 |
| 1:CA:627:G:H2' | 1:CA:628:G:C8 | 2.50 | 0.45 |
| 28:BG:72:ARG:HD3 | 28:BG:85:GLY:HA2 | 1.98 | 0.45 |
| 24:DB:21:G:H2' | 24:DB:22:U:O4' | 2.16 | 0.45 |
| 30:BI:4:ILE:HD11 | 30:BI:44:LEU:HD12 | 1.99 | 0.45 |
| 1:CA:460:G:H1' | 1:CA:472:A:H61 | 1.81 | 0.45 |
| 1:CA:458:C:H2' | 1:CA:460:G:H8 | 1.81 | 0.45 |
| 23:DA:979:G:H3' | 23:DA:980:A:H5'' | 1.98 | 0.45 |
| 23:BA:858:U:O2 | 23:BA:2268:A:H2' | 2.17 | 0.45 |
| 1:AA:436:C:O2' | 1:AA:437:U:P | 2.75 | 0.45 |
| 23:DA:2275:C:H5' | 23:DA:2275:C:C6 | 2.51 | 0.45 |
| 23:DA:2505:G:H2' | 23:DA:2576:G:O6 | 2.17 | 0.45 |
| 1:CA:516:U:C4 | 1:CA:517:G:C6 | 3.04 | 0.45 |
| 1:AA:112:G:C2 | 1:AA:330:C:N4 | 2.84 | 0.45 |
| 5:CE:144:THR:O | 5:CE:148:VAL:HG23 | 2.17 | 0.45 |
| 4:AD:194:LEU:HB3 | 4:AD:196:LEU:HD11 | 1.99 | 0.45 |
| 22:AX:30:TYR:CD2 | 22:AX:30:TYR:N | 2.84 | 0.45 |
| 1:CA:667:G:H4' | 15:CO:51:HIS:CE1 | 2.51 | 0.45 |
| 21:CU:9:ARG:O | 21:CU:13:ILE:HG13 | 2.16 | 0.45 |
| 26:DE:178:GLU:H | 26:DE:178:GLU:CD | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:CL:85:ILE:HA | 12:CL:85:ILE:HD13 | 1.74 | 0.45 |
| 43:BZ:35:ARG:HA | 43:BZ:35:ARG:HD2 | 1.63 | 0.45 |
| 23:DA:850:C:O3' | 47:D3:49:LYS:HE2 | 2.17 | 0.45 |
| 1:CA:953:G:C4 | 1:CA:1229:A:C2 | 3.05 | 0.45 |
| 1:CA:1147:C:H2' | 1:CA:1148:U:H6 | 1.81 | 0.45 |
| 2:AB:28:PHE:CD2 | 2:AB:194:PRO:HG3 | 2.49 | 0.45 |
| 1:AA:1306:A:H2' | 1:AA:1307:U:C6 | 2.52 | 0.45 |
| 1:AA:1061:G:C6 | 1:AA:1197:G:C6 | 3.04 | 0.45 |
| 1:AA:1338:G:H3' | 1:AA:1339:A:C8 | 2.52 | 0.45 |
| 1:AA:1339:A:N6 | 1:AA:1340:A:N3 | 2.64 | 0.45 |
| 23:DA:2137:C:H42 | 23:DA:2154:G:H1 | 1.64 | 0.45 |
| 2:AB:197:VAL:HG12 | 2:AB:198:ASP:H | 1.82 | 0.45 |
| 23:DA:528:A:C2' | 23:DA:529:A:H5' | 2.47 | 0.45 |
| 23:BA:2154:G:H2' | 23:BA:2155:G:C8 | 2.52 | 0.45 |
| 1:AA:1378:C:OP2 | 7:AG:7:ALA:HB3 | 2.16 | 0.45 |
| 1:AA:1250:A:N6 | 1:AA:1251:A:N6 | 2.65 | 0.45 |
| 28:BG:56:ALA:CA | 28:BG:153:ARG:HH21 | 2.29 | 0.45 |
| 41:DX:36:LYS:HG3 | 41:DX:56:THR:HG23 | 1.99 | 0.45 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:CE1 | 2.52 | 0.45 |
| 23:BA:2309:A:N6 | 23:BA:2310:A:N1 | 2.65 | 0.45 |
| 43:DZ:48:PHE:O | 43:DZ:52:SER:N | 2.47 | 0.45 |
| 1:AA:957:U:H3 | 1:AA:960:U:H5'' | 1.82 | 0.45 |
| 23:BA:1418:G:OP1 | 23:BA:1588:C:O2' | 2.31 | 0.45 |
| 27:BF:123:LEU:HD11 | 27:BF:194:MET:HE2 | 1.97 | 0.45 |
| 7:CG:113:GLU:CB | 7:CG:118:VAL:HB | 2.45 | 0.45 |
| 33:BP:59:LEU:HD11 | 52:B8:10:ALA:CB | 2.46 | 0.45 |
| 23:BA:2870:C:H2' | 23:BA:2871:C:O4' | 2.16 | 0.45 |
| 24:BB:111:G:H2' | 24:BB:112:U:H6 | 1.81 | 0.45 |
| 3:CC:68:VAL:HG12 | 3:CC:70:VAL:HG23 | 1.99 | 0.45 |
| 1:AA:664:G:H22 | 1:AA:741:G:H1 | 1.65 | 0.45 |
| 23:BA:2854:G:H2' | 23:BA:2855:C:C6 | 2.51 | 0.45 |
| 29:BH:7:LEU:HD12 | 29:BH:8:PRO:CD | 2.47 | 0.45 |
| 1:CA:5:U:H5'' | 1:CA:6:G:C8 | 2.52 | 0.45 |
| 23:BA:2464:C:O2' | 23:BA:2465:C:OP2 | 2.30 | 0.45 |
| 4:CD:24:GLU:O | 4:CD:27:TYR:HD1 | 1.98 | 0.45 |
| 33:BP:101:VAL:HG23 | 33:BP:106:LEU:HB3 | 1.97 | 0.45 |
| 1:CA:1159:U:H5 | 1:CA:1172:C:H5 | 1.65 | 0.45 |
| 23:DA:242:G:O4' | 52:D8:3:LYS:HE3 | 2.17 | 0.45 |
| 33:DP:63:PRO:HG2 | 52:D8:25:MET:HB2 | 1.98 | 0.45 |
| 25:DD:222:ARG:NH1 | 56:DD:402:HOH:O | 2.48 | 0.45 |
| 23:BA:2064:C:H2' | 23:BA:2065:C:C6 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:BB:89:G:OP2 | 24:BB:89:G:H8 | 2.00 | 0.45 |
| 5:CE:36:ASP:OD2 | 5:CE:38:GLN:N | 2.43 | 0.45 |
| 36:DS:66:ALA:HA | 36:DS:69:VAL:CG1 | 2.47 | 0.45 |
| 10:CJ:15:THR:O | 10:CJ:19:SER:OG | 2.34 | 0.45 |
| 49:B5:45:VAL:HA | 49:B5:52:TYR:HB2 | 1.98 | 0.45 |
| 1:CA:1418:A:H5' | 1:CA:1419:G:OP2 | 2.16 | 0.45 |
| 34:BQ:37:LEU:HD21 | 34:BQ:130:LYS:HB2 | 1.98 | 0.45 |
| 23:DA:2615:U:C2 | 49:D5:7:PRO:HA | 2.52 | 0.45 |
| 1:AA:1457:G:N1 | 1:AA:1458:G:C5 | 2.84 | 0.45 |
| 1:AA:1459:C:H2' | 1:AA:1460:A:N7 | 2.31 | 0.45 |
| 23:BA:26:G:C6 | 23:BA:27:G:N1 | 2.85 | 0.45 |
| 1:CA:1399:C:C2 | 1:CA:1401:G:C5 | 3.04 | 0.45 |
| 1:CA:1254:C:H5 | 10:CJ:43:ARG:CZ | 2.29 | 0.45 |
| 23:DA:2133:G:H2' | 23:DA:2158:A:H61 | 1.81 | 0.45 |
| 23:BA:1540:U:H2' | 23:BA:1541:G:O4' | 2.16 | 0.45 |
| 24:BB:20:C:H2' | 24:BB:21:G:H5' | 1.97 | 0.45 |
| 1:AA:327:A:C4 | 1:AA:329:A:C8 | 3.05 | 0.45 |
| 5:CE:75:THR:HA | 5:CE:115:VAL:HG13 | 1.97 | 0.45 |
| 23:DA:2309:A:N6 | 23:DA:2310:A:N1 | 2.64 | 0.45 |
| 23:BA:1287:A:C6 | 23:BA:1288:U:C4 | 3.05 | 0.45 |
| 23:BA:570:G:H2' | 23:BA:2030:A:C5 | 2.52 | 0.45 |
| 23:DA:534:U:O2' | 38:DU:49:HIS:CD2 | 2.70 | 0.45 |
| 1:AA:624:C:O3' | 16:AP:10:GLY:HA2 | 2.16 | 0.45 |
| 33:DP:71:VAL:HG23 | 33:DP:72:PRO:HA | 1.98 | 0.45 |
| 1:AA:741:G:H2' | 1:AA:742:G:C8 | 2.52 | 0.45 |
| 23:DA:1028:A:H61 | 23:DA:1125:G:H2' | 1.82 | 0.45 |
| 23:BA:323:G:H1' | 23:BA:1205:U:O2 | 2.17 | 0.45 |
| 24:DB:2:C:H2' | 24:DB:3:C:H6 | 1.82 | 0.45 |
| 25:DD:130:ALA:C | 25:DD:131:LEU:HD12 | 2.37 | 0.45 |
| 1:AA:667:G:H4' | 15:AO:51:HIS:ND1 | 2.31 | 0.45 |
| 14:CN:26:ARG:HB3 | 14:CN:26:ARG:HE | 1.51 | 0.45 |
| 20:AT:25:ARG:O | 20:AT:29:LYS:HG3 | 2.17 | 0.45 |
| 4:AD:14:ARG:HA | 4:AD:39:PRO:HB3 | 1.98 | 0.45 |
| 20:CT:36:LEU:HD12 | 20:CT:55:ILE:HG23 | 1.98 | 0.45 |
| 4:CD:194:LEU:HB3 | 4:CD:196:LEU:HD11 | 1.97 | 0.45 |
| 23:BA:2056:G:C2 | 23:BA:2057:A:C8 | 3.05 | 0.45 |
| 38:BU:43:GLY:HA3 | 39:BV:73:SER:OG | 2.15 | 0.45 |
| 27:DF:88:VAL:HG21 | 27:DF:91:GLY:HA3 | 1.98 | 0.45 |
| 4:AD:64:LEU:HD12 | 4:AD:68:TYR:HE1 | 1.81 | 0.45 |
| 9:AI:19:LEU:HA | 9:AI:19:LEU:HD23 | 1.66 | 0.45 |
| 1:CA:1092:A:OP1 | 1:CA:1092:A:H8 | 2.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BU:5:LYS:HE3 | 38:BU:5:LYS:HB2 | 1.74 | 0.45 |
| 23:BA:247:G:H4' | 23:BA:386:G:C5 | 2.52 | 0.45 |
| 1:AA:1427:U:H2' | 1:AA:1428:A:C8 | 2.52 | 0.45 |
| 23:DA:2062:A:P | 56:DA:4041:HOH:O | 2.74 | 0.45 |
| 5:CE:7:GLU:OE2 | 5:CE:37:ARG:NH2 | 2.45 | 0.45 |
| 1:CA:1457:G:C2 | 1:CA:1458:G:C8 | 3.05 | 0.45 |
| 23:DA:2820:A:OP1 | 35:DR:4:LEU:HD23 | 2.17 | 0.45 |
| 1:AA:1027:C:H1' | 1:AA:1034:G:H22 | 1.82 | 0.45 |
| 1:AA:1027:C:H2' | 1:AA:1028:C:C5 | 2.51 | 0.45 |
| 8:AH:88:LYS:HB3 | 8:AH:89:PRO:HD2 | 1.99 | 0.45 |
| 1:AA:1317:C:C5 | 1:AA:1318:A:C8 | 3.04 | 0.45 |
| 1:AA:1321:C:C3' | 1:AA:1322:C:H5'' | 2.47 | 0.45 |
| 1:CA:1124:G:O2' | 10:CJ:38:ILE:HD13 | 2.17 | 0.45 |
| 1:CA:675:A:H2' | 1:CA:676:A:C8 | 2.52 | 0.45 |
| 2:CB:51:LEU:HD23 | 2:CB:55:PHE:HE2 | 1.82 | 0.45 |
| 1:CA:9:G:C2 | 1:CA:26:A:N1 | 2.84 | 0.45 |
| 23:DA:2319:G:H22 | 36:DS:3:ARG:CD | 2.29 | 0.45 |
| 1:CA:1252:A:H61 | 1:CA:1285:A:N6 | 2.15 | 0.45 |
| 9:CI:114:TYR:HD2 | 9:CI:114:TYR:N | 2.13 | 0.45 |
| 9:CI:11:LYS:O | 9:CI:12:GLU:HB3 | 2.17 | 0.45 |
| 1:CA:391:G:C6 | 1:CA:392:G:C5 | 3.05 | 0.45 |
| 1:AA:1269:A:OP1 | 21:AU:24:ARG:HG3 | 2.16 | 0.45 |
| 28:DG:106:LEU:HA | 28:DG:110:ALA:HB3 | 1.99 | 0.45 |
| 27:BF:188:ARG:HG3 | 27:BF:188:ARG:H | 1.48 | 0.45 |
| 23:BA:2742:C:OP1 | 53:B9:35:ARG:HD3 | 2.17 | 0.45 |
| 20:AT:77:ALA:O | 20:AT:81:LYS:HG3 | 2.17 | 0.45 |
| 3:AC:140:ARG:CZ | 3:AC:140:ARG:HB2 | 2.47 | 0.45 |
| 23:BA:1287:A:C5 | 23:BA:1288:U:C4 | 3.05 | 0.45 |
| 23:DA:2601:C:H3' | 23:DA:2602:A:C8 | 2.52 | 0.45 |
| 1:CA:872:A:C8 | 1:CA:874:G:C8 | 3.05 | 0.45 |
| 1:CA:375:U:C4 | 1:CA:376:G:N7 | 2.84 | 0.45 |
| 1:AA:502:G:C2 | 1:AA:503:C:C2 | 3.04 | 0.45 |
| 7:AG:108:ALA:O | 7:AG:119:ARG:HG2 | 2.16 | 0.45 |
| 23:DA:652(E):G:O6 | 23:DA:652(T):C:N3 | 2.50 | 0.45 |
| 27:DF:64:ILE:HD12 | 27:DF:65:TRP:CE3 | 2.51 | 0.45 |
| 12:CL:113:ARG:NH2 | 56:CL:201:HOH:O | 2.50 | 0.45 |
| 23:DA:1845:G:OP1 | 25:DD:258:LYS:NZ | 2.39 | 0.45 |
| 1:CA:1221:G:H1' | 19:CS:53:ASN:O | 2.17 | 0.45 |
| 43:DZ:54:HIS:ND1 | 43:DZ:101:PRO:HG3 | 2.31 | 0.45 |
| 2:CB:44:LEU:HA | 2:CB:47:THR:OG1 | 2.17 | 0.45 |
| 26:BE:111:ARG:HD3 | 26:BE:160:TYR:CD1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1651:G:H2' | 23:DA:1652:A:O4' | 2.17 | 0.45 |
| 34:BQ:60:ARG:NH1 | 43:BZ:177:PRO:HG3 | 2.31 | 0.45 |
| 26:DE:179:GLU:HB3 | 26:DE:181:LEU:HD23 | 1.99 | 0.45 |
| 12:CL:11:VAL:HG22 | 17:CQ:29:HIS:CD2 | 2.52 | 0.45 |
| 53:B9:11:CYS:HB3 | 53:B9:32:HIS:CE1 | 2.52 | 0.45 |
| 23:BA:363(D):G:O2' | 23:BA:363(E):U:H5' | 2.16 | 0.45 |
| 23:BA:272(E):G:C2 | 23:BA:364:C:N3 | 2.85 | 0.45 |
| 24:DB:106:G:H5' | 43:DZ:31:ARG:HG2 | 1.99 | 0.45 |
| 38:DU:74:LEU:HD12 | 38:DU:74:LEU:H | 1.82 | 0.45 |
| 38:BU:17:ILE:HD13 | 38:BU:17:ILE:HA | 1.81 | 0.45 |
| 1:AA:256:U:H2' | 1:AA:257:G:C8 | 2.51 | 0.45 |
| 28:DG:33:ARG:HD3 | 28:DG:162:THR:OG1 | 2.17 | 0.45 |
| 23:DA:2203:U:O2 | 23:DA:2221:G:C2 | 2.70 | 0.45 |
| 1:CA:510:A:H5'' | 1:CA:511:C:OP2 | 2.17 | 0.45 |
| 1:CA:949:A:N6 | 1:CA:1232:U:N3 | 2.40 | 0.45 |
| 1:AA:1190:G:OP2 | 3:AC:5:ILE:HB | 2.17 | 0.45 |
| 1:AA:586:C:O2' | 1:AA:878:G:H4' | 2.17 | 0.45 |
| 9:CI:13:ALA:HB3 | 9:CI:72:GLY:HA3 | 1.99 | 0.45 |
| 1:AA:18:C:H5'' | 5:AE:127:ASN:HD21 | 1.81 | 0.45 |
| 23:DA:1903:G:OP1 | 25:DD:241:PRO:HB2 | 2.16 | 0.45 |
| 23:BA:29:U:H2' | 23:BA:30:G:H8 | 1.77 | 0.45 |
| 23:BA:30:G:H2' | 23:BA:31:C:H6 | 1.82 | 0.45 |
| 23:BA:307:G:H21 | 23:BA:330:A:H62 | 1.65 | 0.45 |
| 1:CA:1079:G:C2 | 1:CA:1080:A:C6 | 3.05 | 0.45 |
| 19:CS:20:LEU:HD21 | 19:CS:43:GLU:HG2 | 1.99 | 0.45 |
| 1:CA:1299:A:C5 | 1:CA:1301:U:H1' | 2.51 | 0.45 |
| 23:BA:2130:U:OP2 | 23:BA:2132:U:H5 | 2.00 | 0.45 |
| 41:DX:31:HIS:HA | 41:DX:32:PRO:HD3 | 1.83 | 0.45 |
| 1:AA:12:U:O2' | 1:AA:526:C:H4' | 2.17 | 0.45 |
| 48:D4:36:CYS:N | 48:D4:39:CYS:SG | 2.89 | 0.45 |
| 23:BA:1046:A:O2' | 23:BA:1047:G:OP2 | 2.34 | 0.45 |
| 1:CA:1323:G:H8 | 1:CA:1323:G:OP2 | 1.99 | 0.45 |
| 19:CS:7:LYS:HA | 19:CS:7:LYS:HD3 | 1.77 | 0.45 |
| 1:CA:1360:A:C5 | 14:CN:18:VAL:HG11 | 2.51 | 0.45 |
| 3:CC:12:LEU:HB3 | 3:CC:18:TRP:CH2 | 2.52 | 0.45 |
| 13:CM:74:VAL:O | 13:CM:78:ILE:HG12 | 2.17 | 0.45 |
| 2:AB:171:ALA:HA | 2:AB:174:VAL:HB | 1.98 | 0.45 |
| 45:D1:3:LYS:HB2 | 45:D1:61:ARG:NH1 | 2.29 | 0.45 |
| 7:AG:102:ARG:NH1 | 7:AG:103:TRP:HE1 | 2.15 | 0.45 |
| 1:AA:21:G:P | 56:AA:1970:HOH:O | 2.74 | 0.45 |
| 31:DN:137:LYS:O | 31:DN:138:LEU:HD23 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:DW:4:LYS:CB | 40:DW:106:ILE:HG12 | 2.47 | 0.45 |
| 23:BA:1164:G:H2' | 23:BA:1165:U:C6 | 2.52 | 0.45 |
| 1:CA:142:G:N3 | 1:CA:143:A:C8 | 2.85 | 0.45 |
| 1:AA:67:C:H2' | 1:AA:68:G:C8 | 2.52 | 0.45 |
| 1:AA:624:C:H2' | 1:AA:625:G:C8 | 2.52 | 0.45 |
| 40:DW:9:TYR:HA | 40:DW:100:THR:HG23 | 1.99 | 0.45 |
| 1:CA:194:C:C2' | 1:CA:195:A:H5'' | 2.47 | 0.45 |
| 31:DN:73:THR:CG2 | 31:DN:82:LEU:HD11 | 2.47 | 0.45 |
| 2:CB:70:PHE:HB2 | 2:CB:92:TYR:HB3 | 1.98 | 0.45 |
| 37:BT:19:LEU:HA | 37:BT:20:PRO:HD3 | 1.81 | 0.45 |
| 23:DA:1419:A:O2' | 23:DA:1420:U:H5'' | 2.17 | 0.45 |
| 20:AT:69:GLY:O | 20:AT:73:HIS:NE2 | 2.50 | 0.45 |
| 23:BA:1814:G:H2' | 23:BA:1815:A:C8 | 2.52 | 0.45 |
| 12:AL:84:LEU:HD13 | 12:AL:85:ILE:N | 2.32 | 0.45 |
| 23:BA:2607:G:H2' | 23:BA:2608:G:O4' | 2.17 | 0.45 |
| 23:BA:2252:G:H2' | 23:BA:2253:G:O4' | 2.17 | 0.45 |
| 24:BB:104:U:O3' | 43:BZ:72:ARG:NH1 | 2.50 | 0.45 |
| 1:CA:546:G:OP1 | 4:CD:73:ARG:HG2 | 2.17 | 0.45 |
| 20:AT:53:LEU:HA | 20:AT:56:MET:HG2 | 1.99 | 0.45 |
| 23:DA:2290:G:H2' | 23:DA:2291:U:O4' | 2.16 | 0.45 |
| 1:AA:35:G:H2' | 1:AA:36:C:C6 | 2.51 | 0.45 |
| 4:AD:88:VAL:HA | 5:AE:97:GLY:HA2 | 1.99 | 0.45 |
| 1:AA:339:C:OP2 | 32:BO:97:ARG:HD3 | 2.17 | 0.45 |
| 7:AG:118:VAL:HG13 | 7:AG:122:HIS:NE2 | 2.31 | 0.45 |
| 34:BQ:109:VAL:HG22 | 34:BQ:113:GLN:OE1 | 2.17 | 0.45 |
| 32:BO:87:ILE:HG22 | 32:BO:93:PRO:HA | 1.98 | 0.45 |
| 1:CA:1107:C:C4 | 1:CA:1108:G:C8 | 3.04 | 0.45 |
| 23:DA:2563:U:O2 | 23:DA:2565:A:H8 | 2.00 | 0.45 |
| 23:DA:1448:G:H5'' | 23:DA:1542:A:OP1 | 2.17 | 0.45 |
| 23:BA:396:G:O3' | 45:B1:44:PRO:HA | 2.16 | 0.45 |
| 23:BA:1025:G:C4 | 23:BA:1135:C:H1' | 2.52 | 0.45 |
| 23:DA:2581:G:H4' | 23:DA:2582:G:C8 | 2.51 | 0.45 |
| 23:DA:116:C:H2' | 23:DA:117:G:O4' | 2.17 | 0.45 |
| 37:DT:13:ARG:HG2 | 37:DT:13:ARG:H | 1.29 | 0.45 |
| 33:BP:147:LEU:HA | 33:BP:147:LEU:HD22 | 1.83 | 0.45 |
| 23:DA:673:C:H5'' | 27:DF:81:PRO:HD2 | 1.99 | 0.45 |
| 13:CM:108:ARG:O | 13:CM:112:GLY:N | 2.50 | 0.45 |
| 23:DA:2251:G:C6 | 23:DA:2252:G:C5 | 3.05 | 0.45 |
| 47:B3:44:ARG:O | 47:B3:48:GLU:HG3 | 2.17 | 0.45 |
| 7:AG:85:TYR:O | 7:AG:87:VAL:HG23 | 2.17 | 0.45 |
| 1:CA:1230:C:H2' | 1:CA:1231:G:H8 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1169:A:H2' | 1:CA:1170:A:C8 | 2.52 | 0.45 |
| 1:CA:939:G:N2 | 1:CA:1344:C:N3 | 2.56 | 0.45 |
| 16:AP:19:ILE:CG2 | 16:AP:36:ILE:HG13 | 2.36 | 0.45 |
| 23:DA:1357:U:H2' | 23:DA:1358:G:O4' | 2.17 | 0.45 |
| 1:CA:16:A:N3 | 1:CA:1080:A:O2' | 2.45 | 0.45 |
| 23:DA:2741:A:H61 | 23:DA:2763:G:H1' | 1.81 | 0.45 |
| 1:AA:674:G:H2' | 1:AA:675:A:H8 | 1.82 | 0.45 |
| 10:AJ:19:SER:CB | 10:AJ:91:PRO:HG3 | 2.47 | 0.45 |
| 1:CA:1237:C:C2 | 1:CA:1337:G:N2 | 2.83 | 0.45 |
| 1:CA:1224:G:N1 | 1:CA:1322:C:O4' | 2.50 | 0.45 |
| 30:DI:87:LYS:N | 30:DI:122:GLU:HA | 2.27 | 0.45 |
| 1:AA:1345:U:H5'' | 9:AI:120:ARG:NH1 | 2.31 | 0.45 |
| 1:CA:148:G:N2 | 1:CA:175:C:C2 | 2.85 | 0.45 |
| 23:BA:1328:G:H2' | 23:BA:1330:C:C5 | 2.52 | 0.45 |
| 45:B1:3:LYS:HB2 | 45:B1:61:ARG:NH1 | 2.32 | 0.45 |
| 7:AG:138:LYS:HA | 7:AG:141:VAL:HB | 1.99 | 0.45 |
| 5:CE:55:VAL:O | 5:CE:58:ALA:HB3 | 2.17 | 0.45 |
| 50:B6:4:GLU:HG3 | 50:B6:5:VAL:N | 2.31 | 0.45 |
| 33:BP:64:LYS:HA | 52:B8:13:ARG:HB3 | 1.98 | 0.45 |
| 23:DA:1814:G:H2' | 23:DA:1815:A:C8 | 2.52 | 0.45 |
| 23:DA:2186:G:N3 | 23:DA:2186:G:H2' | 2.32 | 0.45 |
| 43:BZ:182:LYS:O | 43:BZ:186:GLU:HG2 | 2.16 | 0.45 |
| 42:BY:85:VAL:HG23 | 42:BY:86:ARG:O | 2.17 | 0.45 |
| 1:CA:276:G:O3' | 17:CQ:68:ARG:NH1 | 2.50 | 0.45 |
| 1:AA:509:A:H3' | 1:AA:509:A:C8 | 2.51 | 0.45 |
| 1:AA:458:C:H2' | 1:AA:460:G:H8 | 1.82 | 0.45 |
| 1:CA:1469:G:H2' | 1:CA:1470:G:H8 | 1.81 | 0.45 |
| 34:BQ:2:LEU:HB3 | 34:BQ:70:PRO:CG | 2.47 | 0.45 |
| 25:DD:147:LEU:HD13 | 25:DD:155:LEU:HD11 | 1.99 | 0.45 |
| 20:CT:36:LEU:HD13 | 20:CT:36:LEU:HA | 1.68 | 0.45 |
| 31:BN:128:HIS:H | 31:BN:128:HIS:CD2 | 2.34 | 0.45 |
| 15:CO:4:THR:H | 15:CO:7:GLU:HB2 | 1.81 | 0.45 |
| 23:BA:455:C:N3 | 23:BA:472:A:H2' | 2.32 | 0.45 |
| 1:CA:724:G:C2 | 1:CA:725:G:C8 | 3.05 | 0.45 |
| 1:AA:1342:C:H1' | 9:AI:124:GLN:HG2 | 1.98 | 0.45 |
| 36:DS:27:SER:HA | 36:DS:88:ASP:HB3 | 1.98 | 0.45 |
| 23:DA:576:U:H5 | 56:DA:3905:HOH:O | 2.00 | 0.45 |
| 23:DA:2674:G:H2' | 23:DA:2675:A:C8 | 2.52 | 0.45 |
| 43:BZ:94:GLU:HB2 | 43:BZ:95:PRO:HD2 | 1.99 | 0.45 |
| 38:BU:74:LEU:H | 38:BU:74:LEU:HD12 | 1.82 | 0.45 |
| 26:BE:178:GLU:CD | 26:BE:178:GLU:H | 2.21 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:991:U:C4 | 1:CA:1212:U:H1' | 2.53 | 0.44 |
| 1:CA:1164:G:H1 | 1:CA:1171:G:H22 | 1.65 | 0.44 |
| 52:B8:23:VAL:HG12 | 52:B8:47:LYS:HB3 | 1.99 | 0.44 |
| 1:AA:1321:C:H5' | 1:AA:1322:C:C5' | 2.44 | 0.44 |
| 1:CA:1344:C:H5'' | 9:CI:120:ARG:HG2 | 1.99 | 0.44 |
| 2:AB:216:SER:OG | 2:AB:217:ARG:N | 2.50 | 0.44 |
| 1:CA:1003:G:H3' | 1:CA:1004:A:H4' | 1.98 | 0.44 |
| 1:CA:966:G:C2 | 1:CA:967:C:C2 | 3.05 | 0.44 |
| 1:CA:9:G:OP1 | 5:CE:122:GLU:HB2 | 2.17 | 0.44 |
| 1:AA:1058:G:H2' | 1:AA:1059:C:O4' | 2.17 | 0.44 |
| 1:CA:1366:C:H2' | 1:CA:1367:C:C6 | 2.53 | 0.44 |
| 23:BA:1319:G:C2 | 23:BA:1334:G:C5 | 3.04 | 0.44 |
| 1:CA:984:C:H2' | 1:CA:985:C:O4' | 2.18 | 0.44 |
| 10:AJ:48:THR:HG23 | 10:AJ:62:HIS:HB3 | 1.99 | 0.44 |
| 1:AA:113:G:O4' | 1:AA:354:G:H4' | 2.17 | 0.44 |
| 1:CA:156:G:C6 | 1:CA:166:G:C6 | 3.05 | 0.44 |
| 7:CG:73:MET:CG | 7:CG:145:ALA:HB1 | 2.42 | 0.44 |
| 23:DA:529:A:H5'' | 56:DA:4762:HOH:O | 2.17 | 0.44 |
| 14:CN:23:ARG:HG3 | 14:CN:24:CYS:O | 2.17 | 0.44 |
| 11:AK:41:THR:HG22 | 11:AK:42:TRP:N | 2.31 | 0.44 |
| 5:AE:135:THR:O | 5:AE:138:ALA:HB3 | 2.16 | 0.44 |
| 9:AI:105:ASP:HB2 | 9:AI:107:ARG:HD3 | 1.99 | 0.44 |
| 1:AA:956:U:H2' | 1:AA:957:U:H5' | 1.99 | 0.44 |
| 1:CA:1002:G:O6 | 1:CA:1038:C:N3 | 2.50 | 0.44 |
| 27:DF:7:TYR:N | 27:DF:22:ALA:HB3 | 2.29 | 0.44 |
| 23:DA:530:G:O6 | 23:DA:2023:G:OP1 | 2.35 | 0.44 |
| 1:AA:1402:C:H2' | 1:AA:1403:C:O4' | 2.17 | 0.44 |
| 29:DH:5:GLY:HA2 | 29:DH:69:ARG:HB3 | 1.99 | 0.44 |
| 10:CJ:61:GLU:OE2 | 14:CN:49:HIS:NE2 | 2.50 | 0.44 |
| 1:AA:614:A:H2' | 1:AA:615:C:C6 | 2.52 | 0.44 |
| 18:CR:30:ASP:HB3 | 18:CR:33:ASP:HB2 | 1.98 | 0.44 |
| 38:BU:83:LEU:HD12 | 38:BU:113:ALA:HB2 | 1.99 | 0.44 |
| 23:DA:986:C:C2' | 23:DA:987:G:H5' | 2.47 | 0.44 |
| 2:CB:21:ARG:O | 2:CB:23:ARG:N | 2.47 | 0.44 |
| 23:DA:186:G:H2' | 23:DA:187:G:H8 | 1.82 | 0.44 |
| 1:AA:292:G:C5 | 1:AA:293:G:H1' | 2.51 | 0.44 |
| 23:BA:979:G:H3' | 23:BA:980:A:H5'' | 1.98 | 0.44 |
| 1:AA:402:G:C6 | 1:AA:403:C:C4 | 3.06 | 0.44 |
| 49:B5:36:CYS:HB3 | 49:B5:49:CYS:HB3 | 1.99 | 0.44 |
| 1:AA:1463:C:OP1 | 37:BT:111:ARG:NE | 2.50 | 0.44 |
| 5:CE:84:PHE:CE1 | 5:CE:133:TYR:HB3 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:BA:195:A:H4' | 23:BA:251:A:O2' | 2.17 | 0.44 |
| 43:DZ:28:MET:HG3 | 43:DZ:35:ARG:HB2 | 1.99 | 0.44 |
| 23:DA:257:A:H2' | 23:DA:258:G:O4' | 2.16 | 0.44 |
| 1:AA:1117:G:H1' | 9:AI:106:ALA:HB1 | 1.99 | 0.44 |
| 1:AA:491:G:H2' | 1:AA:492:G:O4' | 2.16 | 0.44 |
| 33:DP:101:VAL:HA | 33:DP:106:LEU:O | 2.17 | 0.44 |
| 23:DA:272(H):C:H6 | 23:DA:272(H):C:H5'' | 1.81 | 0.44 |
| 43:BZ:100:VAL:HG11 | 43:BZ:134:PRO:HG2 | 2.00 | 0.44 |
| 23:DA:34:C:H41 | 23:DA:447:A:H61 | 1.65 | 0.44 |
| 17:CQ:58:GLU:OE1 | 17:CQ:75:ARG:NH2 | 2.50 | 0.44 |
| 13:AM:52:GLU:HG2 | 13:AM:55:ARG:NH2 | 2.32 | 0.44 |
| 27:DF:20:LEU:HA | 27:DF:20:LEU:HD23 | 1.82 | 0.44 |
| 22:CX:77:LEU:HA | 22:CX:77:LEU:HD23 | 1.81 | 0.44 |
| 15:AO:32:LEU:HA | 15:AO:32:LEU:HD23 | 1.74 | 0.44 |
| 26:DE:171:GLU:O | 26:DE:184:VAL:HG23 | 2.16 | 0.44 |
| 1:CA:690:G:H2' | 1:CA:691:G:O4' | 2.17 | 0.44 |
| 23:DA:1782:C:H2' | 23:DA:2608:G:O2' | 2.17 | 0.44 |
| 4:CD:64:LEU:HD12 | 4:CD:68:TYR:HE1 | 1.82 | 0.44 |
| 1:AA:1065:U:H4' | 1:AA:1066:C:O5' | 2.17 | 0.44 |
| 1:CA:838:G:C2' | 1:CA:839:U:H5'' | 2.47 | 0.44 |
| 7:CG:26:PHE:CD2 | 7:CG:30:ILE:HD11 | 2.52 | 0.44 |
| 2:AB:70:PHE:HB2 | 2:AB:92:TYR:HB3 | 1.99 | 0.44 |
| 1:AA:1240:U:H3 | 7:AG:39:ALA:CB | 2.31 | 0.44 |
| 6:AF:11:ASN:HB3 | 6:AF:14:LEU:HG | 1.99 | 0.44 |
| 23:DA:2228:G:C5 | 23:DA:2229:C:C4 | 3.05 | 0.44 |
| 28:DG:22:ARG:HH21 | 28:DG:175:LEU:HD11 | 1.81 | 0.44 |
| 23:BA:2318:G:O2' | 23:BA:2319:G:H5'' | 2.17 | 0.44 |
| 1:AA:673:G:H5'' | 6:AF:87:ARG:CZ | 2.47 | 0.44 |
| 1:CA:369:C:O2' | 1:CA:370:C:H5' | 2.17 | 0.44 |
| 1:CA:1157:A:C2 | 1:CA:1181:G:N3 | 2.86 | 0.44 |
| 1:AA:1269:A:H1' | 1:AA:1326:C:H1' | 1.99 | 0.44 |
| 1:AA:1295:G:O3' | 13:AM:14:ARG:NH1 | 2.50 | 0.44 |
| 23:BA:1845:G:C2' | 23:BA:1846:G:H5' | 2.47 | 0.44 |
| 23:DA:1566:A:OP1 | 25:DD:211:ARG:NH1 | 2.50 | 0.44 |
| 1:AA:1399:C:C2 | 1:AA:1502:A:N6 | 2.85 | 0.44 |
| 23:DA:300:A:H3' | 42:DY:84:ARG:NH2 | 2.33 | 0.44 |
| 1:AA:138:G:H2' | 1:AA:139:G:O4' | 2.17 | 0.44 |
| 23:BA:996:A:C2 | 23:BA:997:G:C8 | 3.05 | 0.44 |
| 23:BA:997:G:OP1 | 38:BU:92:ARG:HG2 | 2.18 | 0.44 |
| 7:CG:18:TYR:HE1 | 7:CG:58:PRO:HB2 | 1.81 | 0.44 |
| 1:AA:510:A:H1' | 1:AA:543:C:H1' | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1516:G:N1 | 1:AA:1519:A:OP2 | 2.50 | 0.44 |
| 3:CC:50:ALA:HB1 | 3:CC:70:VAL:HG11 | 1.98 | 0.44 |
| 23:BA:2378:A:H4' | 36:BS:23:ARG:HH11 | 1.82 | 0.44 |
| 23:BA:1300:U:H4' | 23:BA:1301:A:H5' | 1.99 | 0.44 |
| 1:CA:609:A:H5' | 16:CP:18:ARG:NH2 | 2.32 | 0.44 |
| 28:BG:111:LEU:HA | 28:BG:114:ILE:HG13 | 1.99 | 0.44 |
| 1:AA:1380:U:H2' | 1:AA:1380:U:OP2 | 2.16 | 0.44 |
| 22:CX:81:LEU:HA | 22:CX:84:GLN:HB2 | 1.98 | 0.44 |
| 1:CA:1429:C:H2' | 1:CA:1430:C:C6 | 2.53 | 0.44 |
| 23:DA:2356:C:O3' | 44:D0:20:ARG:HD3 | 2.17 | 0.44 |
| 46:D2:65:ASN:O | 46:D2:69:ARG:NH1 | 2.50 | 0.44 |
| 23:BA:1464:C:H2' | 23:BA:1465:G:C8 | 2.52 | 0.44 |
| 24:BB:32:C:C2 | 24:BB:51:G:N2 | 2.85 | 0.44 |
| 50:D6:8:LYS:HD3 | 52:D8:34:TRP:CD2 | 2.52 | 0.44 |
| 30:BI:84:GLY:C | 30:BI:86:THR:H | 2.21 | 0.44 |
| 29:BH:144:VAL:O | 29:BH:148:ILE:HG12 | 2.17 | 0.44 |
| 36:DS:36:TYR:N | 36:DS:36:TYR:CD1 | 2.85 | 0.44 |
| 1:AA:260:G:H2' | 1:AA:261:U:C6 | 2.52 | 0.44 |
| 36:DS:53:SER:O | 36:DS:57:LYS:N | 2.50 | 0.44 |
| 26:DE:33:VAL:HG12 | 26:DE:89:ASP:O | 2.16 | 0.44 |
| 38:DU:112:ARG:NH2 | 39:DV:47:VAL:HB | 2.32 | 0.44 |
| 8:AH:26:VAL:HG23 | 8:AH:27:PRO:O | 2.17 | 0.44 |
| 1:AA:1005:A:H1' | 1:AA:1036:G:N2 | 2.31 | 0.44 |
| 1:CA:1096:C:O2' | 1:CA:1097:C:H5' | 2.17 | 0.44 |
| 1:AA:838:G:C2' | 1:AA:839:U:H5'' | 2.48 | 0.44 |
| 10:CJ:50:ILE:HD13 | 14:CN:41:ARG:HH11 | 1.82 | 0.44 |
| 19:AS:51:VAL:HG11 | 19:AS:72:GLY:HA2 | 1.99 | 0.44 |
| 9:CI:13:ALA:HB2 | 9:CI:68:GLY:N | 2.33 | 0.44 |
| 1:AA:560:U:H4' | 1:AA:561:U:O5' | 2.17 | 0.44 |
| 2:AB:55:PHE:CG | 2:AB:58:ILE:HD12 | 2.52 | 0.44 |
| 1:AA:1060:C:C2 | 1:AA:1198:G:N2 | 2.85 | 0.44 |
| 1:CA:1367:C:N4 | 1:CA:1368:G:O6 | 2.50 | 0.44 |
| 23:DA:2130:U:H2' | 23:DA:2131:G:N7 | 2.31 | 0.44 |
| 13:AM:108:ARG:O | 13:AM:113:PRO:HD3 | 2.18 | 0.44 |
| 1:AA:113:G:H2' | 1:AA:114:U:C6 | 2.52 | 0.44 |
| 2:CB:178:ARG:HH22 | 8:CH:68:ARG:NH2 | 2.13 | 0.44 |
| 24:BB:60:C:C2 | 24:BB:61:G:C8 | 3.06 | 0.44 |
| 1:CA:1361:G:H8 | 1:CA:1361:G:O5' | 2.01 | 0.44 |
| 1:CA:152:A:N6 | 1:CA:169:C:N3 | 2.65 | 0.44 |
| 13:CM:23:TYR:HB3 | 13:CM:67:GLU:OE1 | 2.17 | 0.44 |
| 23:BA:2306:C:N3 | 23:BA:2307:G:O6 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 23:BA:271(F):C:H2' | 23:BA:271(G):C:C6 | 2.46 | 0.44 |
| 28:DG:133:LEU:HD12 | 28:DG:134:GLY:N | 2.32 | 0.44 |
| 15:AO:78:TYR:O | 15:AO:82:ILE:HG12 | 2.17 | 0.44 |
| 30:BI:33:ARG:HB2 | 30:BI:35:LEU:HD12 | 1.99 | 0.44 |
| 23:DA:1509(A):A:H3' | 23:DA:1509(B):A:C8 | 2.50 | 0.44 |
| 23:BA:545:G:H4' | 23:BA:545:G:OP1 | 2.17 | 0.44 |
| 43:DZ:111:VAL:C | 43:DZ:113:ALA:H | 2.21 | 0.44 |
| 11:AK:84:VAL:CG1 | 11:AK:91:ARG:HD2 | 2.48 | 0.44 |
| 23:BA:2491:U:O2' | 23:BA:2570:G:OP1 | 2.27 | 0.44 |
| 40:DW:60:ASN:HD22 | 40:DW:60:ASN:H | 1.63 | 0.44 |
| 10:CJ:48:THR:HG23 | 10:CJ:62:HIS:HB3 | 1.98 | 0.44 |
| 24:DB:104:U:O3' | 43:DZ:72:ARG:NH1 | 2.50 | 0.44 |
| 2:CB:24:TRP:CZ3 | 2:CB:29:ALA:HB2 | 2.51 | 0.44 |
| 23:DA:649:G:H2' | 23:DA:650:C:H6 | 1.82 | 0.44 |
| 34:DQ:59:ARG:HB3 | 34:DQ:60:ARG:H | 1.69 | 0.44 |
| 4:AD:119:GLN:HE21 | 4:AD:119:GLN:HB3 | 1.57 | 0.44 |
| 11:AK:73:MET:HE2 | 11:AK:103:LEU:HD13 | 2.00 | 0.44 |
| 32:DO:3:GLN:HB2 | 32:DO:4:PRO:HD2 | 2.00 | 0.44 |
| 23:BA:2208:A:H1' | 23:BA:2219:G:C4 | 2.52 | 0.44 |
| 2:CB:143:GLU:O | 2:CB:146:GLN:HB2 | 2.17 | 0.44 |
| 53:B9:10:ILE:HD12 | 53:B9:32:HIS:HA | 1.99 | 0.44 |
| 11:AK:99:GLN:HG3 | 11:AK:105:VAL:HG11 | 1.99 | 0.44 |
| 23:DA:500:G:N1 | 23:DA:503:A:OP2 | 2.50 | 0.44 |
| 23:BA:1161:C:O2' | 39:BV:8:GLY:HA2 | 2.18 | 0.44 |
| 23:BA:2391:G:O6 | 23:BA:2425:A:H8 | 2.00 | 0.44 |
| 38:BU:106:PHE:O | 38:BU:110:VAL:HG23 | 2.18 | 0.44 |
| 23:BA:1282:U:H2' | 23:BA:1283:G:O4' | 2.17 | 0.44 |
| 23:BA:566:U:H5'' | 33:BP:29:LYS:HE3 | 1.98 | 0.44 |
| 23:DA:2751:G:C4 | 29:DH:2:SER:N | 2.86 | 0.44 |
| 23:DA:646:A:H2' | 23:DA:647:G:O4' | 2.17 | 0.44 |
| 1:AA:1508:G:H2' | 1:AA:1509:C:C6 | 2.53 | 0.44 |
| 28:BG:9:ARG:NH1 | 28:BG:13:GLU:OE1 | 2.46 | 0.44 |
| 23:DA:1108:U:O2 | 23:DA:1108:U:H2' | 2.17 | 0.44 |
| 23:BA:428:A:H8 | 23:BA:428:A:OP2 | 2.00 | 0.44 |
| 1:AA:1431:C:H2' | 1:AA:1432:G:O4' | 2.17 | 0.44 |
| 1:CA:1041:A:H2' | 1:CA:1042:G:O4' | 2.17 | 0.44 |
| 22:AX:53:THR:HA | 22:AX:62:HIS:HB3 | 1.99 | 0.44 |
| 23:DA:2226:C:H3' | 56:DA:4145:HOH:O | 2.18 | 0.44 |
| 1:CA:1128:C:H1' | 1:CA:1146:A:N6 | 2.32 | 0.44 |
| 9:CI:74:ILE:HG22 | 9:CI:75:ASP:OD2 | 2.17 | 0.44 |
| 1:CA:1003:G:C2 | 1:CA:1004:A:H1' | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:782:A:O3' | 1:CA:1515:C:H4' | 2.17 | 0.44 |
| 27:BF:101:LEU:HA | 27:BF:101:LEU:HD12 | 1.74 | 0.44 |
| 23:BA:2319:G:H22 | 36:BS:3:ARG:CD | 2.30 | 0.44 |
| 23:DA:2125:G:H21 | 23:DA:2126:A:N6 | 2.15 | 0.44 |
| 1:CA:1026:G:H2' | 1:CA:1026:G:N3 | 2.31 | 0.44 |
| 1:AA:153:C:H42 | 1:AA:169:C:N4 | 2.15 | 0.44 |
| 48:B4:26:SER:OG | 48:B4:27:THR:N | 2.43 | 0.44 |
| 28:DG:56:ALA:CA | 28:DG:153:ARG:HH21 | 2.31 | 0.44 |
| 7:CG:137:LYS:HA | 7:CG:140:ASP:OD2 | 2.17 | 0.44 |
| 7:CG:70:LYS:HA | 7:CG:71:PRO:HD2 | 1.74 | 0.44 |
| 23:DA:528:A:O2' | 23:DA:529:A:H5' | 2.17 | 0.44 |
| 24:BB:90:A:C5 | 24:BB:91:C:H1' | 2.53 | 0.44 |
| 23:BA:1049:C:H1' | 23:BA:1113:U:H4' | 1.99 | 0.44 |
| 9:AI:71:SER:O | 9:AI:75:ASP:N | 2.28 | 0.44 |
| 36:DS:10:ARG:O | 36:DS:14:VAL:HG12 | 2.17 | 0.44 |
| 1:AA:1251:A:O2' | 1:AA:1370:G:H5' | 2.18 | 0.44 |
| 23:BA:2306:C:H3' | 23:BA:2307:G:H8 | 1.77 | 0.44 |
| 1:AA:1226:C:OP1 | 13:AM:91:ARG:NH1 | 2.50 | 0.44 |
| 36:BS:88:ASP:OD1 | 36:BS:90:GLY:N | 2.47 | 0.44 |
| 5:AE:76:ILE:HD11 | 5:AE:142:LEU:HD11 | 1.99 | 0.44 |
| 28:BG:178:PHE:HB3 | 28:BG:180:PHE:CE1 | 2.53 | 0.44 |
| 23:BA:504:U:H2' | 56:BA:4228:HOH:O | 2.18 | 0.44 |
| 5:CE:32:VAL:HB | 5:CE:58:ALA:HB1 | 1.99 | 0.44 |
| 3:AC:110:ASN:ND2 | 3:AC:140:ARG:HD2 | 2.32 | 0.44 |
| 9:CI:17:VAL:HG11 | 9:CI:81:ILE:CA | 2.47 | 0.44 |
| 1:AA:376:G:OP2 | 16:AP:67:THR:HG21 | 2.17 | 0.44 |
| 42:BY:76:CYS:HA | 42:BY:77:PRO:HD3 | 1.87 | 0.44 |
| 20:AT:16:HIS:O | 20:AT:19:SER:N | 2.50 | 0.44 |
| 23:DA:729:G:H2' | 23:DA:1775:U:H1' | 2.00 | 0.44 |
| 23:DA:627:A:C6 | 23:DA:637:A:C8 | 3.05 | 0.44 |
| 24:DB:20:C:H2' | 24:DB:21:G:H5' | 2.00 | 0.44 |
| 1:AA:1350:A:O2' | 7:AG:33:ASP:OD2 | 2.32 | 0.44 |
| 2:AB:162:ILE:HD11 | 2:AB:184:VAL:HG22 | 1.99 | 0.44 |
| 23:DA:2695:C:H2' | 23:DA:2696:U:C6 | 2.53 | 0.44 |
| 12:AL:38:THR:OG1 | 12:AL:39:VAL:N | 2.51 | 0.44 |
| 23:DA:1804:C:H2' | 23:DA:1805:U:H6 | 1.83 | 0.44 |
| 1:AA:439:A:C4 | 1:AA:496:A:C2 | 3.06 | 0.44 |
| 23:BA:2058:A:H5'' | 23:BA:2059:A:OP2 | 2.17 | 0.44 |
| 23:BA:1949:G:C6 | 23:BA:1950:G:C6 | 3.06 | 0.44 |
| 23:BA:868:U:H2' | 23:BA:869:G:O4' | 2.17 | 0.44 |
| 3:AC:178:LEU:HA | 3:AC:178:LEU:HD13 | 1.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BQ:7:MET:HB2 | 34:BQ:7:MET:HE3 | 1.66 | 0.44 |
| 7:CG:53:LYS:HB3 | 7:CG:53:LYS:HE2 | 1.54 | 0.44 |
| 41:DX:60:ARG:HE | 41:DX:60:ARG:HB3 | 1.45 | 0.44 |
| 31:DN:128:HIS:CD2 | 31:DN:128:HIS:H | 2.36 | 0.44 |
| 37:BT:27:THR:HB | 37:BT:89:VAL:HG23 | 1.98 | 0.44 |
| 15:AO:43:LEU:HD23 | 15:AO:43:LEU:HA | 1.84 | 0.44 |
| 23:DA:389:G:O5' | 23:DA:389:G:H8 | 2.01 | 0.44 |
| 1:AA:997:U:H2' | 1:AA:998:G:O4' | 2.17 | 0.44 |
| 35:DR:85:PRO:O | 35:DR:87:TYR:N | 2.50 | 0.44 |
| 23:DA:1007:C:OP1 | 31:DN:35:ARG:NH1 | 2.50 | 0.44 |
| 1:CA:1459:C:P | 1:CA:1460:A:OP2 | 2.75 | 0.44 |
| 1:AA:1096:C:H2' | 1:AA:1097:C:C6 | 2.53 | 0.44 |
| 1:CA:1225:A:H5' | 1:CA:1226:C:OP2 | 2.17 | 0.44 |
| 23:BA:1171:G:HO2' | 23:BA:1173:G:P | 2.30 | 0.44 |
| 1:CA:1299:A:C8 | 1:CA:1301:U:H1' | 2.52 | 0.44 |
| 1:CA:1155:G:H2' | 1:CA:1156:G:H8 | 1.81 | 0.44 |
| 19:AS:61:TYR:CG | 19:AS:62:ILE:N | 2.86 | 0.44 |
| 1:AA:373:A:H2' | 1:AA:374:A:H8 | 1.82 | 0.44 |
| 3:CC:153:VAL:HG12 | 3:CC:196:LEU:HD12 | 2.00 | 0.44 |
| 1:AA:960:U:C4 | 1:AA:1225:A:H1' | 2.52 | 0.44 |
| 1:CA:1001(A):G:H2' | 1:CA:1002:G:C8 | 2.52 | 0.44 |
| 2:CB:141:GLU:O | 2:CB:145:LEU:HB2 | 2.17 | 0.44 |
| 23:BA:993:G:C6 | 23:BA:994:C:N4 | 2.85 | 0.44 |
| 19:CS:81:ARG:HB2 | 19:CS:81:ARG:NH1 | 2.31 | 0.44 |
| 25:DD:148:GLU:CB | 25:DD:151:LYS:HD2 | 2.47 | 0.44 |
| 1:CA:142:G:H1 | 1:CA:221:C:H42 | 1.64 | 0.44 |
| 25:BD:107:ALA:HA | 25:BD:108:PRO:HD2 | 1.90 | 0.44 |
| 23:BA:1799:G:H5' | 23:BA:1819:A:N6 | 2.32 | 0.44 |
| 2:AB:80:ILE:HG12 | 2:AB:211:ILE:HG22 | 2.00 | 0.44 |
| 7:CG:62:PHE:HD1 | 7:CG:124:LEU:HD21 | 1.82 | 0.44 |
| 1:AA:685:G:C2 | 1:AA:686:U:C4 | 3.06 | 0.44 |
| 28:BG:39:ILE:HG23 | 28:BG:157:ILE:HD13 | 2.00 | 0.44 |
| 27:DF:123:LEU:HD11 | 27:DF:194:MET:HE2 | 2.00 | 0.44 |
| 20:AT:74:LYS:HB2 | 20:AT:75:ASN:H | 1.47 | 0.44 |
| 27:BF:168:ARG:CB | 27:BF:168:ARG:HH11 | 2.31 | 0.44 |
| 23:DA:864:G:C6 | 23:DA:865:C:N4 | 2.86 | 0.44 |
| 26:DE:119:ARG:HG2 | 26:DE:160:TYR:HB2 | 2.00 | 0.44 |
| 29:DH:38:SER:HB2 | 29:DH:64:LEU:HD22 | 1.99 | 0.44 |
| 35:DR:103:ARG:HG2 | 35:DR:103:ARG:NH1 | 2.33 | 0.44 |
| 48:B4:14:ILE:HD11 | 48:B4:24:THR:OG1 | 2.16 | 0.44 |
| 23:BA:1547:C:H2' | 23:BA:1548:C:C6 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:2282:G:H4' | 23:BA:2389:G:O2' | 2.17 | 0.44 |
| 9:AI:99:LEU:HB3 | 9:AI:101:PHE:HD1 | 1.83 | 0.44 |
| 23:DA:1827:C:OP2 | 25:DD:222:ARG:HD2 | 2.17 | 0.44 |
| 25:BD:145:VAL:HG12 | 25:BD:146:GLU:O | 2.18 | 0.44 |
| 23:BA:2496:C:OP1 | 34:BQ:82:ARG:HB3 | 2.18 | 0.44 |
| 23:DA:1717:G:C2 | 23:DA:1718:G:C8 | 3.05 | 0.44 |
| 30:DI:33:ARG:HB2 | 30:DI:35:LEU:HD12 | 1.98 | 0.44 |
| 27:DF:79:GLY:HA2 | 27:DF:86:GLY:HA2 | 1.99 | 0.44 |
| 13:AM:77:ASN:OD1 | 13:AM:77:ASN:N | 2.50 | 0.44 |
| 38:BU:39:LEU:HA | 38:BU:39:LEU:HD23 | 1.74 | 0.44 |
| 29:DH:137:ASP:HB3 | 29:DH:140:LYS:HE2 | 2.00 | 0.44 |
| 19:AS:11:VAL:HG13 | 19:AS:13:ASP:H | 1.82 | 0.44 |
| 23:BA:125:G:C6 | 51:B7:10:ARG:HG3 | 2.52 | 0.44 |
| 1:AA:1441:G:H5' | 1:AA:1442:G:OP1 | 2.17 | 0.44 |
| 1:CA:989:C:N4 | 1:CA:1216:G:N1 | 2.28 | 0.44 |
| 1:AA:1003:G:N2 | 1:AA:1004:A:HO2' | 2.14 | 0.44 |
| 23:DA:848:G:N9 | 23:DA:933:A:H8 | 2.15 | 0.44 |
| 13:CM:10:PRO:HG2 | 13:CM:45:VAL:HG21 | 1.98 | 0.44 |
| 1:CA:1372:U:C4 | 1:CA:1373:G:C6 | 3.05 | 0.44 |
| 23:BA:1530:C:HO2' | 23:BA:1531:C:P | 2.35 | 0.44 |
| 1:AA:1057:G:C5 | 1:AA:1204:A:C2 | 3.05 | 0.44 |
| 28:DG:16:ARG:HB2 | 28:DG:17:PRO:HD3 | 2.00 | 0.44 |
| 1:CA:1296:C:H4' | 1:CA:1302:U:C4 | 2.53 | 0.44 |
| 1:CA:1250:A:C2 | 1:CA:1370:G:H1' | 2.53 | 0.44 |
| 1:CA:427:U:P | 4:CD:13:ARG:HH22 | 2.40 | 0.44 |
| 1:CA:958:A:N6 | 1:CA:959:A:N1 | 2.66 | 0.44 |
| 1:CA:982:U:H4' | 1:CA:983:A:O5' | 2.17 | 0.44 |
| 1:AA:1293:G:C2 | 1:AA:1294:G:C4 | 3.06 | 0.44 |
| 19:CS:12:ASP:C | 19:CS:14:HIS:H | 2.17 | 0.44 |
| 28:DG:178:PHE:HB3 | 28:DG:180:PHE:HE1 | 1.82 | 0.44 |
| 23:DA:83:G:H22 | 23:DA:102:G:H2' | 1.81 | 0.44 |
| 17:AQ:45:HIS:CE1 | 17:AQ:47:PRO:HG3 | 2.53 | 0.44 |
| 13:AM:63:THR:HB | 13:AM:64:TRP:CE3 | 2.53 | 0.44 |
| 10:CJ:51:ARG:NH2 | 10:CJ:61:GLU:HB3 | 2.33 | 0.44 |
| 3:AC:40:ARG:O | 3:AC:44:GLU:N | 2.50 | 0.44 |
| 23:DA:579:G:H2' | 23:DA:580:C:C6 | 2.53 | 0.44 |
| 23:BA:1488:G:N1 | 23:BA:1489:U:O2 | 2.50 | 0.44 |
| 23:DA:921:G:C5 | 23:DA:922:U:C4 | 3.05 | 0.44 |
| 23:BA:2698:U:H2' | 23:BA:2699:C:C6 | 2.52 | 0.44 |
| 23:BA:2150:U:H2' | 23:BA:2151:G:C8 | 2.53 | 0.44 |
| 1:CA:346:G:N2 | 1:CA:347:G:C8 | 2.86 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:BA:1525:G:H2' | 23:BA:1526:G:O4' | 2.17 | 0.44 |
| 13:AM:52:GLU:HG2 | 13:AM:55:ARG:HH22 | 1.82 | 0.44 |
| 12:CL:82:VAL:HG23 | 12:CL:106:ASP:OD2 | 2.17 | 0.44 |
| 24:BB:13:A:N1 | 24:BB:69:G:O2' | 2.40 | 0.44 |
| 23:DA:311:A:C8 | 23:DA:332:A:N7 | 2.86 | 0.44 |
| 42:DY:68:HIS:ND1 | 42:DY:70:SER:HB3 | 2.32 | 0.44 |
| 23:DA:975(A):G:H1' | 23:DA:990:A:C2 | 2.53 | 0.44 |
| 23:BA:272(H):C:H6 | 23:BA:272(H):C:H5'' | 1.82 | 0.44 |
| 35:DR:95:THR:HG22 | 35:DR:116:LEU:HD23 | 1.99 | 0.44 |
| 8:AH:73:ASP:OD2 | 8:AH:75:ARG:HB2 | 2.18 | 0.44 |
| 23:BA:2031:A:C6 | 23:BA:2498:C:H1' | 2.53 | 0.44 |
| 23:DA:1161:C:O2' | 39:DV:8:GLY:HA2 | 2.17 | 0.44 |
| 34:BQ:57:HIS:CD2 | 34:BQ:117:ALA:HB2 | 2.52 | 0.44 |
| 52:B8:62:LEU:HB3 | 52:B8:65:GLU:HG2 | 1.99 | 0.44 |
| 23:DA:297:C:H3' | 56:DA:3761:HOH:O | 2.18 | 0.44 |
| 52:D8:39:LYS:HA | 52:D8:42:ARG:NH1 | 2.33 | 0.44 |
| 33:DP:77:ARG:HB2 | 33:DP:78:PRO:HD2 | 1.99 | 0.44 |
| 40:DW:19:LEU:HD12 | 40:DW:19:LEU:HA | 1.70 | 0.44 |
| 29:DH:27:LYS:HB3 | 29:DH:27:LYS:HE2 | 1.77 | 0.44 |
| 3:CC:71:ALA:HA | 3:CC:106:VAL:N | 2.32 | 0.44 |
| 25:BD:69:ARG:NH2 | 25:BD:128:GLY:O | 2.50 | 0.44 |
| 1:CA:317:G:C6 | 1:CA:318:G:C5 | 3.06 | 0.44 |
| 1:AA:717:C:H4' | 11:AK:117:ASN:HB3 | 1.99 | 0.44 |
| 1:CA:1459:C:H6 | 1:CA:1459:C:H3' | 1.83 | 0.44 |
| 9:CI:73:GLN:O | 9:CI:76:ALA:HB3 | 2.18 | 0.44 |
| 1:AA:9:G:OP1 | 5:AE:122:GLU:HB2 | 2.17 | 0.44 |
| 1:AA:1242:C:H4' | 1:AA:1303:C:O3' | 2.18 | 0.44 |
| 1:CA:1006:C:C2 | 1:CA:1023:G:N1 | 2.86 | 0.44 |
| 1:AA:1291:G:H4' | 9:AI:39:GLY:HA3 | 2.00 | 0.44 |
| 1:AA:1053:G:N7 | 1:AA:1199:U:H3' | 2.33 | 0.44 |
| 28:BG:143:GLU:H | 28:BG:143:GLU:HG2 | 1.55 | 0.44 |
| 28:BG:59:GLU:O | 28:BG:63:ILE:N | 2.46 | 0.44 |
| 33:BP:71:VAL:HG23 | 33:BP:72:PRO:HA | 2.00 | 0.44 |
| 3:AC:22:TRP:O | 10:AJ:11:PHE:HD1 | 2.00 | 0.44 |
| 23:BA:1530:C:H1' | 23:BA:1531:C:OP1 | 2.18 | 0.44 |
| 23:DA:2117:A:N6 | 23:DA:2171:A:C6 | 2.86 | 0.44 |
| 1:AA:1267:C:O2 | 1:AA:1327:C:H4' | 2.17 | 0.44 |
| 48:B4:9:LEU:HD22 | 48:B4:26:SER:HA | 2.00 | 0.44 |
| 1:AA:12:U:H4' | 1:AA:526:C:O2' | 2.18 | 0.44 |
| 20:CT:21:LYS:O | 20:CT:25:ARG:HG3 | 2.17 | 0.44 |
| 10:AJ:50:ILE:HD13 | 14:AN:41:ARG:NH1 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:657:G:H2' | 1:CA:658:G:H8 | 1.82 | 0.44 |
| 2:CB:197:VAL:HG12 | 2:CB:198:ASP:H | 1.82 | 0.44 |
| 1:CA:1323:G:N2 | 1:CA:1361:G:O2' | 2.51 | 0.44 |
| 4:AD:107:ARG:NE | 4:AD:173:TRP:HZ2 | 2.15 | 0.44 |
| 23:BA:2309:A:C6 | 23:BA:2310:A:C2 | 3.05 | 0.44 |
| 23:DA:1557:C:H5'' | 23:DA:1558:A:OP2 | 2.18 | 0.44 |
| 50:B6:47:THR:HG22 | 50:B6:48:VAL:N | 2.31 | 0.44 |
| 1:AA:604:G:C5 | 1:AA:605:U:C5 | 3.06 | 0.44 |
| 5:AE:75:THR:HG23 | 5:AE:76:ILE:O | 2.17 | 0.44 |
| 1:AA:1401:G:C2 | 1:AA:1402:C:H1' | 2.53 | 0.44 |
| 5:CE:76:ILE:HD11 | 5:CE:142:LEU:HD11 | 2.00 | 0.44 |
| 4:CD:31:CYS:SG | 4:CD:31:CYS:O | 2.76 | 0.44 |
| 17:AQ:13:ASP:CG | 17:AQ:14:LYS:N | 2.71 | 0.44 |
| 27:BF:64:ILE:HG13 | 27:BF:65:TRP:N | 2.32 | 0.44 |
| 23:BA:2601:C:H3' | 23:BA:2602:A:C8 | 2.53 | 0.44 |
| 2:AB:97:TRP:CZ2 | 2:AB:101:MET:HB2 | 2.53 | 0.44 |
| 26:BE:9:VAL:HB | 37:BT:3:ARG:HG2 | 1.99 | 0.44 |
| 1:CA:35:G:C2 | 1:CA:550:G:N3 | 2.85 | 0.44 |
| 12:AL:32:PHE:HB3 | 12:AL:84:LEU:HD11 | 1.99 | 0.44 |
| 23:BA:2032:G:O2' | 26:BE:145:LYS:NZ | 2.50 | 0.44 |
| 23:DA:1547:C:H2' | 23:DA:1548:C:C6 | 2.53 | 0.44 |
| 23:BA:335:C:H2' | 23:BA:336:C:C6 | 2.52 | 0.44 |
| 32:BO:17:ARG:HD2 | 32:BO:47:ILE:HG23 | 1.99 | 0.44 |
| 43:DZ:98:MET:O | 43:DZ:125:LEU:HD12 | 2.17 | 0.44 |
| 43:BZ:72:ARG:HD3 | 43:BZ:72:ARG:HA | 1.58 | 0.44 |
| 2:AB:112:VAL:HG22 | 2:AB:149:LEU:HD13 | 1.99 | 0.44 |
| 23:DA:1426:G:N7 | 25:DD:31:LYS:NZ | 2.58 | 0.44 |
| 23:DA:2291:U:O2' | 23:DA:2374:C:O2 | 2.35 | 0.44 |
| 53:B9:32:HIS:O | 53:B9:34:GLN:HG3 | 2.18 | 0.44 |
| 23:BA:2478:A:H5' | 53:B9:31:LYS:HD3 | 2.00 | 0.44 |
| 24:DB:96:U:H2' | 24:DB:97:G:C8 | 2.53 | 0.44 |
| 25:DD:68:LYS:HD2 | 25:DD:70:TRP:CZ2 | 2.52 | 0.44 |
| 1:AA:115:G:H4' | 1:AA:116:A:O5' | 2.17 | 0.44 |
| 1:CA:120:A:H2' | 1:CA:121:C:H4' | 1.98 | 0.44 |
| 23:BA:2881:C:H2' | 23:BA:2882:A:O4' | 2.18 | 0.44 |
| 23:BA:1965:C:H3' | 23:BA:1966:A:H2' | 1.99 | 0.44 |
| 44:D0:24:LYS:O | 44:D0:25:ARG:HD3 | 2.17 | 0.44 |
| 12:AL:60:LEU:HB3 | 12:AL:62:SER:H | 1.82 | 0.44 |
| 10:CJ:96:ILE:H | 10:CJ:96:ILE:HG13 | 1.61 | 0.44 |
| 23:DA:1126:A:OP1 | 23:DA:1126:A:H8 | 2.01 | 0.44 |
| 43:BZ:144:LEU:HA | 43:BZ:144:LEU:HD12 | 1.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 40:BW:36:LEU:HD23 | 40:BW:36:LEU:HA | 1.71 | 0.44 |
| 23:DA:857:C:H4' | 44:D0:23:VAL:HG21 | 1.99 | 0.44 |
| 1:CA:1442(A):G:H2' | 1:CA:1442(B):A:H5'' | 2.00 | 0.44 |
| 23:BA:2336:A:H61 | 44:B0:43:THR:CG2 | 2.29 | 0.44 |
| 7:AG:87:VAL:HA | 7:AG:88:PRO:HD2 | 1.78 | 0.44 |
| 23:BA:36:G:O2' | 23:BA:450:G:H2' | 2.18 | 0.44 |
| 1:AA:1065:U:H5' | 1:AA:1190:G:N2 | 2.33 | 0.44 |
| 14:AN:6:LEU:HD12 | 14:AN:9:LYS:CB | 2.48 | 0.44 |
| 19:AS:36:ARG:NH1 | 19:AS:52:TYR:O | 2.51 | 0.44 |
| 2:AB:55:PHE:HA | 2:AB:58:ILE:CG1 | 2.47 | 0.44 |
| 33:BP:38:GLN:HG3 | 33:BP:45:LEU:HD23 | 1.99 | 0.44 |
| 1:CA:560:U:H4' | 1:CA:561:U:C5' | 2.47 | 0.44 |
| 1:CA:1117:G:C8 | 1:CA:1117:G:H5'' | 2.53 | 0.44 |
| 23:BA:1142(A):A:C4 | 23:BA:1144:G:C8 | 3.05 | 0.44 |
| 23:BA:1790:C:H2' | 23:BA:1791:A:C5 | 2.53 | 0.44 |
| 1:CA:979:C:O2 | 14:CN:19:ARG:HG2 | 2.18 | 0.44 |
| 1:AA:191:G:C6 | 1:AA:192:U:C4 | 3.06 | 0.44 |
| 1:CA:1112:C:H42 | 3:CC:178:LEU:HD23 | 1.83 | 0.44 |
| 23:BA:2169:A:H3' | 23:BA:2170:A:C8 | 2.51 | 0.44 |
| 7:AG:103:TRP:HA | 7:AG:106:GLN:HE21 | 1.82 | 0.44 |
| 23:DA:511:U:C5 | 23:DA:512:G:C5 | 3.05 | 0.44 |
| 5:CE:71:LEU:HD23 | 5:CE:115:VAL:HG22 | 1.99 | 0.44 |
| 23:DA:2748:A:C6 | 23:DA:2749:A:C5 | 3.06 | 0.44 |
| 23:DA:2378:A:H4' | 36:DS:23:ARG:HH11 | 1.83 | 0.44 |
| 27:BF:129:PHE:O | 27:BF:132:VAL:HG13 | 2.18 | 0.44 |
| 33:BP:46:LYS:HE3 | 33:BP:51:PHE:CD1 | 2.53 | 0.44 |
| 23:DA:548:A:H61 | 39:DV:19:LYS:H | 1.65 | 0.44 |
| 43:DZ:111:VAL:O | 43:DZ:112:ARG:HB2 | 2.18 | 0.44 |
| 20:CT:74:LYS:HB2 | 20:CT:75:ASN:H | 1.47 | 0.44 |
| 1:CA:189(B):C:H2' | 1:CA:189(C):C:O4' | 2.18 | 0.44 |
| 48:B4:34:GLU:CD | 48:B4:35:VAL:H | 2.21 | 0.44 |
| 23:DA:2884:U:H1' | 49:D5:53:ALA:HB2 | 2.00 | 0.44 |
| 23:BA:2463:C:H2' | 23:BA:2464:C:H5' | 2.00 | 0.44 |
| 23:BA:141:A:H8 | 23:BA:1408:C:O2' | 1.99 | 0.44 |
| 1:CA:35:G:H2' | 1:CA:36:C:H6 | 1.81 | 0.44 |
| 23:BA:1040:C:O5' | 23:BA:1040:C:H6 | 2.00 | 0.44 |
| 1:CA:1065:U:H6 | 1:CA:1190:G:H21 | 1.64 | 0.44 |
| 4:AD:120:LEU:HB3 | 4:AD:126:ILE:HD11 | 2.00 | 0.44 |
| 7:AG:18:TYR:CZ | 7:AG:58:PRO:HB2 | 2.53 | 0.44 |
| 7:AG:56:GLN:OE1 | 7:AG:61:VAL:HG22 | 2.17 | 0.44 |
| 23:BA:1952:A:N3 | 32:BO:22:ILE:HD12 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 26:BE:111:ARG:HD3 | 26:BE:160:TYR:CE1 | 2.52 | 0.44 |
| 32:BO:117:LEU:HA | 32:BO:117:LEU:HD23 | 1.71 | 0.44 |
| 32:BO:63:VAL:HG12 | 32:BO:106:LEU:HD11 | 2.00 | 0.44 |
| 1:CA:328:C:H4' | 1:CA:329:A:H5' | 1.99 | 0.44 |
| 51:B7:43:THR:HA | 51:B7:44:PRO:HD2 | 1.74 | 0.44 |
| 1:AA:564:C:O2' | 8:AH:91:ARG:NH2 | 2.42 | 0.44 |
| 23:BA:1910:G:O2' | 23:BA:1911:U:H5' | 2.17 | 0.44 |
| 28:DG:47:LYS:HG3 | 28:DG:48:GLU:H | 1.82 | 0.44 |
| 33:DP:2:LYS:HG2 | 33:DP:4:SER:H | 1.83 | 0.44 |
| 23:BA:1108:U:H2' | 23:BA:1108:U:O2 | 2.17 | 0.44 |
| 23:DA:815:C:C2 | 23:DA:1193:G:C2 | 3.06 | 0.44 |
| 23:BA:63:U:OP2 | 56:BA:5009:HOH:O | 2.21 | 0.44 |
| 34:DQ:57:HIS:CD2 | 34:DQ:117:ALA:HB2 | 2.53 | 0.44 |
| 23:DA:733:G:N7 | 56:DA:3799:HOH:O | 2.36 | 0.44 |
| 23:BA:1039:G:H1' | 23:BA:1117:G:N2 | 2.32 | 0.44 |
| 23:DA:2687:U:H2' | 23:DA:2688:U:O4' | 2.18 | 0.44 |
| 1:CA:687:A:H4' | 11:CK:47:VAL:HG13 | 2.00 | 0.44 |
| 43:BZ:150:LEU:O | 43:BZ:171:ILE:HG13 | 2.18 | 0.44 |
| 23:DA:303:U:H2' | 23:DA:304:G:C8 | 2.53 | 0.44 |
| 23:DA:2064:C:H2' | 23:DA:2065:C:C6 | 2.53 | 0.44 |
| 10:CJ:7:LYS:N | 10:CJ:97:GLU:O | 2.48 | 0.44 |
| 5:AE:84:PHE:CE1 | 5:AE:133:TYR:HB3 | 2.53 | 0.44 |
| 11:AK:92:GLU:HB3 | 11:AK:96:ARG:HH12 | 1.82 | 0.44 |
| 28:DG:169:ALA:O | 28:DG:173:LEU:HG | 2.17 | 0.44 |
| 1:AA:1442(A):G:C3' | 1:AA:1442(B):A:H5'' | 2.48 | 0.44 |
| 23:BA:2296:U:C4 | 23:BA:2333:A:H1' | 2.53 | 0.44 |
| 10:CJ:55:LYS:O | 10:CJ:56:HIS:CG | 2.71 | 0.44 |
| 23:BA:1357:U:H2' | 23:BA:1358:G:O4' | 2.18 | 0.44 |
| 1:AA:1308:U:OP1 | 13:AM:97:PRO:HA | 2.18 | 0.44 |
| 5:CE:127:ASN:HA | 5:CE:128:PRO:HD3 | 1.80 | 0.44 |
| 1:CA:1030(C):G:C5 | 1:CA:1030(D):A:N7 | 2.86 | 0.44 |
| 1:CA:1358:U:C5 | 1:CA:1359:C:C4 | 3.06 | 0.44 |
| 23:DA:2119:A:H2' | 23:DA:2119:A:OP1 | 2.18 | 0.44 |
| 23:DA:2133:G:N2 | 23:DA:2158:A:H62 | 2.16 | 0.44 |
| 23:BA:1185:C:H5'' | 23:BA:1186:G:OP1 | 2.18 | 0.44 |
| 34:BQ:12:GLN:HG2 | 34:BQ:73:PRO:HD2 | 1.99 | 0.44 |
| 23:DA:30:G:H2' | 23:DA:31:C:C6 | 2.53 | 0.44 |
| 1:CA:148:G:C2 | 1:CA:175:C:C2 | 3.06 | 0.44 |
| 9:AI:13:ALA:HB2 | 9:AI:68:GLY:CA | 2.47 | 0.44 |
| 23:DA:1153:C:H2' | 23:DA:1154:G:O4' | 2.17 | 0.44 |
| 42:BY:40:GLU:O | 42:BY:42:VAL:HG23 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1478:G:HO2' | 23:DA:1558:A:H2 | 1.63 | 0.44 |
| 23:BA:528:A:O2' | 56:BA:4483:HOH:O | 1.85 | 0.44 |
| 23:DA:484:C:H2' | 23:DA:485:C:H6 | 1.80 | 0.44 |
| 12:AL:27:LEU:C | 12:AL:29:GLY:H | 2.21 | 0.44 |
| 23:BA:493:G:H2' | 23:BA:494:G:O4' | 2.17 | 0.44 |
| 23:BA:570:G:H2' | 23:BA:2030:A:N7 | 2.33 | 0.44 |
| 23:BA:102:G:O2' | 23:BA:103:A:P | 2.76 | 0.44 |
| 10:AJ:13:HIS:HB3 | 10:AJ:68:HIS:HD1 | 1.82 | 0.44 |
| 1:AA:627:G:C2 | 1:AA:628:G:C8 | 3.06 | 0.44 |
| 23:BA:2199:A:H5'' | 23:BA:2200:C:OP2 | 2.18 | 0.44 |
| 1:CA:614:A:H2' | 1:CA:615:C:C6 | 2.53 | 0.44 |
| 28:DG:72:ARG:HD3 | 28:DG:85:GLY:HA2 | 1.99 | 0.44 |
| 18:AR:33:ASP:O | 18:AR:40:LEU:HD11 | 2.17 | 0.44 |
| 1:CA:129(A):G:O2' | 1:CA:189(F):U:OP1 | 2.33 | 0.44 |
| 23:DA:830:G:H4' | 23:DA:831:G:OP2 | 2.18 | 0.44 |
| 1:AA:1418:A:H2 | 23:BA:1948:G:N3 | 2.15 | 0.44 |
| 1:CA:35:G:H22 | 1:CA:550:G:H1' | 1.83 | 0.44 |
| 23:BA:2572:A:C8 | 26:BE:144:ARG:HD2 | 2.52 | 0.44 |
| 23:BA:1648:C:H2' | 23:BA:1649:G:O5' | 2.18 | 0.44 |
| 30:BI:47:LEU:HA | 30:BI:47:LEU:HD23 | 1.88 | 0.44 |
| 15:CO:88:ARG:HA | 15:CO:88:ARG:HD2 | 1.83 | 0.44 |
| 24:BB:7:G:H5'' | 24:BB:7:G:C8 | 2.52 | 0.44 |
| 23:DA:1766:U:H2' | 23:DA:1767:C:C6 | 2.53 | 0.44 |
| 6:CF:25:ILE:HD12 | 6:CF:82:ARG:HE | 1.83 | 0.44 |
| 1:CA:269:C:H2' | 1:CA:270:A:C8 | 2.52 | 0.44 |
| 23:BA:973:A:O4' | 23:BA:1188:U:C6 | 2.71 | 0.44 |
| 23:DA:272(H):C:H5' | 23:DA:272(I):U:OP2 | 2.17 | 0.44 |
| 15:CO:55:GLY:O | 15:CO:59:MET:HG3 | 2.18 | 0.44 |
| 1:AA:926:G:H21 | 22:AX:94:GLN:HE22 | 1.66 | 0.44 |
| 1:AA:493:G:HO2' | 1:AA:494:U:H6 | 1.62 | 0.44 |
| 1:AA:1442(A):G:C5 | 1:AA:1442(B):A:N3 | 2.86 | 0.43 |
| 1:CA:991:U:N3 | 1:CA:1212:U:H1' | 2.32 | 0.43 |
| 23:BA:885:C:C4 | 23:BA:886:C:H1' | 2.53 | 0.43 |
| 1:AA:1010:G:H2' | 1:AA:1010:G:N3 | 2.33 | 0.43 |
| 1:AA:1151:A:O2' | 1:AA:1152:A:H8 | 1.80 | 0.43 |
| 1:AA:1317:C:N3 | 19:AS:37:ARG:NH2 | 2.61 | 0.43 |
| 1:AA:983:A:C2 | 1:AA:984:C:H5' | 2.53 | 0.43 |
| 2:AB:70:PHE:H | 2:AB:92:TYR:HA | 1.83 | 0.43 |
| 1:AA:1241:G:H2' | 1:AA:1241:G:N3 | 2.33 | 0.43 |
| 1:CA:959:A:H61 | 19:CS:78:ARG:CA | 2.29 | 0.43 |
| 1:AA:1267:C:O2' | 21:AU:20:LYS:HD3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:CC:15:THR:HG22 | 3:CC:16:ARG:N | 2.33 | 0.43 |
| 24:DB:38:C:O2 | 24:DB:48:A:H1' | 2.17 | 0.43 |
| 3:CC:134:ILE:CG2 | 3:CC:151:VAL:HB | 2.46 | 0.43 |
| 4:CD:12:CYS:SG | 4:CD:19:LEU:O | 2.76 | 0.43 |
| 23:DA:2305:A:C5' | 28:DG:134:GLY:HA3 | 2.47 | 0.43 |
| 5:AE:43:LEU:HD21 | 5:AE:132:ALA:HB1 | 1.99 | 0.43 |
| 23:BA:102:G:HO2' | 23:BA:103:A:P | 2.40 | 0.43 |
| 2:CB:70:PHE:H | 2:CB:92:TYR:HA | 1.82 | 0.43 |
| 23:BA:275:G:O2' | 23:BA:276:A:H5' | 2.18 | 0.43 |
| 23:DA:980:A:N3 | 23:DA:2037:G:O2' | 2.40 | 0.43 |
| 23:DA:1316:U:H2' | 23:DA:1317:A:H8 | 1.83 | 0.43 |
| 7:AG:16:LEU:HD22 | 9:AI:45:ALA:N | 2.33 | 0.43 |
| 43:BZ:151:HIS:C | 43:BZ:153:SER:H | 2.22 | 0.43 |
| 1:CA:516:U:O4 | 1:CA:517:G:N1 | 2.51 | 0.43 |
| 23:DA:51:G:O2' | 23:DA:119:A:N1 | 2.39 | 0.43 |
| 1:AA:1342:C:O2' | 9:AI:124:GLN:HA | 2.17 | 0.43 |
| 23:DA:1804:C:O5' | 23:DA:1804:C:H6 | 1.99 | 0.43 |
| 23:BA:1956:U:H2' | 23:BA:1957:C:H5' | 2.01 | 0.43 |
| 24:DB:46:A:C5 | 24:DB:47:C:C5 | 3.06 | 0.43 |
| 39:DV:76:LYS:HD2 | 39:DV:81:TYR:CD1 | 2.53 | 0.43 |
| 52:B8:39:LYS:HA | 52:B8:42:ARG:NH1 | 2.33 | 0.43 |
| 1:CA:1087:G:N2 | 1:CA:1099:G:H1' | 2.33 | 0.43 |
| 1:CA:283:C:H2' | 1:CA:284:G:O4' | 2.18 | 0.43 |
| 23:DA:2677:G:H2' | 23:DA:2678:C:C6 | 2.53 | 0.43 |
| 29:BH:13:LYS:HA | 29:BH:14:GLY:HA2 | 1.60 | 0.43 |
| 3:AC:122:GLU:HA | 3:AC:125:GLU:OE2 | 2.18 | 0.43 |
| 7:CG:22:LEU:HD12 | 7:CG:22:LEU:HA | 1.78 | 0.43 |
| 23:DA:2238:G:N7 | 56:DA:4648:HOH:O | 2.36 | 0.43 |
| 24:DB:40:U:H1' | 24:DB:45:A:N6 | 2.33 | 0.43 |
| 23:DA:55:G:N3 | 23:DA:127:A:H2 | 2.15 | 0.43 |
| 31:BN:115:ARG:O | 31:BN:118:LYS:HB2 | 2.18 | 0.43 |
| 15:CO:43:LEU:O | 15:CO:44:LYS:C | 2.57 | 0.43 |
| 23:DA:2176:A:H5' | 23:DA:2177:C:OP2 | 2.18 | 0.43 |
| 1:AA:1221:G:O5' | 1:AA:1221:G:H8 | 2.02 | 0.43 |
| 23:DA:1210:A:H8 | 23:DA:1210:A:C5' | 2.30 | 0.43 |
| 1:CA:713:G:H2' | 1:CA:714:G:C8 | 2.52 | 0.43 |
| 1:CA:559:A:N3 | 1:CA:559:A:H5' | 2.32 | 0.43 |
| 1:AA:73:G:C6 | 1:AA:97:G:C6 | 3.06 | 0.43 |
| 1:CA:957:U:H4' | 19:CS:79:THR:HG23 | 2.00 | 0.43 |
| 21:AU:20:LYS:HB3 | 21:AU:20:LYS:HZ3 | 1.82 | 0.43 |
| 23:DA:1340:U:H4' | 23:DA:1394:U:O2' | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:994:A:O2' | 14:CN:8:GLU:HG2 | 2.18 | 0.43 |
| 23:BA:1740:G:H2' | 23:BA:1741:A:H8 | 1.83 | 0.43 |
| 23:BA:2119:A:N6 | 23:BA:2168:G:H1' | 2.33 | 0.43 |
| 1:AA:1250:A:H1' | 1:AA:1370:G:O2' | 2.17 | 0.43 |
| 1:AA:475:G:H2' | 1:AA:476:G:H8 | 1.82 | 0.43 |
| 23:DA:1364:G:P | 45:D1:3:LYS:HG2 | 2.57 | 0.43 |
| 1:AA:427:U:C4 | 1:AA:428:G:C6 | 3.05 | 0.43 |
| 15:CO:78:TYR:O | 15:CO:82:ILE:HG12 | 2.18 | 0.43 |
| 5:CE:32:VAL:O | 5:CE:43:LEU:HD12 | 2.18 | 0.43 |
| 1:CA:1014:A:H2' | 1:CA:1015:A:N9 | 2.33 | 0.43 |
| 27:BF:64:ILE:HG13 | 27:BF:65:TRP:H | 1.83 | 0.43 |
| 1:CA:1246:C:H2' | 1:CA:1247:U:C6 | 2.53 | 0.43 |
| 1:CA:599:C:H4' | 8:CH:130:GLY:C | 2.38 | 0.43 |
| 6:CF:67:MET:HE3 | 6:CF:75:LEU:HD22 | 1.99 | 0.43 |
| 23:BA:1786:A:OP1 | 56:BA:4757:HOH:O | 2.20 | 0.43 |
| 8:CH:36:LEU:O | 8:CH:45:ILE:HD11 | 2.18 | 0.43 |
| 23:BA:1814:G:H4' | 25:BD:51:VAL:HG21 | 2.01 | 0.43 |
| 1:CA:1193:G:C5 | 1:CA:1194:U:C5 | 3.06 | 0.43 |
| 34:DQ:60:ARG:NH1 | 43:DZ:177:PRO:HG3 | 2.33 | 0.43 |
| 25:DD:77:ALA:HB2 | 25:DD:97:TYR:CD2 | 2.53 | 0.43 |
| 36:DS:74:ALA:CB | 36:DS:108:GLY:HA3 | 2.48 | 0.43 |
| 23:DA:2343:C:HO2' | 23:DA:2373:G:HO2' | 1.64 | 0.43 |
| 43:DZ:35:ARG:HD2 | 43:DZ:35:ARG:HA | 1.64 | 0.43 |
| 23:BA:62:C:OP1 | 56:BA:5009:HOH:O | 2.21 | 0.43 |
| 25:DD:96:HIS:HD2 | 25:DD:102:LYS:HG2 | 1.82 | 0.43 |
| 5:AE:144:THR:O | 5:AE:148:VAL:HG23 | 2.18 | 0.43 |
| 23:BA:296:C:O2' | 23:BA:297:C:H5' | 2.18 | 0.43 |
| 23:DA:354:G:H2' | 23:DA:355:G:O4' | 2.18 | 0.43 |
| 23:BA:2789:C:N3 | 23:BA:2894:G:O6 | 2.51 | 0.43 |
| 1:AA:1046:A:H2' | 1:AA:1047:G:O4' | 2.17 | 0.43 |
| 23:DA:824:A:H1' | 23:DA:2358:G:N7 | 2.34 | 0.43 |
| 23:DA:2685:G:H2' | 23:DA:2686:G:H5'' | 2.00 | 0.43 |
| 39:DV:18:LEU:HD23 | 39:DV:18:LEU:HA | 1.84 | 0.43 |
| 23:DA:54:G:O2' | 51:D7:35:ARG:HD3 | 2.18 | 0.43 |
| 16:CP:14:ASN:OD1 | 16:CP:16:HIS:CE1 | 2.71 | 0.43 |
| 1:AA:636:U:H2' | 1:AA:637:G:H8 | 1.83 | 0.43 |
| 1:AA:363:A:O2' | 1:AA:364:A:H5' | 2.17 | 0.43 |
| 1:AA:981:U:OP1 | 14:AN:6:LEU:HD11 | 2.19 | 0.43 |
| 1:AA:988:G:C2 | 1:AA:1218:C:C2 | 3.05 | 0.43 |
| 1:CA:674:G:H2' | 1:CA:675:A:H8 | 1.83 | 0.43 |
| 2:CB:55:PHE:CG | 2:CB:58:ILE:HD12 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1367:C:H5'' | 9:CI:114:TYR:CB | 2.48 | 0.43 |
| 23:DA:675:A:N6 | 23:DA:676:A:N6 | 2.66 | 0.43 |
| 23:BA:300:A:H3' | 42:BY:84:ARG:NH2 | 2.33 | 0.43 |
| 27:DF:197:ASP:O | 27:DF:201:VAL:HG12 | 2.18 | 0.43 |
| 1:AA:1367:C:H5' | 10:AJ:60:ARG:NH1 | 2.32 | 0.43 |
| 23:BA:1535:A:P | 23:BA:1535:A:H3' | 2.58 | 0.43 |
| 34:BQ:71:ASP:O | 34:BQ:73:PRO:HD3 | 2.18 | 0.43 |
| 23:BA:1050:A:H2' | 23:BA:1051:G:C8 | 2.52 | 0.43 |
| 11:AK:67:ASP:OD2 | 11:AK:71:LYS:HE3 | 2.17 | 0.43 |
| 23:DA:768:G:C5 | 56:DA:3978:HOH:O | 2.67 | 0.43 |
| 4:AD:110:PHE:HD2 | 4:AD:148:VAL:HG22 | 1.84 | 0.43 |
| 36:DS:30:ARG:HG3 | 36:DS:97:ARG:CZ | 2.48 | 0.43 |
| 43:DZ:45:ASP:O | 43:DZ:48:PHE:N | 2.50 | 0.43 |
| 23:DA:1513:C:H2' | 23:DA:1514:U:C6 | 2.53 | 0.43 |
| 36:BS:56:LEU:C | 36:BS:58:LEU:HD22 | 2.38 | 0.43 |
| 17:AQ:65:ILE:HD12 | 17:AQ:69:LYS:O | 2.18 | 0.43 |
| 23:BA:1003:G:N2 | 23:BA:1153:C:C2 | 2.86 | 0.43 |
| 17:CQ:10:VAL:HG13 | 17:CQ:19:VAL:HB | 2.00 | 0.43 |
| 12:CL:86:ARG:HB2 | 12:CL:101:VAL:HG22 | 2.00 | 0.43 |
| 23:BA:652(B):A:O2' | 23:BA:652(C):G:H5' | 2.18 | 0.43 |
| 19:AS:31:ILE:HG23 | 19:AS:49:ILE:HA | 1.99 | 0.43 |
| 18:CR:33:ASP:O | 18:CR:40:LEU:HD11 | 2.18 | 0.43 |
| 23:BA:652(E):G:O6 | 23:BA:652(T):C:N3 | 2.51 | 0.43 |
| 1:CA:1410:G:C4 | 1:CA:1491:G:N2 | 2.87 | 0.43 |
| 35:BR:103:ARG:NH1 | 35:BR:103:ARG:HG2 | 2.33 | 0.43 |
| 12:AL:85:ILE:HD13 | 12:AL:85:ILE:HA | 1.75 | 0.43 |
| 1:AA:1513:A:H2' | 1:AA:1514:C:C6 | 2.53 | 0.43 |
| 23:BA:1632:A:N6 | 23:BA:1633:G:C6 | 2.87 | 0.43 |
| 23:DA:322:A:OP2 | 27:DF:169:ASN:HB2 | 2.17 | 0.43 |
| 37:DT:36:GLU:HB3 | 37:DT:37:GLY:H | 1.72 | 0.43 |
| 23:BA:265:A:H1' | 23:BA:266:G:O4' | 2.19 | 0.43 |
| 49:B5:45:VAL:HG11 | 49:B5:58:LEU:HD13 | 1.99 | 0.43 |
| 23:DA:34:C:H5'' | 23:DA:35:G:OP2 | 2.18 | 0.43 |
| 43:DZ:166:SER:HA | 43:DZ:167:PRO:HD3 | 1.93 | 0.43 |
| 1:CA:256:U:H2' | 1:CA:257:G:C8 | 2.53 | 0.43 |
| 1:CA:582:U:OP1 | 15:CO:64:ARG:NH1 | 2.51 | 0.43 |
| 33:BP:77:ARG:HB2 | 33:BP:78:PRO:HD2 | 2.01 | 0.43 |
| 35:BR:72:ASP:O | 35:BR:76:VAL:HG23 | 2.18 | 0.43 |
| 23:BA:2261:C:O2' | 23:BA:2262:U:H5' | 2.18 | 0.43 |
| 45:D1:98:LEU:HD23 | 45:D1:98:LEU:HA | 1.91 | 0.43 |
| 23:DA:2793:G:N2 | 23:DA:2804:C:H1' | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 12:CL:60:LEU:HB3 | 12:CL:62:SER:H | 1.83 | 0.43 |
| 23:BA:1518:U:H2' | 23:BA:1519:G:O4' | 2.18 | 0.43 |
| 17:AQ:40:LYS:HD3 | 17:AQ:42:TYR:CZ | 2.54 | 0.43 |
| 2:CB:86:GLU:C | 2:CB:89:GLY:H | 2.22 | 0.43 |
| 1:CA:883:C:O2' | 1:CA:884:U:H5' | 2.18 | 0.43 |
| 23:DA:2704:C:H2' | 23:DA:2705:A:O4' | 2.18 | 0.43 |
| 23:DA:2223:G:H2' | 23:DA:2224:G:H5' | 2.00 | 0.43 |
| 1:AA:1442(A):G:C2' | 1:AA:1442(B):A:H5'' | 2.49 | 0.43 |
| 1:AA:1442(A):G:H3' | 1:AA:1442(B):A:C5' | 2.49 | 0.43 |
| 1:CA:1457:G:C6 | 1:CA:1458:G:C6 | 3.06 | 0.43 |
| 1:CA:1443:G:O6 | 1:CA:1459:C:C1' | 2.66 | 0.43 |
| 1:CA:1210:C:H5'' | 1:CA:1211:U:C6 | 2.54 | 0.43 |
| 7:AG:87:VAL:HG11 | 7:AG:154:TYR:O | 2.19 | 0.43 |
| 1:AA:1096:C:HO2' | 1:AA:1170:A:HO2' | 1.61 | 0.43 |
| 13:CM:14:ARG:NH1 | 13:CM:41:PRO:HB2 | 2.32 | 0.43 |
| 1:CA:1379:G:H2' | 1:CA:1380:U:H5' | 2.00 | 0.43 |
| 1:CA:946:A:N1 | 1:CA:1236:A:C2 | 2.87 | 0.43 |
| 28:DG:43:LEU:HB3 | 28:DG:44:GLY:H | 1.64 | 0.43 |
| 1:CA:18:C:H4' | 1:CA:1078:U:O2 | 2.18 | 0.43 |
| 1:CA:1321:C:H3' | 1:CA:1322:C:H2' | 2.00 | 0.43 |
| 1:CA:79:G:N2 | 1:CA:91:C:C2 | 2.87 | 0.43 |
| 1:AA:1324:A:H2' | 1:AA:1325:C:C6 | 2.53 | 0.43 |
| 23:BA:1142(A):A:C4 | 23:BA:1144:G:N7 | 2.87 | 0.43 |
| 1:CA:1362:C:O2' | 1:CA:1363:C:H5' | 2.17 | 0.43 |
| 9:AI:27:THR:O | 9:AI:63:ILE:N | 2.51 | 0.43 |
| 23:DA:842:G:H2' | 23:DA:843:G:O4' | 2.17 | 0.43 |
| 23:BA:2306:C:C4 | 23:BA:2307:G:O6 | 2.72 | 0.43 |
| 23:BA:2309:A:C6 | 23:BA:2310:A:N1 | 2.86 | 0.43 |
| 1:CA:1149:C:O2' | 1:CA:1150:U:H5' | 2.18 | 0.43 |
| 23:DA:2774:C:H2' | 23:DA:2775:A:O4' | 2.19 | 0.43 |
| 23:DA:272(E):G:C2 | 23:DA:364:C:N3 | 2.87 | 0.43 |
| 1:AA:324:G:N2 | 1:AA:327:A:C8 | 2.86 | 0.43 |
| 1:AA:328:C:H4' | 1:AA:329:A:H5' | 2.00 | 0.43 |
| 29:BH:70:THR:HA | 29:BH:73:ALA:CB | 2.47 | 0.43 |
| 7:CG:115:ARG:O | 7:CG:118:VAL:HG23 | 2.18 | 0.43 |
| 41:BX:54:VAL:HG13 | 41:BX:81:VAL:HG12 | 2.01 | 0.43 |
| 8:AH:39:LEU:O | 8:AH:43:GLY:N | 2.51 | 0.43 |
| 11:AK:110:ASP:HB3 | 18:AR:85:LEU:HD12 | 2.00 | 0.43 |
| 26:DE:52:LEU:O | 26:DE:76:ARG:HG2 | 2.18 | 0.43 |
| 1:CA:1270:C:H2' | 1:CA:1271:G:C8 | 2.52 | 0.43 |
| 35:DR:103:ARG:HH11 | 35:DR:103:ARG:HG2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:DR:103:ARG:HH11 | 35:DR:103:ARG:CG | 2.32 | 0.43 |
| 5:AE:100:VAL:O | 5:AE:107:ARG:NH2 | 2.52 | 0.43 |
| 39:BV:76:LYS:HD2 | 39:BV:81:TYR:CD1 | 2.54 | 0.43 |
| 2:CB:158:LEU:HA | 2:CB:159:PRO:HD3 | 1.92 | 0.43 |
| 23:DA:2387:U:OP1 | 44:D0:55:ARG:NH2 | 2.51 | 0.43 |
| 25:DD:145:VAL:HG12 | 25:DD:146:GLU:O | 2.18 | 0.43 |
| 23:BA:2590:A:OP2 | 25:BD:238:GLY:HA2 | 2.18 | 0.43 |
| 1:AA:854:G:H3' | 1:AA:871:U:O4 | 2.18 | 0.43 |
| 3:CC:21:ARG:O | 3:CC:58:GLU:HG3 | 2.18 | 0.43 |
| 9:AI:89:ASN:C | 9:AI:91:ASP:H | 2.21 | 0.43 |
| 23:BA:503:A:O2' | 56:BA:4932:HOH:O | 2.20 | 0.43 |
| 23:DA:2494:G:C4 | 23:DA:2495:G:C8 | 3.06 | 0.43 |
| 45:B1:52:ARG:HA | 45:B1:56:GLN:O | 2.18 | 0.43 |
| 5:AE:32:VAL:HB | 5:AE:58:ALA:HB1 | 2.00 | 0.43 |
| 44:D0:56:ASP:OD2 | 44:D0:56:ASP:N | 2.48 | 0.43 |
| 23:BA:895:U:H6 | 23:BA:895:U:H5'' | 1.84 | 0.43 |
| 41:BX:15:GLU:CD | 41:BX:15:GLU:H | 2.21 | 0.43 |
| 46:D2:10:LEU:HD23 | 46:D2:10:LEU:HA | 1.75 | 0.43 |
| 13:CM:58:GLU:O | 13:CM:61:GLU:HB2 | 2.19 | 0.43 |
| 23:BA:885:C:H3' | 23:BA:886:C:O4' | 2.19 | 0.43 |
| 1:AA:1320:C:H5' | 19:AS:70:LYS:HB2 | 2.00 | 0.43 |
| 1:CA:1348:U:H2' | 1:CA:1349:A:C8 | 2.53 | 0.43 |
| 1:CA:965:A:H4' | 1:CA:966:G:O5' | 2.18 | 0.43 |
| 23:DA:1358:G:O2' | 23:DA:1359:A:H5' | 2.18 | 0.43 |
| 2:CB:28:PHE:CD2 | 2:CB:194:PRO:HG3 | 2.51 | 0.43 |
| 1:AA:675:A:H2' | 1:AA:676:A:C8 | 2.53 | 0.43 |
| 1:CA:1357:A:C8 | 1:CA:1358:U:C5 | 3.07 | 0.43 |
| 17:AQ:76:LEU:HD21 | 17:AQ:79:SER:H | 1.83 | 0.43 |
| 13:AM:68:GLY:H | 13:AM:71:ARG:HE | 1.66 | 0.43 |
| 1:CA:164:U:H2' | 1:CA:165:C:C6 | 2.54 | 0.43 |
| 23:DA:1722:A:C5 | 23:DA:1740:G:C6 | 3.07 | 0.43 |
| 23:DA:1740:G:H2' | 23:DA:1741:A:H8 | 1.83 | 0.43 |
| 28:BG:76:SER:CA | 28:BG:83:ARG:HA | 2.45 | 0.43 |
| 23:BA:2165:G:H2' | 23:BA:2166:G:H8 | 1.83 | 0.43 |
| 23:BA:94:C:H2' | 23:BA:94:C:O2 | 2.17 | 0.43 |
| 33:DP:59:LEU:HD11 | 52:D8:10:ALA:CB | 2.45 | 0.43 |
| 8:AH:9:MET:SD | 8:AH:32:LYS:HB3 | 2.59 | 0.43 |
| 23:BA:769:G:H5' | 23:BA:1379:A:N6 | 2.33 | 0.43 |
| 23:BA:316:C:N4 | 56:BA:5253:HOH:O | 2.50 | 0.43 |
| 23:DA:234:C:H2' | 23:DA:235:U:C6 | 2.54 | 0.43 |
| 17:CQ:13:ASP:CG | 17:CQ:14:LYS:N | 2.71 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:625:G:C6 | 1:AA:626:U:C4 | 3.06 | 0.43 |
| 1:AA:614:A:H2' | 1:AA:615:C:H6 | 1.82 | 0.43 |
| 1:CA:650:G:O2' | 1:CA:651:C:H5' | 2.18 | 0.43 |
| 1:CA:397:A:N3 | 1:CA:397:A:H3' | 2.34 | 0.43 |
| 1:CA:277:C:OP1 | 17:CQ:68:ARG:NH2 | 2.48 | 0.43 |
| 23:DA:2850:A:OP2 | 23:DA:2866:U:H5 | 2.01 | 0.43 |
| 1:CA:384:G:H2' | 1:CA:385:C:H6 | 1.82 | 0.43 |
| 23:BA:729:G:H2' | 23:BA:1775:U:H1' | 1.99 | 0.43 |
| 23:DA:2470:G:C2 | 23:DA:2471:C:C6 | 3.07 | 0.43 |
| 33:BP:106:LEU:HA | 33:BP:106:LEU:HD23 | 1.83 | 0.43 |
| 25:BD:33:LEU:HA | 25:BD:33:LEU:HD23 | 1.63 | 0.43 |
| 1:AA:730:G:C5 | 1:AA:731:G:H1' | 2.53 | 0.43 |
| 33:DP:27:HIS:O | 33:DP:31:ALA:HA | 2.19 | 0.43 |
| 1:CA:445:G:N3 | 1:CA:445:G:H2' | 2.33 | 0.43 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 3.06 | 0.43 |
| 41:DX:50:LYS:HB3 | 41:DX:84:ALA:HB2 | 1.99 | 0.43 |
| 23:DA:2556:C:H2' | 23:DA:2557:G:O4' | 2.19 | 0.43 |
| 23:DA:475:U:C4 | 23:DA:481:G:O6 | 2.71 | 0.43 |
| 40:DW:14:PRO:HG2 | 40:DW:78:GLU:HG2 | 1.99 | 0.43 |
| 38:DU:39:LEU:HD23 | 38:DU:39:LEU:HA | 1.85 | 0.43 |
| 1:AA:1176:A:O5' | 1:AA:1176:A:H8 | 2.02 | 0.43 |
| 1:AA:397:A:N3 | 1:AA:397:A:H3' | 2.34 | 0.43 |
| 4:AD:91:SER:O | 4:AD:95:GLY:N | 2.37 | 0.43 |
| 6:AF:68:PRO:HG2 | 6:AF:71:ARG:HD2 | 2.00 | 0.43 |
| 23:DA:2070:G:C2 | 23:DA:2442:C:C2 | 3.07 | 0.43 |
| 1:AA:1442(A):G:H2' | 1:AA:1442(B):A:H5'' | 2.00 | 0.43 |
| 1:CA:949:A:OP1 | 13:CM:101:GLN:HB3 | 2.19 | 0.43 |
| 8:CH:88:LYS:HB3 | 8:CH:89:PRO:HD2 | 2.01 | 0.43 |
| 7:CG:31:MET:HG3 | 7:CG:35:LYS:O | 2.18 | 0.43 |
| 1:AA:79:G:N2 | 1:AA:91:C:O2 | 2.52 | 0.43 |
| 1:AA:1305:G:H5'' | 21:AU:5:ASP:CA | 2.46 | 0.43 |
| 2:CB:80:ILE:HG12 | 2:CB:211:ILE:HG22 | 2.01 | 0.43 |
| 23:DA:2287:A:C5 | 23:DA:2289:G:C5 | 3.06 | 0.43 |
| 28:DG:19:LEU:HD22 | 28:DG:23:PHE:CE1 | 2.51 | 0.43 |
| 1:CA:1295:G:H2' | 1:CA:1296:C:H5' | 2.01 | 0.43 |
| 1:CA:370:C:H2' | 1:CA:371:G:C8 | 2.53 | 0.43 |
| 9:CI:28:VAL:O | 9:CI:31:GLN:HG2 | 2.18 | 0.43 |
| 19:CS:36:ARG:HG2 | 19:CS:51:VAL:HG12 | 2.00 | 0.43 |
| 23:BA:2125:G:N2 | 23:BA:2126:A:H62 | 2.17 | 0.43 |
| 23:BA:744:G:OP1 | 26:BE:132:HIS:ND1 | 2.50 | 0.43 |
| 25:BD:154:LYS:H | 25:BD:154:LYS:HG2 | 1.70 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:BD:155:LEU:HD23 | 25:BD:177:LEU:HD22 | 1.99 | 0.43 |
| 13:CM:70:LEU:O | 13:CM:74:VAL:HG23 | 2.18 | 0.43 |
| 30:DI:83:ALA:HA | 30:DI:89:TYR:CD2 | 2.54 | 0.43 |
| 25:BD:5:LYS:HB3 | 25:BD:5:LYS:HE3 | 1.77 | 0.43 |
| 23:DA:2760:C:C2' | 23:DA:2761:G:H5'' | 2.45 | 0.43 |
| 1:AA:1391:U:H2' | 1:AA:1392:G:H8 | 1.83 | 0.43 |
| 1:CA:142:G:C4 | 1:CA:143:A:C8 | 3.07 | 0.43 |
| 1:AA:622:A:C8 | 1:AA:623:C:C5 | 3.07 | 0.43 |
| 16:CP:38:TYR:N | 16:CP:38:TYR:CD2 | 2.86 | 0.43 |
| 23:DA:819:A:OP2 | 23:DA:1187:G:N2 | 2.35 | 0.43 |
| 23:DA:2273:A:O2' | 23:DA:2274:A:H5' | 2.19 | 0.43 |
| 1:CA:189(F):U:C5 | 17:CQ:72:ARG:NH2 | 2.86 | 0.43 |
| 41:DX:5:TYR:HB3 | 46:D2:33:MET:HB2 | 2.00 | 0.43 |
| 23:DA:2850:A:OP2 | 23:DA:2866:U:C5 | 2.72 | 0.43 |
| 1:CA:65:U:H5'' | 1:CA:65:U:H6 | 1.83 | 0.43 |
| 23:DA:2259:G:C2 | 23:DA:2282:G:N1 | 2.87 | 0.43 |
| 1:CA:527:G:O2' | 1:CA:535:A:N1 | 2.46 | 0.43 |
| 23:DA:39:C:H2' | 23:DA:40:C:C6 | 2.53 | 0.43 |
| 31:BN:67:LEU:HD22 | 31:BN:67:LEU:HA | 1.73 | 0.43 |
| 33:DP:101:VAL:HG23 | 33:DP:106:LEU:HB3 | 2.00 | 0.43 |
| 23:DA:2695:C:H2' | 23:DA:2696:U:H6 | 1.84 | 0.43 |
| 23:BA:1954:G:O2' | 23:BA:1956:U:O4 | 2.19 | 0.43 |
| 27:BF:32:LEU:HD21 | 27:BF:105:VAL:HG13 | 2.01 | 0.43 |
| 1:CA:441:A:H3' | 1:CA:442:C:C6 | 2.54 | 0.43 |
| 1:AA:687:A:H4' | 11:AK:47:VAL:HG13 | 2.01 | 0.43 |
| 35:DR:29:LEU:HB3 | 35:DR:75:LEU:HD21 | 1.99 | 0.43 |
| 23:BA:1655:A:H3' | 23:BA:1656:C:H6 | 1.84 | 0.43 |
| 32:BO:21:CYS:HB2 | 32:BO:39:ILE:HD12 | 1.99 | 0.43 |
| 23:BA:1842:G:C5 | 23:BA:1843:C:C4 | 3.06 | 0.43 |
| 35:DR:38:VAL:HB | 35:DR:39:PRO:HD3 | 1.99 | 0.43 |
| 29:DH:83:TYR:O | 29:DH:134:SER:HA | 2.19 | 0.43 |
| 23:DA:363(A):A:H2' | 23:DA:363(B):G:H8 | 1.82 | 0.43 |
| 9:CI:18:PHE:HD1 | 9:CI:62:TYR:HD2 | 1.66 | 0.43 |
| 34:DQ:66:ILE:HG12 | 34:DQ:104:PHE:CD2 | 2.53 | 0.43 |
| 23:BA:2290:G:C2 | 23:BA:2343:C:O2 | 2.72 | 0.43 |
| 4:AD:78:LEU:HA | 4:AD:78:LEU:HD23 | 1.77 | 0.43 |
| 16:AP:40:ASP:HA | 16:AP:41:PRO:HD2 | 1.91 | 0.43 |
| 4:AD:106:TYR:CD2 | 4:AD:106:TYR:C | 2.91 | 0.43 |
| 12:AL:93:LEU:HA | 12:AL:93:LEU:HD23 | 1.83 | 0.43 |
| 23:BA:2360:A:H2' | 23:BA:2361:A:O4' | 2.19 | 0.43 |
| 5:CE:30:ALA:O | 5:CE:45:PHE:HD1 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:2315:G:H2' | 23:DA:2316:C:C6 | 2.53 | 0.43 |
| 8:CH:4:ASP:HA | 8:CH:5:PRO:HD3 | 1.91 | 0.43 |
| 1:CA:1350:A:N1 | 1:CA:1372:U:O2 | 2.51 | 0.43 |
| 23:DA:271(H):G:O2' | 23:DA:271(I):G:P | 2.76 | 0.43 |
| 1:AA:1352:C:H5'' | 21:AU:3:LYS:HE2 | 2.00 | 0.43 |
| 1:CA:1005:A:N7 | 1:CA:1024:G:O2' | 2.52 | 0.43 |
| 23:DA:2286:A:OP1 | 50:D6:29:ASN:ND2 | 2.52 | 0.43 |
| 1:CA:1299:A:H2' | 1:CA:1299:A:N3 | 2.33 | 0.43 |
| 1:CA:1178:G:N2 | 1:CA:1181:G:N7 | 2.65 | 0.43 |
| 8:CH:29:SER:HB3 | 8:CH:32:LYS:CG | 2.43 | 0.43 |
| 3:CC:67:THR:HG22 | 3:CC:69:HIS:CE1 | 2.53 | 0.43 |
| 1:CA:267:C:OP2 | 17:CQ:67:LYS:HD2 | 2.19 | 0.43 |
| 15:AO:55:GLY:HA2 | 15:AO:58:MET:HG3 | 1.99 | 0.43 |
| 23:BA:1049:C:H41 | 23:BA:1111:A:H2 | 1.63 | 0.43 |
| 4:AD:173:TRP:CD1 | 4:AD:174:LEU:HG | 2.53 | 0.43 |
| 3:AC:48:TYR:O | 3:AC:50:ALA:N | 2.50 | 0.43 |
| 36:BS:10:ARG:O | 36:BS:14:VAL:HG12 | 2.18 | 0.43 |
| 1:AA:604:G:H2' | 1:AA:605:U:O4' | 2.18 | 0.43 |
| 1:CA:1013:G:O2' | 1:CA:1014:A:C8 | 2.69 | 0.43 |
| 1:AA:327:A:C5 | 1:AA:329:A:C5 | 3.06 | 0.43 |
| 1:CA:187:C:H2' | 1:CA:188:C:C6 | 2.54 | 0.43 |
| 1:CA:1137:C:C5' | 1:CA:1138:G:C6 | 3.01 | 0.43 |
| 8:CH:8:ASP:O | 8:CH:12:ARG:N | 2.43 | 0.43 |
| 23:DA:2301:C:H2' | 23:DA:2302:G:C8 | 2.54 | 0.43 |
| 10:AJ:12:ASP:OD2 | 10:AJ:13:HIS:N | 2.43 | 0.43 |
| 23:DA:1287:A:C5 | 23:DA:1288:U:C4 | 3.07 | 0.43 |
| 7:AG:41:ARG:O | 7:AG:44:TYR:N | 2.50 | 0.43 |
| 1:CA:614:A:C6 | 1:CA:627:G:N1 | 2.87 | 0.43 |
| 43:DZ:151:HIS:C | 43:DZ:153:SER:H | 2.21 | 0.43 |
| 23:DA:1419:A:C8 | 23:DA:1421:G:C6 | 3.06 | 0.43 |
| 23:BA:1693:U:O2' | 23:BA:1695:G:O6 | 2.29 | 0.43 |
| 1:CA:35:G:C6 | 1:CA:550:G:C2 | 3.07 | 0.43 |
| 25:DD:10:THR:OG1 | 25:DD:13:ARG:HB2 | 2.19 | 0.43 |
| 3:CC:53:ALA:CB | 3:CC:112:SER:HB2 | 2.48 | 0.43 |
| 23:DA:566:U:H2' | 23:DA:567:A:O4' | 2.19 | 0.43 |
| 23:DA:2647:U:H2' | 23:DA:2648:C:C6 | 2.54 | 0.43 |
| 7:AG:58:PRO:HA | 7:AG:61:VAL:CG2 | 2.47 | 0.43 |
| 23:BA:857:C:N4 | 23:BA:858:U:O4 | 2.52 | 0.43 |
| 6:CF:10:LEU:HB2 | 6:CF:59:TYR:HB3 | 2.00 | 0.43 |
| 32:BO:98:VAL:HG22 | 32:BO:118:ALA:HA | 2.01 | 0.43 |
| 1:CA:929:G:C6 | 1:CA:930:C:C4 | 3.07 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:CE:7:GLU:HG2 | 5:CE:112:LEU:HD22 | 2.01 | 0.43 |
| 12:AL:62:SER:C | 12:AL:64:TYR:H | 2.21 | 0.43 |
| 23:DA:1893:C:C5 | 23:DA:1894:C:C5 | 3.06 | 0.43 |
| 23:BA:2356:C:O3' | 44:B0:20:ARG:HD3 | 2.18 | 0.43 |
| 1:AA:1044:A:H2' | 1:AA:1045:C:H4' | 2.00 | 0.43 |
| 37:BT:80:SER:HA | 37:BT:81:PRO:HD2 | 1.74 | 0.43 |
| 4:CD:106:TYR:CD2 | 4:CD:106:TYR:C | 2.90 | 0.43 |
| 31:DN:58:ASP:OD1 | 31:DN:58:ASP:N | 2.51 | 0.43 |
| 23:DA:428:A:H8 | 23:DA:428:A:OP2 | 2.02 | 0.43 |
| 43:DZ:93:ASP:HA | 43:DZ:130:PRO:HG2 | 2.00 | 0.43 |
| 23:BA:1042:G:C6 | 23:BA:1043:C:C4 | 3.07 | 0.43 |
| 45:D1:52:ARG:HA | 45:D1:56:GLN:O | 2.18 | 0.43 |
| 23:BA:1169:G:H1 | 23:BA:1180:C:H42 | 1.64 | 0.43 |
| 13:CM:15:VAL:HG13 | 13:CM:43:THR:O | 2.19 | 0.43 |
| 1:CA:941:G:N2 | 9:CI:124:GLN:HE22 | 2.15 | 0.43 |
| 23:DA:1204:A:H2 | 23:DA:1241:A:N6 | 2.04 | 0.43 |
| 19:CS:16:LEU:CB | 19:CS:20:LEU:HD12 | 2.49 | 0.43 |
| 4:CD:155:LEU:HD23 | 4:CD:156:GLU:N | 2.33 | 0.43 |
| 1:CA:1112:C:N4 | 3:CC:178:LEU:HD23 | 2.33 | 0.43 |
| 28:BG:122:PRO:HG3 | 28:BG:180:PHE:HD2 | 1.84 | 0.43 |
| 51:D7:24:THR:O | 51:D7:28:ARG:HG3 | 2.19 | 0.43 |
| 23:DA:188:G:N2 | 23:DA:208:C:N3 | 2.46 | 0.43 |
| 1:CA:352:C:H2' | 1:CA:352:C:O2 | 2.18 | 0.43 |
| 30:BI:59:ALA:HA | 30:BI:62:LYS:HB2 | 2.01 | 0.43 |
| 1:AA:1055:A:H62 | 1:AA:1200:C:N4 | 2.16 | 0.43 |
| 1:AA:1254:C:H5'' | 10:AJ:45:ARG:HH21 | 1.82 | 0.43 |
| 23:BA:527:C:C4 | 23:BA:2779:U:H2' | 2.54 | 0.43 |
| 1:CA:652:U:O4 | 1:CA:752:G:O2' | 2.33 | 0.43 |
| 17:CQ:45:HIS:CE1 | 17:CQ:47:PRO:HG3 | 2.54 | 0.43 |
| 1:AA:863:U:H2' | 1:AA:865:A:OP2 | 2.18 | 0.43 |
| 1:CA:1415:G:C6 | 1:CA:1486:G:C6 | 3.06 | 0.43 |
| 1:CA:741:G:H2' | 1:CA:742:G:C8 | 2.53 | 0.43 |
| 1:AA:762:C:H2' | 1:AA:763:G:H8 | 1.84 | 0.43 |
| 23:DA:221:A:N1 | 23:DA:265:A:O2' | 2.47 | 0.43 |
| 1:AA:189(B):C:H2' | 1:AA:189(C):C:O4' | 2.18 | 0.43 |
| 43:DZ:44:PHE:CE2 | 43:DZ:86:VAL:HG11 | 2.54 | 0.43 |
| 35:DR:103:ARG:NH1 | 35:DR:108:GLY:O | 2.52 | 0.43 |
| 16:AP:71:ARG:O | 16:AP:75:ARG:N | 2.52 | 0.43 |
| 39:BV:52:VAL:HG23 | 39:BV:52:VAL:O | 2.18 | 0.43 |
| 43:BZ:137:ILE:HG23 | 43:BZ:156:LYS:HD2 | 2.01 | 0.43 |
| 24:BB:28:C:OP1 | 36:BS:36:TYR:OH | 2.23 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 43:DZ:28:MET:HG2 | 43:DZ:37:VAL:HG11 | 2.00 | 0.43 |
| 12:AL:11:VAL:HG22 | 17:AQ:29:HIS:CD2 | 2.53 | 0.43 |
| 26:DE:5:LEU:HD21 | 26:DE:79:ARG:HB2 | 2.01 | 0.43 |
| 23:BA:451:C:H5' | 56:BA:4580:HOH:O | 2.19 | 0.43 |
| 23:BA:2801(A):A:H1' | 23:BA:2895:U:H1' | 2.00 | 0.43 |
| 23:BA:2028:U:H2' | 23:BA:2029:G:O4' | 2.18 | 0.43 |
| 1:AA:671:G:H2' | 1:AA:672:U:C6 | 2.53 | 0.43 |
| 23:DA:533:G:H5' | 38:DU:24:TYR:CD2 | 2.53 | 0.43 |
| 23:BA:757:U:H2' | 23:BA:758:C:O4' | 2.19 | 0.43 |
| 23:DA:1169:G:N2 | 23:DA:1181:C:C2 | 2.87 | 0.43 |
| 23:BA:760:G:H2' | 23:BA:761:A:O4' | 2.19 | 0.43 |
| 23:BA:219:G:C6 | 56:BA:3973:HOH:O | 2.72 | 0.43 |
| 30:DI:108:THR:OG1 | 30:DI:109:ILE:N | 2.51 | 0.43 |
| 28:DG:98:ARG:HB2 | 28:DG:98:ARG:NH1 | 2.33 | 0.43 |
| 32:DO:106:LEU:HD23 | 32:DO:106:LEU:HA | 1.75 | 0.43 |
| 52:D8:54:GLU:O | 52:D8:58:ILE:HG12 | 2.19 | 0.43 |
| 23:BA:1341:U:OP2 | 23:BA:1394:U:O2' | 2.26 | 0.43 |
| 8:AH:25:ASP:HA | 8:AH:59:LEU:O | 2.19 | 0.43 |
| 8:AH:4:ASP:HB2 | 8:AH:89:PRO:HG3 | 2.01 | 0.43 |
| 9:CI:9:ARG:HG3 | 9:CI:14:VAL:HG22 | 2.01 | 0.43 |
| 48:B4:40:HIS:HA | 48:B4:41:PRO:HD3 | 1.81 | 0.43 |
| 1:CA:1003:G:O2' | 1:CA:1024:G:N2 | 2.52 | 0.43 |
| 1:AA:970:C:C2 | 1:AA:1231:G:H1' | 2.54 | 0.43 |
| 23:BA:557:U:H2' | 23:BA:558:G:H8 | 1.84 | 0.43 |
| 23:DA:2119:A:N6 | 23:DA:2168:G:H1' | 2.34 | 0.43 |
| 23:BA:2133:G:H2' | 23:BA:2158:A:H61 | 1.83 | 0.43 |
| 1:CA:984:C:H2' | 1:CA:985:C:C6 | 2.53 | 0.43 |
| 1:CA:1026:G:H3' | 1:CA:1027:C:C5' | 2.49 | 0.43 |
| 3:CC:19:GLU:HB3 | 3:CC:40:ARG:NH2 | 2.34 | 0.43 |
| 6:AF:60:PHE:O | 6:AF:61:LEU:HD12 | 2.19 | 0.43 |
| 1:CA:604:G:C6 | 1:CA:605:U:C4 | 3.07 | 0.43 |
| 3:AC:70:VAL:N | 3:AC:104:GLN:O | 2.42 | 0.43 |
| 29:BH:3:ARG:HG3 | 29:BH:3:ARG:NH1 | 2.34 | 0.43 |
| 23:DA:1503:U:H2' | 23:DA:1504:C:C6 | 2.53 | 0.43 |
| 23:DA:1647:G:H3' | 23:DA:1647:G:P | 2.59 | 0.43 |
| 17:CQ:19:VAL:HG23 | 17:CQ:44:ALA:HB3 | 2.01 | 0.43 |
| 13:CM:64:TRP:HB2 | 13:CM:66:LEU:HD23 | 2.00 | 0.43 |
| 6:CF:95:GLU:HA | 6:CF:96:PRO:HD3 | 1.90 | 0.43 |
| 26:BE:9:VAL:HG13 | 26:BE:25:VAL:O | 2.19 | 0.43 |
| 26:DE:52:LEU:HA | 26:DE:53:PRO:HD2 | 1.82 | 0.43 |
| 23:BA:548:A:H61 | 39:BV:19:LYS:H | 1.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1265:G:O2' | 1:CA:1266:G:H5' | 2.18 | 0.43 |
| 1:CA:292:G:C5 | 1:CA:293:G:H1' | 2.53 | 0.43 |
| 1:AA:499:A:H4' | 1:AA:500:G:H5' | 2.00 | 0.43 |
| 43:DZ:137:ILE:HG23 | 43:DZ:156:LYS:HD2 | 2.01 | 0.43 |
| 20:AT:55:ILE:O | 20:AT:58:LYS:N | 2.52 | 0.43 |
| 23:DA:1946:U:H2' | 23:DA:1947:C:C6 | 2.54 | 0.43 |
| 23:DA:328:U:H4' | 42:DY:68:HIS:CD2 | 2.54 | 0.43 |
| 12:AL:53:ARG:HG2 | 12:AL:93:LEU:HD11 | 2.01 | 0.43 |
| 19:AS:35:SER:HB3 | 19:AS:38:SER:HB3 | 2.01 | 0.43 |
| 23:BA:903:C:H2' | 23:BA:904:C:C6 | 2.53 | 0.43 |
| 25:BD:159:ALA:HB1 | 25:BD:198:ASN:O | 2.19 | 0.43 |
| 35:DR:28:LEU:HD12 | 35:DR:48:VAL:HG21 | 2.00 | 0.43 |
| 1:AA:318:G:H2' | 1:AA:319:G:H8 | 1.83 | 0.43 |
| 23:DA:2031:A:C6 | 23:DA:2498:C:H1' | 2.54 | 0.43 |
| 22:AX:4:ASN:HB2 | 22:AX:37:VAL:O | 2.18 | 0.43 |
| 28:BG:10:LYS:O | 28:BG:14:GLU:HB3 | 2.19 | 0.43 |
| 52:D8:62:LEU:HB3 | 52:D8:65:GLU:HG2 | 1.99 | 0.43 |
| 39:BV:65:GLY:HA3 | 39:BV:91:TYR:CZ | 2.54 | 0.43 |
| 23:BA:223:A:O2' | 23:BA:420:C:O2 | 2.35 | 0.43 |
| 5:CE:41:VAL:O | 5:CE:67:VAL:HG12 | 2.17 | 0.43 |
| 8:CH:14:ARG:O | 8:CH:18:ARG:HD3 | 2.19 | 0.43 |
| 1:AA:811:C:H4' | 1:AA:900:A:N6 | 2.34 | 0.43 |
| 22:AX:76:GLY:O | 22:AX:79:ASP:HB3 | 2.19 | 0.43 |
| 1:AA:1442:G:C8 | 1:AA:1442(A):G:C5 | 3.07 | 0.43 |
| 23:BA:2296:U:C4 | 23:BA:2333:A:N3 | 2.87 | 0.43 |
| 1:AA:1237:C:H2' | 1:AA:1335:C:C5' | 2.49 | 0.43 |
| 23:DA:1356:G:C6 | 23:DA:1357:U:C4 | 3.07 | 0.43 |
| 5:CE:126:ARG:HA | 5:CE:131:ILE:HD11 | 2.00 | 0.43 |
| 1:AA:713:G:H2' | 1:AA:714:G:C8 | 2.54 | 0.43 |
| 23:DA:2171:A:H4' | 23:DA:2172:U:O5' | 2.18 | 0.43 |
| 1:CA:1238:A:C8 | 1:CA:1239:A:C8 | 3.07 | 0.43 |
| 1:CA:1010:G:C4 | 1:CA:1011:G:C8 | 3.07 | 0.43 |
| 1:AA:66:G:N2 | 1:AA:172:A:N3 | 2.67 | 0.43 |
| 1:AA:11:G:C6 | 1:AA:12:U:C4 | 3.07 | 0.43 |
| 1:AA:352:C:H2' | 1:AA:352:C:O2 | 2.17 | 0.43 |
| 1:CA:1070:U:H2' | 1:CA:1071:C:H6 | 1.84 | 0.43 |
| 3:CC:13:GLY:HA3 | 14:CN:57:ARG:NH2 | 2.30 | 0.43 |
| 1:CA:902:G:H2' | 1:CA:903:G:H8 | 1.84 | 0.43 |
| 36:DS:96:GLY:N | 36:DS:99:LYS:HB3 | 2.34 | 0.43 |
| 23:BA:2307:G:H5' | 23:BA:2308:G:C2 | 2.53 | 0.43 |
| 10:CJ:39:PRO:HG3 | 10:CJ:70:ARG:HH21 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1035:U:O4 | 56:DA:4641:HOH:O | 2.22 | 0.43 |
| 4:AD:32:ALA:O | 4:AD:36:ARG:N | 2.51 | 0.43 |
| 25:DD:101:GLU:OE1 | 25:DD:103:ARG:NH1 | 2.46 | 0.43 |
| 23:BA:658:C:H2' | 23:BA:659:C:C6 | 2.54 | 0.43 |
| 1:CA:1013:G:N2 | 1:CA:1017:G:C6 | 2.87 | 0.43 |
| 23:BA:1586:A:H2' | 23:BA:1587:A:H5' | 2.01 | 0.43 |
| 23:DA:2593:U:H2' | 23:DA:2594:C:C6 | 2.54 | 0.43 |
| 29:BH:69:ARG:HG3 | 29:BH:70:THR:N | 2.33 | 0.43 |
| 23:BA:1163:G:O2' | 23:BA:1164:G:H5' | 2.18 | 0.43 |
| 23:DA:1586:A:H2' | 23:DA:1587:A:H5' | 2.00 | 0.43 |
| 43:BZ:128:VAL:HG23 | 43:BZ:161:VAL:HG22 | 2.00 | 0.43 |
| 28:BG:124:SER:HB2 | 28:BG:131:TYR:CZ | 2.53 | 0.43 |
| 23:BA:1425:G:H2' | 23:BA:1426:G:C8 | 2.54 | 0.43 |
| 37:BT:90:GLN:HG3 | 37:BT:91:ARG:N | 2.34 | 0.43 |
| 1:AA:707:C:O2' | 1:AA:708:C:H5' | 2.18 | 0.43 |
| 46:D2:50:ILE:O | 46:D2:52:ASP:N | 2.45 | 0.43 |
| 7:AG:26:PHE:CD1 | 7:AG:101:LEU:HD22 | 2.54 | 0.43 |
| 9:AI:20:ARG:HA | 9:AI:21:PRO:HD2 | 1.90 | 0.43 |
| 4:AD:61:LYS:HE3 | 4:AD:62:GLN:OE1 | 2.18 | 0.43 |
| 1:CA:1279:A:O2' | 1:CA:1282:C:N4 | 2.52 | 0.43 |
| 23:BA:1011:G:C4 | 23:BA:1151:G:N2 | 2.87 | 0.43 |
| 13:CM:16:ASP:HB3 | 13:CM:34:LEU:CD1 | 2.48 | 0.43 |
| 37:DT:37:GLY:HA2 | 37:DT:38:ASN:HA | 1.52 | 0.43 |
| 25:BD:112:GLN:O | 25:BD:115:GLN:HG2 | 2.19 | 0.43 |
| 29:DH:90:LYS:O | 29:DH:160:LYS:HA | 2.19 | 0.43 |
| 22:AX:29:GLN:C | 22:AX:30:TYR:HD2 | 2.23 | 0.43 |
| 23:BA:1957:C:H2' | 23:BA:1958:C:C6 | 2.54 | 0.43 |
| 23:BA:272(H):C:H5' | 23:BA:272(I):U:OP2 | 2.18 | 0.43 |
| 23:BA:1804:C:H2' | 23:BA:1805:U:H6 | 1.83 | 0.43 |
| 23:BA:1804:C:H6 | 23:BA:1804:C:O5' | 2.01 | 0.43 |
| 2:AB:25:ASN:HA | 2:AB:26:PRO:HD2 | 1.88 | 0.43 |
| 23:BA:2793:G:N2 | 23:BA:2804:C:H1' | 2.34 | 0.43 |
| 23:DA:2360:A:H2' | 23:DA:2361:A:O4' | 2.18 | 0.43 |
| 43:BZ:124:ILE:HD11 | 43:BZ:165:VAL:HG11 | 2.00 | 0.43 |
| 33:DP:107:LYS:O | 33:DP:110:TYR:HB2 | 2.19 | 0.43 |
| 5:AE:41:VAL:O | 5:AE:67:VAL:HG12 | 2.19 | 0.43 |
| 4:CD:177:ASP:CG | 4:CD:180:GLY:HA3 | 2.39 | 0.43 |
| 40:DW:36:LEU:HD23 | 40:DW:36:LEU:HA | 1.77 | 0.43 |
| 9:AI:48:GLU:OE2 | 9:AI:48:GLU:HA | 2.18 | 0.43 |
| 46:D2:61:LEU:HA | 46:D2:61:LEU:HD23 | 1.84 | 0.43 |
| 53:B9:6:SER:O | 53:B9:6:SER:OG | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:BF:12:LEU:HA | 27:BF:12:LEU:HD22 | 1.73 | 0.43 |
| 23:DA:64:A:O3' | 41:DX:71:GLY:HA3 | 2.19 | 0.43 |
| 23:DA:1042:G:C6 | 23:DA:1043:C:C4 | 3.07 | 0.43 |
| 10:CJ:55:LYS:O | 10:CJ:55:LYS:HG2 | 2.17 | 0.42 |
| 19:AS:36:ARG:HB2 | 19:AS:72:GLY:HA2 | 1.99 | 0.42 |
| 1:CA:1288:A:C6 | 1:CA:1371:G:H1' | 2.54 | 0.42 |
| 2:AB:216:SER:O | 2:AB:219:VAL:N | 2.52 | 0.42 |
| 23:BA:271(K):U:H2' | 23:BA:271(K):U:H6 | 1.60 | 0.42 |
| 1:AA:1240:U:O2 | 7:AG:38:LEU:HD23 | 2.20 | 0.42 |
| 1:CA:1234:C:C4 | 1:CA:1235:U:C4 | 3.07 | 0.42 |
| 13:CM:97:PRO:HG3 | 13:CM:110:ARG:HB3 | 2.00 | 0.42 |
| 23:DA:1359:A:N6 | 23:DA:1372:U:C5 | 2.87 | 0.42 |
| 23:DA:1352:U:P | 56:DA:3935:HOH:O | 2.71 | 0.42 |
| 1:AA:1118:C:N3 | 1:AA:1155:G:N2 | 2.56 | 0.42 |
| 25:BD:118:VAL:N | 25:BD:129:ASN:HD22 | 2.03 | 0.42 |
| 1:CA:1283:G:N2 | 1:CA:1284:C:C2 | 2.87 | 0.42 |
| 28:BG:16:ARG:HB2 | 28:BG:17:PRO:HD3 | 2.01 | 0.42 |
| 1:CA:1050:G:N1 | 1:CA:1208:C:O2 | 2.40 | 0.42 |
| 1:AA:113:G:N3 | 1:AA:353:A:O2' | 2.46 | 0.42 |
| 1:CA:235:C:H2' | 1:CA:236:G:H8 | 1.84 | 0.42 |
| 23:BA:1047:G:H2' | 23:BA:1110:G:C2 | 2.54 | 0.42 |
| 25:BD:85:ASP:OD2 | 25:BD:88:ARG:NH1 | 2.49 | 0.42 |
| 3:CC:12:LEU:HD22 | 3:CC:18:TRP:CE3 | 2.53 | 0.42 |
| 28:DG:5:VAL:HG12 | 48:D4:25:TYR:HE1 | 1.81 | 0.42 |
| 23:DA:2544:G:H2' | 23:DA:2545:G:O4' | 2.19 | 0.42 |
| 11:CK:41:THR:HG22 | 11:CK:42:TRP:N | 2.34 | 0.42 |
| 5:AE:14:ARG:HE | 5:AE:16:THR:HG22 | 1.84 | 0.42 |
| 1:AA:1348:U:C4 | 1:AA:1373:G:N2 | 2.87 | 0.42 |
| 1:AA:1373:G:H5'' | 7:AG:36:LYS:HD2 | 2.00 | 0.42 |
| 34:DQ:137:TYR:HE2 | 43:DZ:49:ARG:NH1 | 2.17 | 0.42 |
| 30:DI:92:VAL:CG1 | 30:DI:120:ILE:HB | 2.49 | 0.42 |
| 29:BH:3:ARG:NH2 | 29:BH:5:GLY:H | 2.17 | 0.42 |
| 17:AQ:45:HIS:O | 17:AQ:73:VAL:HG23 | 2.18 | 0.42 |
| 2:AB:16:HIS:CD2 | 2:AB:213:LEU:HD12 | 2.54 | 0.42 |
| 3:CC:113:ALA:HB1 | 3:CC:200:ALA:HB3 | 2.01 | 0.42 |
| 2:CB:14:GLY:HA3 | 2:CB:16:HIS:HE1 | 1.84 | 0.42 |
| 3:AC:36:ASP:N | 3:AC:36:ASP:OD2 | 2.52 | 0.42 |
| 5:CE:8:GLU:CB | 5:CE:34:VAL:HG23 | 2.49 | 0.42 |
| 50:B6:30:THR:OG1 | 50:B6:30:THR:O | 2.37 | 0.42 |
| 1:CA:565:U:OP2 | 1:CA:566:G:O2' | 2.30 | 0.42 |
| 17:AQ:60:ILE:O | 17:AQ:62:SER:OG | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1205:U:H4' | 23:BA:1206:G:OP2 | 2.19 | 0.42 |
| 31:DN:36:GLY:HA3 | 31:DN:49:GLY:HA2 | 2.01 | 0.42 |
| 28:BG:146:TYR:O | 28:BG:149:VAL:HG12 | 2.19 | 0.42 |
| 23:DA:1488:G:C2 | 23:DA:1489:U:O2 | 2.72 | 0.42 |
| 23:BA:1546:C:H5' | 23:BA:1547:C:H5' | 2.00 | 0.42 |
| 34:BQ:70:PRO:HA | 34:BQ:94:VAL:O | 2.19 | 0.42 |
| 46:B2:56:GLN:O | 46:B2:60:LEU:HG | 2.19 | 0.42 |
| 24:DB:28:C:H2' | 24:DB:29:A:O4' | 2.19 | 0.42 |
| 1:AA:445:G:H3' | 1:AA:446:G:H8 | 1.84 | 0.42 |
| 23:DA:2252:G:H2' | 23:DA:2253:G:O4' | 2.18 | 0.42 |
| 23:DA:2678:C:H2' | 23:DA:2679:A:O4' | 2.19 | 0.42 |
| 1:AA:1044:A:H8 | 1:AA:1044:A:OP2 | 2.02 | 0.42 |
| 25:BD:223:GLY:HA3 | 25:BD:231:HIS:CE1 | 2.54 | 0.42 |
| 29:BH:54:ARG:HA | 29:BH:55:PRO:HD2 | 1.87 | 0.42 |
| 27:DF:41:LEU:O | 27:DF:44:ARG:HG2 | 2.19 | 0.42 |
| 30:BI:40:THR:C | 30:BI:42:SER:N | 2.73 | 0.42 |
| 23:DA:2474:C:H5'' | 23:DA:2475:C:OP2 | 2.18 | 0.42 |
| 34:DQ:63:LYS:HD2 | 34:DQ:65:PHE:CZ | 2.53 | 0.42 |
| 22:CX:30:TYR:N | 22:CX:30:TYR:CD2 | 2.86 | 0.42 |
| 26:BE:134:ILE:HG13 | 26:BE:134:ILE:H | 1.71 | 0.42 |
| 9:AI:113:LYS:N | 9:AI:113:LYS:HD3 | 2.34 | 0.42 |
| 23:DA:12:U:H2' | 23:DA:12:U:O2 | 2.19 | 0.42 |
| 27:BF:140:LEU:HD13 | 27:BF:140:LEU:HA | 1.61 | 0.42 |
| 24:DB:78:A:C2 | 24:DB:100:A:C4 | 3.07 | 0.42 |
| 48:D4:16:CYS:HB3 | 48:D4:20:ASN:HB3 | 2.00 | 0.42 |
| 23:BA:968:G:H2' | 23:BA:969:U:O4' | 2.19 | 0.42 |
| 1:AA:1456:G:O2' | 20:AT:39:LYS:HD3 | 2.19 | 0.42 |
| 1:AA:1004:A:H5' | 1:AA:1025:U:O4 | 2.19 | 0.42 |
| 1:AA:1221:G:H4' | 19:AS:77:THR:HG21 | 2.00 | 0.42 |
| 1:CA:1350:A:C6 | 1:CA:1351:U:C4 | 3.07 | 0.42 |
| 7:CG:26:PHE:CE2 | 7:CG:30:ILE:HD11 | 2.54 | 0.42 |
| 1:CA:1055:A:C8 | 1:CA:1206:G:C2 | 3.07 | 0.42 |
| 1:CA:1055:A:N6 | 1:CA:1206:G:N7 | 2.68 | 0.42 |
| 6:AF:14:LEU:HD22 | 6:AF:18:GLN:CB | 2.49 | 0.42 |
| 23:DA:330:A:H2 | 23:DA:1210:A:C2' | 2.20 | 0.42 |
| 23:DA:807:U:OP2 | 33:DP:41:ARG:NH2 | 2.52 | 0.42 |
| 33:DP:38:GLN:O | 33:DP:39:LYS:HB3 | 2.19 | 0.42 |
| 23:DA:1022:G:C5 | 23:DA:1140:C:C4 | 3.08 | 0.42 |
| 27:BF:106:ARG:HG2 | 27:BF:106:ARG:H | 1.37 | 0.42 |
| 23:DA:2169:A:H3' | 23:DA:2170:A:C8 | 2.54 | 0.42 |
| 1:CA:373:A:H2' | 1:CA:374:A:H8 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:302:C:O2' | 23:BA:303:U:H5' | 2.20 | 0.42 |
| 13:AM:69:GLU:C | 13:AM:71:ARG:H | 2.21 | 0.42 |
| 25:BD:154:LYS:HB2 | 25:BD:155:LEU:HD12 | 2.01 | 0.42 |
| 1:CA:151:A:C2 | 1:CA:152:A:H1' | 2.54 | 0.42 |
| 23:DA:1046:A:O2' | 23:DA:1047:G:OP2 | 2.31 | 0.42 |
| 1:CA:429:U:H3' | 4:CD:22:LYS:HZ1 | 1.84 | 0.42 |
| 4:CD:111:ALA:HB1 | 4:CD:116:GLN:OE1 | 2.19 | 0.42 |
| 1:CA:132:C:H2' | 1:CA:133:U:O4' | 2.19 | 0.42 |
| 31:DN:15:LEU:HD12 | 31:DN:137:LYS:HG2 | 1.99 | 0.42 |
| 23:DA:1823:G:OP1 | 25:DD:54:ARG:NH1 | 2.53 | 0.42 |
| 5:AE:8:GLU:CB | 5:AE:34:VAL:HG23 | 2.49 | 0.42 |
| 20:CT:74:LYS:HE2 | 20:CT:74:LYS:HB3 | 1.84 | 0.42 |
| 23:BA:1488:G:H5'' | 23:BA:1489:U:OP2 | 2.18 | 0.42 |
| 23:DA:1649:G:N1 | 23:DA:2009:G:C6 | 2.87 | 0.42 |
| 23:DA:588:U:O4 | 23:DA:670:A:H1' | 2.20 | 0.42 |
| 17:AQ:63:ARG:HA | 17:AQ:64:PRO:HD3 | 1.86 | 0.42 |
| 23:BA:686:G:N2 | 23:BA:788:A:H61 | 2.17 | 0.42 |
| 23:DA:190:A:O5' | 23:DA:205:G:N2 | 2.51 | 0.42 |
| 2:AB:158:LEU:HA | 2:AB:159:PRO:HD3 | 1.97 | 0.42 |
| 30:BI:140:LEU:HA | 30:BI:140:LEU:HD23 | 1.82 | 0.42 |
| 9:CI:27:THR:CG2 | 9:CI:30:GLY:H | 2.33 | 0.42 |
| 20:AT:21:LYS:O | 20:AT:25:ARG:HG3 | 2.18 | 0.42 |
| 1:CA:1093:A:C2 | 1:CA:1095:U:H5' | 2.54 | 0.42 |
| 23:DA:2580:U:C5 | 23:DA:2581:G:C6 | 3.07 | 0.42 |
| 43:DZ:27:VAL:HA | 43:DZ:35:ARG:O | 2.19 | 0.42 |
| 23:DA:2684:U:C4 | 23:DA:2685:G:N7 | 2.87 | 0.42 |
| 17:AQ:29:HIS:HB3 | 17:AQ:33:GLY:N | 2.34 | 0.42 |
| 23:DA:236:C:H2' | 23:DA:237:C:C6 | 2.54 | 0.42 |
| 23:DA:817:C:O2' | 23:DA:839:U:H5'' | 2.20 | 0.42 |
| 23:DA:839:U:H2' | 23:DA:840:C:C6 | 2.54 | 0.42 |
| 27:BF:88:VAL:HG21 | 27:BF:91:GLY:HA3 | 2.01 | 0.42 |
| 23:BA:39:C:H2' | 23:BA:40:C:H6 | 1.83 | 0.42 |
| 23:BA:2302:G:O2' | 28:BG:126:ASP:O | 2.32 | 0.42 |
| 23:DA:479:A:H4' | 23:DA:480:A:OP1 | 2.17 | 0.42 |
| 23:BA:673:C:H5'' | 27:BF:81:PRO:HD2 | 2.01 | 0.42 |
| 23:DA:866:A:C6 | 23:DA:914:C:C5 | 3.07 | 0.42 |
| 47:B3:8:LEU:HD13 | 47:B3:31:LEU:HD23 | 2.00 | 0.42 |
| 46:B2:61:LEU:HD23 | 46:B2:61:LEU:HA | 1.76 | 0.42 |
| 23:BA:1891:G:H8 | 23:BA:1891:G:O5' | 2.03 | 0.42 |
| 26:BE:170:LEU:HD12 | 26:BE:170:LEU:HA | 1.77 | 0.42 |
| 23:BA:2079:U:O3' | 45:B1:35:THR:OG1 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:DE:21:VAL:HA | 26:DE:22:PRO:HD2 | 1.94 | 0.42 |
| 16:CP:22:THR:HA | 16:CP:33:ILE:HG12 | 2.01 | 0.42 |
| 31:BN:62:VAL:CG1 | 31:BN:66:LYS:HB2 | 2.49 | 0.42 |
| 23:DA:2706:G:O2' | 35:DR:64:ARG:HD3 | 2.19 | 0.42 |
| 1:AA:237:C:H5'' | 17:AQ:25:ARG:CZ | 2.49 | 0.42 |
| 1:AA:1095:U:H2' | 1:AA:1096:C:H6 | 1.83 | 0.42 |
| 1:CA:1378:C:OP2 | 7:CG:2:ALA:HB2 | 2.19 | 0.42 |
| 1:CA:1263:C:N3 | 1:CA:1272:G:O6 | 2.51 | 0.42 |
| 1:AA:1238:A:H2' | 1:AA:1239:A:H8 | 1.83 | 0.42 |
| 1:AA:1297:C:O2' | 7:AG:114:ARG:NH2 | 2.52 | 0.42 |
| 1:CA:1198:G:H2' | 1:CA:1199:U:C6 | 2.55 | 0.42 |
| 1:AA:1099:G:H3' | 1:AA:1100:C:C6 | 2.53 | 0.42 |
| 23:BA:2298:A:H2' | 23:BA:2299:G:O4' | 2.19 | 0.42 |
| 10:CJ:9:ARG:HG2 | 10:CJ:69:ASN:CG | 2.39 | 0.42 |
| 1:CA:1250:A:N1 | 1:CA:1251:A:C2 | 2.87 | 0.42 |
| 1:CA:1321:C:H5'' | 1:CA:1322:C:H2' | 2.01 | 0.42 |
| 28:DG:138:GLN:HE21 | 28:DG:144:ILE:HD13 | 1.83 | 0.42 |
| 1:AA:5:U:H5'' | 1:AA:6:G:C8 | 2.54 | 0.42 |
| 1:AA:1309:G:C6 | 1:AA:1310:G:C5 | 3.07 | 0.42 |
| 12:CL:114:LYS:O | 12:CL:117:ARG:HG3 | 2.20 | 0.42 |
| 23:BA:2791:C:N4 | 23:BA:2893:G:O4' | 2.52 | 0.42 |
| 15:CO:57:LEU:O | 15:CO:60:VAL:N | 2.52 | 0.42 |
| 2:CB:132:LYS:O | 2:CB:135:GLN:HG2 | 2.19 | 0.42 |
| 23:DA:248:G:H5' | 23:DA:250:G:N7 | 2.35 | 0.42 |
| 22:AX:67:GLY:HA3 | 22:AX:72:ALA:HB3 | 2.00 | 0.42 |
| 48:D4:1:MET:HB3 | 48:D4:6:HIS:CD2 | 2.53 | 0.42 |
| 19:AS:33:THR:HG21 | 19:AS:49:ILE:HG23 | 2.01 | 0.42 |
| 25:DD:180:GLY:HA3 | 25:DD:275:LYS:HG2 | 2.00 | 0.42 |
| 25:DD:180:GLY:HA3 | 25:DD:275:LYS:CG | 2.49 | 0.42 |
| 17:CQ:66:SER:HB3 | 17:CQ:69:LYS:HD3 | 2.00 | 0.42 |
| 17:AQ:5:VAL:HG22 | 17:AQ:60:ILE:HG13 | 2.01 | 0.42 |
| 43:DZ:128:VAL:HG23 | 43:DZ:161:VAL:HG22 | 2.01 | 0.42 |
| 7:AG:113:GLU:O | 7:AG:119:ARG:HD3 | 2.19 | 0.42 |
| 24:BB:9:G:OP1 | 36:BS:25:ARG:NH2 | 2.52 | 0.42 |
| 26:BE:52:LEU:HA | 26:BE:53:PRO:HD2 | 1.83 | 0.42 |
| 35:BR:103:ARG:HG2 | 35:BR:103:ARG:HH11 | 1.85 | 0.42 |
| 12:AL:33:ARG:HD2 | 12:AL:33:ARG:HA | 1.76 | 0.42 |
| 1:CA:1192:C:C6 | 1:CA:1192:C:H3' | 2.54 | 0.42 |
| 25:BD:136:ILE:HA | 25:BD:137:PRO:HD3 | 1.92 | 0.42 |
| 48:B4:14:ILE:HG23 | 48:B4:31:ILE:HB | 2.01 | 0.42 |
| 37:DT:19:LEU:HA | 37:DT:20:PRO:HD3 | 1.79 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BN:36:GLY:O | 31:BN:42:TRP:HD1 | 2.03 | 0.42 |
| 7:AG:16:LEU:HD22 | 9:AI:44:VAL:O | 2.19 | 0.42 |
| 32:BO:3:GLN:HB2 | 32:BO:4:PRO:HD2 | 2.01 | 0.42 |
| 43:BZ:24:LEU:HD22 | 43:BZ:41:LEU:HD23 | 2.01 | 0.42 |
| 39:DV:52:VAL:HG21 | 39:DV:55:ALA:HB3 | 2.01 | 0.42 |
| 23:DA:311:A:C6 | 23:DA:328:U:C4 | 3.07 | 0.42 |
| 34:DQ:66:ILE:HG12 | 34:DQ:104:PHE:HD2 | 1.84 | 0.42 |
| 1:AA:818:G:HO2' | 1:AA:820:U:H6 | 1.64 | 0.42 |
| 23:DA:623:G:H2' | 23:DA:624:C:C6 | 2.54 | 0.42 |
| 2:AB:110:GLN:HG3 | 2:AB:110:GLN:H | 1.51 | 0.42 |
| 23:DA:362:U:O2' | 23:DA:363:G:H5'' | 2.20 | 0.42 |
| 1:AA:405:U:O4 | 4:AD:2:GLY:N | 2.53 | 0.42 |
| 23:BA:1031:G:H1 | 23:BA:1123:C:H42 | 1.66 | 0.42 |
| 23:DA:2683:C:O2 | 32:DO:70:LYS:NZ | 2.29 | 0.42 |
| 23:DA:744:G:OP1 | 26:DE:132:HIS:ND1 | 2.50 | 0.42 |
| 23:DA:1292:U:H2' | 23:DA:1293:C:C6 | 2.54 | 0.42 |
| 45:D1:32:LYS:HB3 | 45:D1:32:LYS:HE2 | 1.90 | 0.42 |
| 26:BE:40:GLU:CD | 26:BE:40:GLU:H | 2.22 | 0.42 |
| 43:BZ:61:LEU:HD13 | 43:BZ:61:LEU:HA | 1.72 | 0.42 |
| 32:DO:11:ALA:O | 32:DO:99:PHE:N | 2.40 | 0.42 |
| 4:CD:100:ARG:NH1 | 4:CD:137:SER:HA | 2.35 | 0.42 |
| 4:AD:128:VAL:HA | 4:AD:145:GLU:O | 2.20 | 0.42 |
| 46:D2:9:GLN:HE22 | 46:D2:56:GLN:HG2 | 1.84 | 0.42 |
| 1:AA:1111:A:N1 | 3:AC:177:THR:HG23 | 2.34 | 0.42 |
| 1:CA:1345:U:C5 | 1:CA:1377:A:C2 | 3.08 | 0.42 |
| 2:CB:32:ILE:HD11 | 2:CB:40:HIS:HB3 | 2.00 | 0.42 |
| 2:AB:165:VAL:O | 2:AB:187:LEU:HB3 | 2.20 | 0.42 |
| 1:AA:1053:G:C6 | 1:AA:1199:U:H2' | 2.54 | 0.42 |
| 1:AA:1363:C:H5' | 1:AA:1363(A):A:O5' | 2.19 | 0.42 |
| 1:AA:950:U:N3 | 1:AA:951:G:N7 | 2.67 | 0.42 |
| 28:DG:143:GLU:H | 28:DG:143:GLU:HG2 | 1.51 | 0.42 |
| 1:AA:1277:C:C2' | 1:AA:1279:A:H8 | 2.32 | 0.42 |
| 1:AA:1255:G:H3' | 1:AA:1279:A:N6 | 2.34 | 0.42 |
| 33:DP:52:GLU:CD | 52:D8:57:ARG:HH12 | 2.22 | 0.42 |
| 1:CA:1251:A:N6 | 1:CA:1285:A:C6 | 2.85 | 0.42 |
| 1:CA:1366:C:OP1 | 9:CI:117:HIS:ND1 | 2.52 | 0.42 |
| 1:CA:1157:A:OP1 | 1:CA:1158:C:C5 | 2.72 | 0.42 |
| 1:AA:1172:C:C2 | 1:AA:1173:G:C8 | 3.07 | 0.42 |
| 1:CA:748:C:H6 | 1:CA:748:C:O5' | 2.03 | 0.42 |
| 23:DA:279:C:H42 | 23:DA:361:G:H1 | 1.66 | 0.42 |
| 23:BA:674:G:H1' | 27:BF:74:ARG:CD | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CC:11:ARG:HB2 | 3:CC:11:ARG:NH1 | 2.31 | 0.42 |
| 36:DS:95:HIS:C | 36:DS:99:LYS:HB3 | 2.39 | 0.42 |
| 26:DE:93:VAL:HG13 | 56:DE:402:HOH:O | 2.19 | 0.42 |
| 23:BA:528:A:C2' | 23:BA:529:A:H5' | 2.49 | 0.42 |
| 1:CA:1150:U:O2' | 10:CJ:39:PRO:HB2 | 2.19 | 0.42 |
| 23:BA:1352:U:O2 | 23:BA:1570:A:H2 | 2.02 | 0.42 |
| 23:BA:1434:A:O2' | 23:BA:1435:G:H5' | 2.19 | 0.42 |
| 4:CD:18:LYS:HD2 | 4:CD:33:MET:HB2 | 2.02 | 0.42 |
| 2:CB:78:GLN:C | 2:CB:94:ASN:HD21 | 2.22 | 0.42 |
| 1:CA:827:U:H5'' | 1:CA:828:A:OP2 | 2.19 | 0.42 |
| 12:AL:114:LYS:O | 12:AL:117:ARG:HG3 | 2.19 | 0.42 |
| 1:CA:624:C:H2' | 1:CA:625:G:H8 | 1.85 | 0.42 |
| 23:DA:2235:G:H2' | 23:DA:2236:C:C6 | 2.54 | 0.42 |
| 1:AA:62:U:H5'' | 1:AA:385:C:O2 | 2.20 | 0.42 |
| 31:DN:34:LEU:HD12 | 31:DN:34:LEU:HA | 1.76 | 0.42 |
| 24:DB:7:G:C8 | 24:DB:7:G:H5'' | 2.54 | 0.42 |
| 1:CA:512:U:H2' | 1:CA:513:C:C6 | 2.53 | 0.42 |
| 23:BA:2065:C:H2' | 23:BA:2066:C:C6 | 2.54 | 0.42 |
| 23:DA:2202:C:H2' | 23:DA:2203:U:O4' | 2.19 | 0.42 |
| 23:DA:576:U:H2' | 23:DA:577:G:C8 | 2.54 | 0.42 |
| 23:BA:362:U:O2' | 23:BA:363:G:H5'' | 2.19 | 0.42 |
| 38:DU:83:LEU:HD12 | 38:DU:113:ALA:HB2 | 2.01 | 0.42 |
| 23:BA:2584:U:H2' | 23:BA:2585:U:H2' | 2.00 | 0.42 |
| 5:CE:89:ILE:HD13 | 5:CE:90:VAL:N | 2.34 | 0.42 |
| 2:CB:52:GLU:HG2 | 2:CB:56:ARG:NH1 | 2.35 | 0.42 |
| 3:AC:164:ARG:HB2 | 3:AC:164:ARG:HE | 1.38 | 0.42 |
| 37:BT:13:ARG:HG2 | 37:BT:13:ARG:H | 1.27 | 0.42 |
| 40:DW:65:LEU:HA | 40:DW:65:LEU:HD23 | 1.86 | 0.42 |
| 31:BN:12:ARG:HD3 | 31:BN:50:ASP:OD2 | 2.19 | 0.42 |
| 1:AA:716:A:N3 | 11:AK:118:GLY:HA2 | 2.35 | 0.42 |
| 22:CX:31:PHE:CG | 22:CX:85:LEU:HB3 | 2.54 | 0.42 |
| 47:D3:8:LEU:HD13 | 47:D3:31:LEU:HD23 | 2.02 | 0.42 |
| 26:DE:35:GLN:HG3 | 26:DE:36:ARG:N | 2.35 | 0.42 |
| 23:BA:340:A:H2' | 23:BA:341:G:O4' | 2.19 | 0.42 |
| 1:AA:1443:G:O6 | 1:AA:1459:C:C2 | 2.72 | 0.42 |
| 10:CJ:50:ILE:HD12 | 10:CJ:50:ILE:N | 2.31 | 0.42 |
| 13:CM:15:VAL:O | 13:CM:18:ALA:HB3 | 2.19 | 0.42 |
| 2:AB:19:HIS:HE1 | 2:AB:205:ASP:OD1 | 2.02 | 0.42 |
| 1:AA:1237:C:C4 | 1:AA:1336:C:C2 | 3.08 | 0.42 |
| 1:CA:1003:G:H2' | 1:CA:1004:A:H4' | 2.01 | 0.42 |
| 1:CA:1306:A:H62 | 1:CA:1331:G:N2 | 2.17 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:DG:43:LEU:HD22 | 28:DG:90:LEU:HG | 2.01 | 0.42 |
| 45:B1:82:LEU:CA | 45:B1:85:LEU:HD23 | 2.36 | 0.42 |
| 31:DN:23:LEU:HB2 | 31:DN:60:ILE:HG12 | 2.00 | 0.42 |
| 23:DA:2114:A:H3' | 23:DA:2115:G:C8 | 2.55 | 0.42 |
| 23:BA:2070:G:C2 | 23:BA:2442:C:C2 | 3.08 | 0.42 |
| 4:CD:158:ILE:O | 4:CD:162:LEU:HD12 | 2.19 | 0.42 |
| 23:DA:1913:A:P | 23:DA:1913:A:H3' | 2.59 | 0.42 |
| 1:CA:1105:A:N1 | 1:CA:1106:G:C5 | 2.87 | 0.42 |
| 23:BA:1912:A:HO2' | 23:BA:1913:A:P | 2.43 | 0.42 |
| 3:CC:12:LEU:O | 14:CN:57:ARG:NH1 | 2.52 | 0.42 |
| 23:BA:2632:A:O2' | 23:BA:2811:G:O2' | 2.21 | 0.42 |
| 4:AD:108:LEU:CB | 4:AD:110:PHE:HE1 | 2.33 | 0.42 |
| 1:AA:1373:G:H5'' | 7:AG:36:LYS:CD | 2.50 | 0.42 |
| 4:CD:112:VAL:HG22 | 4:CD:116:GLN:OE1 | 2.19 | 0.42 |
| 13:AM:96:LEU:C | 13:AM:110:ARG:HD3 | 2.40 | 0.42 |
| 23:DA:2309:A:C6 | 23:DA:2310:A:C2 | 3.08 | 0.42 |
| 30:BI:5:LEU:HD11 | 30:BI:19:VAL:HG22 | 2.01 | 0.42 |
| 23:BA:571:A:H5' | 23:BA:2030:A:N7 | 2.35 | 0.42 |
| 36:DS:56:LEU:O | 36:DS:58:LEU:HD22 | 2.20 | 0.42 |
| 1:AA:1137:C:C5' | 1:AA:1138:G:C6 | 3.02 | 0.42 |
| 27:BF:64:ILE:HD11 | 27:BF:75:HIS:HB2 | 2.02 | 0.42 |
| 23:DA:1288:U:O2' | 23:DA:1647:G:N2 | 2.52 | 0.42 |
| 9:CI:46:ALA:CB | 9:CI:77:ILE:HB | 2.48 | 0.42 |
| 1:CA:617:G:C2 | 1:CA:618:C:C5 | 3.08 | 0.42 |
| 1:CA:1203:C:P | 14:CN:3:ARG:HH12 | 2.42 | 0.42 |
| 23:DA:2273:A:H2' | 23:DA:2274:A:H8 | 1.83 | 0.42 |
| 1:AA:684:A:N6 | 56:AA:2047:HOH:O | 2.46 | 0.42 |
| 28:BG:47:LYS:HA | 28:BG:88:ILE:HG22 | 2.01 | 0.42 |
| 23:DA:1638:C:H4' | 23:DA:2710:C:O2 | 2.19 | 0.42 |
| 23:BA:322:A:H4' | 23:BA:323:G:OP2 | 2.20 | 0.42 |
| 1:AA:1501:C:N4 | 1:AA:1504:G:C2 | 2.87 | 0.42 |
| 1:CA:384:G:H2' | 1:CA:385:C:C6 | 2.54 | 0.42 |
| 23:DA:566:U:OP1 | 33:DP:29:LYS:HD2 | 2.19 | 0.42 |
| 23:DA:916:G:H5' | 23:DA:917:A:OP1 | 2.20 | 0.42 |
| 23:DA:1799:G:H5' | 23:DA:1819:A:N6 | 2.33 | 0.42 |
| 30:BI:39:ALA:HB1 | 30:BI:44:LEU:HD11 | 2.01 | 0.42 |
| 1:CA:1057:G:H2' | 1:CA:1058:G:H8 | 1.85 | 0.42 |
| 23:DA:2755:C:C4 | 53:D9:19:ARG:NH1 | 2.87 | 0.42 |
| 23:DA:1489:U:C6 | 23:DA:1489:U:H3' | 2.53 | 0.42 |
| 41:DX:11:PRO:HD3 | 46:D2:37:PHE:CE2 | 2.55 | 0.42 |
| 23:DA:2664:G:H3' | 56:DA:3746:HOH:O | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:DA:323:G:OP1 | 23:DA:338:G:N2 | 2.48 | 0.42 |
| 2:CB:114:ARG:HD2 | 2:CB:114:ARG:O | 2.19 | 0.42 |
| 23:DA:2290:G:O2' | 23:DA:2381:C:H1' | 2.20 | 0.42 |
| 23:BA:2065:C:H2' | 23:BA:2066:C:H6 | 1.85 | 0.42 |
| 17:CQ:29:HIS:HB3 | 17:CQ:33:GLY:N | 2.34 | 0.42 |
| 34:BQ:110:THR:HG23 | 34:BQ:113:GLN:HB2 | 2.00 | 0.42 |
| 23:BA:1107:G:N7 | 23:BA:1108:U:C5 | 2.88 | 0.42 |
| 38:DU:82:GLY:HA3 | 38:DU:113:ALA:HB1 | 2.00 | 0.42 |
| 25:DD:39:LYS:NZ | 25:DD:57:GLY:O | 2.53 | 0.42 |
| 23:BA:1441:G:H2' | 23:BA:1442:G:C8 | 2.55 | 0.42 |
| 1:CA:773:G:H4' | 25:DD:202:LYS:HE2 | 2.01 | 0.42 |
| 23:DA:719:C:H2' | 23:DA:720:C:C6 | 2.54 | 0.42 |
| 23:BA:479:A:H4' | 23:BA:480:A:OP1 | 2.20 | 0.42 |
| 23:DA:2018:G:H2' | 23:DA:2019:A:O4' | 2.19 | 0.42 |
| 23:BA:824:A:H1' | 23:BA:2358:G:N7 | 2.34 | 0.42 |
| 37:DT:27:THR:HB | 37:DT:89:VAL:HG23 | 2.02 | 0.42 |
| 13:AM:106:ASN:HB3 | 13:AM:107:ALA:H | 1.68 | 0.42 |
| 23:DA:656:G:H2' | 23:DA:657:U:O4' | 2.19 | 0.42 |
| 47:B3:4:LEU:HA | 47:B3:4:LEU:HD23 | 1.88 | 0.42 |
| 4:AD:97:LEU:HD23 | 4:AD:97:LEU:HA | 1.78 | 0.42 |
| 42:BY:51:VAL:HG12 | 42:BY:51:VAL:O | 2.20 | 0.42 |
| 10:AJ:17:ASP:O | 10:AJ:21:GLN:HB2 | 2.20 | 0.42 |
| 23:BA:705:A:C2 | 23:BA:727:A:H1' | 2.55 | 0.42 |
| 1:CA:1459:C:H2' | 1:CA:1460:A:C8 | 2.55 | 0.42 |
| 37:DT:118:ARG:NE | 37:DT:118:ARG:HA | 2.34 | 0.42 |
| 1:CA:1166:G:N2 | 1:CA:1169:A:H3' | 2.35 | 0.42 |
| 3:AC:11:ARG:HD3 | 3:AC:15:THR:HG21 | 2.01 | 0.42 |
| 3:AC:153:VAL:HG13 | 3:AC:197:GLY:O | 2.20 | 0.42 |
| 2:AB:70:PHE:CD2 | 2:AB:163:PHE:HB3 | 2.54 | 0.42 |
| 1:AA:951:G:N1 | 1:AA:1231:G:N7 | 2.67 | 0.42 |
| 14:AN:53:LEU:HA | 14:AN:54:PRO:HD3 | 1.69 | 0.42 |
| 1:CA:1160:G:O6 | 1:CA:1181:G:C6 | 2.73 | 0.42 |
| 21:AU:12:LYS:CE | 21:AU:19:GLY:HA3 | 2.48 | 0.42 |
| 1:AA:167:G:H2' | 1:AA:168:G:C8 | 2.54 | 0.42 |
| 1:AA:353:A:C8 | 1:AA:353:A:H5' | 2.51 | 0.42 |
| 23:DA:271(S):G:C6 | 23:DA:271(T):C:C4 | 3.07 | 0.42 |
| 1:CA:170:U:O2' | 1:CA:171:A:H5' | 2.20 | 0.42 |
| 1:AA:1248:A:H2 | 1:AA:1289:A:H62 | 1.67 | 0.42 |
| 26:DE:29:GLY:HA3 | 56:DE:402:HOH:O | 2.20 | 0.42 |
| 33:DP:59:LEU:HD23 | 33:DP:59:LEU:HA | 1.70 | 0.42 |
| 23:DA:674:G:H1' | 27:DF:74:ARG:CD | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DB:91:C:C2' | 24:DB:92:C:H5' | 2.49 | 0.42 |
| 23:DA:2309:A:C6 | 23:DA:2310:A:N1 | 2.88 | 0.42 |
| 3:AC:43:LEU:HA | 3:AC:43:LEU:HD23 | 1.67 | 0.42 |
| 23:BA:1166:C:O2 | 23:BA:1184:G:C2 | 2.73 | 0.42 |
| 23:BA:248:G:H5' | 23:BA:250:G:N7 | 2.34 | 0.42 |
| 23:DA:1287:A:H5'' | 23:DA:1288:U:OP2 | 2.19 | 0.42 |
| 28:BG:110:ALA:HA | 28:BG:140:ILE:O | 2.19 | 0.42 |
| 23:BA:2273:A:O2' | 23:BA:2274:A:H5' | 2.18 | 0.42 |
| 1:AA:741:G:H2' | 1:AA:742:G:H8 | 1.85 | 0.42 |
| 53:D9:32:HIS:O | 53:D9:34:GLN:HG3 | 2.19 | 0.42 |
| 23:BA:1489:U:H3' | 23:BA:1489:U:H6 | 1.83 | 0.42 |
| 23:DA:922:U:H2' | 23:DA:923:C:C6 | 2.55 | 0.42 |
| 33:DP:82:GLY:HA2 | 33:DP:113:LYS:O | 2.20 | 0.42 |
| 23:DA:2836:U:H2' | 23:DA:2837:G:C8 | 2.55 | 0.42 |
| 23:BA:2464:C:O2' | 23:BA:2465:C:H5'' | 2.19 | 0.42 |
| 25:BD:130:ALA:HA | 25:BD:192:THR:HA | 2.01 | 0.42 |
| 23:DA:229:A:OP1 | 23:DA:229:A:C8 | 2.73 | 0.42 |
| 34:BQ:39:PRO:HA | 34:BQ:97:VAL:O | 2.19 | 0.42 |
| 1:AA:1067:A:H1' | 1:AA:1068:G:O4' | 2.19 | 0.42 |
| 23:DA:1849:G:H2' | 23:DA:1850:G:C8 | 2.55 | 0.42 |
| 23:BA:1259:G:O2' | 23:BA:1260:G:H5' | 2.20 | 0.42 |
| 25:BD:146:GLU:HB2 | 25:BD:189:CYS:HB3 | 2.02 | 0.42 |
| 1:AA:819:A:H4' | 1:AA:820:U:OP2 | 2.20 | 0.42 |
| 6:AF:25:ILE:HD12 | 6:AF:82:ARG:HE | 1.84 | 0.42 |
| 32:BO:115:VAL:HG13 | 32:BO:121:VAL:HG21 | 2.02 | 0.42 |
| 23:DA:663:G:C6 | 23:DA:664:C:C4 | 3.08 | 0.42 |
| 23:BA:853:G:H1 | 23:BA:924:C:H42 | 1.67 | 0.42 |
| 23:BA:1747(A):G:N7 | 56:BA:5107:HOH:O | 2.36 | 0.42 |
| 23:BA:1749:A:N6 | 56:BA:5361:HOH:O | 2.53 | 0.42 |
| 3:CC:179:ARG:HG3 | 3:CC:206:GLU:OE1 | 2.20 | 0.42 |
| 23:BA:764:A:OP1 | 25:BD:208:LYS:HE2 | 2.19 | 0.42 |
| 23:DA:1927:A:H2' | 23:DA:1928:A:C8 | 2.54 | 0.42 |
| 13:AM:88:ARG:HG2 | 13:AM:88:ARG:O | 2.19 | 0.42 |
| 23:DA:2420:C:H6 | 23:DA:2420:C:O5' | 2.02 | 0.42 |
| 1:AA:571:U:O5' | 1:AA:571:U:H6 | 2.03 | 0.42 |
| 23:BA:928:G:O5' | 23:BA:928:G:H8 | 2.03 | 0.42 |
| 27:DF:112:MET:HB2 | 27:DF:112:MET:HE2 | 1.86 | 0.42 |
| 29:BH:94:TYR:CD1 | 29:BH:94:TYR:N | 2.87 | 0.42 |
| 24:BB:79:C:O5' | 24:BB:79:C:H6 | 2.02 | 0.42 |
| 16:AP:9:PHE:CD2 | 16:AP:18:ARG:HG3 | 2.54 | 0.42 |
| 23:BA:2821:A:H2' | 23:BA:2822:G:O4' | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:BA:586:A:C2 | 23:BA:1254:A:C2 | 3.08 | 0.42 |
| 1:CA:1460:A:H2' | 1:CA:1461:G:O4' | 2.19 | 0.42 |
| 1:AA:1207:G:O2' | 1:AA:1208:C:H5' | 2.20 | 0.42 |
| 1:AA:958:A:OP1 | 1:AA:958:A:H8 | 2.02 | 0.42 |
| 23:BA:1356:G:C5 | 23:BA:1357:U:C5 | 3.07 | 0.42 |
| 1:CA:1128:C:H1' | 1:CA:1146:A:N1 | 2.35 | 0.42 |
| 2:AB:70:PHE:HB2 | 2:AB:92:TYR:CB | 2.49 | 0.42 |
| 1:AA:1299:A:H2' | 1:AA:1301:U:H1' | 2.01 | 0.42 |
| 1:AA:1305:G:H2' | 21:AU:5:ASP:HA | 2.02 | 0.42 |
| 1:CA:1309:G:C6 | 1:CA:1329:A:N6 | 2.87 | 0.42 |
| 23:BA:2304:G:O6 | 23:BA:2312:U:O4 | 2.37 | 0.42 |
| 33:DP:55:ARG:HA | 56:DP:309:HOH:O | 2.20 | 0.42 |
| 23:BA:804:A:H5'' | 23:BA:805:G:OP1 | 2.20 | 0.42 |
| 1:CA:1286:A:H2 | 21:CU:22:ARG:NH2 | 2.09 | 0.42 |
| 23:BA:2161:C:C5 | 23:BA:2162:G:N7 | 2.88 | 0.42 |
| 1:CA:235:C:H2' | 1:CA:236:G:C8 | 2.55 | 0.42 |
| 7:CG:43:PHE:CD1 | 7:CG:43:PHE:O | 2.73 | 0.42 |
| 23:DA:2005:A:H5'' | 23:DA:2006:C:OP2 | 2.20 | 0.42 |
| 1:AA:184:G:H5' | 1:AA:224:C:O2' | 2.20 | 0.42 |
| 23:DA:860:U:C2 | 23:DA:2268:A:C8 | 3.08 | 0.42 |
| 28:BG:138:GLN:HE22 | 28:BG:153:ARG:NH2 | 2.18 | 0.42 |
| 1:AA:1077:G:N2 | 1:AA:1079:G:H3' | 2.35 | 0.42 |
| 1:CA:1151:A:C4 | 1:CA:1152:A:C8 | 3.08 | 0.42 |
| 1:CA:1001(A):G:N2 | 1:CA:1040:U:C2 | 2.88 | 0.42 |
| 13:AM:91:ARG:HB2 | 13:AM:98:VAL:HG13 | 2.01 | 0.42 |
| 37:BT:64:ARG:HB2 | 37:BT:73:GLU:HG2 | 2.00 | 0.42 |
| 1:CA:331:G:O4' | 56:CA:1860:HOH:O | 2.21 | 0.42 |
| 1:AA:1134:G:H2' | 1:AA:1135:U:H5' | 2.01 | 0.42 |
| 2:AB:14:GLY:HA3 | 2:AB:16:HIS:HE1 | 1.85 | 0.42 |
| 23:BA:1153:C:H2' | 23:BA:1154:G:O4' | 2.19 | 0.42 |
| 10:AJ:66:ARG:HB3 | 10:AJ:68:HIS:NE2 | 2.34 | 0.42 |
| 16:AP:20:VAL:HG21 | 16:AP:32:TYR:CG | 2.55 | 0.42 |
| 1:AA:502:G:OP1 | 12:AL:117:ARG:N | 2.52 | 0.42 |
| 1:AA:709:G:H2' | 1:AA:710:G:C8 | 2.55 | 0.42 |
| 2:AB:77:ALA:HB1 | 2:AB:211:ILE:HG21 | 2.00 | 0.42 |
| 23:DA:2561:A:H2' | 23:DA:2562:U:O4' | 2.19 | 0.42 |
| 27:DF:64:ILE:HG13 | 27:DF:65:TRP:H | 1.85 | 0.42 |
| 23:DA:1300:U:H4' | 23:DA:1301:A:H5' | 2.02 | 0.42 |
| 30:DI:9:LEU:HB3 | 30:DI:12:LEU:HB2 | 2.01 | 0.42 |
| 32:DO:17:ARG:HD2 | 32:DO:47:ILE:HG23 | 2.02 | 0.42 |
| 43:DZ:152:ALA:HA | 43:DZ:155:LEU:HB2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1063:C:OP2 | 1:AA:1064:G:O2' | 2.37 | 0.42 |
| 1:CA:472:A:H4' | 16:CP:80:PHE:O | 2.20 | 0.42 |
| 29:BH:137:ASP:HB3 | 29:BH:140:LYS:CB | 2.49 | 0.42 |
| 1:AA:757:U:OP1 | 1:AA:822:C:O2' | 2.34 | 0.42 |
| 17:CQ:86:GLU:O | 17:CQ:90:ILE:HG13 | 2.18 | 0.42 |
| 23:DA:335:C:H2' | 23:DA:336:C:C6 | 2.55 | 0.42 |
| 33:BP:101:VAL:HG12 | 33:BP:102:ARG:N | 2.34 | 0.42 |
| 34:DQ:70:PRO:HA | 34:DQ:94:VAL:O | 2.19 | 0.42 |
| 43:BZ:27:VAL:HA | 43:BZ:35:ARG:O | 2.19 | 0.42 |
| 24:DB:96:U:H2' | 24:DB:97:G:H8 | 1.85 | 0.42 |
| 1:AA:116:A:C8 | 1:AA:116:A:OP2 | 2.73 | 0.42 |
| 24:DB:40:U:H1' | 24:DB:45:A:H61 | 1.83 | 0.42 |
| 23:BA:219:G:O6 | 56:BA:3973:HOH:O | 2.22 | 0.42 |
| 23:BA:1717:G:C2 | 23:BA:1718:G:C8 | 3.08 | 0.42 |
| 23:DA:696:G:O2' | 23:DA:697:C:H5' | 2.20 | 0.42 |
| 23:DA:1932:A:H2' | 23:DA:1933:G:O4' | 2.19 | 0.42 |
| 1:CA:439:A:C4 | 1:CA:496:A:C2 | 3.08 | 0.42 |
| 23:DA:1844:C:OP1 | 25:DD:257:LEU:HD23 | 2.19 | 0.42 |
| 6:CF:68:PRO:HG2 | 6:CF:71:ARG:HD2 | 2.01 | 0.42 |
| 23:DA:1577:C:OP2 | 56:DA:4265:HOH:O | 2.21 | 0.42 |
| 12:AL:42:THR:HB | 12:AL:52:LEU:HD12 | 2.01 | 0.42 |
| 1:AA:778:G:H2' | 1:AA:779:C:O4' | 2.20 | 0.42 |
| 23:DA:2862:G:H2' | 23:DA:2863:C:H6 | 1.85 | 0.42 |
| 24:BB:75:G:H5'' | 24:BB:76:G:OP2 | 2.20 | 0.42 |
| 24:BB:78:A:C2 | 24:BB:100:A:C4 | 3.08 | 0.42 |
| 34:DQ:78:PRO:O | 34:DQ:81:VAL:HG13 | 2.20 | 0.42 |
| 38:DU:43:GLY:HA3 | 39:DV:73:SER:OG | 2.18 | 0.42 |
| 16:CP:23:ASP:OD1 | 16:CP:25:ARG:HG3 | 2.20 | 0.42 |
| 1:AA:1004:A:N6 | 1:AA:1034:G:H2' | 2.31 | 0.42 |
| 1:AA:1009:G:N3 | 1:AA:1010:G:H1' | 2.34 | 0.42 |
| 7:CG:31:MET:O | 7:CG:32:ARG:NH1 | 2.53 | 0.42 |
| 1:CA:1379:G:N7 | 7:CG:2:ALA:N | 2.68 | 0.42 |
| 2:AB:69:LEU:HD13 | 2:AB:92:TYR:HA | 2.02 | 0.42 |
| 23:BA:27:G:HO2' | 23:BA:28:A:P | 2.42 | 0.42 |
| 23:BA:330:A:H2 | 23:BA:1210:A:C2' | 2.24 | 0.42 |
| 1:CA:1306:A:H1' | 1:CA:1332:A:N3 | 2.35 | 0.42 |
| 1:CA:1309:G:OP1 | 13:CM:92:HIS:CE1 | 2.73 | 0.42 |
| 1:CA:1309:G:O3' | 13:CM:77:ASN:HB3 | 2.20 | 0.42 |
| 23:DA:1022:G:C6 | 23:DA:1140:C:C4 | 3.08 | 0.42 |
| 3:AC:23:TYR:CD1 | 10:AJ:10:GLY:HA2 | 2.55 | 0.42 |
| 23:DA:2114:A:C6 | 23:DA:2115:G:C2 | 3.07 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:71:A:H5'' | 23:DA:73:A:C8 | 2.54 | 0.42 |
| 1:AA:346:G:N2 | 1:AA:347:G:C8 | 2.88 | 0.42 |
| 24:BB:21:G:H2' | 24:BB:22:U:O4' | 2.20 | 0.42 |
| 23:BA:2117:A:H61 | 23:BA:2166:G:N2 | 2.12 | 0.42 |
| 5:CE:43:LEU:HD21 | 5:CE:132:ALA:HB1 | 2.01 | 0.42 |
| 23:BA:2741:A:H61 | 23:BA:2763:G:H1' | 1.85 | 0.42 |
| 23:DA:2833:G:C3' | 23:DA:2834:G:H5' | 2.48 | 0.42 |
| 30:BI:9:LEU:HD21 | 30:BI:35:LEU:CD2 | 2.50 | 0.42 |
| 29:BH:5:GLY:HA2 | 29:BH:69:ARG:HB3 | 2.01 | 0.42 |
| 3:CC:30:ARG:HG3 | 3:CC:31:HIS:HD2 | 1.85 | 0.42 |
| 3:CC:31:HIS:H | 3:CC:31:HIS:CD2 | 2.36 | 0.42 |
| 1:AA:922:G:C6 | 1:AA:923:A:C6 | 3.07 | 0.42 |
| 23:DA:1833:U:O2' | 23:DA:1969:A:N1 | 2.34 | 0.42 |
| 30:BI:77:LEU:HD22 | 30:BI:77:LEU:HA | 1.78 | 0.42 |
| 1:AA:602:A:C6 | 1:AA:603:U:N3 | 2.88 | 0.42 |
| 42:DY:90:LEU:C | 42:DY:92:ASN:H | 2.21 | 0.42 |
| 46:D2:50:ILE:C | 46:D2:52:ASP:N | 2.72 | 0.42 |
| 23:BA:1488:G:C6 | 23:BA:1489:U:N3 | 2.87 | 0.42 |
| 1:CA:1521:G:H2' | 1:CA:1522:U:H6 | 1.85 | 0.42 |
| 1:CA:646:U:H2' | 1:CA:647:C:C6 | 2.55 | 0.42 |
| 29:BH:38:SER:HB2 | 29:BH:64:LEU:HD22 | 2.02 | 0.42 |
| 23:DA:1525:G:H2' | 23:DA:1526:G:O4' | 2.19 | 0.42 |
| 23:BA:1011:G:C2 | 23:BA:1151:G:C2 | 3.07 | 0.42 |
| 23:BA:1467:C:C5 | 23:BA:1546:C:H2' | 2.54 | 0.42 |
| 1:CA:1201:A:H4' | 1:CA:1202:G:O5' | 2.19 | 0.42 |
| 23:DA:117:G:C6 | 23:DA:119:A:C6 | 3.08 | 0.42 |
| 2:AB:110:GLN:O | 2:AB:114:ARG:HB2 | 2.20 | 0.42 |
| 23:DA:2019:A:H4' | 38:DU:34:LYS:HD2 | 2.01 | 0.42 |
| 1:CA:622:A:C8 | 1:CA:623:C:C5 | 3.07 | 0.42 |
| 23:BA:1376:C:N4 | 23:BA:1377:G:C6 | 2.88 | 0.42 |
| 23:DA:1163:G:O2' | 23:DA:1164:G:H5' | 2.20 | 0.42 |
| 10:CJ:35:SER:HB3 | 10:CJ:73:ASP:HB3 | 2.01 | 0.42 |
| 17:AQ:99:SER:C | 17:AQ:100:LYS:HD3 | 2.40 | 0.42 |
| 23:BA:839:U:H2' | 23:BA:840:C:C6 | 2.54 | 0.42 |
| 29:BH:80:SER:OG | 29:BH:81:GLU:N | 2.53 | 0.42 |
| 31:BN:18:ALA:O | 31:BN:19:GLU:HB3 | 2.18 | 0.42 |
| 23:DA:907:U:O2' | 34:DQ:101:ARG:NH2 | 2.43 | 0.42 |
| 51:D7:1:MET:O | 51:D7:2:LYS:C | 2.57 | 0.42 |
| 2:CB:172:ILE:H | 2:CB:172:ILE:HG13 | 1.43 | 0.42 |
| 27:BF:179:GLU:H | 27:BF:179:GLU:CD | 2.23 | 0.42 |
| 23:BA:2279:G:O6 | 44:B0:14:ARG:HD2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:CK:120:ARG:HA | 11:CK:121:PRO:HD3 | 1.85 | 0.42 |
| 52:B8:8:LYS:HB3 | 52:B8:12:LYS:HE3 | 2.02 | 0.42 |
| 1:AA:1440:C:H2' | 1:AA:1441:G:O4' | 2.20 | 0.42 |
| 1:CA:1348:U:H4' | 9:CI:120:ARG:HD2 | 2.02 | 0.42 |
| 1:CA:1375:A:H4' | 7:CG:29:LYS:HZ3 | 1.85 | 0.42 |
| 1:CA:1378:C:H6 | 1:CA:1378:C:O5' | 2.02 | 0.42 |
| 23:DA:271(I):G:H2' | 23:DA:271(J):C:C6 | 2.55 | 0.42 |
| 21:AU:13:ILE:N | 21:AU:22:ARG:HD2 | 2.35 | 0.42 |
| 1:CA:1003:G:C2 | 1:CA:1004:A:O2' | 2.70 | 0.42 |
| 10:AJ:8:LEU:O | 10:AJ:69:ASN:HA | 2.20 | 0.42 |
| 10:AJ:8:LEU:O | 10:AJ:70:ARG:N | 2.43 | 0.42 |
| 1:CA:560:U:H4' | 1:CA:561:U:O5' | 2.18 | 0.42 |
| 1:CA:1357:A:C5 | 1:CA:1358:U:C4 | 3.08 | 0.42 |
| 1:AA:1157:A:H1' | 1:AA:1181:G:C2 | 2.55 | 0.42 |
| 1:CA:1070:U:O2 | 1:CA:1106:G:C2 | 2.72 | 0.42 |
| 14:CN:25:VAL:N | 14:CN:39:LEU:HD23 | 2.34 | 0.42 |
| 28:DG:105:LYS:HZ1 | 48:D4:26:SER:HB2 | 1.84 | 0.42 |
| 23:BA:1324:G:C5 | 23:BA:1328:G:O6 | 2.73 | 0.42 |
| 23:BA:2791:C:OP2 | 23:BA:2791:C:H3' | 2.19 | 0.42 |
| 4:CD:108:LEU:HB3 | 4:CD:110:PHE:HE1 | 1.84 | 0.42 |
| 23:BA:2782:G:C8 | 56:BA:4087:HOH:O | 2.70 | 0.42 |
| 1:AA:309:G:O2' | 1:AA:607:A:N1 | 2.52 | 0.42 |
| 23:DA:2022:U:O2' | 23:DA:2617:C:H5' | 2.20 | 0.42 |
| 23:DA:7:G:H4' | 31:DN:13:TRP:CH2 | 2.55 | 0.42 |
| 5:CE:10:MET:HG2 | 5:CE:13:ILE:HD11 | 2.02 | 0.42 |
| 23:BA:627:A:H62 | 33:BP:84:ASN:HD21 | 1.68 | 0.42 |
| 35:BR:50:HIS:O | 35:BR:54:LEU:HD22 | 2.20 | 0.42 |
| 23:DA:652(E):G:C2 | 23:DA:652(U):G:C2 | 3.08 | 0.42 |
| 46:B2:50:ILE:O | 46:B2:52:ASP:N | 2.45 | 0.42 |
| 1:CA:1496:C:H2' | 1:CA:1497:G:O4' | 2.20 | 0.42 |
| 2:AB:21:ARG:HE | 2:AB:21:ARG:H | 1.66 | 0.42 |
| 1:CA:1191:A:O5' | 1:CA:1191:A:H8 | 2.03 | 0.42 |
| 19:CS:53:ASN:ND2 | 19:CS:77:THR:O | 2.49 | 0.42 |
| 23:BA:2838:G:C6 | 23:BA:2839:G:C5 | 3.08 | 0.42 |
| 23:BA:1952:A:C2 | 32:BO:22:ILE:HD12 | 2.55 | 0.42 |
| 23:BA:863:A:H2' | 23:BA:864:G:H8 | 1.83 | 0.42 |
| 23:DA:1179:C:H2' | 23:DA:1180:C:C6 | 2.55 | 0.42 |
| 36:DS:34:HIS:ND1 | 36:DS:53:SER:OG | 2.52 | 0.42 |
| 23:BA:2565:A:H5'' | 23:BA:2566:A:OP2 | 2.19 | 0.42 |
| 23:DA:2525:G:C2 | 23:DA:2539:C:C2 | 3.08 | 0.42 |
| 15:CO:50:HIS:O | 15:CO:53:HIS:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:900:A:H2' | 23:BA:901:A:H8 | 1.85 | 0.42 |
| 18:AR:71:LYS:HA | 18:AR:74:ARG:HD2 | 2.02 | 0.42 |
| 1:CA:45:U:H2' | 1:CA:46:G:C8 | 2.55 | 0.42 |
| 20:CT:38:LYS:O | 20:CT:41:ILE:HG13 | 2.19 | 0.42 |
| 1:AA:791:G:C6 | 1:AA:792:A:N7 | 2.88 | 0.42 |
| 23:BA:2178:C:H2' | 23:BA:2179:C:O4' | 2.19 | 0.42 |
| 26:BE:181:LEU:HD13 | 26:BE:181:LEU:HA | 1.74 | 0.42 |
| 23:BA:1138:G:O2' | 31:BN:105:GLY:HA3 | 2.19 | 0.42 |
| 38:DU:106:PHE:O | 38:DU:110:VAL:HG23 | 2.20 | 0.42 |
| 1:AA:1002:G:C2 | 1:AA:1039:C:C2 | 3.08 | 0.42 |
| 23:BA:2121:G:O6 | 23:BA:2176:A:N6 | 2.53 | 0.42 |
| 1:AA:1316:G:HO2' | 1:AA:1318:A:H8 | 1.64 | 0.42 |
| 1:CA:1123:A:H2' | 1:CA:1124:G:O4' | 2.19 | 0.42 |
| 2:CB:216:SER:O | 2:CB:219:VAL:N | 2.53 | 0.42 |
| 1:CA:1262:C:N4 | 1:CA:1273:G:N1 | 2.39 | 0.42 |
| 23:DA:2304:G:O6 | 23:DA:2312:U:O4 | 2.38 | 0.42 |
| 1:CA:1084:G:C5 | 1:CA:1085:U:C4 | 3.07 | 0.42 |
| 1:CA:1074:G:C4 | 1:CA:1102:A:C2 | 3.08 | 0.42 |
| 24:BB:91:C:O2' | 24:BB:92:C:H5' | 2.19 | 0.42 |
| 1:AA:448:A:H2' | 1:AA:449:C:C6 | 2.55 | 0.42 |
| 1:AA:1347:G:H5'' | 9:AI:107:ARG:CB | 2.49 | 0.42 |
| 7:AG:99:LEU:H | 7:AG:99:LEU:HG | 1.69 | 0.42 |
| 15:CO:56:LEU:O | 15:CO:60:VAL:HG23 | 2.20 | 0.42 |
| 23:BA:635:C:O2' | 23:BA:639:U:OP1 | 2.33 | 0.42 |
| 50:B6:9:LEU:CD2 | 50:B6:25:LYS:HB3 | 2.50 | 0.42 |
| 1:CA:683:G:C6 | 1:CA:684:A:C5 | 3.08 | 0.42 |
| 1:CA:1338:G:H2' | 1:CA:1339:A:O4' | 2.19 | 0.42 |
| 23:BA:1889:A:N1 | 23:BA:2234:G:H1' | 2.35 | 0.42 |
| 23:DA:1319:G:C6 | 23:DA:1320:C:N4 | 2.87 | 0.42 |
| 7:AG:51:GLN:HG2 | 7:AG:58:PRO:HD3 | 2.02 | 0.42 |
| 37:DT:110:ILE:H | 37:DT:110:ILE:HG12 | 1.58 | 0.42 |
| 48:D4:13:ARG:N | 48:D4:29:PRO:O | 2.37 | 0.42 |
| 8:CH:25:ASP:HB2 | 8:CH:58:TYR:CD2 | 2.55 | 0.42 |
| 32:DO:70:LYS:HB3 | 32:DO:70:LYS:HE2 | 1.76 | 0.42 |
| 23:DA:1518:U:H2' | 23:DA:1519:G:O4' | 2.20 | 0.42 |
| 1:CA:909:A:H2' | 1:CA:910:C:O4' | 2.20 | 0.42 |
| 23:DA:21:A:O2' | 23:DA:22:C:H5' | 2.20 | 0.42 |
| 50:D6:19:ARG:H | 50:D6:19:ARG:HD2 | 1.85 | 0.42 |
| 30:BI:121:LYS:HD3 | 30:BI:121:LYS:HA | 1.91 | 0.42 |
| 43:DZ:6:LYS:HE2 | 43:DZ:6:LYS:HB3 | 1.88 | 0.42 |
| 24:DB:32:C:C2 | 24:DB:51:G:N2 | 2.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DA:2516:G:C6 | 23:DA:2517:C:C4 | 3.08 | 0.42 |
| 23:BA:19:C:H2' | 23:BA:20:C:H6 | 1.84 | 0.42 |
| 1:CA:1048:G:O4' | 1:CA:1215:G:H5'' | 2.20 | 0.41 |
| 1:AA:1096:C:O2' | 1:AA:1170:A:O2' | 2.33 | 0.41 |
| 1:AA:1219:U:N3 | 1:AA:1220:G:N7 | 2.68 | 0.41 |
| 1:AA:984:C:N3 | 1:AA:1222:G:C2 | 2.88 | 0.41 |
| 1:AA:1316:G:C2 | 1:AA:1318:A:H5'' | 2.55 | 0.41 |
| 1:CA:1124:G:H1' | 10:CJ:38:ILE:CG2 | 2.50 | 0.41 |
| 9:CI:9:ARG:N | 9:CI:76:ALA:HA | 2.35 | 0.41 |
| 1:AA:1237:C:N4 | 1:AA:1336:C:C2 | 2.88 | 0.41 |
| 23:DA:675:A:C8 | 23:DA:804:A:C6 | 3.08 | 0.41 |
| 3:CC:136:GLN:CG | 3:CC:140:ARG:HD2 | 2.50 | 0.41 |
| 1:CA:1071:C:H5'' | 5:CE:49:PRO:CG | 2.50 | 0.41 |
| 1:AA:184:G:O4' | 1:AA:224:C:H4' | 2.19 | 0.41 |
| 1:CA:706:A:C5 | 1:CA:707:C:C5 | 3.08 | 0.41 |
| 4:AD:148:VAL:HG11 | 4:AD:158:ILE:HG13 | 2.02 | 0.41 |
| 1:AA:392:G:H5' | 16:AP:13:HIS:CE1 | 2.55 | 0.41 |
| 1:AA:1348:U:N3 | 1:AA:1374:A:C8 | 2.84 | 0.41 |
| 27:BF:7:TYR:N | 27:BF:22:ALA:HB3 | 2.30 | 0.41 |
| 1:CA:1325:C:H4' | 21:CU:17:THR:HG21 | 2.02 | 0.41 |
| 23:DA:816:C:P | 56:DA:4440:HOH:O | 2.77 | 0.41 |
| 23:DA:2748:A:N6 | 23:DA:2749:A:C6 | 2.88 | 0.41 |
| 17:AQ:66:SER:HB3 | 17:AQ:69:LYS:HD3 | 2.01 | 0.41 |
| 23:BA:1405:U:H2' | 23:BA:1406:U:H6 | 1.80 | 0.41 |
| 23:BA:1797:C:C2' | 23:BA:1798:U:H5' | 2.50 | 0.41 |
| 23:DA:2293:C:H2' | 23:DA:2294:C:H6 | 1.83 | 0.41 |
| 1:CA:611:A:N6 | 1:CA:629:G:H1 | 2.16 | 0.41 |
| 7:AG:113:GLU:HG2 | 7:AG:119:ARG:CB | 2.50 | 0.41 |
| 23:DA:2464:C:O2' | 23:DA:2465:C:P | 2.78 | 0.41 |
| 23:BA:1814:G:O3' | 25:BD:54:ARG:NH2 | 2.53 | 0.41 |
| 23:BA:2574:G:O2' | 26:BE:143:ASN:HB3 | 2.20 | 0.41 |
| 23:DA:565:C:H2' | 23:DA:566:U:O4' | 2.20 | 0.41 |
| 28:BG:19:LEU:HD22 | 28:BG:23:PHE:CE1 | 2.53 | 0.41 |
| 23:BA:907:U:O2' | 34:BQ:101:ARG:NH2 | 2.45 | 0.41 |
| 23:BA:12:U:C2' | 23:BA:12:U:O2 | 2.68 | 0.41 |
| 26:BE:14:ILE:HG13 | 26:BE:21:VAL:HG13 | 2.02 | 0.41 |
| 36:DS:66:ALA:O | 36:DS:69:VAL:N | 2.53 | 0.41 |
| 15:CO:43:LEU:HD23 | 15:CO:43:LEU:HA | 1.86 | 0.41 |
| 50:B6:40:CYS:HA | 50:B6:41:PRO:HD3 | 1.68 | 0.41 |
| 29:DH:13:LYS:HA | 29:DH:14:GLY:HA2 | 1.59 | 0.41 |
| 7:CG:63:LYS:HA | 7:CG:67:GLU:OE2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DX:61:GLY:HA3 | 41:DX:73:ARG:O | 2.20 | 0.41 |
| 34:DQ:11:LYS:HE2 | 34:DQ:88:GLY:O | 2.20 | 0.41 |
| 23:BA:593:G:N2 | 23:BA:665:C:C2 | 2.87 | 0.41 |
| 38:DU:5:LYS:HB2 | 38:DU:5:LYS:HE3 | 1.83 | 0.41 |
| 34:BQ:34:LEU:HA | 34:BQ:34:LEU:HD12 | 1.86 | 0.41 |
| 45:B1:32:LYS:HB3 | 45:B1:32:LYS:HE2 | 1.93 | 0.41 |
| 29:BH:87:LEU:HA | 29:BH:87:LEU:HD23 | 1.84 | 0.41 |
| 41:DX:72:LYS:HE3 | 41:DX:72:LYS:HB3 | 1.92 | 0.41 |
| 46:B2:35:LEU:HA | 46:B2:35:LEU:HD23 | 1.71 | 0.41 |
| 12:AL:123:LYS:HG2 | 12:AL:123:LYS:H | 1.59 | 0.41 |
| 26:BE:4:ILE:HG12 | 26:BE:5:LEU:O | 2.20 | 0.41 |
| 16:CP:6:LEU:HG | 16:CP:17:TYR:HB3 | 2.01 | 0.41 |
| 1:CA:1442:G:N7 | 1:CA:1442(A):G:O6 | 2.53 | 0.41 |
| 1:CA:877:C:H5'' | 8:CH:88:LYS:HD3 | 2.02 | 0.41 |
| 1:CA:1288:A:H1' | 1:CA:1353:G:H4' | 2.01 | 0.41 |
| 21:AU:3:LYS:HA | 21:AU:10:ARG:HB3 | 2.01 | 0.41 |
| 1:AA:1290:G:H3' | 1:AA:1291:G:C8 | 2.51 | 0.41 |
| 1:CA:17:U:O2' | 1:CA:1079:G:N3 | 2.49 | 0.41 |
| 23:DA:1530:C:O2' | 23:DA:1531:C:H6 | 2.03 | 0.41 |
| 1:CA:1116:C:H2' | 1:CA:1117:G:O4' | 2.20 | 0.41 |
| 21:AU:15:ARG:CA | 21:AU:15:ARG:HE | 2.33 | 0.41 |
| 27:DF:101:LEU:HB3 | 27:DF:106:ARG:HD3 | 2.01 | 0.41 |
| 13:AM:71:ARG:HG3 | 13:AM:71:ARG:H | 1.58 | 0.41 |
| 23:DA:1912:A:HO2' | 23:DA:1913:A:P | 2.43 | 0.41 |
| 3:CC:148:GLY:HA3 | 3:CC:172:ARG:O | 2.20 | 0.41 |
| 9:AI:71:SER:O | 9:AI:74:ILE:N | 2.53 | 0.41 |
| 30:DI:44:LEU:HA | 30:DI:44:LEU:HD12 | 1.74 | 0.41 |
| 1:CA:1313:U:OP1 | 19:CS:7:LYS:NZ | 2.53 | 0.41 |
| 23:DA:1740:G:H2' | 23:DA:1741:A:C8 | 2.55 | 0.41 |
| 3:CC:12:LEU:HA | 3:CC:16:ARG:O | 2.20 | 0.41 |
| 1:CA:101:A:C6 | 1:CA:102:G:N7 | 2.88 | 0.41 |
| 16:AP:6:LEU:HG | 16:AP:17:TYR:CB | 2.50 | 0.41 |
| 16:AP:6:LEU:HD12 | 16:AP:6:LEU:HA | 1.83 | 0.41 |
| 1:AA:611:A:N6 | 1:AA:629:G:H1 | 2.17 | 0.41 |
| 2:AB:141:GLU:O | 2:AB:145:LEU:HB2 | 2.19 | 0.41 |
| 48:D4:1:MET:HB3 | 48:D4:6:HIS:NE2 | 2.35 | 0.41 |
| 2:AB:97:TRP:CZ2 | 2:AB:173:ALA:HA | 2.55 | 0.41 |
| 31:DN:24:GLY:HA2 | 31:DN:27:ALA:CB | 2.50 | 0.41 |
| 46:D2:50:ILE:O | 46:D2:51:ARG:HB3 | 2.20 | 0.41 |
| 2:CB:70:PHE:HB2 | 2:CB:92:TYR:CB | 2.50 | 0.41 |
| 23:BA:2193:G:H2' | 23:BA:2194:G:H8 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:575:G:C5 | 1:AA:881:G:C2 | 3.08 | 0.41 |
| 26:BE:32:PRO:HD2 | 26:BE:50:GLY:O | 2.21 | 0.41 |
| 20:AT:73:HIS:O | 20:AT:76:ALA:HB3 | 2.20 | 0.41 |
| 56:DA:4439:HOH:O | 33:DP:16:ARG:HG3 | 2.20 | 0.41 |
| 23:BA:857:C:H4' | 44:B0:23:VAL:HG21 | 2.02 | 0.41 |
| 1:CA:1445:C:H2' | 1:CA:1446:U:H5' | 2.02 | 0.41 |
| 40:BW:107:LEU:HA | 40:BW:107:LEU:HD12 | 1.85 | 0.41 |
| 23:BA:1925:C:C2' | 23:BA:1926:U:H5' | 2.49 | 0.41 |
| 23:DA:323:G:H1' | 23:DA:1205:U:O2 | 2.19 | 0.41 |
| 24:BB:46:A:C5 | 24:BB:47:C:C4 | 3.08 | 0.41 |
| 23:BA:916:G:H5' | 23:BA:917:A:OP1 | 2.20 | 0.41 |
| 24:DB:28:C:H2' | 24:DB:29:A:H8 | 1.85 | 0.41 |
| 1:CA:1095:U:P | 1:CA:1108:G:H22 | 2.42 | 0.41 |
| 1:CA:445:G:H3' | 1:CA:446:G:H8 | 1.85 | 0.41 |
| 1:AA:1043:C:H2' | 1:AA:1044:A:C8 | 2.55 | 0.41 |
| 23:BA:236:C:H2' | 23:BA:237:C:C6 | 2.54 | 0.41 |
| 23:BA:817:C:O2' | 23:BA:839:U:H5'' | 2.20 | 0.41 |
| 23:BA:656:G:H2' | 23:BA:657:U:O4' | 2.21 | 0.41 |
| 38:BU:32:PHE:O | 38:BU:35:ALA:HB3 | 2.21 | 0.41 |
| 23:BA:666:G:O2' | 23:BA:667:U:H5' | 2.20 | 0.41 |
| 1:AA:124:G:H2' | 1:AA:125:U:O4' | 2.20 | 0.41 |
| 27:BF:150:GLY:HA2 | 27:BF:172:TRP:CD2 | 2.55 | 0.41 |
| 40:DW:10:VAL:HG21 | 40:DW:103:ILE:HD12 | 2.02 | 0.41 |
| 23:DA:44:G:H5'' | 23:DA:45:C:OP1 | 2.20 | 0.41 |
| 14:CN:13:THR:HG21 | 14:CN:20:ALA:HB2 | 2.02 | 0.41 |
| 1:CA:585:G:N3 | 1:CA:879:C:H4' | 2.36 | 0.41 |
| 23:BA:1313:U:H3' | 23:BA:1314:C:H5' | 2.02 | 0.41 |
| 29:DH:87:LEU:HD23 | 29:DH:87:LEU:HA | 1.87 | 0.41 |
| 1:CA:417:C:O5' | 1:CA:417:C:H6 | 2.03 | 0.41 |
| 13:CM:111:LYS:HE2 | 13:CM:111:LYS:HB3 | 1.60 | 0.41 |
| 24:DB:89:G:H8 | 24:DB:89:G:OP2 | 2.03 | 0.41 |
| 4:CD:97:LEU:HD23 | 4:CD:97:LEU:HA | 1.86 | 0.41 |
| 1:CA:961:U:OP2 | 1:CA:1223:C:O2' | 2.12 | 0.41 |
| 1:CA:792:A:H4' | 1:CA:793:U:H5'' | 2.02 | 0.41 |
| 1:CA:990:C:C4 | 1:CA:991:U:O4 | 2.73 | 0.41 |
| 23:DA:2821:A:H2' | 23:DA:2822:G:O4' | 2.19 | 0.41 |
| 23:DA:849:A:H5'' | 23:DA:850:C:OP2 | 2.19 | 0.41 |
| 8:AH:87:SER:HA | 8:AH:93:VAL:HG23 | 2.03 | 0.41 |
| 1:AA:9:G:H2' | 1:AA:10:A:C8 | 2.55 | 0.41 |
| 2:AB:187:LEU:CD1 | 2:AB:205:ASP:HA | 2.50 | 0.41 |
| 1:AA:1305:G:H5' | 21:AU:4:GLY:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1194:U:H2' | 1:AA:1195:C:C6 | 2.54 | 0.41 |
| 1:AA:951:G:C6 | 1:AA:952:U:C4 | 3.08 | 0.41 |
| 1:CA:1308:U:O2' | 1:CA:1309:G:H5' | 2.20 | 0.41 |
| 1:CA:1305:G:C8 | 21:CU:5:ASP:HA | 2.53 | 0.41 |
| 2:CB:48:MET:HA | 2:CB:51:LEU:HD12 | 2.03 | 0.41 |
| 1:AA:1275:A:O2' | 1:AA:1276:G:H5' | 2.20 | 0.41 |
| 1:CA:1050:G:C6 | 1:CA:1208:C:N3 | 2.87 | 0.41 |
| 23:DA:945:A:C4 | 23:DA:2448:A:C2 | 3.07 | 0.41 |
| 1:CA:748:C:H4' | 1:CA:749:C:O5' | 2.20 | 0.41 |
| 1:CA:165:C:H2' | 1:CA:166:G:H8 | 1.86 | 0.41 |
| 1:CA:484:G:O2' | 1:CA:485:G:P | 2.78 | 0.41 |
| 23:DA:860:U:H1' | 23:DA:2268:A:H5' | 2.02 | 0.41 |
| 23:BA:2811:G:N2 | 23:BA:2891:G:H1' | 2.36 | 0.41 |
| 1:AA:1126:U:O2 | 1:AA:1126:U:H2' | 2.20 | 0.41 |
| 25:DD:107:ALA:HA | 25:DD:108:PRO:HD2 | 1.94 | 0.41 |
| 1:AA:1226:C:H5' | 19:AS:80:TYR:CE1 | 2.55 | 0.41 |
| 1:AA:427:U:OP1 | 4:AD:13:ARG:NH2 | 2.53 | 0.41 |
| 42:DY:23:ARG:NH1 | 42:DY:23:ARG:HB2 | 2.35 | 0.41 |
| 20:CT:53:LEU:HA | 20:CT:56:MET:HG2 | 2.03 | 0.41 |
| 13:AM:5:ALA:HB1 | 13:AM:66:LEU:HD12 | 2.02 | 0.41 |
| 16:AP:17:TYR:N | 16:AP:17:TYR:CD1 | 2.87 | 0.41 |
| 1:CA:1063:C:OP2 | 1:CA:1063:C:H6 | 2.04 | 0.41 |
| 1:CA:684:A:C6 | 1:CA:685:G:C6 | 3.08 | 0.41 |
| 1:CA:1339:A:C5 | 1:CA:1340:A:H1' | 2.55 | 0.41 |
| 23:DA:2321:G:C2' | 23:DA:2321:G:N3 | 2.81 | 0.41 |
| 37:DT:53:ARG:NH1 | 37:DT:60:THR:OG1 | 2.53 | 0.41 |
| 23:BA:1488:G:C2 | 23:BA:1489:U:O2 | 2.73 | 0.41 |
| 35:BR:94:TYR:O | 35:BR:117:VAL:HG23 | 2.20 | 0.41 |
| 23:DA:2464:C:O2' | 23:DA:2465:C:OP2 | 2.34 | 0.41 |
| 4:CD:61:LYS:HE3 | 4:CD:62:GLN:OE1 | 2.20 | 0.41 |
| 23:BA:141:A:OP2 | 56:BA:3981:HOH:O | 2.22 | 0.41 |
| 23:DA:900:A:H2' | 23:DA:901:A:H8 | 1.85 | 0.41 |
| 23:DA:1925:C:C2' | 23:DA:1926:U:H5' | 2.50 | 0.41 |
| 43:DZ:100:VAL:HG11 | 43:DZ:134:PRO:HG2 | 2.03 | 0.41 |
| 5:CE:137:GLU:HA | 5:CE:140:ARG:HB3 | 2.02 | 0.41 |
| 39:BV:91:TYR:CD1 | 39:BV:91:TYR:C | 2.94 | 0.41 |
| 38:DU:106:PHE:O | 38:DU:109:LEU:HB2 | 2.20 | 0.41 |
| 28:DG:125:PHE:CZ | 28:DG:170:ARG:HA | 2.55 | 0.41 |
| 50:D6:10:LEU:HG | 50:D6:54:ILE:HD12 | 2.03 | 0.41 |
| 1:CA:1431:C:H2' | 1:CA:1432:G:O4' | 2.20 | 0.41 |
| 23:DA:2554:U:H2' | 23:DA:2555:U:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:CC:51:GLY:O | 3:CC:52:LEU:HD22 | 2.20 | 0.41 |
| 30:DI:25:TYR:CD1 | 30:DI:30:LEU:HD11 | 2.55 | 0.41 |
| 1:AA:1212:U:H5' | 1:AA:1213:A:OP1 | 2.20 | 0.41 |
| 23:DA:2016:U:H2' | 23:DA:2017:U:C6 | 2.55 | 0.41 |
| 41:DX:24:GLY:O | 41:DX:83:VAL:HG22 | 2.20 | 0.41 |
| 23:BA:2435:A:H2' | 23:BA:2436:G:O5' | 2.21 | 0.41 |
| 9:AI:41:VAL:HG12 | 9:AI:42:ARG:N | 2.35 | 0.41 |
| 1:AA:1190:G:H3' | 1:AA:1190:G:C8 | 2.56 | 0.41 |
| 8:CH:87:SER:HB2 | 8:CH:93:VAL:HB | 2.01 | 0.41 |
| 1:AA:1313:U:H2' | 1:AA:1314:C:C6 | 2.56 | 0.41 |
| 1:AA:560:U:H2' | 1:AA:560:U:H6 | 1.61 | 0.41 |
| 1:AA:9:G:H2' | 1:AA:10:A:H8 | 1.85 | 0.41 |
| 2:AB:163:PHE:HA | 2:AB:185:ILE:O | 2.18 | 0.41 |
| 33:BP:38:GLN:HA | 33:BP:41:ARG:CG | 2.50 | 0.41 |
| 2:CB:165:VAL:O | 2:CB:187:LEU:HB3 | 2.21 | 0.41 |
| 1:AA:1277:C:H2' | 1:AA:1279:A:C8 | 2.55 | 0.41 |
| 10:AJ:52:GLY:HA2 | 10:AJ:53:PRO:HD2 | 1.56 | 0.41 |
| 23:DA:2742:C:OP1 | 53:D9:35:ARG:HD3 | 2.20 | 0.41 |
| 23:DA:1530:C:H42 | 23:DA:1539:G:H1 | 1.68 | 0.41 |
| 23:DA:2173:A:C3' | 23:DA:2174:C:H5' | 2.50 | 0.41 |
| 1:CA:1368:G:O2' | 1:CA:1369:C:H5' | 2.20 | 0.41 |
| 23:BA:2126:A:C2 | 23:BA:2162:G:N3 | 2.88 | 0.41 |
| 1:AA:170:U:O2' | 1:AA:171:A:H5' | 2.20 | 0.41 |
| 1:AA:148:G:C2 | 1:AA:175:C:C2 | 3.09 | 0.41 |
| 23:DA:2153:G:H2' | 23:DA:2154:G:O4' | 2.21 | 0.41 |
| 1:CA:1083:U:C5 | 1:CA:1084:G:C6 | 3.08 | 0.41 |
| 1:CA:994:A:C2 | 14:CN:4:LYS:HD3 | 2.52 | 0.41 |
| 23:BA:1740:G:H2' | 23:BA:1741:A:C8 | 2.55 | 0.41 |
| 23:BA:1759:A:H1' | 23:BA:2711:A:C2 | 2.55 | 0.41 |
| 26:DE:47:VAL:CG1 | 26:DE:86:PRO:HD2 | 2.47 | 0.41 |
| 1:AA:187:C:H2' | 1:AA:188:C:C6 | 2.56 | 0.41 |
| 1:AA:872:A:C4 | 1:AA:874:G:N7 | 2.88 | 0.41 |
| 23:DA:2261:C:O2' | 23:DA:2262:U:H5' | 2.21 | 0.41 |
| 1:CA:509:A:C8 | 1:CA:509:A:H3' | 2.55 | 0.41 |
| 7:AG:40:ALA:O | 7:AG:44:TYR:N | 2.53 | 0.41 |
| 1:CA:618:C:H5' | 1:CA:619:U:H5'' | 2.03 | 0.41 |
| 1:AA:384:G:H2' | 1:AA:385:C:C6 | 2.55 | 0.41 |
| 23:BA:1040:C:H2' | 23:BA:1041:C:O4' | 2.20 | 0.41 |
| 23:BA:229:A:OP1 | 23:BA:229:A:C8 | 2.73 | 0.41 |
| 1:CA:409:G:OP1 | 4:CD:25:ARG:N | 2.35 | 0.41 |
| 6:AF:55:ASP:HA | 6:AF:56:PRO:HD2 | 1.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:37:ARG:HH21 | 8:AH:38:ILE:CD1 | 2.33 | 0.41 |
| 43:BZ:28:MET:HG3 | 43:BZ:35:ARG:HB2 | 2.02 | 0.41 |
| 23:BA:541:C:O2' | 23:BA:542:C:H5' | 2.21 | 0.41 |
| 23:BA:1453:U:O2' | 23:BA:1455:G:N7 | 2.46 | 0.41 |
| 23:BA:1368:G:C2 | 23:BA:1369:G:C8 | 3.08 | 0.41 |
| 25:DD:210:GLY:O | 25:DD:213:ARG:N | 2.53 | 0.41 |
| 24:BB:33:G:C2 | 24:BB:50:G:C2 | 3.09 | 0.41 |
| 1:CA:721:G:H4' | 1:CA:722:A:O4' | 2.20 | 0.41 |
| 23:BA:1742:G:H2' | 23:BA:1743:C:O4' | 2.21 | 0.41 |
| 9:CI:82:ALA:HB2 | 9:CI:101:PHE:HB3 | 2.02 | 0.41 |
| 40:DW:97:LYS:HE3 | 40:DW:99:ARG:NH2 | 2.35 | 0.41 |
| 23:DA:1783:A:C2 | 23:DA:2587:A:C5 | 3.09 | 0.41 |
| 8:CH:86:ILE:HG21 | 8:CH:133:LEU:HD13 | 2.01 | 0.41 |
| 30:BI:61:ARG:HA | 30:BI:61:ARG:HH11 | 1.85 | 0.41 |
| 1:CA:1442:G:C8 | 1:CA:1442(A):G:C5 | 3.09 | 0.41 |
| 8:CH:4:ASP:HB2 | 8:CH:89:PRO:HG3 | 2.03 | 0.41 |
| 1:CA:936:C:H3' | 1:CA:937:A:H8 | 1.85 | 0.41 |
| 1:AA:1306:A:H1' | 1:AA:1332:A:C5 | 2.55 | 0.41 |
| 1:CA:1003:G:C3' | 1:CA:1004:A:H4' | 2.51 | 0.41 |
| 1:AA:1195:C:N3 | 1:AA:1197:G:C8 | 2.88 | 0.41 |
| 23:BA:1536:C:C5 | 23:BA:1537:G:C5 | 3.09 | 0.41 |
| 1:CA:1030:C:H2' | 1:CA:1030(A):G:H5' | 2.00 | 0.41 |
| 1:AA:1202:G:H2' | 1:AA:1203:C:O4' | 2.20 | 0.41 |
| 27:BF:101:LEU:HD12 | 27:BF:102:PRO:HD2 | 2.02 | 0.41 |
| 23:DA:2299:G:N1 | 23:DA:2318:G:C8 | 2.89 | 0.41 |
| 23:BA:2161:C:H5 | 23:BA:2161:C:OP2 | 1.97 | 0.41 |
| 1:AA:164:U:H2' | 1:AA:165:C:C6 | 2.56 | 0.41 |
| 3:CC:35:GLU:OE2 | 3:CC:59:ARG:NH2 | 2.53 | 0.41 |
| 1:AA:1164:G:C6 | 1:AA:1173:G:C6 | 3.08 | 0.41 |
| 23:BA:910:A:C6 | 23:BA:911:A:C6 | 3.09 | 0.41 |
| 14:CN:23:ARG:HG3 | 14:CN:24:CYS:N | 2.34 | 0.41 |
| 3:CC:18:TRP:NE1 | 14:CN:55:GLY:N | 2.69 | 0.41 |
| 13:CM:23:TYR:HE1 | 13:CM:71:ARG:HG2 | 1.85 | 0.41 |
| 1:AA:520:A:OP2 | 12:AL:51:ALA:HB1 | 2.20 | 0.41 |
| 34:BQ:32:TYR:HE2 | 34:BQ:133:ARG:HE | 1.69 | 0.41 |
| 7:AG:69:VAL:O | 7:AG:138:LYS:HG3 | 2.20 | 0.41 |
| 7:AG:71:PRO:HD2 | 7:AG:99:LEU:HD13 | 2.02 | 0.41 |
| 36:BS:7:TYR:CE1 | 36:BS:91:PRO:HG3 | 2.55 | 0.41 |
| 3:AC:140:ARG:HH11 | 3:AC:140:ARG:HB2 | 1.84 | 0.41 |
| 29:DH:3:ARG:NH2 | 29:DH:5:GLY:H | 2.19 | 0.41 |
| 23:DA:1051:G:H2' | 23:DA:1051:G:N3 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:CQ:91:ARG:HB2 | 17:CQ:91:ARG:HE | 1.55 | 0.41 |
| 1:CA:766:A:H2 | 1:CA:1525:G:N3 | 2.19 | 0.41 |
| 5:AE:12:LEU:HD22 | 5:AE:13:ILE:H | 1.85 | 0.41 |
| 1:CA:130:A:C8 | 17:CQ:63:ARG:HG3 | 2.56 | 0.41 |
| 17:CQ:63:ARG:HA | 17:CQ:64:PRO:HD3 | 1.89 | 0.41 |
| 25:BD:275:LYS:HG3 | 25:BD:275:LYS:O | 2.21 | 0.41 |
| 16:CP:20:VAL:HG21 | 16:CP:32:TYR:CG | 2.54 | 0.41 |
| 23:BA:962:G:C6 | 23:BA:963:U:C4 | 3.08 | 0.41 |
| 23:BA:1028:A:H61 | 23:BA:1125:G:H2' | 1.86 | 0.41 |
| 1:AA:1113:C:H2' | 1:AA:1114:C:H6 | 1.86 | 0.41 |
| 3:AC:123:GLN:HA | 3:AC:126:ARG:HD2 | 2.02 | 0.41 |
| 2:CB:110:GLN:HG3 | 2:CB:110:GLN:H | 1.49 | 0.41 |
| 41:BX:11:PRO:HG2 | 41:BX:13:LEU:HD21 | 2.02 | 0.41 |
| 39:DV:76:LYS:HB2 | 39:DV:81:TYR:HB3 | 2.03 | 0.41 |
| 23:DA:286:C:H42 | 23:DA:355:G:H1 | 1.68 | 0.41 |
| 8:AH:25:ASP:HB2 | 8:AH:58:TYR:CD2 | 2.55 | 0.41 |
| 1:AA:317:G:C6 | 1:AA:318:G:C5 | 3.09 | 0.41 |
| 23:DA:478:A:C6 | 23:DA:480:A:C6 | 3.08 | 0.41 |
| 1:CA:1437:C:H2' | 1:CA:1438:G:C8 | 2.56 | 0.41 |
| 11:AK:30:VAL:HG21 | 11:AK:65:ALA:HA | 2.02 | 0.41 |
| 23:DA:2812:G:C2 | 23:DA:2813:A:C4 | 3.08 | 0.41 |
| 32:DO:7:TYR:OH | 32:DO:44:LYS:HG3 | 2.20 | 0.41 |
| 23:DA:2092:U:H4' | 23:DA:2093:G:O5' | 2.21 | 0.41 |
| 7:AG:72:ARG:HB3 | 7:AG:96:GLN:HE22 | 1.86 | 0.41 |
| 32:DO:9:GLU:HB2 | 32:DO:83:ALA:HB2 | 2.03 | 0.41 |
| 29:DH:35:VAL:HA | 29:DH:36:PRO:HD2 | 1.77 | 0.41 |
| 41:BX:21:PHE:CZ | 41:BX:92:LEU:HD12 | 2.56 | 0.41 |
| 23:DA:909:A:C6 | 23:DA:912:C:C2 | 3.08 | 0.41 |
| 26:DE:137:HIS:HB3 | 26:DE:138:PRO:HD2 | 2.02 | 0.41 |
| 23:BA:2415:G:H2' | 23:BA:2416:C:C6 | 2.55 | 0.41 |
| 43:DZ:106:GLY:HA3 | 43:DZ:142:SER:OG | 2.21 | 0.41 |
| 31:BN:28:THR:HG22 | 31:BN:29:LYS:N | 2.35 | 0.41 |
| 11:AK:82:VAL:CG1 | 11:AK:108:ILE:HG12 | 2.50 | 0.41 |
| 39:BV:70:ILE:HD13 | 39:BV:70:ILE:HA | 1.78 | 0.41 |
| 30:DI:139:GLN:HA | 30:DI:139:GLN:HE21 | 1.85 | 0.41 |
| 39:BV:82:ARG:HD2 | 39:BV:82:ARG:N | 2.36 | 0.41 |
| 33:BP:6:LEU:HD23 | 33:BP:6:LEU:HA | 1.61 | 0.41 |
| 4:AD:176:LEU:HD12 | 4:AD:176:LEU:HA | 1.84 | 0.41 |
| 34:DQ:54:MET:HB2 | 34:DQ:54:MET:HE2 | 1.86 | 0.41 |
| 23:DA:2239:G:H5' | 25:DD:251:GLY:HA3 | 2.02 | 0.41 |
| 1:CA:1416:G:H2' | 1:CA:1417:G:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:CJ:57:LYS:O | 10:CJ:60:ARG:HG3 | 2.21 | 0.41 |
| 1:AA:1168:A:C6 | 1:AA:1169:A:C6 | 3.09 | 0.41 |
| 1:AA:1169:A:C2' | 1:AA:1170:A:C8 | 3.01 | 0.41 |
| 48:B4:40:HIS:O | 48:B4:42:PHE:N | 2.49 | 0.41 |
| 1:AA:1300:G:H4' | 1:AA:1301:U:H6 | 1.85 | 0.41 |
| 1:AA:971:G:N2 | 1:AA:1363(A):A:O4' | 2.51 | 0.41 |
| 23:DA:2127:G:H1' | 23:DA:2173:A:C2 | 2.56 | 0.41 |
| 23:BA:1319:G:C6 | 23:BA:1320:C:N4 | 2.89 | 0.41 |
| 23:DA:2130:U:O3' | 23:DA:2133:G:H4' | 2.20 | 0.41 |
| 28:DG:138:GLN:HE22 | 28:DG:153:ARG:NH2 | 2.19 | 0.41 |
| 9:AI:14:VAL:O | 9:AI:65:VAL:HA | 2.20 | 0.41 |
| 9:AI:31:GLN:HG2 | 9:AI:36:TYR:CD1 | 2.55 | 0.41 |
| 1:CA:1176:A:C6 | 1:CA:1177:G:O6 | 2.73 | 0.41 |
| 1:AA:373:A:C2 | 1:AA:374:A:C8 | 3.08 | 0.41 |
| 1:AA:476:G:N2 | 1:AA:477:A:C4 | 2.88 | 0.41 |
| 3:AC:186:PHE:CZ | 3:AC:188:LEU:HB2 | 2.55 | 0.41 |
| 4:CD:173:TRP:CD1 | 4:CD:174:LEU:HG | 2.56 | 0.41 |
| 2:AB:135:GLN:O | 2:AB:139:LYS:N | 2.44 | 0.41 |
| 1:AA:59:A:H2' | 1:AA:59:A:N3 | 2.35 | 0.41 |
| 4:AD:13:ARG:NH2 | 4:AD:36:ARG:HH21 | 2.19 | 0.41 |
| 37:DT:55:ASN:H | 37:DT:59:THR:HB | 1.84 | 0.41 |
| 23:BA:1832:C:N4 | 23:BA:1833:U:C4 | 2.88 | 0.41 |
| 20:CT:53:LEU:HD12 | 20:CT:99:LEU:O | 2.20 | 0.41 |
| 1:CA:102:G:C4 | 1:CA:103:C:C5 | 3.09 | 0.41 |
| 36:BS:99:LYS:HE2 | 36:BS:103:GLU:OE2 | 2.20 | 0.41 |
| 1:CA:832:C:O2' | 1:CA:833:U:P | 2.79 | 0.41 |
| 30:BI:139:GLN:NE2 | 30:BI:139:GLN:HA | 2.31 | 0.41 |
| 25:BD:111:LEU:HD23 | 25:BD:111:LEU:HA | 1.67 | 0.41 |
| 12:CL:27:LEU:C | 12:CL:29:GLY:H | 2.24 | 0.41 |
| 16:CP:45:THR:O | 16:CP:48:TRP:HB3 | 2.21 | 0.41 |
| 28:DG:66:GLN:HG2 | 48:D4:1:MET:CE | 2.51 | 0.41 |
| 25:BD:148:GLU:CB | 25:BD:151:LYS:HD2 | 2.49 | 0.41 |
| 24:DB:73:A:C4 | 24:DB:105:A:C2 | 3.08 | 0.41 |
| 1:CA:1265:G:N2 | 1:CA:1271:G:N3 | 2.69 | 0.41 |
| 2:CB:24:TRP:CZ2 | 2:CB:26:PRO:HB3 | 2.55 | 0.41 |
| 23:DA:1253:A:C5 | 56:DA:4450:HOH:O | 2.72 | 0.41 |
| 23:BA:2516:G:O2' | 23:BA:2517:C:H5' | 2.20 | 0.41 |
| 27:DF:158:THR:HG1 | 27:DF:160:ASN:H | 1.59 | 0.41 |
| 37:DT:20:PRO:HG2 | 37:DT:86:ILE:O | 2.20 | 0.41 |
| 34:DQ:72:LYS:HB3 | 34:DQ:94:VAL:HG23 | 2.03 | 0.41 |
| 23:BA:2537:U:H2' | 23:BA:2538:C:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:512:U:H2' | 1:AA:513:C:C6 | 2.55 | 0.41 |
| 32:BO:106:LEU:HD23 | 32:BO:106:LEU:HA | 1.84 | 0.41 |
| 23:DA:2528:U:H2' | 23:DA:2530:A:O5' | 2.21 | 0.41 |
| 3:CC:130:VAL:HA | 3:CC:133:ALA:HB3 | 2.02 | 0.41 |
| 23:DA:2178:C:H2' | 23:DA:2179:C:O4' | 2.20 | 0.41 |
| 26:DE:7:VAL:HG12 | 26:DE:51:PHE:CE1 | 2.55 | 0.41 |
| 26:DE:51:PHE:O | 26:DE:75:VAL:HG13 | 2.21 | 0.41 |
| 31:DN:102:ALA:O | 31:DN:106:MET:HG3 | 2.21 | 0.41 |
| 40:DW:64:MET:HE3 | 40:DW:109:GLU:HG3 | 2.02 | 0.41 |
| 28:BG:129:GLY:HA2 | 28:BG:166:ASP:HA | 2.02 | 0.41 |
| 28:DG:8:LYS:O | 28:DG:12:TYR:HD1 | 2.03 | 0.41 |
| 40:BW:10:VAL:HG21 | 40:BW:103:ILE:HD12 | 2.03 | 0.41 |
| 1:CA:124:G:H2' | 1:CA:125:U:O4' | 2.20 | 0.41 |
| 8:CH:75:ARG:HA | 8:CH:76:PRO:HD2 | 1.68 | 0.41 |
| 12:CL:36:VAL:O | 12:CL:58:VAL:HG13 | 2.20 | 0.41 |
| 1:AA:690:G:H2' | 1:AA:691:G:O4' | 2.19 | 0.41 |
| 23:BA:1686:C:C2' | 23:BA:1687:G:H5' | 2.50 | 0.41 |
| 23:BA:2051:A:C6 | 23:BA:2614:A:C5 | 3.08 | 0.41 |
| 4:AD:113:SER:O | 4:AD:117:ALA:N | 2.46 | 0.41 |
| 50:B6:19:ARG:HD2 | 50:B6:19:ARG:H | 1.85 | 0.41 |
| 23:DA:2233:U:H2' | 23:DA:2234:G:C8 | 2.56 | 0.41 |
| 23:DA:2791:C:H2' | 23:DA:2792:G:C8 | 2.55 | 0.41 |
| 4:CD:63:LYS:O | 4:CD:67:ILE:HG13 | 2.21 | 0.41 |
| 1:AA:1025:U:C2 | 1:AA:1036:G:O6 | 2.68 | 0.41 |
| 1:CA:1004:A:N3 | 1:CA:1037:C:N3 | 2.69 | 0.41 |
| 1:AA:992:U:O2 | 1:AA:993:G:N2 | 2.54 | 0.41 |
| 28:DG:82:LEU:HD22 | 28:DG:86:MET:CB | 2.51 | 0.41 |
| 2:CB:55:PHE:HA | 2:CB:58:ILE:CG1 | 2.51 | 0.41 |
| 23:DA:826:U:C4' | 33:DP:55:ARG:HB2 | 2.51 | 0.41 |
| 23:DA:2165:G:H2' | 23:DA:2166:G:H8 | 1.84 | 0.41 |
| 23:BA:303:U:H2' | 23:BA:304:G:C8 | 2.56 | 0.41 |
| 7:CG:69:VAL:HG11 | 7:CG:104:LEU:HB2 | 2.02 | 0.41 |
| 23:DA:528:A:C2 | 23:DA:2043:C:H4' | 2.55 | 0.41 |
| 19:CS:62:ILE:H | 19:CS:62:ILE:HD12 | 1.86 | 0.41 |
| 1:CA:67:C:H2' | 1:CA:68:G:C8 | 2.55 | 0.41 |
| 23:BA:2114:A:H3' | 23:BA:2115:G:C8 | 2.55 | 0.41 |
| 23:BA:2117:A:H2' | 23:BA:2118:U:H3' | 2.02 | 0.41 |
| 23:BA:269:U:C5 | 23:BA:271(Y):U:C5 | 3.08 | 0.41 |
| 1:CA:734:G:C5 | 1:CA:735:C:C4 | 3.09 | 0.41 |
| 28:DG:106:LEU:O | 28:DG:111:LEU:HG | 2.21 | 0.41 |
| 1:AA:546:G:OP1 | 4:AD:73:ARG:HG2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1014:A:H5' | 19:CS:14:HIS:CD2 | 2.56 | 0.41 |
| 28:DG:174:GLU:HG2 | 28:DG:180:PHE:CD1 | 2.56 | 0.41 |
| 29:DH:3:ARG:HG2 | 29:DH:6:ARG:CZ | 2.49 | 0.41 |
| 10:CJ:61:GLU:OE2 | 14:CN:45:ARG:HG2 | 2.20 | 0.41 |
| 10:CJ:63:PHE:CD1 | 14:CN:58:LYS:HA | 2.51 | 0.41 |
| 23:DA:1814:G:H4' | 25:DD:51:VAL:HG21 | 2.03 | 0.41 |
| 1:CA:855:G:C6 | 1:CA:856:C:C4 | 3.08 | 0.41 |
| 30:DI:106:GLY:HA2 | 30:DI:107:VAL:HB | 2.03 | 0.41 |
| 7:AG:45:ASP:HB2 | 7:AG:117:ALA:HB1 | 2.03 | 0.41 |
| 1:AA:623:C:C4 | 1:AA:624:C:C5 | 3.08 | 0.41 |
| 1:CA:627:G:O2' | 1:CA:628:G:H5' | 2.21 | 0.41 |
| 1:CA:737:A:H2' | 1:CA:738:C:H6 | 1.84 | 0.41 |
| 23:DA:928:G:H8 | 23:DA:928:G:O5' | 2.04 | 0.41 |
| 28:DG:72:ARG:NH1 | 28:DG:87:PRO:HG3 | 2.34 | 0.41 |
| 30:BI:77:LEU:HB3 | 30:BI:142:VAL:CG1 | 2.50 | 0.41 |
| 13:CM:53:VAL:HA | 13:CM:56:LEU:HD12 | 2.03 | 0.41 |
| 23:BA:2321:G:C2' | 23:BA:2321:G:N3 | 2.84 | 0.41 |
| 1:AA:1371:G:O3' | 9:AI:69:GLY:HA3 | 2.20 | 0.41 |
| 23:DA:1648:C:H2' | 23:DA:1649:G:O5' | 2.20 | 0.41 |
| 31:DN:96:GLU:HB2 | 31:DN:122:VAL:HG12 | 2.03 | 0.41 |
| 29:BH:137:ASP:HB3 | 29:BH:140:LYS:HB3 | 2.02 | 0.41 |
| 1:CA:189(J):G:H2' | 1:CA:189(K):U:C6 | 2.55 | 0.41 |
| 48:B4:1:MET:HB3 | 48:B4:6:HIS:CD2 | 2.56 | 0.41 |
| 1:AA:65:U:H5'' | 1:AA:65:U:H6 | 1.86 | 0.41 |
| 1:AA:688:G:H2' | 1:AA:689:C:C6 | 2.56 | 0.41 |
| 23:DA:725:G:H8 | 23:DA:725:G:O5' | 2.04 | 0.41 |
| 1:CA:881:G:H2' | 1:CA:882:C:O4' | 2.19 | 0.41 |
| 23:BA:54:G:O2' | 51:B7:35:ARG:HD3 | 2.21 | 0.41 |
| 3:AC:123:GLN:O | 3:AC:126:ARG:HB2 | 2.21 | 0.41 |
| 23:BA:2099:U:H3 | 23:BA:2190:G:H1 | 1.69 | 0.41 |
| 23:DA:647:G:H2' | 23:DA:648:G:O4' | 2.21 | 0.41 |
| 1:CA:317:G:C6 | 1:CA:318:G:N7 | 2.89 | 0.41 |
| 23:BA:1106:G:H2' | 23:BA:1107:G:H21 | 1.85 | 0.41 |
| 23:BA:1453:U:OP1 | 35:BR:77:ARG:NH1 | 2.53 | 0.41 |
| 8:CH:86:ILE:CB | 8:CH:133:LEU:HD22 | 2.51 | 0.41 |
| 26:BE:120:TRP:CD1 | 26:BE:155:LYS:HB3 | 2.56 | 0.41 |
| 23:DA:2091:U:O2' | 45:D1:47:GLN:HG3 | 2.21 | 0.41 |
| 2:AB:52:GLU:HG2 | 2:AB:56:ARG:NH1 | 2.36 | 0.41 |
| 23:DA:1709:U:H2' | 23:DA:1710:C:C6 | 2.56 | 0.41 |
| 23:BA:1936:A:C8 | 23:BA:1940:U:O2 | 2.74 | 0.41 |
| 24:BB:77:U:OP1 | 43:BZ:19:ARG:NH2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:AP:11:SER:OG | 16:AP:12:LYS:N | 2.51 | 0.41 |
| 30:BI:94:ALA:HA | 30:BI:97:ILE:HG13 | 2.03 | 0.41 |
| 4:AD:146:ILE:N | 4:AD:146:ILE:HD12 | 2.36 | 0.41 |
| 34:DQ:34:LEU:HA | 34:DQ:34:LEU:HD12 | 1.77 | 0.41 |
| 5:AE:116:THR:HG23 | 5:AE:117:ASP:OD2 | 2.21 | 0.41 |
| 1:AA:27:G:H2' | 1:AA:28:G:O4' | 2.21 | 0.41 |
| 23:DA:401:A:H2' | 23:DA:402:A:O4' | 2.21 | 0.41 |
| 23:DA:224:G:H2' | 23:DA:225:A:O4' | 2.21 | 0.41 |
| 1:AA:1442(B):A:N7 | 37:BT:118:ARG:CZ | 2.83 | 0.41 |
| 1:CA:1443:G:H1 | 1:CA:1459:C:H2' | 1.86 | 0.41 |
| 1:CA:1098:C:C5' | 1:CA:1169:A:H1' | 2.49 | 0.41 |
| 1:AA:1206:G:C4 | 1:AA:1207:G:C8 | 3.09 | 0.41 |
| 1:CA:954:G:N1 | 1:CA:1226:C:C2 | 2.88 | 0.41 |
| 1:AA:1052:U:H5'' | 1:AA:1053:G:OP2 | 2.21 | 0.41 |
| 1:AA:963:G:O2' | 1:AA:1199:U:H5'' | 2.21 | 0.41 |
| 1:AA:1128:C:H1' | 1:AA:1146:A:N1 | 2.36 | 0.41 |
| 23:BA:28:A:C5 | 23:BA:29:U:C5 | 3.09 | 0.41 |
| 23:BA:1537:G:O2' | 23:BA:1538:G:H5' | 2.21 | 0.41 |
| 1:CA:560:U:H2' | 1:CA:560:U:H6 | 1.61 | 0.41 |
| 1:CA:1368:G:OP2 | 9:CI:112:LYS:HG3 | 2.21 | 0.41 |
| 23:BA:2172:U:H4' | 23:BA:2173:A:OP2 | 2.21 | 0.41 |
| 1:AA:1015:A:H8 | 1:AA:1015:A:O5' | 2.03 | 0.41 |
| 28:BG:5:VAL:HG11 | 28:BG:101:ILE:HG12 | 2.02 | 0.41 |
| 23:BA:1022:G:C6 | 23:BA:1140:C:C4 | 3.09 | 0.41 |
| 36:DS:11:LYS:HD3 | 36:DS:15:ARG:NH2 | 2.36 | 0.41 |
| 2:AB:137:ARG:H | 2:AB:137:ARG:HG3 | 1.71 | 0.41 |
| 26:BE:36:ARG:NH1 | 26:BE:86:PRO:O | 2.37 | 0.41 |
| 1:AA:1126:U:H1' | 1:AA:1280:A:C6 | 2.56 | 0.41 |
| 36:BS:27:SER:HA | 36:BS:88:ASP:HB3 | 2.02 | 0.41 |
| 23:DA:272(E):G:C2 | 23:DA:364:C:C2 | 3.08 | 0.41 |
| 1:AA:1502:A:C2 | 1:AA:1505:G:N1 | 2.76 | 0.41 |
| 1:CA:997:U:N3 | 1:CA:1044:A:C2 | 2.89 | 0.41 |
| 28:DG:39:ILE:HG23 | 28:DG:157:ILE:HD13 | 2.02 | 0.41 |
| 23:BA:1827:C:OP2 | 25:BD:222:ARG:HD2 | 2.21 | 0.41 |
| 23:DA:534:U:H5' | 38:DU:42:ALA:HB1 | 2.03 | 0.41 |
| 5:CE:100:VAL:O | 5:CE:107:ARG:NH2 | 2.53 | 0.41 |
| 23:DA:1188:U:O2' | 23:DA:1189:A:H5' | 2.20 | 0.41 |
| 23:DA:1131:G:H21 | 31:DN:73:THR:CG2 | 2.34 | 0.41 |
| 23:DA:2463:C:H2' | 23:DA:2464:C:H5' | 2.03 | 0.41 |
| 1:CA:22:G:H2' | 1:CA:23:C:C6 | 2.56 | 0.41 |
| 43:DZ:72:ARG:HA | 43:DZ:72:ARG:HD3 | 1.61 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 23:DA:918:A:C5 | 23:DA:919:G:H1' | 2.56 | 0.41 |
| 3:CC:57:ILE:HG23 | 3:CC:66:VAL:HA | 2.03 | 0.41 |
| 3:CC:66:VAL:O | 3:CC:102:ASN:HB3 | 2.21 | 0.41 |
| 43:DZ:39:VAL:CG2 | 43:DZ:44:PHE:HB2 | 2.51 | 0.41 |
| 11:CK:34:ASP:HB3 | 11:CK:40:ILE:HD11 | 2.03 | 0.41 |
| 34:BQ:26:TYR:HE1 | 34:BQ:28:ALA:HB2 | 1.85 | 0.41 |
| 1:CA:269:C:H2' | 1:CA:270:A:H8 | 1.84 | 0.41 |
| 23:DA:1441:G:H2' | 23:DA:1442:G:H8 | 1.85 | 0.41 |
| 38:BU:74:LEU:N | 38:BU:74:LEU:HD12 | 2.36 | 0.41 |
| 1:CA:329:A:C2 | 1:CA:332:G:C8 | 3.09 | 0.41 |
| 29:BH:12:PRO:O | 29:BH:14:GLY:HA2 | 2.20 | 0.41 |
| 26:DE:4:ILE:HG12 | 26:DE:5:LEU:O | 2.20 | 0.41 |
| 16:CP:6:LEU:HG | 16:CP:17:TYR:CB | 2.50 | 0.41 |
| 35:BR:38:VAL:HB | 35:BR:39:PRO:HD3 | 2.02 | 0.41 |
| 23:BA:65:C:O2' | 23:BA:456:C:O2 | 2.38 | 0.41 |
| 25:DD:26:LYS:HE2 | 25:DD:28:GLU:O | 2.21 | 0.41 |
| 23:BA:1947:C:N3 | 23:BA:1960:A:C2 | 2.89 | 0.41 |
| 36:BS:78:LEU:HD13 | 36:BS:78:LEU:HA | 1.82 | 0.41 |
| 12:CL:46:LYS:H | 12:CL:46:LYS:HG2 | 1.69 | 0.41 |
| 39:DV:2:PHE:CZ | 39:DV:41:GLY:HA3 | 2.56 | 0.41 |
| 15:AO:74:ASP:OD1 | 15:AO:76:GLU:HB2 | 2.21 | 0.41 |
| 1:AA:1457:G:C6 | 1:AA:1458:G:C6 | 3.08 | 0.41 |
| 1:AA:1459:C:H5' | 1:AA:1460:A:OP2 | 2.21 | 0.41 |
| 1:AA:1442(B):A:N7 | 37:BT:118:ARG:NH1 | 2.68 | 0.41 |
| 1:CA:1442(A):G:C2' | 1:CA:1442(B):A:H5'' | 2.50 | 0.41 |
| 1:CA:1442(A):G:H3' | 1:CA:1442(B):A:C5' | 2.51 | 0.41 |
| 23:BA:2335:A:N6 | 23:BA:2337:G:H1' | 2.35 | 0.41 |
| 23:BA:890:A:H3' | 23:BA:892:G:C8 | 2.56 | 0.41 |
| 1:AA:1004:A:H3' | 1:AA:1025:U:H3 | 1.86 | 0.41 |
| 23:DA:563:G:H5' | 23:DA:572:A:H4' | 2.02 | 0.41 |
| 8:CH:87:SER:HB2 | 8:CH:93:VAL:H | 1.86 | 0.41 |
| 1:CA:1126:U:H2' | 1:CA:1126:U:O2 | 2.21 | 0.41 |
| 1:CA:1380:U:H5 | 7:CG:3:ARG:HA | 1.85 | 0.41 |
| 21:AU:13:ILE:HA | 21:AU:22:ARG:HH11 | 1.82 | 0.41 |
| 7:AG:27:ILE:O | 7:AG:30:ILE:HG13 | 2.20 | 0.41 |
| 23:BA:330:A:O2' | 23:BA:331:A:H8 | 2.04 | 0.41 |
| 1:CA:1308:U:H5' | 13:CM:110:ARG:NH1 | 2.36 | 0.41 |
| 23:DA:1376:C:N4 | 23:DA:1377:G:C6 | 2.89 | 0.41 |
| 33:DP:38:GLN:HG3 | 33:DP:45:LEU:HD23 | 2.02 | 0.41 |
| 1:AA:1261:A:C4 | 1:AA:1275:A:C2 | 3.09 | 0.41 |
| 45:D1:82:LEU:CA | 45:D1:85:LEU:HD23 | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BA:1473:G:H2' | 23:BA:1474:C:O4' | 2.21 | 0.41 |
| 10:CJ:9:ARG:HG2 | 10:CJ:69:ASN:ND2 | 2.36 | 0.41 |
| 1:CA:373:A:C2 | 1:CA:374:A:C8 | 3.09 | 0.41 |
| 1:CA:1154:G:C2 | 1:CA:1155:G:C5 | 3.09 | 0.41 |
| 3:CC:136:GLN:HG2 | 3:CC:140:ARG:HD2 | 2.01 | 0.41 |
| 3:CC:19:GLU:HA | 3:CC:54:ARG:NH1 | 2.36 | 0.41 |
| 9:CI:44:VAL:HA | 9:CI:45:ALA:HA | 1.58 | 0.41 |
| 1:AA:657:G:C2 | 1:AA:750:G:C5 | 3.08 | 0.41 |
| 1:CA:657:G:C2 | 1:CA:750:G:C5 | 3.09 | 0.41 |
| 1:CA:1072:G:O6 | 1:CA:1102:A:N6 | 2.53 | 0.41 |
| 1:AA:448:A:P | 1:AA:485:G:H22 | 2.43 | 0.41 |
| 14:CN:23:ARG:HH11 | 14:CN:30:ALA:HB2 | 1.85 | 0.41 |
| 25:BD:147:LEU:HD13 | 25:BD:155:LEU:HD11 | 2.03 | 0.41 |
| 15:CO:21:ASP:OD2 | 15:CO:24:SER:HB3 | 2.20 | 0.41 |
| 3:CC:12:LEU:HD11 | 14:CN:51:GLY:HA2 | 2.03 | 0.41 |
| 23:BA:1224:C:O2' | 39:BV:85:LYS:HA | 2.21 | 0.41 |
| 1:AA:373:A:N3 | 1:AA:374:A:C8 | 2.89 | 0.41 |
| 34:BQ:133:ARG:HG2 | 34:BQ:134:ARG:N | 2.36 | 0.41 |
| 23:DA:1185:C:H5'' | 23:DA:1186:G:OP1 | 2.21 | 0.41 |
| 3:CC:121:ALA:HB2 | 3:CC:198:VAL:HG21 | 2.03 | 0.41 |
| 10:CJ:39:PRO:HG3 | 10:CJ:70:ARG:HE | 1.85 | 0.41 |
| 21:CU:18:TYR:CG | 21:CU:24:ARG:HG3 | 2.55 | 0.41 |
| 23:BA:606:U:H4' | 23:BA:658:C:C4' | 2.49 | 0.41 |
| 23:BA:2887:U:O2' | 23:BA:2888:C:H5' | 2.21 | 0.41 |
| 23:DA:2305:A:H2' | 23:DA:2306:C:O4' | 2.20 | 0.41 |
| 29:BH:5:GLY:HA3 | 29:BH:65:HIS:CD2 | 2.56 | 0.41 |
| 33:BP:59:LEU:HD23 | 33:BP:59:LEU:HA | 1.73 | 0.41 |
| 36:BS:99:LYS:O | 36:BS:102:ALA:HB3 | 2.20 | 0.41 |
| 1:AA:123:C:OP1 | 1:AA:311:C:O2' | 2.24 | 0.41 |
| 23:DA:2572:A:N7 | 26:DE:144:ARG:HD2 | 2.35 | 0.41 |
| 23:BA:2869:G:H2' | 23:BA:2870:C:O4' | 2.20 | 0.41 |
| 48:D4:14:ILE:HD12 | 48:D4:22:ILE:HB | 2.03 | 0.41 |
| 1:CA:584:G:OP1 | 17:CQ:91:ARG:NH2 | 2.54 | 0.41 |
| 13:CM:60:VAL:HG13 | 13:CM:64:TRP:HZ3 | 1.86 | 0.41 |
| 1:CA:626:U:H4' | 16:CP:38:TYR:CZ | 2.56 | 0.41 |
| 23:DA:928:G:O6 | 56:DA:3686:HOH:O | 2.22 | 0.41 |
| 7:CG:62:PHE:HA | 7:CG:124:LEU:CD2 | 2.50 | 0.41 |
| 23:BA:2615:U:N1 | 49:B5:7:PRO:HA | 2.35 | 0.41 |
| 6:CF:55:ASP:HA | 6:CF:56:PRO:HD2 | 1.78 | 0.41 |
| 1:CA:575:G:O2' | 1:CA:821:G:H5' | 2.21 | 0.41 |
| 7:AG:9:VAL:HG21 | 7:AG:94:ARG:NE | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:CJ:62:HIS:HD2 | 10:CJ:62:HIS:H | 1.68 | 0.41 |
| 1:AA:918:A:H2' | 1:AA:919:A:H8 | 1.84 | 0.41 |
| 30:DI:12:LEU:HA | 30:DI:12:LEU:HD23 | 1.88 | 0.41 |
| 1:CA:499:A:H4' | 1:CA:500:G:H5' | 2.02 | 0.41 |
| 35:BR:103:ARG:CG | 35:BR:103:ARG:HH11 | 2.33 | 0.41 |
| 15:AO:88:ARG:HA | 15:AO:88:ARG:HD2 | 1.85 | 0.41 |
| 12:AL:84:LEU:HA | 12:AL:84:LEU:HD22 | 1.93 | 0.41 |
| 25:DD:136:ILE:HA | 25:DD:137:PRO:HD3 | 1.95 | 0.41 |
| 34:BQ:101:ARG:HG3 | 34:BQ:102:VAL:N | 2.36 | 0.41 |
| 1:CA:1065:U:O2' | 1:CA:1066:C:OP2 | 2.27 | 0.41 |
| 23:BA:2872:G:HO2' | 23:BA:2873:A:H5' | 1.85 | 0.41 |
| 4:AD:101:LEU:CD2 | 4:AD:121:VAL:HG11 | 2.51 | 0.41 |
| 12:CL:6:THR:O | 12:CL:9:GLN:HB2 | 2.20 | 0.41 |
| 29:DH:22:GLY:HA2 | 29:DH:37:VAL:O | 2.20 | 0.41 |
| 28:BG:98:ARG:HE | 48:B4:1:MET:HE3 | 1.85 | 0.41 |
| 8:CH:48:TYR:HA | 8:CH:60:ARG:O | 2.20 | 0.41 |
| 42:BY:6:HIS:H | 42:BY:6:HIS:HD2 | 1.68 | 0.41 |
| 23:BA:2202:C:H2' | 23:BA:2203:U:O4' | 2.20 | 0.41 |
| 1:CA:420:U:HO2' | 1:CA:421:U:H6 | 1.67 | 0.41 |
| 23:DA:1668:A:OP1 | 32:DO:5:GLN:HG3 | 2.21 | 0.41 |
| 23:DA:708:C:H5' | 23:DA:709:U:OP2 | 2.21 | 0.41 |
| 2:CB:180:LEU:HD23 | 2:CB:180:LEU:HA | 1.79 | 0.41 |
| 1:CA:968:A:C8 | 1:CA:1062:U:H4' | 2.55 | 0.41 |
| 23:BA:2278:A:OP1 | 34:BQ:11:LYS:HD2 | 2.20 | 0.41 |
| 23:DA:794:G:H2' | 23:DA:795:C:C6 | 2.55 | 0.41 |
| 23:DA:1171:G:OP2 | 23:DA:1171:G:H8 | 2.03 | 0.41 |
| 2:AB:142:LEU:HG | 2:AB:146:GLN:HE21 | 1.86 | 0.41 |
| 1:AA:1012:U:H6 | 1:AA:1012:U:O5' | 2.04 | 0.41 |
| 10:CJ:15:THR:HG22 | 10:CJ:91:PRO:HB2 | 2.03 | 0.41 |
| 23:DA:2203:U:O2' | 23:DA:2205:C:H5' | 2.20 | 0.41 |
| 31:BN:128:HIS:O | 31:BN:131:GLN:NE2 | 2.40 | 0.41 |
| 23:DA:2607:G:H2' | 23:DA:2608:G:O4' | 2.21 | 0.41 |
| 23:DA:127:A:H5'' | 23:DA:128:C:C6 | 2.54 | 0.41 |
| 24:DB:46:A:C5 | 24:DB:47:C:C4 | 3.09 | 0.41 |
| 23:DA:285:C:H2' | 23:DA:286:C:H6 | 1.86 | 0.41 |
| 16:CP:9:PHE:HB2 | 16:CP:16:HIS:O | 2.21 | 0.41 |
| 23:DA:2498:C:O2' | 23:DA:2499:C:H5' | 2.21 | 0.41 |
| 26:DE:14:ILE:HG13 | 26:DE:21:VAL:HG13 | 2.03 | 0.41 |
| 1:AA:283:C:H2' | 1:AA:284:G:O4' | 2.21 | 0.41 |
| 8:CH:30:ARG:O | 8:CH:34:GLU:HB2 | 2.20 | 0.41 |
| 50:D6:40:CYS:SG | 50:D6:42:TRP:N | 2.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:458:G:O2' | 51:D7:39:ARG:HD3 | 2.20 | 0.41 |
| 23:BA:2695:C:H2' | 23:BA:2696:U:H6 | 1.86 | 0.41 |
| 14:AN:23:ARG:CZ | 14:AN:30:ALA:HB2 | 2.50 | 0.41 |
| 23:BA:116:C:H2' | 23:BA:117:G:O4' | 2.21 | 0.41 |
| 36:BS:77:ALA:O | 36:BS:80:LEU:N | 2.48 | 0.41 |
| 17:AQ:10:VAL:HG13 | 17:AQ:19:VAL:HB | 2.02 | 0.41 |
| 23:DA:1742:G:H2' | 23:DA:1743:C:O4' | 2.20 | 0.41 |
| 36:BS:82:ILE:HA | 36:BS:83:LYS:CB | 2.51 | 0.41 |
| 12:AL:124:LYS:HA | 12:AL:125:PRO:HD3 | 1.88 | 0.41 |
| 15:AO:57:LEU:HA | 15:AO:57:LEU:HD23 | 1.83 | 0.41 |
| 23:DA:271(Y):U:H2' | 23:DA:271(Y):U:H6 | 1.69 | 0.41 |
| 1:AA:528:C:H41 | 12:AL:49:ASN:CG | 2.23 | 0.41 |
| 29:DH:143:GLN:HG3 | 29:DH:147:ASN:ND2 | 2.36 | 0.41 |
| 36:DS:77:ALA:O | 36:DS:80:LEU:N | 2.48 | 0.41 |
| 37:DT:35:LYS:HA | 37:DT:40:THR:HG22 | 2.03 | 0.41 |
| 9:AI:50:LEU:HA | 9:AI:53:VAL:O | 2.20 | 0.41 |
| 43:DZ:124:ILE:HD11 | 43:DZ:165:VAL:HG11 | 2.03 | 0.41 |
| 25:DD:221:VAL:HG22 | 25:DD:226:MET:CE | 2.51 | 0.41 |
| 23:DA:1712:C:H2' | 23:DA:1713:U:C6 | 2.55 | 0.41 |
| 22:CX:79:ASP:O | 22:CX:82:ALA:HB3 | 2.21 | 0.41 |
| 12:AL:82:VAL:HG23 | 12:AL:106:ASP:OD2 | 2.21 | 0.41 |
| 31:DN:12:ARG:HG3 | 31:DN:14:VAL:HG23 | 2.03 | 0.41 |
| 16:AP:38:TYR:CD2 | 16:AP:38:TYR:N | 2.88 | 0.41 |
| 2:CB:111:ARG:HA | 2:CB:111:ARG:HD3 | 1.52 | 0.41 |
| 4:CD:146:ILE:N | 4:CD:146:ILE:HD12 | 2.36 | 0.41 |
| 22:CX:78:ILE:HA | 22:CX:78:ILE:HD13 | 1.83 | 0.41 |
| 40:BW:64:MET:HE3 | 40:BW:109:GLU:HG3 | 2.02 | 0.41 |
| 27:DF:167:ALA:HB1 | 27:DF:173:VAL:HG11 | 2.02 | 0.41 |
| 41:DX:25:LYS:HG3 | 41:DX:82:GLN:OE1 | 2.21 | 0.41 |
| 1:AA:32:A:C6 | 1:AA:33:A:C6 | 3.09 | 0.41 |
| 1:AA:1170:A:C2 | 1:AA:1171:G:H1' | 2.56 | 0.41 |
| 1:AA:1359:C:O2' | 1:AA:1361:G:N7 | 2.53 | 0.41 |
| 1:AA:1219:U:P | 14:AN:19:ARG:HH22 | 2.42 | 0.41 |
| 13:CM:19:LEU:HA | 13:CM:22:ILE:CD1 | 2.51 | 0.41 |
| 13:CM:25:ILE:HG23 | 13:CM:29:ARG:CB | 2.51 | 0.41 |
| 9:CI:109:VAL:HG22 | 9:CI:110:GLU:H | 1.86 | 0.41 |
| 1:AA:1235:U:H4' | 21:AU:4:GLY:H | 1.84 | 0.41 |
| 23:DA:2115:G:H4' | 23:DA:2167:U:C4' | 2.45 | 0.41 |
| 1:CA:436:C:O2' | 1:CA:437:U:P | 2.79 | 0.41 |
| 1:CA:437:U:C4 | 1:CA:438:G:C6 | 3.09 | 0.41 |
| 23:BA:2108:C:H42 | 23:BA:2181:G:H1 | 1.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:1507:A:O2' | 23:DA:1508:A:C8 | 2.63 | 0.41 |
| 1:CA:148:G:C2 | 1:CA:149:A:N7 | 2.88 | 0.41 |
| 23:BA:2893:G:H2' | 23:BA:2893:G:N3 | 2.36 | 0.41 |
| 9:AI:76:ALA:O | 9:AI:80:GLY:N | 2.29 | 0.41 |
| 4:AD:156:GLU:OE1 | 4:AD:156:GLU:N | 2.53 | 0.41 |
| 28:BG:139:LEU:HB3 | 28:BG:144:ILE:HG22 | 2.03 | 0.41 |
| 3:CC:150:LYS:O | 3:CC:201:TYR:N | 2.54 | 0.41 |
| 28:BG:174:GLU:HG2 | 28:BG:180:PHE:CD1 | 2.56 | 0.41 |
| 1:CA:1292:U:O2' | 1:CA:1293:G:H5' | 2.20 | 0.41 |
| 1:CA:1268:A:O2' | 1:CA:1326:C:H4' | 2.21 | 0.41 |
| 23:DA:198:C:H5' | 23:DA:2244:U:OP1 | 2.21 | 0.41 |
| 1:CA:836:G:C6 | 1:CA:851:G:C6 | 3.09 | 0.41 |
| 2:CB:74:LYS:H | 2:CB:74:LYS:HG2 | 1.58 | 0.41 |
| 3:CC:184:TYR:HA | 3:CC:200:ALA:O | 2.21 | 0.41 |
| 1:AA:375:U:H4' | 16:AP:17:TYR:CE2 | 2.55 | 0.41 |
| 3:AC:40:ARG:O | 3:AC:44:GLU:HB2 | 2.20 | 0.41 |
| 40:DW:79:GLY:CA | 40:DW:100:THR:HG22 | 2.49 | 0.41 |
| 1:CA:685:G:C2 | 1:CA:686:U:C4 | 3.09 | 0.41 |
| 1:CA:627:G:N3 | 1:CA:628:G:C8 | 2.88 | 0.41 |
| 2:AB:215:LEU:HD23 | 2:AB:215:LEU:HA | 1.68 | 0.41 |
| 43:BZ:152:ALA:HA | 43:BZ:155:LEU:HB2 | 2.02 | 0.41 |
| 1:AA:933:G:P | 7:AG:4:ARG:HE | 2.41 | 0.41 |
| 7:AG:75:VAL:HG11 | 7:AG:144:MET:HB3 | 2.02 | 0.41 |
| 23:DA:322:A:H4' | 23:DA:323:G:OP2 | 2.21 | 0.41 |
| 23:DA:189:G:H2' | 23:DA:205:G:N2 | 2.36 | 0.41 |
| 44:B0:25:ARG:HD2 | 44:B0:29:GLN:NE2 | 2.36 | 0.41 |
| 34:BQ:72:LYS:HB3 | 34:BQ:94:VAL:HG23 | 2.03 | 0.41 |
| 23:BA:1257:C:O2' | 27:BF:84:VAL:HG23 | 2.20 | 0.41 |
| 23:DA:481:G:H1' | 23:DA:507:A:N1 | 2.36 | 0.41 |
| 12:AL:53:ARG:NH1 | 12:AL:92:ASP:OD2 | 2.54 | 0.41 |
| 23:DA:410:G:C2 | 23:DA:418:G:C2 | 3.09 | 0.41 |
| 26:BE:37:ARG:HB2 | 26:BE:46:ALA:N | 2.36 | 0.41 |
| 1:AA:200:G:H2' | 1:AA:201:C:O4' | 2.21 | 0.41 |
| 23:BA:2330:G:H2' | 23:BA:2331:G:O4' | 2.21 | 0.41 |
| 34:DQ:110:THR:HG23 | 34:DQ:113:GLN:HB2 | 2.02 | 0.41 |
| 28:BG:169:ALA:O | 28:BG:173:LEU:HG | 2.21 | 0.41 |
| 27:BF:196:LEU:HA | 27:BF:196:LEU:HD23 | 1.72 | 0.41 |
| 27:BF:112:MET:HE2 | 27:BF:112:MET:HB2 | 1.91 | 0.41 |
| 28:BG:128:ARG:HE | 28:BG:128:ARG:HB2 | 1.55 | 0.41 |
| 39:BV:18:LEU:HA | 39:BV:18:LEU:HD23 | 1.84 | 0.41 |
| 23:BA:1336:A:H2' | 23:BA:1337:G:C8 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:2338:G:O2' | 23:DA:2339:G:H5' | 2.21 | 0.41 |
| 23:DA:1957:C:H2' | 23:DA:1958:C:C6 | 2.56 | 0.41 |
| 23:DA:862:G:OP2 | 56:DA:4349:HOH:O | 2.21 | 0.41 |
| 47:D3:36:VAL:O | 47:D3:37:LEU:HD23 | 2.20 | 0.41 |
| 24:DB:113:G:H2' | 24:DB:114:C:O4' | 2.21 | 0.41 |
| 23:BA:883:G:O5' | 23:BA:883:G:H8 | 2.04 | 0.40 |
| 1:AA:1008:C:H2' | 1:AA:1009:G:O4' | 2.21 | 0.40 |
| 9:CI:9:ARG:HA | 9:CI:14:VAL:HA | 2.03 | 0.40 |
| 1:AA:78:G:O2' | 1:AA:79:G:OP2 | 2.36 | 0.40 |
| 2:AB:70:PHE:HE2 | 2:AB:163:PHE:HD2 | 1.69 | 0.40 |
| 23:DA:1971:A:H5'' | 56:DA:4209:HOH:O | 2.19 | 0.40 |
| 1:AA:951:G:N3 | 1:AA:970:C:O2' | 2.50 | 0.40 |
| 1:CA:1204:A:H5'' | 1:CA:1205:U:OP2 | 2.21 | 0.40 |
| 1:CA:1206:G:C2' | 1:CA:1207:G:H5' | 2.51 | 0.40 |
| 33:DP:38:GLN:C | 33:DP:40:SER:N | 2.74 | 0.40 |
| 1:AA:1255:G:H3' | 1:AA:1279:A:H61 | 1.87 | 0.40 |
| 1:AA:1099:G:H5' | 1:AA:1100:C:OP2 | 2.21 | 0.40 |
| 1:AA:1202:G:H1' | 14:AN:42:ILE:HD13 | 2.02 | 0.40 |
| 10:AJ:91:PRO:CG | 10:AJ:94:VAL:HB | 2.42 | 0.40 |
| 23:BA:2125:G:N2 | 23:BA:2126:A:N6 | 2.69 | 0.40 |
| 3:CC:54:ARG:HB3 | 3:CC:69:HIS:CD2 | 2.57 | 0.40 |
| 13:AM:3:ARG:CZ | 13:AM:3:ARG:HB2 | 2.51 | 0.40 |
| 23:DA:26:G:H1' | 23:DA:515:A:H61 | 1.86 | 0.40 |
| 23:BA:2791:C:C4 | 23:BA:2893:G:O4' | 2.73 | 0.40 |
| 4:AD:98:GLU:O | 4:AD:104:VAL:HG23 | 2.21 | 0.40 |
| 1:CA:1318:A:H4' | 19:CS:10:PHE:CD2 | 2.56 | 0.40 |
| 2:CB:94:ASN:HB3 | 2:CB:95:GLN:NE2 | 2.36 | 0.40 |
| 6:AF:97:PHE:CD2 | 18:AR:31:LEU:HD21 | 2.50 | 0.40 |
| 1:AA:622:A:C8 | 1:AA:623:C:C6 | 3.09 | 0.40 |
| 1:CA:628:G:O2' | 1:CA:629:G:H5' | 2.21 | 0.40 |
| 23:DA:2110:G:C6 | 23:DA:2120:G:C8 | 3.09 | 0.40 |
| 23:BA:652(T):C:H2' | 23:BA:652(U):G:C8 | 2.56 | 0.40 |
| 23:DA:2464:C:N3 | 23:DA:2487:G:C2 | 2.89 | 0.40 |
| 23:DA:652(B):A:O2' | 23:DA:652(C):G:H5' | 2.21 | 0.40 |
| 1:AA:832:C:N3 | 1:AA:855:G:C6 | 2.89 | 0.40 |
| 2:CB:25:ASN:HA | 2:CB:26:PRO:HD2 | 1.93 | 0.40 |
| 23:DA:1790:C:H2' | 23:DA:1791:A:C5 | 2.56 | 0.40 |
| 1:AA:357:G:C2 | 1:AA:358:U:C5 | 3.09 | 0.40 |
| 23:BA:288:C:H2' | 23:BA:289:A:C8 | 2.56 | 0.40 |
| 23:BA:2251:G:C6 | 23:BA:2252:G:C6 | 3.09 | 0.40 |
| 34:BQ:59:ARG:HB3 | 34:BQ:60:ARG:H | 1.73 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:DD:146:GLU:HG2 | 25:DD:152:GLY:C | 2.41 | 0.40 |
| 1:CA:1091:U:C2 | 1:CA:1095:U:C4 | 3.09 | 0.40 |
| 1:CA:1095:U:OP2 | 1:CA:1108:G:N1 | 2.50 | 0.40 |
| 23:BA:19:C:H2' | 23:BA:20:C:C6 | 2.57 | 0.40 |
| 23:DA:2791:C:OP2 | 23:DA:2791:C:H3' | 2.21 | 0.40 |
| 23:DA:1417:C:H2' | 23:DA:1418:G:O4' | 2.21 | 0.40 |
| 18:AR:56:THR:HB | 18:AR:58:LEU:HD13 | 2.03 | 0.40 |
| 2:AB:37:ASN:O | 2:AB:39:ILE:HD12 | 2.21 | 0.40 |
| 2:AB:38:GLY:O | 2:AB:39:ILE:HG13 | 2.21 | 0.40 |
| 34:DQ:30:GLY:HA2 | 34:DQ:107:ALA:HB2 | 2.03 | 0.40 |
| 19:CS:35:SER:HA | 19:CS:37:ARG:HG2 | 2.03 | 0.40 |
| 23:BA:224:G:H2' | 23:BA:225:A:O4' | 2.22 | 0.40 |
| 35:DR:62:ALA:O | 35:DR:66:VAL:HG23 | 2.21 | 0.40 |
| 1:CA:489:C:C4 | 1:CA:490:G:N7 | 2.89 | 0.40 |
| 1:AA:134:A:H1' | 1:AA:325:A:C5 | 2.56 | 0.40 |
| 8:CH:134:ILE:HG22 | 8:CH:135:CYS:SG | 2.61 | 0.40 |
| 23:DA:1655:A:H3' | 23:DA:1656:C:H6 | 1.86 | 0.40 |
| 1:CA:115:G:H4' | 1:CA:116:A:O5' | 2.19 | 0.40 |
| 33:DP:147:LEU:HD22 | 33:DP:147:LEU:HA | 1.87 | 0.40 |
| 4:AD:94:LEU:HD23 | 4:AD:94:LEU:HA | 1.89 | 0.40 |
| 27:BF:103:LYS:HG3 | 27:BF:103:LYS:H | 1.74 | 0.40 |
| 28:BG:36:LYS:HE3 | 28:BG:160:VAL:HG21 | 2.03 | 0.40 |
| 1:CA:875:C:H5'' | 1:CA:876:G:OP2 | 2.21 | 0.40 |
| 1:CA:693:G:H2' | 1:CA:694:A:C8 | 2.56 | 0.40 |
| 23:DA:686:G:N2 | 23:DA:788:A:H61 | 2.20 | 0.40 |
| 1:CA:145:G:C6 | 1:CA:146:G:C5 | 3.09 | 0.40 |
| 17:CQ:99:SER:C | 17:CQ:100:LYS:HD3 | 2.41 | 0.40 |
| 1:AA:1189:C:OP1 | 10:AJ:51:ARG:NH2 | 2.51 | 0.40 |
| 1:AA:1452:C:H6 | 1:AA:1452:C:H5'' | 1.86 | 0.40 |
| 1:CA:1089:G:C6 | 1:CA:1090:U:C4 | 3.09 | 0.40 |
| 23:BA:2228:G:C5 | 23:BA:2229:C:C4 | 3.09 | 0.40 |
| 23:BA:271(H):G:O2' | 23:BA:271(I):G:P | 2.79 | 0.40 |
| 23:DA:1971:A:C4 | 25:DD:241:PRO:HD3 | 2.56 | 0.40 |
| 1:CA:1308:U:H5' | 13:CM:110:ARG:CZ | 2.51 | 0.40 |
| 33:BP:127:ALA:C | 33:BP:148:LEU:HD23 | 2.40 | 0.40 |
| 1:CA:1287:A:N6 | 1:CA:1370:G:H21 | 2.18 | 0.40 |
| 1:CA:959:A:H2' | 1:CA:960:U:H4' | 2.02 | 0.40 |
| 1:CA:78:G:H1 | 1:CA:91:C:H42 | 1.68 | 0.40 |
| 24:BB:90:A:N7 | 24:BB:91:C:H1' | 2.36 | 0.40 |
| 23:DA:28:A:C5 | 23:DA:29:U:C5 | 3.09 | 0.40 |
| 23:DA:31:C:C4 | 23:DA:32:C:C5 | 3.10 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:BA:1817:G:H2' | 23:BA:1818:U:H5' | 2.03 | 0.40 |
| 1:AA:1345:U:OP1 | 9:AI:120:ARG:NH1 | 2.54 | 0.40 |
| 23:BA:2892:A:C2' | 23:BA:2893:G:H5' | 2.51 | 0.40 |
| 23:BA:1224:C:O5' | 23:BA:1224:C:H6 | 2.04 | 0.40 |
| 23:DA:1512:U:H2' | 23:DA:1513:C:H6 | 1.87 | 0.40 |
| 1:CA:997:U:O5' | 1:CA:997:U:H6 | 2.04 | 0.40 |
| 23:BA:2561:A:H2' | 23:BA:2562:U:O4' | 2.21 | 0.40 |
| 1:CA:918:A:H2' | 1:CA:919:A:O4' | 2.21 | 0.40 |
| 5:CE:102:ALA:O | 5:CE:107:ARG:NH1 | 2.54 | 0.40 |
| 10:CJ:45:ARG:HD3 | 10:CJ:65:LEU:HD23 | 2.02 | 0.40 |
| 23:BA:1450:G:H2' | 23:BA:1450(A):C:C6 | 2.56 | 0.40 |
| 1:CA:377:G:H2' | 1:CA:378:G:H8 | 1.82 | 0.40 |
| 23:BA:1876:A:OP2 | 23:BA:1876:A:H8 | 2.04 | 0.40 |
| 23:BA:7:G:H2' | 23:BA:8:A:O4' | 2.20 | 0.40 |
| 25:DD:275:LYS:HG3 | 25:DD:275:LYS:O | 2.21 | 0.40 |
| 11:AK:91:ARG:NH1 | 11:AK:110:ASP:OD1 | 2.55 | 0.40 |
| 23:DA:2492:U:H2' | 23:DA:2493:U:H6 | 1.83 | 0.40 |
| 2:CB:70:PHE:HE2 | 2:CB:163:PHE:HD2 | 1.69 | 0.40 |
| 25:BD:180:GLY:HA3 | 25:BD:275:LYS:HG2 | 2.03 | 0.40 |
| 1:CA:536:C:H2' | 1:CA:537:G:C8 | 2.56 | 0.40 |
| 33:DP:86:LYS:HB3 | 33:DP:117:GLU:O | 2.22 | 0.40 |
| 16:CP:39:TYR:CG | 16:CP:73:LEU:HD13 | 2.56 | 0.40 |
| 1:CA:333:G:H4' | 20:CT:16:HIS:CE1 | 2.56 | 0.40 |
| 1:AA:189(C):C:H2' | 1:AA:189(D):C:O4' | 2.21 | 0.40 |
| 1:AA:1445:C:H2' | 1:AA:1446:U:H5' | 2.04 | 0.40 |
| 1:AA:693:G:H2' | 1:AA:694:A:C8 | 2.56 | 0.40 |
| 43:BZ:44:PHE:CE2 | 43:BZ:86:VAL:HG11 | 2.56 | 0.40 |
| 30:DI:45:LYS:O | 30:DI:48:GLU:N | 2.54 | 0.40 |
| 1:AA:35:G:H2' | 1:AA:36:C:H6 | 1.86 | 0.40 |
| 23:DA:610:G:N2 | 23:DA:619:G:H1' | 2.35 | 0.40 |
| 1:CA:318:G:H2' | 1:CA:319:G:H8 | 1.85 | 0.40 |
| 23:DA:2360:A:H8 | 23:DA:2360:A:O5' | 2.05 | 0.40 |
| 23:DA:478:A:N6 | 23:DA:502:A:N6 | 2.69 | 0.40 |
| 23:DA:719:C:H2' | 23:DA:720:C:H6 | 1.87 | 0.40 |
| 1:AA:789:U:O2 | 1:AA:791:G:C8 | 2.74 | 0.40 |
| 1:AA:690:G:C6 | 1:AA:691:G:C6 | 3.09 | 0.40 |
| 31:DN:12:ARG:HD3 | 31:DN:50:ASP:OD2 | 2.21 | 0.40 |
| 23:DA:2714:G:O2' | 23:DA:2715:C:H5' | 2.20 | 0.40 |
| 8:CH:38:ILE:HG13 | 8:CH:118:VAL:HG12 | 2.03 | 0.40 |
| 1:CA:620:C:H2' | 1:CA:621:A:O4' | 2.21 | 0.40 |
| 23:BA:1194:A:N7 | 56:BA:5296:HOH:O | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AH:81:HIS:N | 8:AH:138:TRP:O | 2.54 | 0.40 |
| 1:AA:1496:C:H2' | 1:AA:1497:G:O4' | 2.21 | 0.40 |
| 27:DF:202:PHE:O | 27:DF:205:ARG:HB3 | 2.21 | 0.40 |
| 23:DA:2100:G:C6 | 23:DA:2101:G:C5 | 3.09 | 0.40 |
| 24:BB:24:G:N7 | 24:BB:56:G:H2' | 2.36 | 0.40 |
| 23:DA:2584:U:H2' | 23:DA:2585:U:H2' | 2.02 | 0.40 |
| 23:BA:2241:A:N7 | 56:BA:4293:HOH:O | 2.37 | 0.40 |
| 23:BA:2709:G:N2 | 56:BA:4848:HOH:O | 2.54 | 0.40 |
| 4:AD:111:ALA:HB1 | 4:AD:116:GLN:OE1 | 2.21 | 0.40 |
| 23:BA:2349:G:OP1 | 56:BA:3933:HOH:O | 2.22 | 0.40 |
| 23:BA:719:C:O5' | 23:BA:719:C:H6 | 2.04 | 0.40 |
| 23:DA:895:U:H6 | 23:DA:895:U:H5'' | 1.86 | 0.40 |
| 27:DF:93:LYS:HD3 | 27:DF:93:LYS:HA | 1.85 | 0.40 |
| 25:BD:67:PHE:HB3 | 25:BD:153:ALA:H | 1.86 | 0.40 |
| 20:CT:89:ARG:HH22 | 20:CT:104:LEU:H | 1.67 | 0.40 |
| 23:BA:1247:A:OP1 | 27:BF:95:ARG:NH2 | 2.46 | 0.40 |
| 23:BA:2342:C:O2' | 23:BA:2374:C:H5'' | 2.21 | 0.40 |
| 29:BH:35:VAL:HA | 29:BH:36:PRO:HD2 | 1.74 | 0.40 |
| 1:AA:634:C:H2' | 1:AA:635:G:H8 | 1.86 | 0.40 |
| 23:BA:2296:U:N3 | 23:BA:2333:A:C2 | 2.89 | 0.40 |
| 23:BA:884:C:H2' | 23:BA:885:C:O4' | 2.22 | 0.40 |
| 1:AA:1002:G:C2 | 1:AA:1003:G:H1' | 2.57 | 0.40 |
| 4:AD:22:LYS:HB3 | 4:AD:26:CYS:HB2 | 2.02 | 0.40 |
| 1:AA:1121:U:O2' | 1:AA:1122:U:H5' | 2.20 | 0.40 |
| 1:AA:91:C:H6 | 1:AA:91:C:O5' | 2.04 | 0.40 |
| 9:AI:5:TYR:HE1 | 9:AI:16:ARG:HA | 1.87 | 0.40 |
| 1:CA:1392:G:N2 | 1:CA:1502:A:H8 | 2.19 | 0.40 |
| 13:CM:86:CYS:SG | 13:CM:88:ARG:HG2 | 2.62 | 0.40 |
| 23:DA:2286:A:H4' | 23:DA:2287:A:O4' | 2.22 | 0.40 |
| 1:AA:1074:G:N3 | 1:AA:1102:A:C2 | 2.90 | 0.40 |
| 23:BA:2317:C:C2' | 23:BA:2318:G:H5' | 2.39 | 0.40 |
| 1:CA:1300:G:O2' | 1:CA:1301:U:O5' | 2.33 | 0.40 |
| 1:CA:1296:C:H4' | 1:CA:1302:U:C5 | 2.56 | 0.40 |
| 1:CA:1300:G:O6 | 1:CA:1334:G:H3' | 2.21 | 0.40 |
| 1:CA:1250:A:N1 | 1:CA:1251:A:N1 | 2.70 | 0.40 |
| 23:BA:1022:G:C5 | 23:BA:1140:C:C4 | 3.09 | 0.40 |
| 1:AA:267:C:OP2 | 17:AQ:67:LYS:HD2 | 2.21 | 0.40 |
| 1:AA:1030(C):G:H3' | 1:AA:1030(C):G:H8 | 1.86 | 0.40 |
| 36:BS:32:LEU:HA | 36:BS:32:LEU:HD23 | 1.85 | 0.40 |
| 28:DG:97:ASP:O | 28:DG:101:ILE:HG13 | 2.22 | 0.40 |
| 23:BA:1996:C:H4' | 23:BA:1997:G:OP1 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:DA:996:A:N6 | 23:DA:1160:G:C6 | 2.90 | 0.40 |
| 23:DA:1558:A:N3 | 23:DA:1558:A:O4' | 2.52 | 0.40 |
| 23:DA:123:G:H2' | 23:DA:124:G:O4' | 2.21 | 0.40 |
| 4:CD:18:LYS:HG3 | 4:CD:31:CYS:SG | 2.60 | 0.40 |
| 23:BA:530:G:O6 | 23:BA:2023:G:OP1 | 2.39 | 0.40 |
| 8:AH:36:LEU:O | 8:AH:45:ILE:HD11 | 2.21 | 0.40 |
| 11:AK:110:ASP:CB | 18:AR:85:LEU:HD12 | 2.52 | 0.40 |
| 40:DW:59:VAL:HG12 | 40:DW:60:ASN:HD22 | 1.86 | 0.40 |
| 7:AG:108:ALA:O | 7:AG:111:ARG:HB2 | 2.22 | 0.40 |
| 7:AG:113:GLU:O | 7:AG:119:ARG:HB2 | 2.20 | 0.40 |
| 24:BB:8:U:H5' | 24:BB:9:G:OP2 | 2.21 | 0.40 |
| 23:DA:275:G:H2' | 23:DA:276:A:H5' | 2.04 | 0.40 |
| 46:B2:50:ILE:C | 46:B2:52:ASP:N | 2.73 | 0.40 |
| 1:AA:855:G:C6 | 1:AA:856:C:C4 | 3.09 | 0.40 |
| 24:DB:60:C:C2 | 24:DB:61:G:C8 | 3.09 | 0.40 |
| 1:CA:1265:G:N2 | 1:CA:1271:G:C4 | 2.90 | 0.40 |
| 1:CA:1270:C:H6 | 1:CA:1270:C:O5' | 2.05 | 0.40 |
| 27:BF:34:TRP:NE1 | 33:BP:8:PRO:HD3 | 2.36 | 0.40 |
| 31:DN:67:LEU:O | 31:DN:88:GLU:HG3 | 2.21 | 0.40 |
| 23:BA:704:G:H1' | 23:BA:726:G:N2 | 2.37 | 0.40 |
| 41:BX:84:ALA:HB3 | 41:BX:87:GLN:CD | 2.41 | 0.40 |
| 11:CK:34:ASP:OD2 | 11:CK:38:ASN:N | 2.54 | 0.40 |
| 23:DA:414:C:O2' | 23:DA:415:A:H5' | 2.22 | 0.40 |
| 20:AT:53:LEU:O | 20:AT:56:MET:HG3 | 2.21 | 0.40 |
| 1:CA:665:A:H2' | 1:CA:725:G:N2 | 2.36 | 0.40 |
| 33:DP:106:LEU:HD23 | 33:DP:106:LEU:HA | 1.88 | 0.40 |
| 1:CA:1429:C:H2' | 1:CA:1430:C:H6 | 1.86 | 0.40 |
| 1:CA:1429:C:O2' | 23:DA:1704:G:H5' | 2.21 | 0.40 |
| 23:DA:303:U:H2' | 23:DA:304:G:H8 | 1.86 | 0.40 |
| 23:BA:2301:C:H2' | 23:BA:2302:G:H8 | 1.86 | 0.40 |
| 3:CC:52:LEU:O | 3:CC:52:LEU:HD23 | 2.21 | 0.40 |
| 49:D5:36:CYS:O | 49:D5:37:LYS:HD3 | 2.22 | 0.40 |
| 1:AA:566:G:H4' | 1:AA:567:G:OP1 | 2.21 | 0.40 |
| 35:BR:53:HIS:O | 35:BR:56:LYS:HB2 | 2.20 | 0.40 |
| 26:DE:203:LYS:CB | 26:DE:204:ALA:HA | 2.51 | 0.40 |
| 28:BG:20:ILE:O | 28:BG:24:GLY:N | 2.46 | 0.40 |
| 1:CA:729:A:H2' | 1:CA:730:G:H8 | 1.87 | 0.40 |
| 1:CA:127:G:O2' | 17:CQ:2:PRO:O | 2.39 | 0.40 |
| 9:AI:78:LYS:O | 9:AI:82:ALA:HB3 | 2.22 | 0.40 |
| 18:CR:53:ARG:HE | 18:CR:59:SER:C | 2.25 | 0.40 |
| 25:BD:183:ARG:HG3 | 25:BD:270:ILE:HG12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 37:BT:99:LEU:HD22 | 37:BT:101:PHE:HE1 | 1.85 | 0.40 |
| 1:AA:875:C:C4 | 1:AA:876:G:N7 | 2.90 | 0.40 |
| 23:BA:1213:A:N3 | 23:BA:1238:G:O2' | 2.45 | 0.40 |
| 35:DR:67:LEU:HD13 | 35:DR:67:LEU:HA | 1.72 | 0.40 |
| 23:BA:1647:G:H3' | 23:BA:1647:G:P | 2.60 | 0.40 |
| 43:BZ:76:LEU:HD12 | 43:BZ:76:LEU:HA | 1.64 | 0.40 |
| 43:DZ:92:SER:HB2 | 43:DZ:94:GLU:HG2 | 2.03 | 0.40 |
| 23:DA:1864:U:H5'' | 23:DA:2410:G:O2' | 2.22 | 0.40 |
| 27:DF:170:LEU:HA | 27:DF:171:PRO:HD3 | 1.90 | 0.40 |
| 1:AA:127:G:O2' | 17:AQ:2:PRO:O | 2.39 | 0.40 |
| 1:CA:1442(A):G:C3' | 1:CA:1442(B):A:H5'' | 2.51 | 0.40 |
| 35:BR:2:ARG:CZ | 35:BR:2:ARG:HB3 | 2.46 | 0.40 |
| 1:AA:1005:A:C8 | 1:AA:1005:A:OP2 | 2.75 | 0.40 |
| 1:AA:1151:A:C5' | 10:AJ:41:PRO:HA | 2.51 | 0.40 |
| 1:AA:1097:C:H1' | 1:AA:1170:A:H1' | 2.03 | 0.40 |
| 19:AS:36:ARG:HH22 | 19:AS:76:PRO:HA | 1.87 | 0.40 |
| 5:AE:127:ASN:HA | 5:AE:128:PRO:HD3 | 1.85 | 0.40 |
| 23:DA:2287:A:N6 | 23:DA:2344:U:N3 | 2.56 | 0.40 |
| 28:DG:16:ARG:NE | 28:DG:31:VAL:HG21 | 2.33 | 0.40 |
| 23:DA:2427:C:H5'' | 23:DA:2428:G:OP1 | 2.22 | 0.40 |
| 23:BA:921:G:H2' | 23:BA:922:U:C6 | 2.57 | 0.40 |
| 7:CG:38:LEU:O | 7:CG:42:ILE:HG12 | 2.22 | 0.40 |
| 28:BG:97:ASP:O | 28:BG:101:ILE:HG13 | 2.22 | 0.40 |
| 1:AA:1030(D):A:H62 | 1:AA:1031:G:H21 | 1.70 | 0.40 |
| 23:DA:1606:G:H5'' | 23:DA:1607:C:OP1 | 2.21 | 0.40 |
| 31:DN:47:ALA:HB2 | 31:DN:112:LEU:CD1 | 2.45 | 0.40 |
| 1:CA:1072:G:C2 | 1:CA:1104:G:C2 | 3.10 | 0.40 |
| 23:DA:1722:A:C2 | 23:DA:1740:G:C8 | 3.09 | 0.40 |
| 5:AE:90:VAL:HG23 | 5:AE:121:LYS:O | 2.21 | 0.40 |
| 1:CA:68:G:N2 | 1:CA:152:A:O2' | 2.55 | 0.40 |
| 48:D4:9:LEU:HD22 | 48:D4:26:SER:HA | 2.02 | 0.40 |
| 1:CA:1175:G:C2 | 1:CA:1176:A:C4 | 3.10 | 0.40 |
| 1:AA:519:C:H2' | 1:AA:520:A:C8 | 2.55 | 0.40 |
| 23:BA:528:A:N1 | 23:BA:2043:C:O5' | 2.55 | 0.40 |
| 23:BA:563:G:H5' | 23:BA:572:A:H4' | 2.04 | 0.40 |
| 1:CA:1256:A:H5'' | 1:CA:1257:U:OP1 | 2.21 | 0.40 |
| 15:AO:21:ASP:OD2 | 15:AO:24:SER:HB3 | 2.21 | 0.40 |
| 26:DE:9:VAL:HB | 37:DT:3:ARG:HG2 | 2.02 | 0.40 |
| 1:AA:827:U:H5'' | 1:AA:828:A:OP2 | 2.20 | 0.40 |
| 17:CQ:13:ASP:HB3 | 17:CQ:19:VAL:HG12 | 2.03 | 0.40 |
| 23:BA:2628:C:H5'' | 23:BA:2629:A:O5' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:628:G:O2' | 1:AA:629:G:H5' | 2.21 | 0.40 |
| 23:DA:994:C:OP1 | 38:DU:53:ARG:NH2 | 2.53 | 0.40 |
| 23:DA:315:G:H2' | 23:DA:316:C:H6 | 1.87 | 0.40 |
| 23:DA:1602:U:O4 | 56:DA:3939:HOH:O | 2.21 | 0.40 |
| 1:AA:663:A:C2' | 1:AA:664:G:H5' | 2.51 | 0.40 |
| 1:AA:683:G:C2 | 1:AA:708:C:C2 | 3.09 | 0.40 |
| 34:DQ:42:ILE:CG2 | 34:DQ:47:ILE:HG13 | 2.51 | 0.40 |
| 1:CA:35:G:N3 | 12:CL:118:SER:HB2 | 2.37 | 0.40 |
| 3:AC:30:ARG:HH21 | 14:AN:35:ARG:HA | 1.86 | 0.40 |
| 1:CA:1446:U:H4' | 1:CA:1447:A:C6 | 2.56 | 0.40 |
| 44:D0:14:ARG:HG3 | 44:D0:14:ARG:NH1 | 2.36 | 0.40 |
| 23:DA:1579:A:H2' | 23:DA:1580:A:C8 | 2.56 | 0.40 |
| 23:DA:2099:U:H3 | 23:DA:2190:G:H1 | 1.68 | 0.40 |
| 26:DE:179:GLU:HB3 | 26:DE:181:LEU:CD2 | 2.51 | 0.40 |
| 34:DQ:35:VAL:HG23 | 34:DQ:101:ARG:O | 2.20 | 0.40 |
| 23:DA:1756:G:H4' | 23:DA:1758:G:O4' | 2.22 | 0.40 |
| 9:CI:52:ALA:HB2 | 9:CI:101:PHE:CE1 | 2.56 | 0.40 |
| 23:BA:1448:G:H5'' | 23:BA:1542:A:OP1 | 2.21 | 0.40 |
| 23:BA:2409:G:C6 | 23:BA:2410:G:C5 | 3.09 | 0.40 |
| 39:DV:24:LYS:HA | 39:DV:92:THR:OG1 | 2.22 | 0.40 |
| 1:AA:870:U:H3' | 56:AA:1963:HOH:O | 2.21 | 0.40 |
| 23:DA:1918:A:O2' | 23:DA:1920:C:N4 | 2.54 | 0.40 |
| 9:AI:103:THR:HG23 | 9:AI:103:THR:O | 2.21 | 0.40 |
| 43:BZ:70:LEU:HD23 | 43:BZ:70:LEU:HA | 1.93 | 0.40 |
| 34:DQ:7:MET:HE3 | 34:DQ:7:MET:HB2 | 1.66 | 0.40 |
| 8:AH:30:ARG:O | 8:AH:34:GLU:HB2 | 2.21 | 0.40 |
| 23:BA:2818:G:O2' | 23:BA:2819:G:H5' | 2.21 | 0.40 |
| 1:CA:784:C:H4' | 23:DA:1837:C:OP1 | 2.21 | 0.40 |
| 23:BA:2466:C:C2 | 23:BA:2485:G:C2 | 3.09 | 0.40 |
| 1:CA:794:A:H2' | 1:CA:795:C:O4' | 2.21 | 0.40 |
| 1:AA:1316:G:H4' | 14:AN:18:VAL:CG1 | 2.51 | 0.40 |
| 1:AA:1360:A:C8 | 14:AN:18:VAL:HG12 | 2.56 | 0.40 |
| 9:CI:66:ARG:C | 9:CI:73:GLN:HE21 | 2.25 | 0.40 |
| 1:AA:560:U:H4' | 1:AA:561:U:C5' | 2.51 | 0.40 |
| 1:CA:1346:A:H4' | 1:CA:1347:G:OP1 | 2.21 | 0.40 |
| 1:CA:1262:C:H2' | 1:CA:1263:C:C6 | 2.56 | 0.40 |
| 23:BA:515:A:H1' | 23:BA:581:C:H1' | 2.04 | 0.40 |
| 1:CA:947:G:O2' | 1:CA:1306:A:H4' | 2.21 | 0.40 |
| 2:CB:205:ASP:C | 2:CB:211:ILE:HD11 | 2.42 | 0.40 |
| 2:CB:80:ILE:HG21 | 2:CB:208:ILE:CG2 | 2.51 | 0.40 |
| 23:DA:1204:A:N6 | 23:DA:1240:U:H2' | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:BI:37:VAL:HG12 | 30:BI:38:LEU:N | 2.36 | 0.40 |
| 10:CJ:40:LEU:HG | 10:CJ:69:ASN:O | 2.21 | 0.40 |
| 1:CA:1336:C:H4' | 1:CA:1337:G:O4' | 2.22 | 0.40 |
| 23:BA:1019:U:H3 | 23:BA:1142(A):A:N6 | 2.06 | 0.40 |
| 56:BA:4338:HOH:O | 45:B1:18:ILE:N | 2.48 | 0.40 |
| 23:DA:26:G:C6 | 23:DA:27:G:N1 | 2.89 | 0.40 |
| 1:CA:1313:U:H3 | 1:CA:1324:A:H61 | 1.69 | 0.40 |
| 23:BA:2791:C:H2' | 23:BA:2792:G:C8 | 2.57 | 0.40 |
| 9:AI:67:GLY:O | 9:AI:73:GLN:HG3 | 2.22 | 0.40 |
| 1:CA:126:G:OP1 | 1:CA:605:U:O2' | 2.39 | 0.40 |
| 42:BY:14:LEU:HD12 | 42:BY:23:ARG:O | 2.21 | 0.40 |
| 13:AM:92:HIS:HA | 13:AM:110:ARG:HH22 | 1.86 | 0.40 |
| 13:AM:92:HIS:CE1 | 13:AM:98:VAL:HG21 | 2.56 | 0.40 |
| 23:BA:271(S):G:C6 | 23:BA:271(T):C:C4 | 3.09 | 0.40 |
| 23:BA:314:A:H2' | 23:BA:315:G:H5' | 2.03 | 0.40 |
| 23:BA:2762:G:H2' | 23:BA:2763:G:H5' | 2.04 | 0.40 |
| 23:BA:1406:U:H2' | 23:BA:1407:C:H6 | 1.83 | 0.40 |
| 23:BA:1154:G:O5' | 23:BA:1154:G:H8 | 2.04 | 0.40 |
| 2:CB:14:GLY:HA3 | 2:CB:16:HIS:CE1 | 2.56 | 0.40 |
| 23:DA:94:C:H2' | 23:DA:94:C:O2 | 2.20 | 0.40 |
| 23:DA:2406:U:H6 | 23:DA:2406:U:OP2 | 2.04 | 0.40 |
| 51:D7:47:ARG:HH11 | 51:D7:47:ARG:CG | 2.33 | 0.40 |
| 23:BA:646:A:H5' | 56:BA:5354:HOH:O | 2.21 | 0.40 |
| 24:DB:23:G:H1 | 24:DB:60:C:H42 | 1.69 | 0.40 |
| 1:CA:35:G:O2' | 12:CL:121:GLY:HA2 | 2.21 | 0.40 |
| 23:BA:2291:U:H2' | 23:BA:2292:C:C6 | 2.57 | 0.40 |
| 43:DZ:144:LEU:HD21 | 43:DZ:150:LEU:HG | 2.03 | 0.40 |
| 1:CA:105:G:H2' | 1:CA:106:C:H6 | 1.87 | 0.40 |
| 23:BA:1260:G:C6 | 23:BA:1261:C:C4 | 3.10 | 0.40 |
| 1:AA:1193:G:H4' | 5:AE:25:ARG:NH2 | 2.37 | 0.40 |
| 25:DD:154:LYS:HB2 | 25:DD:155:LEU:HD12 | 2.03 | 0.40 |
| 51:D7:48:LYS:HE2 | 51:D7:48:LYS:HB2 | 1.88 | 0.40 |
| 23:DA:2576:G:O2' | 23:DA:2579:C:OP2 | 2.29 | 0.40 |
| 1:CA:319:G:C2 | 1:CA:320:C:C2 | 3.10 | 0.40 |
| 23:DA:2070:G:H2' | 23:DA:2071:A:C8 | 2.57 | 0.40 |
| 8:CH:112:LEU:HB3 | 8:CH:133:LEU:HA | 2.03 | 0.40 |
| 11:AK:82:VAL:O | 11:AK:109:VAL:HG23 | 2.21 | 0.40 |
| 24:BB:77:U:H4' | 43:BZ:84:GLU:OE1 | 2.22 | 0.40 |
| 18:AR:56:THR:CB | 18:AR:58:LEU:HD13 | 2.52 | 0.40 |
| 16:CP:40:ASP:HA | 16:CP:41:PRO:HD2 | 1.93 | 0.40 |
| 23:DA:2139:C:H2' | 23:DA:2140:C:O4' | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:AD:7:PRO:HB2 | 4:AD:10:ARG:HD2 | 2.03 | 0.40 |
| 23:DA:2729:G:H2' | 23:DA:2730:C:C6 | 2.56 | 0.40 |
| 26:BE:97:LYS:HA | 26:BE:98:PRO:HD3 | 1.96 | 0.40 |
| 28:BG:125:PHE:CE1 | 28:BG:170:ARG:HG2 | 2.57 | 0.40 |
| 22:CX:68:GLN:O | 22:CX:72:ALA:HB3 | 2.22 | 0.40 |
| 3:AC:134:ILE:HG22 | 3:AC:168:ALA:HB3 | 2.03 | 0.40 |
| 23:DA:705:A:C2 | 23:DA:727:A:H1' | 2.57 | 0.40 |
| 23:DA:65:C:O2' | 23:DA:456:C:O2 | 2.39 | 0.40 |
| 1:AA:1041:A:C2' | 1:AA:1042:G:H5' | 2.52 | 0.40 |
| 23:DA:2028:U:H2' | 23:DA:2029:G:O4' | 2.22 | 0.40 |
| 23:DA:194:G:H2' | 23:DA:195:A:O4' | 2.21 | 0.40 |
| 26:BE:38:THR:O | 26:BE:42:ASP:N | 2.51 | 0.40 |
| 2:CB:100:GLY:HA3 | 2:CB:104:ASN:HB3 | 2.03 | 0.40 |
| 24:BB:117:G:O5' | 24:BB:117:G:H8 | 2.04 | 0.40 |
| 23:DA:1676:A:C8 | 56:DA:4368:HOH:O | 2.72 | 0.40 |
| 13:CM:105:THR:OG1 | 13:CM:106:ASN:N | 2.52 | 0.40 |
| 26:BE:203:LYS:CB | 26:BE:204:ALA:HA | 2.52 | 0.40 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 23:BA:1594:G:OP1 | 56:BB:323:HOH:O[1_455] | 2.18 | 0.02 |
| 30:BI:91:SER:OG | 1:CA:368:U:OP1[3_654] | 2.19 | 0.01 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AB | 228/256 (89%) | 199 (87%) | 28 (12%) | 1 (0%) | 39 | 75 |
| 2 | CB | 227/256 (89%) | 197 (87%) | 29 (13%) | 1 (0%) | 39 | 75 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | AC | 204/239 (85%) | 175 (86%) | 28 (14%) | 1 (0%) | 34 | 72 |
| 3 | CC | 204/239 (85%) | 177 (87%) | 27 (13%) | 0 | 100 | 100 |
| 4 | AD | 206/209 (99%) | 190 (92%) | 16 (8%) | 0 | 100 | 100 |
| 4 | CD | 206/209 (99%) | 190 (92%) | 16 (8%) | 0 | 100 | 100 |
| 5 | AE | 146/162 (90%) | 134 (92%) | 12 (8%) | 0 | 100 | 100 |
| 5 | CE | 146/162 (90%) | 135 (92%) | 10 (7%) | 1 (1%) | 26 | 65 |
| 6 | AF | 98/101 (97%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | CF | 98/101 (97%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 7 | AG | 153/156 (98%) | 138 (90%) | 13 (8%) | 2 (1%) | 15 | 50 |
| 7 | CG | 153/156 (98%) | 132 (86%) | 20 (13%) | 1 (1%) | 26 | 65 |
| 8 | AH | 136/138 (99%) | 131 (96%) | 5 (4%) | 0 | 100 | 100 |
| 8 | CH | 136/138 (99%) | 131 (96%) | 5 (4%) | 0 | 100 | 100 |
| 9 | AI | 123/128 (96%) | 112 (91%) | 10 (8%) | 1 (1%) | 24 | 63 |
| 9 | CI | 123/128 (96%) | 111 (90%) | 11 (9%) | 1 (1%) | 24 | 63 |
| 10 | AJ | 94/105 (90%) | 78 (83%) | 13 (14%) | 3 (3%) | 5 | 26 |
| 10 | CJ | 94/105 (90%) | 76 (81%) | 16 (17%) | 2 (2%) | 9 | 37 |
| 11 | AK | 112/129 (87%) | 106 (95%) | 6 (5%) | 0 | 100 | 100 |
| 11 | CK | 112/129 (87%) | 106 (95%) | 6 (5%) | 0 | 100 | 100 |
| 12 | AL | 120/132 (91%) | 110 (92%) | 9 (8%) | 1 (1%) | 24 | 63 |
| 12 | CL | 120/132 (91%) | 109 (91%) | 10 (8%) | 1 (1%) | 24 | 63 |
| 13 | AM | 112/126 (89%) | 89 (80%) | 21 (19%) | 2 (2%) | 11 | 42 |
| 13 | CM | 112/126 (89%) | 87 (78%) | 21 (19%) | 4 (4%) | 4 | 24 |
| 14 | AN | 58/61 (95%) | 47 (81%) | 9 (16%) | 2 (3%) | 5 | 25 |
| 14 | CN | 58/61 (95%) | 52 (90%) | 6 (10%) | 0 | 100 | 100 |
| 15 | AO | 86/89 (97%) | 75 (87%) | 9 (10%) | 2 (2%) | 8 | 35 |
| 15 | CO | 86/89 (97%) | 75 (87%) | 9 (10%) | 2 (2%) | 8 | 35 |
| 16 | AP | 80/88 (91%) | 75 (94%) | 4 (5%) | 1 (1%) | 15 | 50 |
| 16 | CP | 80/88 (91%) | 74 (92%) | 5 (6%) | 1 (1%) | 15 | 50 |
| 17 | AQ | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 17 | CQ | 97/105 (92%) | 89 (92%) | 8 (8%) | 0 | 100 | 100 |
| 18 | AR | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 18 | CR | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 19 | AS | 79/93 (85%) | 67 (85%) | 11 (14%) | 1 (1%) | 15 | 50 |
| 19 | CS | 79/93 (85%) | 65 (82%) | 13 (16%) | 1 (1%) | 15 | 50 |
| 20 | AT | 85/106 (80%) | 78 (92%) | 7 (8%) | 0 | 100 | 100 |
| 20 | CT | 95/106 (90%) | 84 (88%) | 8 (8%) | 3 (3%) | 5 | 26 |
| 21 | AU | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 21 | CU | 21/27 (78%) | 20 (95%) | 1 (5%) | 0 | 100 | 100 |
| 22 | AX | 93/101 (92%) | 79 (85%) | 13 (14%) | 1 (1%) | 17 | 55 |
| 22 | CX | 93/101 (92%) | 84 (90%) | 9 (10%) | 0 | 100 | 100 |
| 25 | BD | 273/276 (99%) | 260 (95%) | 12 (4%) | 1 (0%) | 39 | 75 |
| 25 | DD | 273/276 (99%) | 259 (95%) | 13 (5%) | 1 (0%) | 39 | 75 |
| 26 | BE | 202/206 (98%) | 190 (94%) | 10 (5%) | 2 (1%) | 19 | 58 |
| 26 | DE | 202/206 (98%) | 188 (93%) | 12 (6%) | 2 (1%) | 19 | 58 |
| 27 | BF | 201/210 (96%) | 195 (97%) | 6 (3%) | 0 | 100 | 100 |
| 27 | DF | 201/210 (96%) | 193 (96%) | 7 (4%) | 1 (0%) | 34 | 72 |
| 28 | BG | 179/182 (98%) | 150 (84%) | 28 (16%) | 1 (1%) | 30 | 68 |
| 28 | DG | 179/182 (98%) | 150 (84%) | 29 (16%) | 0 | 100 | 100 |
| 29 | BH | 172/180 (96%) | 163 (95%) | 8 (5%) | 1 (1%) | 30 | 68 |
| 29 | DH | 172/180 (96%) | 162 (94%) | 9 (5%) | 1 (1%) | 30 | 68 |
| 30 | BI | 144/148 (97%) | 121 (84%) | 21 (15%) | 2 (1%) | 14 | 48 |
| 30 | DI | 144/148 (97%) | 123 (85%) | 19 (13%) | 2 (1%) | 14 | 48 |
| 31 | BN | 138/140 (99%) | 129 (94%) | 6 (4%) | 3 (2%) | 8 | 36 |
| 31 | DN | 138/140 (99%) | 128 (93%) | 7 (5%) | 3 (2%) | 8 | 36 |
| 32 | BO | 120/122 (98%) | 117 (98%) | 3 (2%) | 0 | 100 | 100 |
| 32 | DO | 120/122 (98%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 33 | BP | 147/150 (98%) | 137 (93%) | 10 (7%) | 0 | 100 | 100 |
| 33 | DP | 147/150 (98%) | 136 (92%) | 11 (8%) | 0 | 100 | 100 |
| 34 | BQ | 139/141 (99%) | 130 (94%) | 8 (6%) | 1 (1%) | 26 | 65 |
| 34 | DQ | 139/141 (99%) | 130 (94%) | 8 (6%) | 1 (1%) | 26 | 65 |
| 35 | BR | 116/118 (98%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 35 | DR | 116/118 (98%) | 110 (95%) | 6 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 36 | BS | 108/112 (96%) | 101 (94%) | 7 (6%) | 0 | 100 | 100 |
| 36 | DS | 108/112 (96%) | 101 (94%) | 7 (6%) | 0 | 100 | 100 |
| 37 | BT | 129/146 (88%) | 127 (98%) | 2 (2%) | 0 | 100 | 100 |
| 37 | DT | 129/146 (88%) | 126 (98%) | 3 (2%) | 0 | 100 | 100 |
| 38 | BU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 38 | DU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 39 | BV | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 | 100 |
| 39 | DV | 99/101 (98%) | 94 (95%) | 5 (5%) | 0 | 100 | 100 |
| 40 | BW | 110/113 (97%) | 108 (98%) | 1 (1%) | 1 (1%) | 21 | 61 |
| 40 | DW | 110/113 (97%) | 107 (97%) | 3 (3%) | 0 | 100 | 100 |
| 41 | BX | 93/96 (97%) | 88 (95%) | 5 (5%) | 0 | 100 | 100 |
| 41 | DX | 93/96 (97%) | 88 (95%) | 5 (5%) | 0 | 100 | 100 |
| 42 | BY | 105/110 (96%) | 94 (90%) | 10 (10%) | 1 (1%) | 19 | 58 |
| 42 | DY | 105/110 (96%) | 94 (90%) | 10 (10%) | 1 (1%) | 19 | 58 |
| 43 | BZ | 199/206 (97%) | 183 (92%) | 14 (7%) | 2 (1%) | 19 | 58 |
| 43 | DZ | 196/206 (95%) | 180 (92%) | 14 (7%) | 2 (1%) | 19 | 58 |
| 44 | B0 | 74/85 (87%) | 72 (97%) | 2 (3%) | 0 | 100 | 100 |
| 44 | D0 | 74/85 (87%) | 73 (99%) | 1 (1%) | 0 | 100 | 100 |
| 45 | B1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 17 | 55 |
| 45 | D1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 17 | 55 |
| 46 | B2 | 68/72 (94%) | 64 (94%) | 4 (6%) | 0 | 100 | 100 |
| 46 | D2 | 68/72 (94%) | 63 (93%) | 5 (7%) | 0 | 100 | 100 |
| 47 | B3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 47 | D3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 48 | B4 | 44/71 (62%) | 36 (82%) | 8 (18%) | 0 | 100 | 100 |
| 48 | D4 | 44/71 (62%) | 36 (82%) | 8 (18%) | 0 | 100 | 100 |
| 49 | B5 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 49 | D5 | 57/60 (95%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 50 | B6 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 50 | D6 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 51 | B7 | 46/49 (94%) | 43 (94%) | 2 (4%) | 1 (2%) | 8 | 36 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 51 | D7 | 46/49 (94%) | 43 (94%) | 2 (4%) | 1 (2%) | 8 | 36 |
| 52 | B8 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 52 | D8 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 53 | B9 | 34/37 (92%) | 34 (100%) | 0 | 0 | 100 | 100 |
| 53 | D9 | 34/37 (92%) | 33 (97%) | 1 (3%) | 0 | 100 | 100 |
| All | All | 11552/12330 (94%) | 10628 (92%) | 855 (7%) | 69 (1%) | 30 | 68 |

All (69) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CT | 100 | ILE |
| 12 | AL | 28 | LYS |
| 14 | AN | 15 | LYS |
| 16 | AP | 79 | VAL |
| 12 | CL | 28 | LYS |
| 16 | CP | 79 | VAL |
| 15 | AO | 75 | PRO |
| 19 | AS | 13 | ASP |
| 31 | BN | 5 | VAL |
| 34 | BQ | 135 | ASP |
| 9 | CI | 102 | LEU |
| 10 | CJ | 80 | LYS |
| 13 | CM | 88 | ARG |
| 15 | CO | 75 | PRO |
| 31 | DN | 18 | ALA |
| 34 | DQ | 135 | ASP |
| 7 | AG | 56 | GLN |
| 9 | AI | 119 | ALA |
| 10 | AJ | 34 | VAL |
| 15 | AO | 76 | GLU |
| 30 | BI | 86 | THR |
| 31 | BN | 4 | TYR |
| 43 | BZ | 192 | ALA |
| 45 | B1 | 3 | LYS |
| 51 | B7 | 46 | VAL |
| 2 | CB | 150 | SER |
| 15 | CO | 76 | GLU |
| 31 | DN | 4 | TYR |
| 31 | DN | 5 | VAL |
| 43 | DZ | 192 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | D1 | 3 | LYS |
| 51 | D7 | 46 | VAL |
| 2 | AB | 150 | SER |
| 14 | AN | 17 | LYS |
| 29 | BH | 170 | ARG |
| 31 | BN | 18 | ALA |
| 7 | CG | 100 | ALA |
| 10 | CJ | 41 | PRO |
| 13 | CM | 87 | TYR |
| 29 | DH | 170 | ARG |
| 30 | DI | 10 | GLU |
| 3 | AC | 62 | ASP |
| 7 | AG | 100 | ALA |
| 30 | BI | 107 | VAL |
| 5 | CE | 21 | ALA |
| 20 | CT | 71 | THR |
| 27 | DF | 130 | ALA |
| 10 | AJ | 75 | ILE |
| 19 | CS | 45 | VAL |
| 30 | DI | 107 | VAL |
| 22 | AX | 56 | VAL |
| 26 | BE | 52 | LEU |
| 26 | BE | 72 | VAL |
| 26 | DE | 52 | LEU |
| 26 | DE | 72 | VAL |
| 13 | AM | 84 | ILE |
| 25 | BD | 3 | VAL |
| 40 | BW | 80 | PRO |
| 42 | BY | 3 | VAL |
| 13 | CM | 10 | PRO |
| 25 | DD | 3 | VAL |
| 42 | DY | 3 | VAL |
| 28 | BG | 87 | PRO |
| 13 | CM | 7 | VAL |
| 43 | DZ | 161 | VAL |
| 10 | AJ | 90 | LEU |
| 13 | AM | 7 | VAL |
| 43 | BZ | 161 | VAL |
| 20 | CT | 98 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | AB | 178/220 (81%) | 133 (75%) | 45 (25%) | 1 | 2 |
| 2 | CB | 177/220 (80%) | 133 (75%) | 44 (25%) | 1 | 3 |
| 3 | AC | 114/188 (61%) | 79 (69%) | 35 (31%) | 0 | 1 |
| 3 | CC | 114/188 (61%) | 92 (81%) | 22 (19%) | 2 | 8 |
| 4 | AD | 141/181 (78%) | 118 (84%) | 23 (16%) | 3 | 12 |
| 4 | CD | 141/181 (78%) | 119 (84%) | 22 (16%) | 3 | 14 |
| 5 | AE | 108/123 (88%) | 87 (81%) | 21 (19%) | 2 | 7 |
| 5 | CE | 108/123 (88%) | 87 (81%) | 21 (19%) | 2 | 7 |
| 6 | AF | 76/90 (84%) | 61 (80%) | 15 (20%) | 1 | 7 |
| 6 | CF | 76/90 (84%) | 58 (76%) | 18 (24%) | 1 | 3 |
| 7 | AG | 103/127 (81%) | 73 (71%) | 30 (29%) | 0 | 1 |
| 7 | CG | 103/127 (81%) | 68 (66%) | 35 (34%) | 0 | 0 |
| 8 | AH | 103/119 (87%) | 82 (80%) | 21 (20%) | 1 | 6 |
| 8 | CH | 103/119 (87%) | 83 (81%) | 20 (19%) | 2 | 7 |
| 9 | AI | 62/99 (63%) | 47 (76%) | 15 (24%) | 1 | 3 |
| 9 | CI | 62/99 (63%) | 47 (76%) | 15 (24%) | 1 | 3 |
| 10 | AJ | 53/92 (58%) | 38 (72%) | 15 (28%) | 0 | 1 |
| 10 | CJ | 53/92 (58%) | 39 (74%) | 14 (26%) | 0 | 2 |
| 11 | AK | 81/99 (82%) | 71 (88%) | 10 (12%) | 6 | 23 |
| 11 | CK | 81/99 (82%) | 70 (86%) | 11 (14%) | 5 | 19 |
| 12 | AL | 91/109 (84%) | 80 (88%) | 11 (12%) | 6 | 24 |
| 12 | CL | 91/109 (84%) | 81 (89%) | 10 (11%) | 8 | 30 |
| 13 | AM | 64/101 (63%) | 48 (75%) | 16 (25%) | 1 | 2 |
| 13 | CM | 64/101 (63%) | 49 (77%) | 15 (23%) | 1 | 4 |
| 14 | AN | 46/50 (92%) | 36 (78%) | 10 (22%) | 1 | 5 |
| 14 | CN | 46/50 (92%) | 32 (70%) | 14 (30%) | 0 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 15 | AO | 77/80 (96%) | 68 (88%) | 9 (12%) | 7 | 26 |
| 15 | CO | 77/80 (96%) | 68 (88%) | 9 (12%) | 7 | 26 |
| 16 | AP | 63/74 (85%) | 46 (73%) | 17 (27%) | 0 | 1 |
| 16 | CP | 63/74 (85%) | 44 (70%) | 19 (30%) | 0 | 1 |
| 17 | AQ | 94/97 (97%) | 80 (85%) | 14 (15%) | 4 | 15 |
| 17 | CQ | 94/97 (97%) | 81 (86%) | 13 (14%) | 4 | 19 |
| 18 | AR | 49/77 (64%) | 44 (90%) | 5 (10%) | 9 | 33 |
| 18 | CR | 49/77 (64%) | 44 (90%) | 5 (10%) | 9 | 33 |
| 19 | AS | 43/80 (54%) | 26 (60%) | 17 (40%) | 0 | 0 |
| 19 | CS | 43/80 (54%) | 32 (74%) | 11 (26%) | 0 | 2 |
| 20 | AT | 64/82 (78%) | 55 (86%) | 9 (14%) | 4 | 18 |
| 20 | CT | 65/82 (79%) | 55 (85%) | 10 (15%) | 3 | 14 |
| 21 | AU | 18/22 (82%) | 13 (72%) | 5 (28%) | 0 | 1 |
| 21 | CU | 18/22 (82%) | 11 (61%) | 7 (39%) | 0 | 0 |
| 22 | AX | 45/87 (52%) | 34 (76%) | 11 (24%) | 1 | 3 |
| 22 | CX | 38/87 (44%) | 29 (76%) | 9 (24%) | 1 | 3 |
| 25 | BD | 215/218 (99%) | 182 (85%) | 33 (15%) | 3 | 14 |
| 25 | DD | 215/218 (99%) | 183 (85%) | 32 (15%) | 4 | 15 |
| 26 | BE | 163/166 (98%) | 135 (83%) | 28 (17%) | 2 | 11 |
| 26 | DE | 163/166 (98%) | 137 (84%) | 26 (16%) | 3 | 13 |
| 27 | BF | 159/166 (96%) | 135 (85%) | 24 (15%) | 3 | 15 |
| 27 | DF | 159/166 (96%) | 134 (84%) | 25 (16%) | 3 | 13 |
| 28 | BG | 128/156 (82%) | 109 (85%) | 19 (15%) | 4 | 16 |
| 28 | DG | 128/156 (82%) | 109 (85%) | 19 (15%) | 4 | 16 |
| 29 | BH | 141/148 (95%) | 123 (87%) | 18 (13%) | 5 | 21 |
| 29 | DH | 141/148 (95%) | 123 (87%) | 18 (13%) | 5 | 21 |
| 30 | BI | 98/124 (79%) | 81 (83%) | 17 (17%) | 2 | 11 |
| 30 | DI | 74/124 (60%) | 60 (81%) | 14 (19%) | 2 | 8 |
| 31 | BN | 117/119 (98%) | 98 (84%) | 19 (16%) | 3 | 12 |
| 31 | DN | 117/119 (98%) | 98 (84%) | 19 (16%) | 3 | 12 |
| 32 | BO | 98/100 (98%) | 82 (84%) | 16 (16%) | 3 | 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 32 | DO | 98/100 (98%) | 83 (85%) | 15 (15%) | 3 | 14 |
| 33 | BP | 114/116 (98%) | 99 (87%) | 15 (13%) | 5 | 20 |
| 33 | DP | 114/116 (98%) | 99 (87%) | 15 (13%) | 5 | 20 |
| 34 | BQ | 111/111 (100%) | 96 (86%) | 15 (14%) | 5 | 20 |
| 34 | DQ | 111/111 (100%) | 96 (86%) | 15 (14%) | 5 | 20 |
| 35 | BR | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 | 5 |
| 35 | DR | 101/101 (100%) | 77 (76%) | 24 (24%) | 1 | 3 |
| 36 | BS | 84/88 (96%) | 67 (80%) | 17 (20%) | 1 | 7 |
| 36 | DS | 84/88 (96%) | 68 (81%) | 16 (19%) | 2 | 8 |
| 37 | BT | 110/127 (87%) | 98 (89%) | 12 (11%) | 8 | 30 |
| 37 | DT | 110/127 (87%) | 95 (86%) | 15 (14%) | 5 | 19 |
| 38 | BU | 93/94 (99%) | 82 (88%) | 11 (12%) | 6 | 25 |
| 38 | DU | 93/94 (99%) | 83 (89%) | 10 (11%) | 8 | 30 |
| 39 | BV | 80/82 (98%) | 63 (79%) | 17 (21%) | 1 | 6 |
| 39 | DV | 80/82 (98%) | 63 (79%) | 17 (21%) | 1 | 6 |
| 40 | BW | 89/92 (97%) | 81 (91%) | 8 (9%) | 12 | 41 |
| 40 | DW | 89/92 (97%) | 78 (88%) | 11 (12%) | 6 | 23 |
| 41 | BX | 75/78 (96%) | 71 (95%) | 4 (5%) | 28 | 64 |
| 41 | DX | 75/78 (96%) | 70 (93%) | 5 (7%) | 20 | 56 |
| 42 | BY | 80/91 (88%) | 64 (80%) | 16 (20%) | 1 | 7 |
| 42 | DY | 80/91 (88%) | 63 (79%) | 17 (21%) | 1 | 6 |
| 43 | BZ | 159/179 (89%) | 137 (86%) | 22 (14%) | 4 | 19 |
| 43 | DZ | 159/179 (89%) | 139 (87%) | 20 (13%) | 5 | 22 |
| 44 | B0 | 59/67 (88%) | 51 (86%) | 8 (14%) | 5 | 19 |
| 44 | D0 | 59/67 (88%) | 50 (85%) | 9 (15%) | 3 | 14 |
| 45 | B1 | 78/83 (94%) | 63 (81%) | 15 (19%) | 2 | 8 |
| 45 | D1 | 78/83 (94%) | 66 (85%) | 12 (15%) | 3 | 14 |
| 46 | B2 | 65/67 (97%) | 54 (83%) | 11 (17%) | 2 | 11 |
| 46 | D2 | 65/67 (97%) | 55 (85%) | 10 (15%) | 3 | 14 |
| 47 | B3 | 49/52 (94%) | 44 (90%) | 5 (10%) | 9 | 33 |
| 47 | D3 | 49/52 (94%) | 44 (90%) | 5 (10%) | 9 | 33 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 48 | B4 | 39/63 (62%) | 33 (85%) | 6 (15%) | 3 | 14 |
| 48 | D4 | 39/63 (62%) | 33 (85%) | 6 (15%) | 3 | 14 |
| 49 | B5 | 50/52 (96%) | 42 (84%) | 8 (16%) | 3 | 13 |
| 49 | D5 | 50/52 (96%) | 41 (82%) | 9 (18%) | 2 | 10 |
| 50 | B6 | 50/52 (96%) | 39 (78%) | 11 (22%) | 1 | 5 |
| 50 | D6 | 50/52 (96%) | 40 (80%) | 10 (20%) | 1 | 7 |
| 51 | B7 | 41/42 (98%) | 34 (83%) | 7 (17%) | 2 | 11 |
| 51 | D7 | 41/42 (98%) | 34 (83%) | 7 (17%) | 2 | 11 |
| 52 | B8 | 52/55 (94%) | 42 (81%) | 10 (19%) | 2 | 8 |
| 52 | D8 | 52/55 (94%) | 42 (81%) | 10 (19%) | 2 | 8 |
| 53 | B9 | 32/34 (94%) | 28 (88%) | 4 (12%) | 6 | 22 |
| 53 | D9 | 32/34 (94%) | 28 (88%) | 4 (12%) | 6 | 22 |
| All | All | 8775/10240 (86%) | 7244 (83%) | 1531 (17%) | 2 | 11 |

All (1531) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 15 | VAL |
| 2 | AB | 16 | HIS |
| 2 | AB | 17 | PHE |
| 2 | AB | 21 | ARG |
| 2 | AB | 24 | TRP |
| 2 | AB | 47 | THR |
| 2 | AB | 51 | LEU |
| 2 | AB | 67 | THR |
| 2 | AB | 69 | LEU |
| 2 | AB | 74 | LYS |
| 2 | AB | 80 | ILE |
| 2 | AB | 82 | ARG |
| 2 | AB | 86 | GLU |
| 2 | AB | 87 | ARG |
| 2 | AB | 93 | VAL |
| 2 | AB | 94 | ASN |
| 2 | AB | 110 | GLN |
| 2 | AB | 113 | HIS |
| 2 | AB | 114 | ARG |
| 2 | AB | 117 | GLU |
| 2 | AB | 121 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 124 | SER |
| 2 | AB | 133 | LYS |
| 2 | AB | 137 | ARG |
| 2 | AB | 139 | LYS |
| 2 | AB | 140 | HIS |
| 2 | AB | 150 | SER |
| 2 | AB | 153 | ARG |
| 2 | AB | 155 | LEU |
| 2 | AB | 157 | ARG |
| 2 | AB | 160 | ASP |
| 2 | AB | 163 | PHE |
| 2 | AB | 170 | GLU |
| 2 | AB | 185 | ILE |
| 2 | AB | 187 | LEU |
| 2 | AB | 191 | ASP |
| 2 | AB | 197 | VAL |
| 2 | AB | 200 | ILE |
| 2 | AB | 205 | ASP |
| 2 | AB | 208 | ILE |
| 2 | AB | 209 | ARG |
| 2 | AB | 210 | SER |
| 2 | AB | 212 | GLN |
| 2 | AB | 221 | LEU |
| 2 | AB | 230 | VAL |
| 3 | AC | 3 | ASN |
| 3 | AC | 6 | HIS |
| 3 | AC | 8 | ILE |
| 3 | AC | 15 | THR |
| 3 | AC | 17 | ASP |
| 3 | AC | 20 | SER |
| 3 | AC | 22 | TRP |
| 3 | AC | 29 | TYR |
| 3 | AC | 30 | ARG |
| 3 | AC | 36 | ASP |
| 3 | AC | 37 | GLN |
| 3 | AC | 38 | ARG |
| 3 | AC | 40 | ARG |
| 3 | AC | 44 | GLU |
| 3 | AC | 46 | GLU |
| 3 | AC | 47 | LEU |
| 3 | AC | 49 | SER |
| 3 | AC | 54 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 70 | VAL |
| 3 | AC | 112 | SER |
| 3 | AC | 118 | GLN |
| 3 | AC | 127 | ARG |
| 3 | AC | 128 | PHE |
| 3 | AC | 131 | ARG |
| 3 | AC | 140 | ARG |
| 3 | AC | 144 | SER |
| 3 | AC | 172 | ARG |
| 3 | AC | 175 | LEU |
| 3 | AC | 179 | ARG |
| 3 | AC | 191 | THR |
| 3 | AC | 192 | THR |
| 3 | AC | 193 | TYR |
| 3 | AC | 196 | LEU |
| 3 | AC | 202 | ILE |
| 3 | AC | 207 | VAL |
| 4 | AD | 11 | LEU |
| 4 | AD | 12 | CYS |
| 4 | AD | 13 | ARG |
| 4 | AD | 20 | TYR |
| 4 | AD | 36 | ARG |
| 4 | AD | 52 | SER |
| 4 | AD | 53 | ASP |
| 4 | AD | 57 | ARG |
| 4 | AD | 70 | ILE |
| 4 | AD | 76 | ARG |
| 4 | AD | 83 | SER |
| 4 | AD | 91 | SER |
| 4 | AD | 101 | LEU |
| 4 | AD | 106 | TYR |
| 4 | AD | 113 | SER |
| 4 | AD | 119 | GLN |
| 4 | AD | 122 | ARG |
| 4 | AD | 127 | THR |
| 4 | AD | 135 | LEU |
| 4 | AD | 138 | TYR |
| 4 | AD | 158 | ILE |
| 4 | AD | 170 | VAL |
| 4 | AD | 193 | ASP |
| 5 | AE | 11 | ILE |
| 5 | AE | 12 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 14 | ARG |
| 5 | AE | 16 | THR |
| 5 | AE | 41 | VAL |
| 5 | AE | 47 | LYS |
| 5 | AE | 51 | VAL |
| 5 | AE | 60 | TYR |
| 5 | AE | 63 | ARG |
| 5 | AE | 65 | ASN |
| 5 | AE | 76 | ILE |
| 5 | AE | 78 | HIS |
| 5 | AE | 79 | GLU |
| 5 | AE | 84 | PHE |
| 5 | AE | 87 | SER |
| 5 | AE | 89 | ILE |
| 5 | AE | 91 | LEU |
| 5 | AE | 98 | THR |
| 5 | AE | 107 | ARG |
| 5 | AE | 147 | ASP |
| 5 | AE | 152 | ARG |
| 6 | AF | 7 | ASN |
| 6 | AF | 22 | GLU |
| 6 | AF | 36 | ARG |
| 6 | AF | 40 | VAL |
| 6 | AF | 48 | LEU |
| 6 | AF | 57 | GLN |
| 6 | AF | 63 | TYR |
| 6 | AF | 69 | GLU |
| 6 | AF | 72 | VAL |
| 6 | AF | 73 | ASN |
| 6 | AF | 74 | ASP |
| 6 | AF | 75 | LEU |
| 6 | AF | 89 | MET |
| 6 | AF | 94 | GLN |
| 6 | AF | 98 | LEU |
| 7 | AG | 4 | ARG |
| 7 | AG | 6 | ARG |
| 7 | AG | 21 | VAL |
| 7 | AG | 30 | ILE |
| 7 | AG | 38 | LEU |
| 7 | AG | 53 | LYS |
| 7 | AG | 56 | GLN |
| 7 | AG | 59 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 72 | ARG |
| 7 | AG | 74 | GLU |
| 7 | AG | 75 | VAL |
| 7 | AG | 80 | VAL |
| 7 | AG | 89 | MET |
| 7 | AG | 94 | ARG |
| 7 | AG | 96 | GLN |
| 7 | AG | 99 | LEU |
| 7 | AG | 103 | TRP |
| 7 | AG | 104 | LEU |
| 7 | AG | 109 | ASN |
| 7 | AG | 114 | ARG |
| 7 | AG | 120 | ILE |
| 7 | AG | 123 | GLU |
| 7 | AG | 124 | LEU |
| 7 | AG | 125 | MET |
| 7 | AG | 135 | VAL |
| 7 | AG | 138 | LYS |
| 7 | AG | 139 | GLU |
| 7 | AG | 142 | GLU |
| 7 | AG | 144 | MET |
| 7 | AG | 155 | ARG |
| 8 | AH | 2 | LEU |
| 8 | AH | 21 | LYS |
| 8 | AH | 25 | ASP |
| 8 | AH | 37 | ARG |
| 8 | AH | 49 | GLU |
| 8 | AH | 52 | ASP |
| 8 | AH | 54 | ASP |
| 8 | AH | 60 | ARG |
| 8 | AH | 63 | LEU |
| 8 | AH | 77 | GLU |
| 8 | AH | 78 | GLN |
| 8 | AH | 83 | ILE |
| 8 | AH | 84 | ARG |
| 8 | AH | 85 | ARG |
| 8 | AH | 91 | ARG |
| 8 | AH | 95 | VAL |
| 8 | AH | 109 | ILE |
| 8 | AH | 115 | SER |
| 8 | AH | 119 | LEU |
| 8 | AH | 120 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | AH | 127 | LEU |
| 9 | AI | 3 | GLN |
| 9 | AI | 9 | ARG |
| 9 | AI | 16 | ARG |
| 9 | AI | 17 | VAL |
| 9 | AI | 20 | ARG |
| 9 | AI | 27 | THR |
| 9 | AI | 34 | ASN |
| 9 | AI | 36 | TYR |
| 9 | AI | 37 | PHE |
| 9 | AI | 48 | GLU |
| 9 | AI | 62 | TYR |
| 9 | AI | 71 | SER |
| 9 | AI | 74 | ILE |
| 9 | AI | 99 | LEU |
| 9 | AI | 113 | LYS |
| 10 | AJ | 8 | LEU |
| 10 | AJ | 16 | LEU |
| 10 | AJ | 19 | SER |
| 10 | AJ | 21 | GLN |
| 10 | AJ | 42 | THR |
| 10 | AJ | 45 | ARG |
| 10 | AJ | 54 | PHE |
| 10 | AJ | 55 | LYS |
| 10 | AJ | 58 | ASP |
| 10 | AJ | 63 | PHE |
| 10 | AJ | 66 | ARG |
| 10 | AJ | 67 | THR |
| 10 | AJ | 69 | ASN |
| 10 | AJ | 73 | ASP |
| 10 | AJ | 100 | THR |
| 11 | AK | 14 | VAL |
| 11 | AK | 16 | SER |
| 11 | AK | 29 | ILE |
| 11 | AK | 30 | VAL |
| 11 | AK | 32 | ILE |
| 11 | AK | 47 | VAL |
| 11 | AK | 96 | ARG |
| 11 | AK | 103 | LEU |
| 11 | AK | 109 | VAL |
| 11 | AK | 117 | ASN |
| 12 | AL | 11 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 33 | ARG |
| 12 | AL | 44 | THR |
| 12 | AL | 52 | LEU |
| 12 | AL | 60 | LEU |
| 12 | AL | 66 | VAL |
| 12 | AL | 82 | VAL |
| 12 | AL | 97 | ARG |
| 12 | AL | 114 | LYS |
| 12 | AL | 115 | LYS |
| 12 | AL | 119 | LYS |
| 13 | AM | 3 | ARG |
| 13 | AM | 16 | ASP |
| 13 | AM | 20 | THR |
| 13 | AM | 43 | THR |
| 13 | AM | 45 | VAL |
| 13 | AM | 56 | LEU |
| 13 | AM | 59 | TYR |
| 13 | AM | 63 | THR |
| 13 | AM | 66 | LEU |
| 13 | AM | 70 | LEU |
| 13 | AM | 71 | ARG |
| 13 | AM | 77 | ASN |
| 13 | AM | 88 | ARG |
| 13 | AM | 91 | ARG |
| 13 | AM | 98 | VAL |
| 13 | AM | 114 | ARG |
| 14 | AN | 7 | ILE |
| 14 | AN | 8 | GLU |
| 14 | AN | 16 | PHE |
| 14 | AN | 18 | VAL |
| 14 | AN | 22 | THR |
| 14 | AN | 29 | ARG |
| 14 | AN | 33 | VAL |
| 14 | AN | 35 | ARG |
| 14 | AN | 41 | ARG |
| 14 | AN | 61 | TRP |
| 15 | AO | 3 | ILE |
| 15 | AO | 4 | THR |
| 15 | AO | 13 | GLN |
| 15 | AO | 24 | SER |
| 15 | AO | 26 | GLU |
| 15 | AO | 39 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AO | 66 | LEU |
| 15 | AO | 72 | ARG |
| 15 | AO | 87 | ILE |
| 16 | AP | 1 | MET |
| 16 | AP | 2 | VAL |
| 16 | AP | 6 | LEU |
| 16 | AP | 11 | SER |
| 16 | AP | 21 | VAL |
| 16 | AP | 25 | ARG |
| 16 | AP | 27 | LYS |
| 16 | AP | 29 | ASP |
| 16 | AP | 36 | ILE |
| 16 | AP | 38 | TYR |
| 16 | AP | 43 | LYS |
| 16 | AP | 45 | THR |
| 16 | AP | 62 | VAL |
| 16 | AP | 65 | GLN |
| 16 | AP | 67 | THR |
| 16 | AP | 69 | THR |
| 16 | AP | 76 | GLN |
| 17 | AQ | 11 | VAL |
| 17 | AQ | 34 | LYS |
| 17 | AQ | 43 | LEU |
| 17 | AQ | 45 | HIS |
| 17 | AQ | 50 | LYS |
| 17 | AQ | 57 | VAL |
| 17 | AQ | 59 | ILE |
| 17 | AQ | 65 | ILE |
| 17 | AQ | 72 | ARG |
| 17 | AQ | 74 | LEU |
| 17 | AQ | 86 | GLU |
| 17 | AQ | 96 | GLU |
| 17 | AQ | 99 | SER |
| 17 | AQ | 100 | LYS |
| 18 | AR | 35 | ARG |
| 18 | AR | 36 | ASN |
| 18 | AR | 76 | LEU |
| 18 | AR | 79 | LEU |
| 18 | AR | 85 | LEU |
| 19 | AS | 9 | VAL |
| 19 | AS | 10 | PHE |
| 19 | AS | 11 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 19 | AS | 12 | ASP |
| 19 | AS | 14 | HIS |
| 19 | AS | 20 | LEU |
| 19 | AS | 31 | ILE |
| 19 | AS | 33 | THR |
| 19 | AS | 37 | ARG |
| 19 | AS | 44 | MET |
| 19 | AS | 51 | VAL |
| 19 | AS | 62 | ILE |
| 19 | AS | 63 | THR |
| 19 | AS | 66 | MET |
| 19 | AS | 70 | LYS |
| 19 | AS | 77 | THR |
| 19 | AS | 78 | ARG |
| 20 | AT | 10 | LEU |
| 20 | AT | 13 | LEU |
| 20 | AT | 36 | LEU |
| 20 | AT | 39 | LYS |
| 20 | AT | 62 | LEU |
| 20 | AT | 71 | THR |
| 20 | AT | 72 | LEU |
| 20 | AT | 73 | HIS |
| 20 | AT | 74 | LYS |
| 21 | AU | 6 | ARG |
| 21 | AU | 8 | THR |
| 21 | AU | 9 | ARG |
| 21 | AU | 10 | ARG |
| 21 | AU | 15 | ARG |
| 22 | AX | 2 | GLN |
| 22 | AX | 23 | LYS |
| 22 | AX | 53 | THR |
| 22 | AX | 54 | LEU |
| 22 | AX | 62 | HIS |
| 22 | AX | 69 | ASP |
| 22 | AX | 77 | LEU |
| 22 | AX | 90 | ASP |
| 22 | AX | 91 | LYS |
| 22 | AX | 92 | LEU |
| 22 | AX | 93 | LYS |
| 25 | BD | 12 | SER |
| 25 | BD | 13 | ARG |
| 25 | BD | 18 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | BD | 24 | ILE |
| 25 | BD | 27 | THR |
| 25 | BD | 54 | ARG |
| 25 | BD | 83 | GLU |
| 25 | BD | 94 | LEU |
| 25 | BD | 103 | ARG |
| 25 | BD | 106 | ILE |
| 25 | BD | 111 | LEU |
| 25 | BD | 117 | VAL |
| 25 | BD | 126 | GLN |
| 25 | BD | 141 | VAL |
| 25 | BD | 150 | LYS |
| 25 | BD | 154 | LYS |
| 25 | BD | 157 | ARG |
| 25 | BD | 173 | VAL |
| 25 | BD | 192 | THR |
| 25 | BD | 200 | ASP |
| 25 | BD | 211 | ARG |
| 25 | BD | 212 | SER |
| 25 | BD | 217 | ARG |
| 25 | BD | 218 | ARG |
| 25 | BD | 221 | VAL |
| 25 | BD | 229 | VAL |
| 25 | BD | 254 | THR |
| 25 | BD | 257 | LEU |
| 25 | BD | 259 | THR |
| 25 | BD | 260 | ARG |
| 25 | BD | 271 | ILE |
| 25 | BD | 273 | ARG |
| 25 | BD | 274 | ARG |
| 26 | BE | 7 | VAL |
| 26 | BE | 12 | THR |
| 26 | BE | 21 | VAL |
| 26 | BE | 24 | THR |
| 26 | BE | 33 | VAL |
| 26 | BE | 34 | VAL |
| 26 | BE | 40 | GLU |
| 26 | BE | 47 | VAL |
| 26 | BE | 49 | LEU |
| 26 | BE | 52 | LEU |
| 26 | BE | 61 | ARG |
| 26 | BE | 69 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BE | 72 | VAL |
| 26 | BE | 75 | VAL |
| 26 | BE | 77 | ILE |
| 26 | BE | 82 | ARG |
| 26 | BE | 92 | THR |
| 26 | BE | 111 | ARG |
| 26 | BE | 116 | VAL |
| 26 | BE | 119 | ARG |
| 26 | BE | 128 | SER |
| 26 | BE | 144 | ARG |
| 26 | BE | 154 | LYS |
| 26 | BE | 167 | VAL |
| 26 | BE | 170 | LEU |
| 26 | BE | 179 | GLU |
| 26 | BE | 181 | LEU |
| 26 | BE | 195 | LEU |
| 27 | BF | 12 | LEU |
| 27 | BF | 18 | ARG |
| 27 | BF | 20 | LEU |
| 27 | BF | 24 | LEU |
| 27 | BF | 33 | LEU |
| 27 | BF | 38 | ARG |
| 27 | BF | 41 | LEU |
| 27 | BF | 50 | SER |
| 27 | BF | 57 | VAL |
| 27 | BF | 69 | HIS |
| 27 | BF | 77 | ASP |
| 27 | BF | 88 | VAL |
| 27 | BF | 106 | ARG |
| 27 | BF | 110 | LEU |
| 27 | BF | 112 | MET |
| 27 | BF | 132 | VAL |
| 27 | BF | 137 | LYS |
| 27 | BF | 140 | LEU |
| 27 | BF | 158 | THR |
| 27 | BF | 168 | ARG |
| 27 | BF | 170 | LEU |
| 27 | BF | 175 | THR |
| 27 | BF | 188 | ARG |
| 27 | BF | 192 | LEU |
| 28 | BG | 3 | LEU |
| 28 | BG | 5 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BG | 7 | LEU |
| 28 | BG | 21 | ARG |
| 28 | BG | 28 | VAL |
| 28 | BG | 35 | GLU |
| 28 | BG | 47 | LYS |
| 28 | BG | 98 | ARG |
| 28 | BG | 128 | ARG |
| 28 | BG | 136 | ARG |
| 28 | BG | 139 | LEU |
| 28 | BG | 140 | ILE |
| 28 | BG | 143 | GLU |
| 28 | BG | 146 | TYR |
| 28 | BG | 149 | VAL |
| 28 | BG | 155 | MET |
| 28 | BG | 161 | THR |
| 28 | BG | 170 | ARG |
| 28 | BG | 175 | LEU |
| 29 | BH | 3 | ARG |
| 29 | BH | 6 | ARG |
| 29 | BH | 7 | LEU |
| 29 | BH | 15 | VAL |
| 29 | BH | 24 | VAL |
| 29 | BH | 41 | MET |
| 29 | BH | 44 | VAL |
| 29 | BH | 49 | VAL |
| 29 | BH | 51 | ARG |
| 29 | BH | 58 | GLU |
| 29 | BH | 68 | THR |
| 29 | BH | 69 | ARG |
| 29 | BH | 98 | LEU |
| 29 | BH | 113 | VAL |
| 29 | BH | 122 | THR |
| 29 | BH | 134 | SER |
| 29 | BH | 139 | GLN |
| 29 | BH | 169 | VAL |
| 30 | BI | 1 | MET |
| 30 | BI | 9 | LEU |
| 30 | BI | 47 | LEU |
| 30 | BI | 51 | ILE |
| 30 | BI | 54 | GLN |
| 30 | BI | 61 | ARG |
| 30 | BI | 68 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | BI | 75 | LEU |
| 30 | BI | 77 | LEU |
| 30 | BI | 78 | THR |
| 30 | BI | 81 | VAL |
| 30 | BI | 92 | VAL |
| 30 | BI | 117 | GLU |
| 30 | BI | 123 | LEU |
| 30 | BI | 140 | LEU |
| 30 | BI | 142 | VAL |
| 30 | BI | 144 | VAL |
| 31 | BN | 1 | MET |
| 31 | BN | 5 | VAL |
| 31 | BN | 12 | ARG |
| 31 | BN | 28 | THR |
| 31 | BN | 33 | LEU |
| 31 | BN | 34 | LEU |
| 31 | BN | 38 | HIS |
| 31 | BN | 46 | VAL |
| 31 | BN | 48 | MET |
| 31 | BN | 62 | VAL |
| 31 | BN | 67 | LEU |
| 31 | BN | 68 | GLU |
| 31 | BN | 85 | ILE |
| 31 | BN | 99 | LEU |
| 31 | BN | 112 | LEU |
| 31 | BN | 120 | LEU |
| 31 | BN | 130 | HIS |
| 31 | BN | 133 | GLN |
| 31 | BN | 140 | VAL |
| 32 | BO | 8 | LEU |
| 32 | BO | 10 | VAL |
| 32 | BO | 17 | ARG |
| 32 | BO | 21 | CYS |
| 32 | BO | 24 | VAL |
| 32 | BO | 25 | LEU |
| 32 | BO | 26 | LYS |
| 32 | BO | 29 | ASN |
| 32 | BO | 32 | TYR |
| 32 | BO | 52 | VAL |
| 32 | BO | 53 | LYS |
| 32 | BO | 58 | VAL |
| 32 | BO | 94 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | BO | 98 | VAL |
| 32 | BO | 104 | ARG |
| 32 | BO | 113 | LYS |
| 33 | BP | 21 | ARG |
| 33 | BP | 32 | THR |
| 33 | BP | 40 | SER |
| 33 | BP | 42 | SER |
| 33 | BP | 45 | LEU |
| 33 | BP | 55 | ARG |
| 33 | BP | 59 | LEU |
| 33 | BP | 65 | ARG |
| 33 | BP | 71 | VAL |
| 33 | BP | 83 | VAL |
| 33 | BP | 86 | LYS |
| 33 | BP | 95 | VAL |
| 33 | BP | 106 | LEU |
| 33 | BP | 112 | LEU |
| 33 | BP | 125 | VAL |
| 34 | BQ | 1 | MET |
| 34 | BQ | 5 | ARG |
| 34 | BQ | 7 | MET |
| 34 | BQ | 16 | ARG |
| 34 | BQ | 45 | GLN |
| 34 | BQ | 55 | VAL |
| 34 | BQ | 56 | ARG |
| 34 | BQ | 59 | ARG |
| 34 | BQ | 63 | LYS |
| 34 | BQ | 75 | THR |
| 34 | BQ | 81 | VAL |
| 34 | BQ | 109 | VAL |
| 34 | BQ | 110 | THR |
| 34 | BQ | 134 | ARG |
| 34 | BQ | 138 | ASP |
| 35 | BR | 1 | MET |
| 35 | BR | 2 | ARG |
| 35 | BR | 6 | SER |
| 35 | BR | 15 | SER |
| 35 | BR | 18 | LEU |
| 35 | BR | 24 | GLN |
| 35 | BR | 28 | LEU |
| 35 | BR | 29 | LEU |
| 35 | BR | 33 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | BR | 44 | LEU |
| 35 | BR | 54 | LEU |
| 35 | BR | 60 | LEU |
| 35 | BR | 65 | LEU |
| 35 | BR | 67 | LEU |
| 35 | BR | 79 | LEU |
| 35 | BR | 86 | ARG |
| 35 | BR | 100 | LEU |
| 35 | BR | 103 | ARG |
| 35 | BR | 111 | LEU |
| 35 | BR | 113 | LEU |
| 35 | BR | 114 | VAL |
| 35 | BR | 117 | VAL |
| 36 | BS | 3 | ARG |
| 36 | BS | 8 | GLU |
| 36 | BS | 12 | PHE |
| 36 | BS | 13 | ARG |
| 36 | BS | 20 | ARG |
| 36 | BS | 30 | ARG |
| 36 | BS | 36 | TYR |
| 36 | BS | 50 | SER |
| 36 | BS | 52 | SER |
| 36 | BS | 57 | LYS |
| 36 | BS | 58 | LEU |
| 36 | BS | 69 | VAL |
| 36 | BS | 75 | GLU |
| 36 | BS | 78 | LEU |
| 36 | BS | 84 | GLN |
| 36 | BS | 85 | VAL |
| 36 | BS | 95 | HIS |
| 37 | BT | 13 | ARG |
| 37 | BT | 16 | ARG |
| 37 | BT | 17 | THR |
| 37 | BT | 36 | GLU |
| 37 | BT | 39 | ARG |
| 37 | BT | 49 | VAL |
| 37 | BT | 64 | ARG |
| 37 | BT | 74 | ARG |
| 37 | BT | 82 | LEU |
| 37 | BT | 96 | ARG |
| 37 | BT | 107 | ASP |
| 37 | BT | 118 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 38 | BU | 5 | LYS |
| 38 | BU | 8 | VAL |
| 38 | BU | 30 | LYS |
| 38 | BU | 31 | SER |
| 38 | BU | 36 | ARG |
| 38 | BU | 59 | ARG |
| 38 | BU | 60 | LEU |
| 38 | BU | 74 | LEU |
| 38 | BU | 85 | LYS |
| 38 | BU | 104 | GLN |
| 38 | BU | 108 | GLU |
| 39 | BV | 7 | THR |
| 39 | BV | 12 | TYR |
| 39 | BV | 18 | LEU |
| 39 | BV | 21 | ARG |
| 39 | BV | 28 | GLU |
| 39 | BV | 32 | THR |
| 39 | BV | 33 | VAL |
| 39 | BV | 57 | VAL |
| 39 | BV | 61 | VAL |
| 39 | BV | 62 | LEU |
| 39 | BV | 72 | VAL |
| 39 | BV | 73 | SER |
| 39 | BV | 79 | VAL |
| 39 | BV | 85 | LYS |
| 39 | BV | 89 | GLN |
| 39 | BV | 95 | LEU |
| 39 | BV | 100 | ARG |
| 40 | BW | 4 | LYS |
| 40 | BW | 11 | ARG |
| 40 | BW | 19 | LEU |
| 40 | BW | 23 | LEU |
| 40 | BW | 27 | LYS |
| 40 | BW | 51 | LEU |
| 40 | BW | 100 | THR |
| 40 | BW | 107 | LEU |
| 41 | BX | 15 | GLU |
| 41 | BX | 57 | LEU |
| 41 | BX | 65 | ARG |
| 41 | BX | 76 | ARG |
| 42 | BY | 2 | ARG |
| 42 | BY | 3 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | BY | 6 | HIS |
| 42 | BY | 9 | LYS |
| 42 | BY | 23 | ARG |
| 42 | BY | 45 | VAL |
| 42 | BY | 49 | VAL |
| 42 | BY | 55 | TYR |
| 42 | BY | 72 | VAL |
| 42 | BY | 90 | LEU |
| 42 | BY | 91 | GLU |
| 42 | BY | 92 | ASN |
| 42 | BY | 97 | ARG |
| 42 | BY | 101 | LYS |
| 42 | BY | 102 | CYS |
| 42 | BY | 107 | ASP |
| 43 | BZ | 5 | LEU |
| 43 | BZ | 10 | ARG |
| 43 | BZ | 11 | GLU |
| 43 | BZ | 19 | ARG |
| 43 | BZ | 24 | LEU |
| 43 | BZ | 37 | VAL |
| 43 | BZ | 42 | VAL |
| 43 | BZ | 52 | SER |
| 43 | BZ | 56 | VAL |
| 43 | BZ | 66 | SER |
| 43 | BZ | 72 | ARG |
| 43 | BZ | 76 | LEU |
| 43 | BZ | 82 | ARG |
| 43 | BZ | 91 | LEU |
| 43 | BZ | 97 | GLU |
| 43 | BZ | 118 | GLN |
| 43 | BZ | 126 | VAL |
| 43 | BZ | 155 | LEU |
| 43 | BZ | 156 | LYS |
| 43 | BZ | 165 | VAL |
| 43 | BZ | 179 | ASP |
| 43 | BZ | 185 | GLU |
| 44 | B0 | 9 | SER |
| 44 | B0 | 10 | THR |
| 44 | B0 | 20 | ARG |
| 44 | B0 | 38 | VAL |
| 44 | B0 | 55 | ARG |
| 44 | B0 | 74 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | B0 | 77 | ARG |
| 44 | B0 | 83 | PRO |
| 45 | B1 | 4 | VAL |
| 45 | B1 | 5 | CYS |
| 45 | B1 | 14 | VAL |
| 45 | B1 | 21 | ARG |
| 45 | B1 | 39 | LYS |
| 45 | B1 | 40 | ARG |
| 45 | B1 | 46 | LEU |
| 45 | B1 | 51 | VAL |
| 45 | B1 | 58 | ILE |
| 45 | B1 | 59 | THR |
| 45 | B1 | 76 | ARG |
| 45 | B1 | 82 | LEU |
| 45 | B1 | 83 | GLU |
| 45 | B1 | 86 | SER |
| 45 | B1 | 95 | LEU |
| 46 | B2 | 17 | SER |
| 46 | B2 | 28 | LYS |
| 46 | B2 | 32 | LEU |
| 46 | B2 | 34 | GLU |
| 46 | B2 | 43 | GLN |
| 46 | B2 | 44 | LEU |
| 46 | B2 | 47 | ASN |
| 46 | B2 | 53 | LEU |
| 46 | B2 | 55 | ARG |
| 46 | B2 | 68 | ARG |
| 46 | B2 | 70 | GLN |
| 47 | B3 | 8 | LEU |
| 47 | B3 | 18 | ASP |
| 47 | B3 | 23 | LEU |
| 47 | B3 | 31 | LEU |
| 47 | B3 | 40 | THR |
| 48 | B4 | 14 | ILE |
| 48 | B4 | 16 | CYS |
| 48 | B4 | 27 | THR |
| 48 | B4 | 34 | GLU |
| 48 | B4 | 43 | TYR |
| 48 | B4 | 46 | GLN |
| 49 | B5 | 6 | VAL |
| 49 | B5 | 8 | LYS |
| 49 | B5 | 9 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 49 | B5 | 23 | HIS |
| 49 | B5 | 29 | THR |
| 49 | B5 | 37 | LYS |
| 49 | B5 | 40 | LYS |
| 49 | B5 | 58 | LEU |
| 50 | B6 | 4 | GLU |
| 50 | B6 | 6 | ARG |
| 50 | B6 | 13 | CYS |
| 50 | B6 | 14 | THR |
| 50 | B6 | 23 | THR |
| 50 | B6 | 28 | ARG |
| 50 | B6 | 30 | THR |
| 50 | B6 | 34 | LEU |
| 50 | B6 | 38 | LYS |
| 50 | B6 | 40 | CYS |
| 50 | B6 | 44 | ARG |
| 51 | B7 | 1 | MET |
| 51 | B7 | 4 | THR |
| 51 | B7 | 8 | ASN |
| 51 | B7 | 9 | ARG |
| 51 | B7 | 23 | ARG |
| 51 | B7 | 32 | LYS |
| 51 | B7 | 47 | ARG |
| 52 | B8 | 6 | THR |
| 52 | B8 | 11 | LYS |
| 52 | B8 | 14 | VAL |
| 52 | B8 | 23 | VAL |
| 52 | B8 | 31 | HIS |
| 52 | B8 | 32 | LEU |
| 52 | B8 | 34 | TRP |
| 52 | B8 | 35 | GLN |
| 52 | B8 | 41 | ILE |
| 52 | B8 | 49 | VAL |
| 53 | B9 | 6 | SER |
| 53 | B9 | 7 | VAL |
| 53 | B9 | 17 | ILE |
| 53 | B9 | 26 | ILE |
| 2 | CB | 15 | VAL |
| 2 | CB | 17 | PHE |
| 2 | CB | 21 | ARG |
| 2 | CB | 24 | TRP |
| 2 | CB | 47 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CB | 51 | LEU |
| 2 | CB | 67 | THR |
| 2 | CB | 69 | LEU |
| 2 | CB | 74 | LYS |
| 2 | CB | 80 | ILE |
| 2 | CB | 82 | ARG |
| 2 | CB | 86 | GLU |
| 2 | CB | 87 | ARG |
| 2 | CB | 93 | VAL |
| 2 | CB | 94 | ASN |
| 2 | CB | 110 | GLN |
| 2 | CB | 113 | HIS |
| 2 | CB | 114 | ARG |
| 2 | CB | 117 | GLU |
| 2 | CB | 121 | LEU |
| 2 | CB | 124 | SER |
| 2 | CB | 133 | LYS |
| 2 | CB | 137 | ARG |
| 2 | CB | 139 | LYS |
| 2 | CB | 140 | HIS |
| 2 | CB | 150 | SER |
| 2 | CB | 153 | ARG |
| 2 | CB | 157 | ARG |
| 2 | CB | 160 | ASP |
| 2 | CB | 163 | PHE |
| 2 | CB | 170 | GLU |
| 2 | CB | 185 | ILE |
| 2 | CB | 187 | LEU |
| 2 | CB | 191 | ASP |
| 2 | CB | 197 | VAL |
| 2 | CB | 200 | ILE |
| 2 | CB | 205 | ASP |
| 2 | CB | 208 | ILE |
| 2 | CB | 209 | ARG |
| 2 | CB | 210 | SER |
| 2 | CB | 212 | GLN |
| 2 | CB | 221 | LEU |
| 2 | CB | 230 | VAL |
| 2 | CB | 233 | SER |
| 3 | CC | 4 | LYS |
| 3 | CC | 11 | ARG |
| 3 | CC | 26 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CC | 30 | ARG |
| 3 | CC | 31 | HIS |
| 3 | CC | 32 | LEU |
| 3 | CC | 36 | ASP |
| 3 | CC | 47 | LEU |
| 3 | CC | 49 | SER |
| 3 | CC | 52 | LEU |
| 3 | CC | 56 | ASP |
| 3 | CC | 59 | ARG |
| 3 | CC | 104 | GLN |
| 3 | CC | 136 | GLN |
| 3 | CC | 143 | GLU |
| 3 | CC | 154 | SER |
| 3 | CC | 175 | LEU |
| 3 | CC | 176 | HIS |
| 3 | CC | 183 | ASP |
| 3 | CC | 188 | LEU |
| 3 | CC | 195 | VAL |
| 3 | CC | 202 | ILE |
| 4 | CD | 11 | LEU |
| 4 | CD | 12 | CYS |
| 4 | CD | 13 | ARG |
| 4 | CD | 20 | TYR |
| 4 | CD | 36 | ARG |
| 4 | CD | 52 | SER |
| 4 | CD | 53 | ASP |
| 4 | CD | 57 | ARG |
| 4 | CD | 70 | ILE |
| 4 | CD | 76 | ARG |
| 4 | CD | 83 | SER |
| 4 | CD | 106 | TYR |
| 4 | CD | 113 | SER |
| 4 | CD | 119 | GLN |
| 4 | CD | 122 | ARG |
| 4 | CD | 127 | THR |
| 4 | CD | 129 | ASN |
| 4 | CD | 135 | LEU |
| 4 | CD | 138 | TYR |
| 4 | CD | 158 | ILE |
| 4 | CD | 170 | VAL |
| 4 | CD | 193 | ASP |
| 5 | CE | 11 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 12 | LEU |
| 5 | CE | 14 | ARG |
| 5 | CE | 16 | THR |
| 5 | CE | 41 | VAL |
| 5 | CE | 51 | VAL |
| 5 | CE | 60 | TYR |
| 5 | CE | 63 | ARG |
| 5 | CE | 65 | ASN |
| 5 | CE | 76 | ILE |
| 5 | CE | 78 | HIS |
| 5 | CE | 79 | GLU |
| 5 | CE | 83 | GLU |
| 5 | CE | 84 | PHE |
| 5 | CE | 87 | SER |
| 5 | CE | 89 | ILE |
| 5 | CE | 91 | LEU |
| 5 | CE | 98 | THR |
| 5 | CE | 107 | ARG |
| 5 | CE | 147 | ASP |
| 5 | CE | 152 | ARG |
| 6 | CF | 7 | ASN |
| 6 | CF | 22 | GLU |
| 6 | CF | 36 | ARG |
| 6 | CF | 40 | VAL |
| 6 | CF | 45 | LEU |
| 6 | CF | 48 | LEU |
| 6 | CF | 57 | GLN |
| 6 | CF | 63 | TYR |
| 6 | CF | 69 | GLU |
| 6 | CF | 70 | ASP |
| 6 | CF | 72 | VAL |
| 6 | CF | 73 | ASN |
| 6 | CF | 74 | ASP |
| 6 | CF | 75 | LEU |
| 6 | CF | 89 | MET |
| 6 | CF | 94 | GLN |
| 6 | CF | 98 | LEU |
| 6 | CF | 100 | ASN |
| 7 | CG | 3 | ARG |
| 7 | CG | 6 | ARG |
| 7 | CG | 12 | LEU |
| 7 | CG | 17 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CG | 20 | ASP |
| 7 | CG | 23 | VAL |
| 7 | CG | 24 | THR |
| 7 | CG | 26 | PHE |
| 7 | CG | 32 | ARG |
| 7 | CG | 33 | ASP |
| 7 | CG | 36 | LYS |
| 7 | CG | 44 | TYR |
| 7 | CG | 47 | CYS |
| 7 | CG | 56 | GLN |
| 7 | CG | 61 | VAL |
| 7 | CG | 62 | PHE |
| 7 | CG | 67 | GLU |
| 7 | CG | 73 | MET |
| 7 | CG | 75 | VAL |
| 7 | CG | 80 | VAL |
| 7 | CG | 90 | GLU |
| 7 | CG | 96 | GLN |
| 7 | CG | 111 | ARG |
| 7 | CG | 113 | GLU |
| 7 | CG | 118 | VAL |
| 7 | CG | 119 | ARG |
| 7 | CG | 120 | ILE |
| 7 | CG | 125 | MET |
| 7 | CG | 126 | ASP |
| 7 | CG | 135 | VAL |
| 7 | CG | 142 | GLU |
| 7 | CG | 143 | ARG |
| 7 | CG | 148 | ASN |
| 7 | CG | 153 | HIS |
| 7 | CG | 155 | ARG |
| 8 | CH | 2 | LEU |
| 8 | CH | 21 | LYS |
| 8 | CH | 25 | ASP |
| 8 | CH | 37 | ARG |
| 8 | CH | 49 | GLU |
| 8 | CH | 52 | ASP |
| 8 | CH | 54 | ASP |
| 8 | CH | 60 | ARG |
| 8 | CH | 63 | LEU |
| 8 | CH | 77 | GLU |
| 8 | CH | 78 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CH | 83 | ILE |
| 8 | CH | 84 | ARG |
| 8 | CH | 85 | ARG |
| 8 | CH | 91 | ARG |
| 8 | CH | 95 | VAL |
| 8 | CH | 109 | ILE |
| 8 | CH | 119 | LEU |
| 8 | CH | 120 | THR |
| 8 | CH | 127 | LEU |
| 9 | CI | 5 | TYR |
| 9 | CI | 11 | LYS |
| 9 | CI | 62 | TYR |
| 9 | CI | 63 | ILE |
| 9 | CI | 64 | THR |
| 9 | CI | 65 | VAL |
| 9 | CI | 66 | ARG |
| 9 | CI | 74 | ILE |
| 9 | CI | 75 | ASP |
| 9 | CI | 77 | ILE |
| 9 | CI | 88 | TYR |
| 9 | CI | 104 | ARG |
| 9 | CI | 107 | ARG |
| 9 | CI | 108 | VAL |
| 9 | CI | 114 | TYR |
| 10 | CJ | 12 | ASP |
| 10 | CJ | 21 | GLN |
| 10 | CJ | 33 | GLN |
| 10 | CJ | 38 | ILE |
| 10 | CJ | 42 | THR |
| 10 | CJ | 45 | ARG |
| 10 | CJ | 49 | VAL |
| 10 | CJ | 55 | LYS |
| 10 | CJ | 62 | HIS |
| 10 | CJ | 64 | GLU |
| 10 | CJ | 73 | ASP |
| 10 | CJ | 94 | VAL |
| 10 | CJ | 96 | ILE |
| 10 | CJ | 100 | THR |
| 11 | CK | 14 | VAL |
| 11 | CK | 16 | SER |
| 11 | CK | 29 | ILE |
| 11 | CK | 30 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | CK | 32 | ILE |
| 11 | CK | 47 | VAL |
| 11 | CK | 81 | ASP |
| 11 | CK | 96 | ARG |
| 11 | CK | 103 | LEU |
| 11 | CK | 109 | VAL |
| 11 | CK | 117 | ASN |
| 12 | CL | 33 | ARG |
| 12 | CL | 44 | THR |
| 12 | CL | 52 | LEU |
| 12 | CL | 53 | ARG |
| 12 | CL | 60 | LEU |
| 12 | CL | 66 | VAL |
| 12 | CL | 82 | VAL |
| 12 | CL | 97 | ARG |
| 12 | CL | 115 | LYS |
| 12 | CL | 119 | LYS |
| 13 | CM | 3 | ARG |
| 13 | CM | 19 | LEU |
| 13 | CM | 34 | LEU |
| 13 | CM | 45 | VAL |
| 13 | CM | 47 | ASP |
| 13 | CM | 55 | ARG |
| 13 | CM | 56 | LEU |
| 13 | CM | 61 | GLU |
| 13 | CM | 65 | LYS |
| 13 | CM | 66 | LEU |
| 13 | CM | 67 | GLU |
| 13 | CM | 70 | LEU |
| 13 | CM | 71 | ARG |
| 13 | CM | 88 | ARG |
| 13 | CM | 105 | THR |
| 14 | CN | 3 | ARG |
| 14 | CN | 6 | LEU |
| 14 | CN | 7 | ILE |
| 14 | CN | 8 | GLU |
| 14 | CN | 13 | THR |
| 14 | CN | 17 | LYS |
| 14 | CN | 24 | CYS |
| 14 | CN | 25 | VAL |
| 14 | CN | 32 | SER |
| 14 | CN | 33 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | CN | 39 | LEU |
| 14 | CN | 42 | ILE |
| 14 | CN | 45 | ARG |
| 14 | CN | 53 | LEU |
| 15 | CO | 3 | ILE |
| 15 | CO | 4 | THR |
| 15 | CO | 13 | GLN |
| 15 | CO | 24 | SER |
| 15 | CO | 26 | GLU |
| 15 | CO | 39 | LEU |
| 15 | CO | 66 | LEU |
| 15 | CO | 72 | ARG |
| 15 | CO | 87 | ILE |
| 16 | CP | 1 | MET |
| 16 | CP | 2 | VAL |
| 16 | CP | 6 | LEU |
| 16 | CP | 11 | SER |
| 16 | CP | 21 | VAL |
| 16 | CP | 22 | THR |
| 16 | CP | 25 | ARG |
| 16 | CP | 26 | ARG |
| 16 | CP | 27 | LYS |
| 16 | CP | 29 | ASP |
| 16 | CP | 36 | ILE |
| 16 | CP | 38 | TYR |
| 16 | CP | 43 | LYS |
| 16 | CP | 45 | THR |
| 16 | CP | 62 | VAL |
| 16 | CP | 65 | GLN |
| 16 | CP | 67 | THR |
| 16 | CP | 69 | THR |
| 16 | CP | 76 | GLN |
| 17 | CQ | 11 | VAL |
| 17 | CQ | 34 | LYS |
| 17 | CQ | 43 | LEU |
| 17 | CQ | 45 | HIS |
| 17 | CQ | 50 | LYS |
| 17 | CQ | 57 | VAL |
| 17 | CQ | 59 | ILE |
| 17 | CQ | 65 | ILE |
| 17 | CQ | 72 | ARG |
| 17 | CQ | 74 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | CQ | 86 | GLU |
| 17 | CQ | 96 | GLU |
| 17 | CQ | 100 | LYS |
| 18 | CR | 35 | ARG |
| 18 | CR | 36 | ASN |
| 18 | CR | 76 | LEU |
| 18 | CR | 79 | LEU |
| 18 | CR | 85 | LEU |
| 19 | CS | 44 | MET |
| 19 | CS | 47 | HIS |
| 19 | CS | 51 | VAL |
| 19 | CS | 61 | TYR |
| 19 | CS | 62 | ILE |
| 19 | CS | 66 | MET |
| 19 | CS | 67 | VAL |
| 19 | CS | 69 | HIS |
| 19 | CS | 78 | ARG |
| 19 | CS | 79 | THR |
| 19 | CS | 81 | ARG |
| 20 | CT | 10 | LEU |
| 20 | CT | 13 | LEU |
| 20 | CT | 36 | LEU |
| 20 | CT | 39 | LYS |
| 20 | CT | 62 | LEU |
| 20 | CT | 71 | THR |
| 20 | CT | 72 | LEU |
| 20 | CT | 73 | HIS |
| 20 | CT | 74 | LYS |
| 20 | CT | 84 | LEU |
| 21 | CU | 6 | ARG |
| 21 | CU | 7 | ARG |
| 21 | CU | 9 | ARG |
| 21 | CU | 10 | ARG |
| 21 | CU | 12 | LYS |
| 21 | CU | 13 | ILE |
| 21 | CU | 17 | THR |
| 22 | CX | 4 | ASN |
| 22 | CX | 6 | THR |
| 22 | CX | 31 | PHE |
| 22 | CX | 54 | LEU |
| 22 | CX | 62 | HIS |
| 22 | CX | 64 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | CX | 66 | GLU |
| 22 | CX | 77 | LEU |
| 22 | CX | 93 | LYS |
| 25 | DD | 12 | SER |
| 25 | DD | 13 | ARG |
| 25 | DD | 18 | VAL |
| 25 | DD | 24 | ILE |
| 25 | DD | 54 | ARG |
| 25 | DD | 83 | GLU |
| 25 | DD | 94 | LEU |
| 25 | DD | 103 | ARG |
| 25 | DD | 106 | ILE |
| 25 | DD | 111 | LEU |
| 25 | DD | 126 | GLN |
| 25 | DD | 131 | LEU |
| 25 | DD | 138 | VAL |
| 25 | DD | 141 | VAL |
| 25 | DD | 150 | LYS |
| 25 | DD | 154 | LYS |
| 25 | DD | 173 | VAL |
| 25 | DD | 192 | THR |
| 25 | DD | 200 | ASP |
| 25 | DD | 211 | ARG |
| 25 | DD | 212 | SER |
| 25 | DD | 217 | ARG |
| 25 | DD | 218 | ARG |
| 25 | DD | 221 | VAL |
| 25 | DD | 229 | VAL |
| 25 | DD | 254 | THR |
| 25 | DD | 257 | LEU |
| 25 | DD | 259 | THR |
| 25 | DD | 260 | ARG |
| 25 | DD | 271 | ILE |
| 25 | DD | 273 | ARG |
| 25 | DD | 274 | ARG |
| 26 | DE | 7 | VAL |
| 26 | DE | 12 | THR |
| 26 | DE | 21 | VAL |
| 26 | DE | 24 | THR |
| 26 | DE | 33 | VAL |
| 26 | DE | 40 | GLU |
| 26 | DE | 49 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | DE | 52 | LEU |
| 26 | DE | 61 | ARG |
| 26 | DE | 69 | LYS |
| 26 | DE | 72 | VAL |
| 26 | DE | 75 | VAL |
| 26 | DE | 77 | ILE |
| 26 | DE | 82 | ARG |
| 26 | DE | 92 | THR |
| 26 | DE | 111 | ARG |
| 26 | DE | 116 | VAL |
| 26 | DE | 119 | ARG |
| 26 | DE | 128 | SER |
| 26 | DE | 144 | ARG |
| 26 | DE | 154 | LYS |
| 26 | DE | 167 | VAL |
| 26 | DE | 170 | LEU |
| 26 | DE | 179 | GLU |
| 26 | DE | 181 | LEU |
| 26 | DE | 195 | LEU |
| 27 | DF | 12 | LEU |
| 27 | DF | 18 | ARG |
| 27 | DF | 20 | LEU |
| 27 | DF | 24 | LEU |
| 27 | DF | 33 | LEU |
| 27 | DF | 41 | LEU |
| 27 | DF | 50 | SER |
| 27 | DF | 57 | VAL |
| 27 | DF | 69 | HIS |
| 27 | DF | 77 | ASP |
| 27 | DF | 88 | VAL |
| 27 | DF | 96 | ASP |
| 27 | DF | 106 | ARG |
| 27 | DF | 110 | LEU |
| 27 | DF | 112 | MET |
| 27 | DF | 132 | VAL |
| 27 | DF | 137 | LYS |
| 27 | DF | 140 | LEU |
| 27 | DF | 158 | THR |
| 27 | DF | 161 | GLU |
| 27 | DF | 168 | ARG |
| 27 | DF | 170 | LEU |
| 27 | DF | 175 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | DF | 188 | ARG |
| 27 | DF | 192 | LEU |
| 28 | DG | 3 | LEU |
| 28 | DG | 5 | VAL |
| 28 | DG | 7 | LEU |
| 28 | DG | 21 | ARG |
| 28 | DG | 28 | VAL |
| 28 | DG | 35 | GLU |
| 28 | DG | 47 | LYS |
| 28 | DG | 98 | ARG |
| 28 | DG | 128 | ARG |
| 28 | DG | 136 | ARG |
| 28 | DG | 139 | LEU |
| 28 | DG | 140 | ILE |
| 28 | DG | 143 | GLU |
| 28 | DG | 146 | TYR |
| 28 | DG | 149 | VAL |
| 28 | DG | 155 | MET |
| 28 | DG | 161 | THR |
| 28 | DG | 170 | ARG |
| 28 | DG | 175 | LEU |
| 29 | DH | 3 | ARG |
| 29 | DH | 6 | ARG |
| 29 | DH | 7 | LEU |
| 29 | DH | 15 | VAL |
| 29 | DH | 24 | VAL |
| 29 | DH | 41 | MET |
| 29 | DH | 44 | VAL |
| 29 | DH | 49 | VAL |
| 29 | DH | 51 | ARG |
| 29 | DH | 58 | GLU |
| 29 | DH | 68 | THR |
| 29 | DH | 69 | ARG |
| 29 | DH | 88 | LEU |
| 29 | DH | 98 | LEU |
| 29 | DH | 113 | VAL |
| 29 | DH | 122 | THR |
| 29 | DH | 134 | SER |
| 29 | DH | 139 | GLN |
| 30 | DI | 1 | MET |
| 30 | DI | 42 | SER |
| 30 | DI | 44 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | DI | 45 | LYS |
| 30 | DI | 47 | LEU |
| 30 | DI | 81 | VAL |
| 30 | DI | 101 | LEU |
| 30 | DI | 120 | ILE |
| 30 | DI | 123 | LEU |
| 30 | DI | 129 | THR |
| 30 | DI | 130 | TYR |
| 30 | DI | 139 | GLN |
| 30 | DI | 142 | VAL |
| 30 | DI | 145 | VAL |
| 31 | DN | 1 | MET |
| 31 | DN | 5 | VAL |
| 31 | DN | 12 | ARG |
| 31 | DN | 28 | THR |
| 31 | DN | 33 | LEU |
| 31 | DN | 34 | LEU |
| 31 | DN | 38 | HIS |
| 31 | DN | 46 | VAL |
| 31 | DN | 48 | MET |
| 31 | DN | 62 | VAL |
| 31 | DN | 67 | LEU |
| 31 | DN | 68 | GLU |
| 31 | DN | 85 | ILE |
| 31 | DN | 99 | LEU |
| 31 | DN | 112 | LEU |
| 31 | DN | 120 | LEU |
| 31 | DN | 130 | HIS |
| 31 | DN | 133 | GLN |
| 31 | DN | 140 | VAL |
| 32 | DO | 8 | LEU |
| 32 | DO | 10 | VAL |
| 32 | DO | 17 | ARG |
| 32 | DO | 24 | VAL |
| 32 | DO | 25 | LEU |
| 32 | DO | 26 | LYS |
| 32 | DO | 29 | ASN |
| 32 | DO | 32 | TYR |
| 32 | DO | 52 | VAL |
| 32 | DO | 53 | LYS |
| 32 | DO | 58 | VAL |
| 32 | DO | 94 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | DO | 98 | VAL |
| 32 | DO | 104 | ARG |
| 32 | DO | 113 | LYS |
| 33 | DP | 21 | ARG |
| 33 | DP | 32 | THR |
| 33 | DP | 40 | SER |
| 33 | DP | 42 | SER |
| 33 | DP | 45 | LEU |
| 33 | DP | 55 | ARG |
| 33 | DP | 59 | LEU |
| 33 | DP | 65 | ARG |
| 33 | DP | 71 | VAL |
| 33 | DP | 83 | VAL |
| 33 | DP | 86 | LYS |
| 33 | DP | 95 | VAL |
| 33 | DP | 106 | LEU |
| 33 | DP | 112 | LEU |
| 33 | DP | 125 | VAL |
| 34 | DQ | 1 | MET |
| 34 | DQ | 5 | ARG |
| 34 | DQ | 7 | MET |
| 34 | DQ | 16 | ARG |
| 34 | DQ | 45 | GLN |
| 34 | DQ | 55 | VAL |
| 34 | DQ | 56 | ARG |
| 34 | DQ | 59 | ARG |
| 34 | DQ | 63 | LYS |
| 34 | DQ | 75 | THR |
| 34 | DQ | 81 | VAL |
| 34 | DQ | 109 | VAL |
| 34 | DQ | 110 | THR |
| 34 | DQ | 134 | ARG |
| 34 | DQ | 138 | ASP |
| 35 | DR | 1 | MET |
| 35 | DR | 2 | ARG |
| 35 | DR | 6 | SER |
| 35 | DR | 9 | LYS |
| 35 | DR | 15 | SER |
| 35 | DR | 18 | LEU |
| 35 | DR | 24 | GLN |
| 35 | DR | 28 | LEU |
| 35 | DR | 29 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DR | 33 | ARG |
| 35 | DR | 44 | LEU |
| 35 | DR | 54 | LEU |
| 35 | DR | 57 | ARG |
| 35 | DR | 60 | LEU |
| 35 | DR | 63 | ARG |
| 35 | DR | 65 | LEU |
| 35 | DR | 67 | LEU |
| 35 | DR | 79 | LEU |
| 35 | DR | 86 | ARG |
| 35 | DR | 100 | LEU |
| 35 | DR | 103 | ARG |
| 35 | DR | 111 | LEU |
| 35 | DR | 113 | LEU |
| 35 | DR | 117 | VAL |
| 36 | DS | 3 | ARG |
| 36 | DS | 8 | GLU |
| 36 | DS | 12 | PHE |
| 36 | DS | 13 | ARG |
| 36 | DS | 20 | ARG |
| 36 | DS | 30 | ARG |
| 36 | DS | 36 | TYR |
| 36 | DS | 50 | SER |
| 36 | DS | 57 | LYS |
| 36 | DS | 58 | LEU |
| 36 | DS | 69 | VAL |
| 36 | DS | 75 | GLU |
| 36 | DS | 78 | LEU |
| 36 | DS | 84 | GLN |
| 36 | DS | 85 | VAL |
| 36 | DS | 95 | HIS |
| 37 | DT | 6 | LEU |
| 37 | DT | 13 | ARG |
| 37 | DT | 16 | ARG |
| 37 | DT | 17 | THR |
| 37 | DT | 36 | GLU |
| 37 | DT | 39 | ARG |
| 37 | DT | 49 | VAL |
| 37 | DT | 64 | ARG |
| 37 | DT | 74 | ARG |
| 37 | DT | 82 | LEU |
| 37 | DT | 95 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | DT | 96 | ARG |
| 37 | DT | 107 | ASP |
| 37 | DT | 111 | ARG |
| 37 | DT | 118 | ARG |
| 38 | DU | 8 | VAL |
| 38 | DU | 30 | LYS |
| 38 | DU | 31 | SER |
| 38 | DU | 36 | ARG |
| 38 | DU | 59 | ARG |
| 38 | DU | 60 | LEU |
| 38 | DU | 74 | LEU |
| 38 | DU | 101 | ARG |
| 38 | DU | 104 | GLN |
| 38 | DU | 108 | GLU |
| 39 | DV | 7 | THR |
| 39 | DV | 12 | TYR |
| 39 | DV | 13 | ARG |
| 39 | DV | 18 | LEU |
| 39 | DV | 21 | ARG |
| 39 | DV | 28 | GLU |
| 39 | DV | 32 | THR |
| 39 | DV | 33 | VAL |
| 39 | DV | 57 | VAL |
| 39 | DV | 61 | VAL |
| 39 | DV | 62 | LEU |
| 39 | DV | 72 | VAL |
| 39 | DV | 73 | SER |
| 39 | DV | 79 | VAL |
| 39 | DV | 85 | LYS |
| 39 | DV | 95 | LEU |
| 39 | DV | 100 | ARG |
| 40 | DW | 11 | ARG |
| 40 | DW | 15 | ARG |
| 40 | DW | 19 | LEU |
| 40 | DW | 23 | LEU |
| 40 | DW | 27 | LYS |
| 40 | DW | 41 | LYS |
| 40 | DW | 51 | LEU |
| 40 | DW | 60 | ASN |
| 40 | DW | 77 | ASP |
| 40 | DW | 100 | THR |
| 40 | DW | 107 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DX | 15 | GLU |
| 41 | DX | 25 | LYS |
| 41 | DX | 57 | LEU |
| 41 | DX | 65 | ARG |
| 41 | DX | 76 | ARG |
| 42 | DY | 2 | ARG |
| 42 | DY | 3 | VAL |
| 42 | DY | 6 | HIS |
| 42 | DY | 9 | LYS |
| 42 | DY | 23 | ARG |
| 42 | DY | 45 | VAL |
| 42 | DY | 49 | VAL |
| 42 | DY | 55 | TYR |
| 42 | DY | 61 | ILE |
| 42 | DY | 72 | VAL |
| 42 | DY | 90 | LEU |
| 42 | DY | 91 | GLU |
| 42 | DY | 92 | ASN |
| 42 | DY | 97 | ARG |
| 42 | DY | 101 | LYS |
| 42 | DY | 102 | CYS |
| 42 | DY | 107 | ASP |
| 43 | DZ | 5 | LEU |
| 43 | DZ | 10 | ARG |
| 43 | DZ | 11 | GLU |
| 43 | DZ | 19 | ARG |
| 43 | DZ | 24 | LEU |
| 43 | DZ | 42 | VAL |
| 43 | DZ | 52 | SER |
| 43 | DZ | 56 | VAL |
| 43 | DZ | 66 | SER |
| 43 | DZ | 76 | LEU |
| 43 | DZ | 82 | ARG |
| 43 | DZ | 97 | GLU |
| 43 | DZ | 98 | MET |
| 43 | DZ | 118 | GLN |
| 43 | DZ | 126 | VAL |
| 43 | DZ | 155 | LEU |
| 43 | DZ | 156 | LYS |
| 43 | DZ | 165 | VAL |
| 43 | DZ | 179 | ASP |
| 43 | DZ | 185 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | D0 | 10 | THR |
| 44 | D0 | 19 | LYS |
| 44 | D0 | 20 | ARG |
| 44 | D0 | 38 | VAL |
| 44 | D0 | 49 | LYS |
| 44 | D0 | 55 | ARG |
| 44 | D0 | 74 | ARG |
| 44 | D0 | 77 | ARG |
| 44 | D0 | 83 | PRO |
| 45 | D1 | 4 | VAL |
| 45 | D1 | 5 | CYS |
| 45 | D1 | 14 | VAL |
| 45 | D1 | 21 | ARG |
| 45 | D1 | 40 | ARG |
| 45 | D1 | 46 | LEU |
| 45 | D1 | 51 | VAL |
| 45 | D1 | 58 | ILE |
| 45 | D1 | 82 | LEU |
| 45 | D1 | 83 | GLU |
| 45 | D1 | 86 | SER |
| 45 | D1 | 95 | LEU |
| 46 | D2 | 17 | SER |
| 46 | D2 | 32 | LEU |
| 46 | D2 | 34 | GLU |
| 46 | D2 | 43 | GLN |
| 46 | D2 | 44 | LEU |
| 46 | D2 | 47 | ASN |
| 46 | D2 | 53 | LEU |
| 46 | D2 | 55 | ARG |
| 46 | D2 | 68 | ARG |
| 46 | D2 | 70 | GLN |
| 47 | D3 | 8 | LEU |
| 47 | D3 | 18 | ASP |
| 47 | D3 | 23 | LEU |
| 47 | D3 | 31 | LEU |
| 47 | D3 | 40 | THR |
| 48 | D4 | 14 | ILE |
| 48 | D4 | 16 | CYS |
| 48 | D4 | 27 | THR |
| 48 | D4 | 34 | GLU |
| 48 | D4 | 43 | TYR |
| 48 | D4 | 46 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | D5 | 6 | VAL |
| 49 | D5 | 8 | LYS |
| 49 | D5 | 9 | LYS |
| 49 | D5 | 23 | HIS |
| 49 | D5 | 29 | THR |
| 49 | D5 | 37 | LYS |
| 49 | D5 | 40 | LYS |
| 49 | D5 | 46 | CYS |
| 49 | D5 | 58 | LEU |
| 50 | D6 | 4 | GLU |
| 50 | D6 | 6 | ARG |
| 50 | D6 | 13 | CYS |
| 50 | D6 | 14 | THR |
| 50 | D6 | 28 | ARG |
| 50 | D6 | 30 | THR |
| 50 | D6 | 34 | LEU |
| 50 | D6 | 38 | LYS |
| 50 | D6 | 40 | CYS |
| 50 | D6 | 44 | ARG |
| 51 | D7 | 1 | MET |
| 51 | D7 | 4 | THR |
| 51 | D7 | 8 | ASN |
| 51 | D7 | 9 | ARG |
| 51 | D7 | 23 | ARG |
| 51 | D7 | 32 | LYS |
| 51 | D7 | 47 | ARG |
| 52 | D8 | 6 | THR |
| 52 | D8 | 11 | LYS |
| 52 | D8 | 14 | VAL |
| 52 | D8 | 23 | VAL |
| 52 | D8 | 31 | HIS |
| 52 | D8 | 32 | LEU |
| 52 | D8 | 34 | TRP |
| 52 | D8 | 35 | GLN |
| 52 | D8 | 41 | ILE |
| 52 | D8 | 49 | VAL |
| 53 | D9 | 6 | SER |
| 53 | D9 | 7 | VAL |
| 53 | D9 | 17 | ILE |
| 53 | D9 | 26 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 94 | ASN |
| 2 | AB | 110 | GLN |
| 2 | AB | 146 | GLN |
| 2 | AB | 212 | GLN |
| 3 | AC | 6 | HIS |
| 3 | AC | 31 | HIS |
| 5 | AE | 78 | HIS |
| 6 | AF | 64 | GLN |
| 6 | AF | 73 | ASN |
| 6 | AF | 94 | GLN |
| 7 | AG | 28 | ASN |
| 7 | AG | 64 | GLN |
| 7 | AG | 106 | GLN |
| 7 | AG | 109 | ASN |
| 9 | AI | 3 | GLN |
| 9 | AI | 38 | GLN |
| 10 | AJ | 21 | GLN |
| 10 | AJ | 56 | HIS |
| 16 | AP | 13 | HIS |
| 16 | AP | 16 | HIS |
| 16 | AP | 65 | GLN |
| 18 | AR | 36 | ASN |
| 19 | AS | 57 | HIS |
| 20 | AT | 16 | HIS |
| 22 | AX | 2 | GLN |
| 22 | AX | 35 | ASN |
| 22 | AX | 94 | GLN |
| 22 | AX | 95 | HIS |
| 25 | BD | 112 | GLN |
| 25 | BD | 129 | ASN |
| 25 | BD | 143 | HIS |
| 26 | BE | 143 | ASN |
| 27 | BF | 75 | HIS |
| 28 | BG | 40 | ASN |
| 28 | BG | 66 | GLN |
| 28 | BG | 108 | ASN |
| 28 | BG | 138 | GLN |
| 29 | BH | 74 | ASN |
| 29 | BH | 111 | HIS |
| 30 | BI | 74 | ASN |
| 30 | BI | 133 | HIS |
| 30 | BI | 139 | GLN |
| 31 | BN | 128 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31 | BN | 133 | GLN |
| 32 | BO | 3 | GLN |
| 33 | BP | 84 | ASN |
| 34 | BQ | 12 | GLN |
| 36 | BS | 68 | GLN |
| 38 | BU | 49 | HIS |
| 38 | BU | 72 | HIS |
| 39 | BV | 80 | GLN |
| 40 | BW | 60 | ASN |
| 40 | BW | 61 | ASN |
| 41 | BX | 31 | HIS |
| 46 | B2 | 9 | GLN |
| 48 | B4 | 46 | GLN |
| 50 | B6 | 20 | ASN |
| 50 | B6 | 49 | HIS |
| 2 | CB | 94 | ASN |
| 2 | CB | 110 | GLN |
| 2 | CB | 140 | HIS |
| 2 | CB | 146 | GLN |
| 2 | CB | 212 | GLN |
| 3 | CC | 31 | HIS |
| 3 | CC | 37 | GLN |
| 3 | CC | 69 | HIS |
| 3 | CC | 136 | GLN |
| 5 | CE | 65 | ASN |
| 5 | CE | 78 | HIS |
| 5 | CE | 130 | ASN |
| 6 | CF | 64 | GLN |
| 6 | CF | 73 | ASN |
| 6 | CF | 94 | GLN |
| 7 | CG | 96 | GLN |
| 7 | CG | 148 | ASN |
| 9 | CI | 3 | GLN |
| 10 | CJ | 68 | HIS |
| 13 | CM | 77 | ASN |
| 14 | CN | 52 | GLN |
| 16 | CP | 16 | HIS |
| 16 | CP | 65 | GLN |
| 17 | CQ | 45 | HIS |
| 18 | CR | 36 | ASN |
| 19 | CS | 83 | HIS |
| 22 | CX | 94 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | DD | 112 | GLN |
| 25 | DD | 129 | ASN |
| 25 | DD | 143 | HIS |
| 28 | DG | 40 | ASN |
| 28 | DG | 66 | GLN |
| 28 | DG | 108 | ASN |
| 28 | DG | 138 | GLN |
| 29 | DH | 74 | ASN |
| 29 | DH | 147 | ASN |
| 30 | DI | 105 | HIS |
| 30 | DI | 139 | GLN |
| 31 | DN | 128 | HIS |
| 31 | DN | 133 | GLN |
| 32 | DO | 3 | GLN |
| 33 | DP | 84 | ASN |
| 36 | DS | 68 | GLN |
| 37 | DT | 58 | ASN |
| 38 | DU | 49 | HIS |
| 40 | DW | 61 | ASN |
| 41 | DX | 31 | HIS |
| 43 | DZ | 151 | HIS |
| 46 | D2 | 9 | GLN |
| 48 | D4 | 46 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1499/1522 (98%) | 385 (25%) | 33 (2%) |
| 1 | CA | 1495/1522 (98%) | 396 (26%) | 34 (2%) |
| 23 | BA | 2833/2913 (97%) | 609 (21%) | 60 (2%) |
| 23 | DA | 2807/2913 (96%) | 600 (21%) | 56 (1%) |
| 24 | BB | 119/122 (97%) | 25 (21%) | 0 |
| 24 | DB | 119/122 (97%) | 26 (21%) | 0 |
| All | All | 8872/9114 (97%) | 2041 (23%) | 183 (2%) |

All (2041) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 5 | U |
| 1 | AA | 6 | G |
| 1 | AA | 7 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 9 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 50 | A |
| 1 | AA | 51 | A |
| 1 | AA | 53 | A |
| 1 | AA | 60 | A |
| 1 | AA | 61 | G |
| 1 | AA | 62 | U |
| 1 | AA | 65 | U |
| 1 | AA | 66 | G |
| 1 | AA | 67 | C |
| 1 | AA | 70 | G |
| 1 | AA | 77 | G |
| 1 | AA | 78 | G |
| 1 | AA | 79 | G |
| 1 | AA | 89 | C |
| 1 | AA | 90 | U |
| 1 | AA | 91 | C |
| 1 | AA | 93 | G |
| 1 | AA | 96 | U |
| 1 | AA | 97 | G |
| 1 | AA | 115 | G |
| 1 | AA | 116 | A |
| 1 | AA | 121 | C |
| 1 | AA | 131 | C |
| 1 | AA | 142 | G |
| 1 | AA | 150 | C |
| 1 | AA | 163 | C |
| 1 | AA | 173 | U |
| 1 | AA | 182 | U |
| 1 | AA | 189(G) | G |
| 1 | AA | 189(H) | G |
| 1 | AA | 195 | A |
| 1 | AA | 197 | A |
| 1 | AA | 201 | C |
| 1 | AA | 203 | U |
| 1 | AA | 204 | U |
| 1 | AA | 216 | G |
| 1 | AA | 227 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 243 | A |
| 1 | AA | 244 | U |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 289 | G |
| 1 | AA | 306 | G |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 332 | G |
| 1 | AA | 341 | C |
| 1 | AA | 342 | C |
| 1 | AA | 343 | U |
| 1 | AA | 344 | A |
| 1 | AA | 345 | C |
| 1 | AA | 351 | G |
| 1 | AA | 352 | C |
| 1 | AA | 353 | A |
| 1 | AA | 354 | G |
| 1 | AA | 365 | U |
| 1 | AA | 367 | U |
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 388 | G |
| 1 | AA | 392 | G |
| 1 | AA | 397 | A |
| 1 | AA | 398 | C |
| 1 | AA | 406 | G |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 414 | A |
| 1 | AA | 422 | C |
| 1 | AA | 423 | G |
| 1 | AA | 424 | G |
| 1 | AA | 429 | U |
| 1 | AA | 435 | C |
| 1 | AA | 437 | U |
| 1 | AA | 439 | A |
| 1 | AA | 442 | C |
| 1 | AA | 445 | G |
| 1 | AA | 446 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 452 | A |
| 1 | AA | 457 | C |
| 1 | AA | 461 | A |
| 1 | AA | 484 | G |
| 1 | AA | 485 | G |
| 1 | AA | 493 | G |
| 1 | AA | 496 | A |
| 1 | AA | 498 | U |
| 1 | AA | 505 | G |
| 1 | AA | 509 | A |
| 1 | AA | 510 | A |
| 1 | AA | 511 | C |
| 1 | AA | 518 | C |
| 1 | AA | 520 | A |
| 1 | AA | 521 | G |
| 1 | AA | 524 | G |
| 1 | AA | 527 | G |
| 1 | AA | 531 | U |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 547 | A |
| 1 | AA | 559 | A |
| 1 | AA | 560 | U |
| 1 | AA | 561 | U |
| 1 | AA | 562 | C |
| 1 | AA | 563 | A |
| 1 | AA | 570 | G |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 575 | G |
| 1 | AA | 576 | G |
| 1 | AA | 577 | G |
| 1 | AA | 588 | G |
| 1 | AA | 596 | C |
| 1 | AA | 607 | A |
| 1 | AA | 618 | C |
| 1 | AA | 623 | C |
| 1 | AA | 629 | G |
| 1 | AA | 630 | G |
| 1 | AA | 631 | G |
| 1 | AA | 632 | A |
| 1 | AA | 633 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 653 | A |
| 1 | AA | 661 | G |
| 1 | AA | 665 | A |
| 1 | AA | 666 | G |
| 1 | AA | 680 | C |
| 1 | AA | 687 | A |
| 1 | AA | 688 | G |
| 1 | AA | 690 | G |
| 1 | AA | 724 | G |
| 1 | AA | 731 | G |
| 1 | AA | 749 | C |
| 1 | AA | 755 | G |
| 1 | AA | 766 | A |
| 1 | AA | 774 | G |
| 1 | AA | 777 | A |
| 1 | AA | 786 | G |
| 1 | AA | 787 | A |
| 1 | AA | 792 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 796 | C |
| 1 | AA | 802 | A |
| 1 | AA | 816 | A |
| 1 | AA | 817 | C |
| 1 | AA | 818 | G |
| 1 | AA | 821 | G |
| 1 | AA | 827 | U |
| 1 | AA | 828 | A |
| 1 | AA | 833 | U |
| 1 | AA | 836 | G |
| 1 | AA | 839 | U |
| 1 | AA | 840 | C |
| 1 | AA | 841 | U |
| 1 | AA | 848 | C |
| 1 | AA | 859 | A |
| 1 | AA | 870 | U |
| 1 | AA | 875 | C |
| 1 | AA | 876 | G |
| 1 | AA | 902 | G |
| 1 | AA | 914 | A |
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 932 | C |
| 1 | AA | 934 | C |
| 1 | AA | 935 | A |
| 1 | AA | 939 | G |
| 1 | AA | 943 | U |
| 1 | AA | 944 | G |
| 1 | AA | 945 | G |
| 1 | AA | 946 | A |
| 1 | AA | 948 | C |
| 1 | AA | 958 | A |
| 1 | AA | 960 | U |
| 1 | AA | 961 | U |
| 1 | AA | 964 | A |
| 1 | AA | 968 | A |
| 1 | AA | 969 | A |
| 1 | AA | 971 | G |
| 1 | AA | 974 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 978 | A |
| 1 | AA | 979 | C |
| 1 | AA | 980 | C |
| 1 | AA | 981 | U |
| 1 | AA | 983 | A |
| 1 | AA | 984 | C |
| 1 | AA | 985 | C |
| 1 | AA | 990 | C |
| 1 | AA | 991 | U |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 996 | A |
| 1 | AA | 997 | U |
| 1 | AA | 1000 | U |
| 1 | AA | 1001(A) | G |
| 1 | AA | 1003 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1005 | A |
| 1 | AA | 1006 | C |
| 1 | AA | 1010 | G |
| 1 | AA | 1011 | G |
| 1 | AA | 1013 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1014 | A |
| 1 | AA | 1016 | A |
| 1 | AA | 1021 | G |
| 1 | AA | 1022 | G |
| 1 | AA | 1023 | G |
| 1 | AA | 1026 | G |
| 1 | AA | 1027 | C |
| 1 | AA | 1030(A) | G |
| 1 | AA | 1031 | G |
| 1 | AA | 1034 | G |
| 1 | AA | 1035 | A |
| 1 | AA | 1036 | G |
| 1 | AA | 1042 | G |
| 1 | AA | 1044 | A |
| 1 | AA | 1045 | C |
| 1 | AA | 1046 | A |
| 1 | AA | 1051 | C |
| 1 | AA | 1053 | G |
| 1 | AA | 1054 | C |
| 1 | AA | 1055 | A |
| 1 | AA | 1056 | U |
| 1 | AA | 1065 | U |
| 1 | AA | 1066 | C |
| 1 | AA | 1068 | G |
| 1 | AA | 1070 | U |
| 1 | AA | 1073 | U |
| 1 | AA | 1074 | G |
| 1 | AA | 1081 | G |
| 1 | AA | 1082 | G |
| 1 | AA | 1084 | G |
| 1 | AA | 1085 | U |
| 1 | AA | 1090 | U |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1101 | A |
| 1 | AA | 1113 | C |
| 1 | AA | 1117 | G |
| 1 | AA | 1121 | U |
| 1 | AA | 1122 | U |
| 1 | AA | 1124 | G |
| 1 | AA | 1125 | U |
| 1 | AA | 1126 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 1127 | G |
| 1 | AA | 1129 | C |
| 1 | AA | 1131 | G |
| 1 | AA | 1134 | G |
| 1 | AA | 1136 | U |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1140 | C |
| 1 | AA | 1144 | G |
| 1 | AA | 1145 | C |
| 1 | AA | 1149 | C |
| 1 | AA | 1152 | A |
| 1 | AA | 1153 | C |
| 1 | AA | 1154 | G |
| 1 | AA | 1155 | G |
| 1 | AA | 1157 | A |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1164 | G |
| 1 | AA | 1175 | G |
| 1 | AA | 1184 | G |
| 1 | AA | 1190 | G |
| 1 | AA | 1196 | U |
| 1 | AA | 1197 | G |
| 1 | AA | 1199 | U |
| 1 | AA | 1201 | A |
| 1 | AA | 1202 | G |
| 1 | AA | 1206 | G |
| 1 | AA | 1207 | G |
| 1 | AA | 1211 | U |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1214 | C |
| 1 | AA | 1220 | G |
| 1 | AA | 1225 | A |
| 1 | AA | 1226 | C |
| 1 | AA | 1227 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1239 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1241 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1242 | C |
| 1 | AA | 1244 | C |
| 1 | AA | 1246 | C |
| 1 | AA | 1247 | U |
| 1 | AA | 1250 | A |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | U |
| 1 | AA | 1258 | G |
| 1 | AA | 1260 | C |
| 1 | AA | 1266 | G |
| 1 | AA | 1270 | C |
| 1 | AA | 1275 | A |
| 1 | AA | 1277 | C |
| 1 | AA | 1278 | U |
| 1 | AA | 1280 | A |
| 1 | AA | 1282 | C |
| 1 | AA | 1285 | A |
| 1 | AA | 1286 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1294 | G |
| 1 | AA | 1297 | C |
| 1 | AA | 1298 | C |
| 1 | AA | 1300 | G |
| 1 | AA | 1301 | U |
| 1 | AA | 1302 | U |
| 1 | AA | 1304 | G |
| 1 | AA | 1305 | G |
| 1 | AA | 1306 | A |
| 1 | AA | 1308 | U |
| 1 | AA | 1312 | G |
| 1 | AA | 1316 | G |
| 1 | AA | 1318 | A |
| 1 | AA | 1319 | A |
| 1 | AA | 1320 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1325 | C |
| 1 | AA | 1328 | C |
| 1 | AA | 1330 | U |
| 1 | AA | 1331 | G |
| 1 | AA | 1332 | A |
| 1 | AA | 1333 | A |
| 1 | AA | 1334 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | AA | 1335 | C |
| 1 | AA | 1336 | C |
| 1 | AA | 1337 | G |
| 1 | AA | 1338 | G |
| 1 | AA | 1339 | A |
| 1 | AA | 1345 | U |
| 1 | AA | 1346 | A |
| 1 | AA | 1347 | G |
| 1 | AA | 1349 | A |
| 1 | AA | 1355 | G |
| 1 | AA | 1360 | A |
| 1 | AA | 1363 | C |
| 1 | AA | 1363(A) | A |
| 1 | AA | 1364 | U |
| 1 | AA | 1365 | G |
| 1 | AA | 1369 | C |
| 1 | AA | 1378 | C |
| 1 | AA | 1379 | G |
| 1 | AA | 1380 | U |
| 1 | AA | 1388 | C |
| 1 | AA | 1395 | C |
| 1 | AA | 1398 | A |
| 1 | AA | 1401 | G |
| 1 | AA | 1419 | G |
| 1 | AA | 1441 | G |
| 1 | AA | 1442 | G |
| 1 | AA | 1442(B) | A |
| 1 | AA | 1446 | U |
| 1 | AA | 1447 | A |
| 1 | AA | 1452 | C |
| 1 | AA | 1456 | G |
| 1 | AA | 1457 | G |
| 1 | AA | 1459 | C |
| 1 | AA | 1487 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1493 | A |
| 1 | AA | 1494 | G |
| 1 | AA | 1495 | U |
| 1 | AA | 1497 | G |
| 1 | AA | 1504 | G |
| 1 | AA | 1505 | G |
| 1 | AA | 1506 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 1517 | G |
| 1 | AA | 1520 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 23 | BA | 10 | G |
| 23 | BA | 12 | U |
| 23 | BA | 15 | G |
| 23 | BA | 34 | C |
| 23 | BA | 36 | G |
| 23 | BA | 45 | C |
| 23 | BA | 55 | G |
| 23 | BA | 69 | C |
| 23 | BA | 71 | A |
| 23 | BA | 72 | U |
| 23 | BA | 74 | A |
| 23 | BA | 75 | G |
| 23 | BA | 82 | G |
| 23 | BA | 84 | A |
| 23 | BA | 90 | U |
| 23 | BA | 94 | C |
| 23 | BA | 95 | G |
| 23 | BA | 100 | G |
| 23 | BA | 102 | G |
| 23 | BA | 103 | A |
| 23 | BA | 118 | A |
| 23 | BA | 119 | A |
| 23 | BA | 120 | U |
| 23 | BA | 131 | G |
| 23 | BA | 141 | A |
| 23 | BA | 154 | G |
| 23 | BA | 154(A) | C |
| 23 | BA | 157 | U |
| 23 | BA | 181 | A |
| 23 | BA | 182 | A |
| 23 | BA | 188 | G |
| 23 | BA | 196 | A |
| 23 | BA | 199 | A |
| 23 | BA | 200 | U |
| 23 | BA | 201 | C |
| 23 | BA | 204 | A |
| 23 | BA | 205 | G |
| 23 | BA | 214 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 215 | G |
| 23 | BA | 216 | A |
| 23 | BA | 221 | A |
| 23 | BA | 222 | A |
| 23 | BA | 225 | A |
| 23 | BA | 229 | A |
| 23 | BA | 233 | A |
| 23 | BA | 248 | G |
| 23 | BA | 250 | G |
| 23 | BA | 266 | G |
| 23 | BA | 269 | U |
| 23 | BA | 271(I) | G |
| 23 | BA | 271(K) | U |
| 23 | BA | 271(L) | U |
| 23 | BA | 271(M) | G |
| 23 | BA | 271(N) | U |
| 23 | BA | 271(Y) | U |
| 23 | BA | 272(B) | G |
| 23 | BA | 272(G) | C |
| 23 | BA | 272(H) | C |
| 23 | BA | 272(I) | U |
| 23 | BA | 272(J) | C |
| 23 | BA | 276 | A |
| 23 | BA | 277 | C |
| 23 | BA | 278 | A |
| 23 | BA | 279 | C |
| 23 | BA | 280 | C |
| 23 | BA | 286 | C |
| 23 | BA | 311 | A |
| 23 | BA | 315 | G |
| 23 | BA | 316 | C |
| 23 | BA | 324 | A |
| 23 | BA | 329 | G |
| 23 | BA | 330 | A |
| 23 | BA | 331 | A |
| 23 | BA | 332 | A |
| 23 | BA | 333 | G |
| 23 | BA | 335 | C |
| 23 | BA | 342 | G |
| 23 | BA | 352 | G |
| 23 | BA | 353 | G |
| 23 | BA | 363 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | BA | 363(C) | G |
| 23 | BA | 363(F) | A |
| 23 | BA | 386 | G |
| 23 | BA | 404 | C |
| 23 | BA | 405 | U |
| 23 | BA | 407 | G |
| 23 | BA | 411 | G |
| 23 | BA | 412 | A |
| 23 | BA | 428 | A |
| 23 | BA | 444 | C |
| 23 | BA | 448 | U |
| 23 | BA | 457 | A |
| 23 | BA | 460 | A |
| 23 | BA | 470 | A |
| 23 | BA | 471 | A |
| 23 | BA | 481 | G |
| 23 | BA | 482 | A |
| 23 | BA | 505 | A |
| 23 | BA | 509 | C |
| 23 | BA | 512 | G |
| 23 | BA | 513 | A |
| 23 | BA | 529 | A |
| 23 | BA | 530 | G |
| 23 | BA | 531 | C |
| 23 | BA | 532 | A |
| 23 | BA | 533 | G |
| 23 | BA | 543 | C |
| 23 | BA | 545 | G |
| 23 | BA | 546 | C |
| 23 | BA | 547 | A |
| 23 | BA | 548 | A |
| 23 | BA | 563 | G |
| 23 | BA | 573 | G |
| 23 | BA | 575 | A |
| 23 | BA | 586 | A |
| 23 | BA | 587 | C |
| 23 | BA | 588 | U |
| 23 | BA | 602 | G |
| 23 | BA | 603 | A |
| 23 | BA | 604 | G |
| 23 | BA | 607 | U |
| 23 | BA | 614(A) | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | BA | 614(B) | G |
| 23 | BA | 614(C) | A |
| 23 | BA | 615 | G |
| 23 | BA | 620 | G |
| 23 | BA | 627 | A |
| 23 | BA | 632 | A |
| 23 | BA | 637 | A |
| 23 | BA | 645 | C |
| 23 | BA | 646 | A |
| 23 | BA | 647 | G |
| 23 | BA | 652(A) | A |
| 23 | BA | 652(B) | A |
| 23 | BA | 652(C) | G |
| 23 | BA | 652(E) | G |
| 23 | BA | 652(F) | G |
| 23 | BA | 652(J) | G |
| 23 | BA | 652(Q) | G |
| 23 | BA | 652(R) | C |
| 23 | BA | 652(T) | C |
| 23 | BA | 652(U) | G |
| 23 | BA | 668 | G |
| 23 | BA | 669 | G |
| 23 | BA | 686 | G |
| 23 | BA | 701 | G |
| 23 | BA | 708 | C |
| 23 | BA | 709 | U |
| 23 | BA | 715 | G |
| 23 | BA | 717 | G |
| 23 | BA | 730 | C |
| 23 | BA | 752 | A |
| 23 | BA | 753 | C |
| 23 | BA | 762 | U |
| 23 | BA | 764 | A |
| 23 | BA | 765 | G |
| 23 | BA | 771 | G |
| 23 | BA | 775 | G |
| 23 | BA | 776 | G |
| 23 | BA | 782 | A |
| 23 | BA | 784 | A |
| 23 | BA | 785 | G |
| 23 | BA | 792 | G |
| 23 | BA | 805 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | BA | 810 | U |
| 23 | BA | 812 | C |
| 23 | BA | 819 | A |
| 23 | BA | 827 | U |
| 23 | BA | 828 | U |
| 23 | BA | 830 | G |
| 23 | BA | 857 | C |
| 23 | BA | 859 | G |
| 23 | BA | 879 | G |
| 23 | BA | 882 | G |
| 23 | BA | 884 | C |
| 23 | BA | 885 | C |
| 23 | BA | 886 | C |
| 23 | BA | 888 | C |
| 23 | BA | 889 | C |
| 23 | BA | 890 | A |
| 23 | BA | 895 | U |
| 23 | BA | 896 | A |
| 23 | BA | 897 | C |
| 23 | BA | 900 | A |
| 23 | BA | 901 | A |
| 23 | BA | 910 | A |
| 23 | BA | 914 | C |
| 23 | BA | 917 | A |
| 23 | BA | 932 | G |
| 23 | BA | 938 | G |
| 23 | BA | 941 | A |
| 23 | BA | 945 | A |
| 23 | BA | 946 | G |
| 23 | BA | 953 | A |
| 23 | BA | 958 | U |
| 23 | BA | 959 | A |
| 23 | BA | 961 | C |
| 23 | BA | 974 | G |
| 23 | BA | 975 | C |
| 23 | BA | 975(A) | G |
| 23 | BA | 983 | A |
| 23 | BA | 990 | A |
| 23 | BA | 991 | C |
| 23 | BA | 994 | C |
| 23 | BA | 996 | A |
| 23 | BA | 1005 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1012 | U |
| 23 | BA | 1013 | C |
| 23 | BA | 1020 | A |
| 23 | BA | 1022 | G |
| 23 | BA | 1023 | U |
| 23 | BA | 1025 | G |
| 23 | BA | 1026 | U |
| 23 | BA | 1027 | A |
| 23 | BA | 1033 | U |
| 23 | BA | 1038 | C |
| 23 | BA | 1039 | G |
| 23 | BA | 1040 | C |
| 23 | BA | 1041 | C |
| 23 | BA | 1042 | G |
| 23 | BA | 1043 | C |
| 23 | BA | 1045 | A |
| 23 | BA | 1046 | A |
| 23 | BA | 1047 | G |
| 23 | BA | 1048 | A |
| 23 | BA | 1049 | C |
| 23 | BA | 1050 | A |
| 23 | BA | 1052 | C |
| 23 | BA | 1107 | G |
| 23 | BA | 1109 | C |
| 23 | BA | 1110 | G |
| 23 | BA | 1112 | G |
| 23 | BA | 1115 | G |
| 23 | BA | 1128 | A |
| 23 | BA | 1129 | A |
| 23 | BA | 1130 | U |
| 23 | BA | 1135 | C |
| 23 | BA | 1136 | G |
| 23 | BA | 1139 | G |
| 23 | BA | 1141 | U |
| 23 | BA | 1154 | G |
| 23 | BA | 1155 | A |
| 23 | BA | 1170 | G |
| 23 | BA | 1171 | G |
| 23 | BA | 1173 | G |
| 23 | BA | 1174 | A |
| 23 | BA | 1175 | U |
| 23 | BA | 1176 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BA | 1177 | A |
| 23 | BA | 1188 | U |
| 23 | BA | 1210 | A |
| 23 | BA | 1211 | U |
| 23 | BA | 1224 | C |
| 23 | BA | 1244 | G |
| 23 | BA | 1252 | G |
| 23 | BA | 1253 | A |
| 23 | BA | 1256 | G |
| 23 | BA | 1267 | U |
| 23 | BA | 1271 | G |
| 23 | BA | 1272 | A |
| 23 | BA | 1273 | U |
| 23 | BA | 1292 | U |
| 23 | BA | 1300 | U |
| 23 | BA | 1301 | A |
| 23 | BA | 1305 | C |
| 23 | BA | 1314 | C |
| 23 | BA | 1320 | C |
| 23 | BA | 1321 | A |
| 23 | BA | 1329 | U |
| 23 | BA | 1345 | C |
| 23 | BA | 1352 | U |
| 23 | BA | 1359 | A |
| 23 | BA | 1360 | A |
| 23 | BA | 1365 | A |
| 23 | BA | 1368 | G |
| 23 | BA | 1370 | C |
| 23 | BA | 1373 | A |
| 23 | BA | 1374 | G |
| 23 | BA | 1378 | A |
| 23 | BA | 1379 | A |
| 23 | BA | 1380 | G |
| 23 | BA | 1383 | C |
| 23 | BA | 1384 | A |
| 23 | BA | 1385 | G |
| 23 | BA | 1386 | C |
| 23 | BA | 1395 | A |
| 23 | BA | 1405 | U |
| 23 | BA | 1416 | G |
| 23 | BA | 1417 | C |
| 23 | BA | 1419 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 23 | BA | 1420 | U |
| 23 | BA | 1421 | G |
| 23 | BA | 1427 | A |
| 23 | BA | 1428 | C |
| 23 | BA | 1429 | G |
| 23 | BA | 1437 | C |
| 23 | BA | 1445 | A |
| 23 | BA | 1449 | A |
| 23 | BA | 1455 | G |
| 23 | BA | 1459 | G |
| 23 | BA | 1467 | C |
| 23 | BA | 1471 | A |
| 23 | BA | 1482 | G |
| 23 | BA | 1488 | G |
| 23 | BA | 1490 | A |
| 23 | BA | 1493 | C |
| 23 | BA | 1497 | U |
| 23 | BA | 1507 | A |
| 23 | BA | 1508 | A |
| 23 | BA | 1509 | C |
| 23 | BA | 1509(A) | A |
| 23 | BA | 1510 | G |
| 23 | BA | 1520 | G |
| 23 | BA | 1531 | C |
| 23 | BA | 1533 | G |
| 23 | BA | 1534 | U |
| 23 | BA | 1535 | A |
| 23 | BA | 1536 | C |
| 23 | BA | 1537 | G |
| 23 | BA | 1539 | G |
| 23 | BA | 1540 | U |
| 23 | BA | 1542 | A |
| 23 | BA | 1543 | C |
| 23 | BA | 1545 | A |
| 23 | BA | 1548 | C |
| 23 | BA | 1554 | A |
| 23 | BA | 1558 | A |
| 23 | BA | 1559 | G |
| 23 | BA | 1560 | G |
| 23 | BA | 1566 | A |
| 23 | BA | 1569 | A |
| 23 | BA | 1578 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1579 | A |
| 23 | BA | 1580 | A |
| 23 | BA | 1581 | G |
| 23 | BA | 1584 | C |
| 23 | BA | 1586 | A |
| 23 | BA | 1598 | C |
| 23 | BA | 1608 | A |
| 23 | BA | 1609 | A |
| 23 | BA | 1610 | A |
| 23 | BA | 1617 | C |
| 23 | BA | 1635 | G |
| 23 | BA | 1640 | C |
| 23 | BA | 1647 | G |
| 23 | BA | 1648 | C |
| 23 | BA | 1652 | A |
| 23 | BA | 1654 | A |
| 23 | BA | 1674 | G |
| 23 | BA | 1675 | C |
| 23 | BA | 1696 | G |
| 23 | BA | 1698 | A |
| 23 | BA | 1700 | A |
| 23 | BA | 1701 | A |
| 23 | BA | 1703 | G |
| 23 | BA | 1721 | G |
| 23 | BA | 1722 | A |
| 23 | BA | 1746 | G |
| 23 | BA | 1763 | G |
| 23 | BA | 1764 | G |
| 23 | BA | 1773 | A |
| 23 | BA | 1780 | A |
| 23 | BA | 1782 | C |
| 23 | BA | 1791 | A |
| 23 | BA | 1799 | G |
| 23 | BA | 1800 | C |
| 23 | BA | 1801 | G |
| 23 | BA | 1812 | A |
| 23 | BA | 1816 | G |
| 23 | BA | 1819 | A |
| 23 | BA | 1820 | U |
| 23 | BA | 1826 | G |
| 23 | BA | 1828 | G |
| 23 | BA | 1829 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BA | 1835 | G |
| 23 | BA | 1838 | C |
| 23 | BA | 1840 | G |
| 23 | BA | 1847 | A |
| 23 | BA | 1848 | A |
| 23 | BA | 1858 | G |
| 23 | BA | 1865 | G |
| 23 | BA | 1866 | C |
| 23 | BA | 1877 | A |
| 23 | BA | 1878 | G |
| 23 | BA | 1881 | C |
| 23 | BA | 1882 | C |
| 23 | BA | 1896 | G |
| 23 | BA | 1900 | A |
| 23 | BA | 1905 | C |
| 23 | BA | 1906 | G |
| 23 | BA | 1912 | A |
| 23 | BA | 1913 | A |
| 23 | BA | 1914 | C |
| 23 | BA | 1929 | G |
| 23 | BA | 1930 | G |
| 23 | BA | 1931 | U |
| 23 | BA | 1936 | A |
| 23 | BA | 1937 | A |
| 23 | BA | 1938 | A |
| 23 | BA | 1939 | U |
| 23 | BA | 1952 | A |
| 23 | BA | 1955 | U |
| 23 | BA | 1963 | U |
| 23 | BA | 1964 | G |
| 23 | BA | 1967 | C |
| 23 | BA | 1969 | A |
| 23 | BA | 1970 | A |
| 23 | BA | 1971 | A |
| 23 | BA | 1972 | A |
| 23 | BA | 1982 | C |
| 23 | BA | 1991 | U |
| 23 | BA | 1993 | U |
| 23 | BA | 1997 | G |
| 23 | BA | 2005 | A |
| 23 | BA | 2020 | A |
| 23 | BA | 2023 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BA | 2031 | A |
| 23 | BA | 2032 | G |
| 23 | BA | 2033 | A |
| 23 | BA | 2036 | C |
| 23 | BA | 2043 | C |
| 23 | BA | 2049 | G |
| 23 | BA | 2055 | C |
| 23 | BA | 2056 | G |
| 23 | BA | 2060 | A |
| 23 | BA | 2061 | G |
| 23 | BA | 2062 | A |
| 23 | BA | 2069 | G |
| 23 | BA | 2099 | U |
| 23 | BA | 2100 | G |
| 23 | BA | 2103 | C |
| 23 | BA | 2104 | G |
| 23 | BA | 2108 | C |
| 23 | BA | 2110 | G |
| 23 | BA | 2111 | C |
| 23 | BA | 2112 | G |
| 23 | BA | 2115 | G |
| 23 | BA | 2116 | G |
| 23 | BA | 2117 | A |
| 23 | BA | 2119 | A |
| 23 | BA | 2123 | G |
| 23 | BA | 2126 | A |
| 23 | BA | 2127 | G |
| 23 | BA | 2128 | C |
| 23 | BA | 2131 | G |
| 23 | BA | 2133 | G |
| 23 | BA | 2134 | A |
| 23 | BA | 2135 | A |
| 23 | BA | 2136 | C |
| 23 | BA | 2146 | C |
| 23 | BA | 2147 | G |
| 23 | BA | 2150 | U |
| 23 | BA | 2159 | G |
| 23 | BA | 2160 | G |
| 23 | BA | 2161 | C |
| 23 | BA | 2162 | G |
| 23 | BA | 2164 | C |
| 23 | BA | 2169 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BA | 2170 | A |
| 23 | BA | 2172 | U |
| 23 | BA | 2173 | A |
| 23 | BA | 2174 | C |
| 23 | BA | 2176 | A |
| 23 | BA | 2179 | C |
| 23 | BA | 2180 | U |
| 23 | BA | 2183 | C |
| 23 | BA | 2185 | C |
| 23 | BA | 2186 | G |
| 23 | BA | 2187 | G |
| 23 | BA | 2188 | C |
| 23 | BA | 2191 | G |
| 23 | BA | 2192 | G |
| 23 | BA | 2193 | G |
| 23 | BA | 2198 | A |
| 23 | BA | 2199 | A |
| 23 | BA | 2200 | C |
| 23 | BA | 2206 | G |
| 23 | BA | 2207 | G |
| 23 | BA | 2208 | A |
| 23 | BA | 2225 | A |
| 23 | BA | 2234 | G |
| 23 | BA | 2238 | G |
| 23 | BA | 2239 | G |
| 23 | BA | 2240 | C |
| 23 | BA | 2248 | C |
| 23 | BA | 2249 | U |
| 23 | BA | 2252 | G |
| 23 | BA | 2268 | A |
| 23 | BA | 2273 | A |
| 23 | BA | 2275 | C |
| 23 | BA | 2278 | A |
| 23 | BA | 2283 | C |
| 23 | BA | 2287 | A |
| 23 | BA | 2288 | A |
| 23 | BA | 2289 | G |
| 23 | BA | 2291 | U |
| 23 | BA | 2294 | C |
| 23 | BA | 2305 | A |
| 23 | BA | 2306 | C |
| 23 | BA | 2308 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 2309 | A |
| 23 | BA | 2311 | A |
| 23 | BA | 2316 | C |
| 23 | BA | 2319 | G |
| 23 | BA | 2320 | A |
| 23 | BA | 2321 | G |
| 23 | BA | 2325 | G |
| 23 | BA | 2334 | G |
| 23 | BA | 2336 | A |
| 23 | BA | 2343 | C |
| 23 | BA | 2347 | C |
| 23 | BA | 2350 | C |
| 23 | BA | 2354 | G |
| 23 | BA | 2379 | G |
| 23 | BA | 2383 | G |
| 23 | BA | 2385 | C |
| 23 | BA | 2388 | A |
| 23 | BA | 2400 | G |
| 23 | BA | 2406 | U |
| 23 | BA | 2410 | G |
| 23 | BA | 2414 | G |
| 23 | BA | 2418 | A |
| 23 | BA | 2422 | A |
| 23 | BA | 2425 | A |
| 23 | BA | 2429 | G |
| 23 | BA | 2430 | A |
| 23 | BA | 2435 | A |
| 23 | BA | 2439 | A |
| 23 | BA | 2441 | C |
| 23 | BA | 2448 | A |
| 23 | BA | 2465 | C |
| 23 | BA | 2469 | A |
| 23 | BA | 2470 | G |
| 23 | BA | 2472 | G |
| 23 | BA | 2474 | C |
| 23 | BA | 2476 | A |
| 23 | BA | 2477 | C |
| 23 | BA | 2486 | G |
| 23 | BA | 2487 | G |
| 23 | BA | 2502 | G |
| 23 | BA | 2504 | U |
| 23 | BA | 2505 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 23 | BA | 2506 | U |
| 23 | BA | 2518 | A |
| 23 | BA | 2520 | C |
| 23 | BA | 2525 | G |
| 23 | BA | 2529 | G |
| 23 | BA | 2535 | G |
| 23 | BA | 2554 | U |
| 23 | BA | 2564 | A |
| 23 | BA | 2566 | A |
| 23 | BA | 2567 | G |
| 23 | BA | 2573 | C |
| 23 | BA | 2582 | G |
| 23 | BA | 2585 | U |
| 23 | BA | 2586 | C |
| 23 | BA | 2602 | A |
| 23 | BA | 2603 | G |
| 23 | BA | 2604 | U |
| 23 | BA | 2608 | G |
| 23 | BA | 2609 | U |
| 23 | BA | 2610 | C |
| 23 | BA | 2611 | U |
| 23 | BA | 2612 | C |
| 23 | BA | 2615 | U |
| 23 | BA | 2628 | C |
| 23 | BA | 2629 | A |
| 23 | BA | 2630 | G |
| 23 | BA | 2654 | A |
| 23 | BA | 2663 | G |
| 23 | BA | 2672 | G |
| 23 | BA | 2674 | G |
| 23 | BA | 2686 | G |
| 23 | BA | 2690 | C |
| 23 | BA | 2691 | C |
| 23 | BA | 2702 | U |
| 23 | BA | 2703 | C |
| 23 | BA | 2707 | G |
| 23 | BA | 2712(A) | A |
| 23 | BA | 2713 | A |
| 23 | BA | 2714 | G |
| 23 | BA | 2726 | U |
| 23 | BA | 2733 | A |
| 23 | BA | 2739 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BA | 2744 | G |
| 23 | BA | 2758 | A |
| 23 | BA | 2761 | G |
| 23 | BA | 2765 | A |
| 23 | BA | 2766 | G |
| 23 | BA | 2778 | A |
| 23 | BA | 2790 | A |
| 23 | BA | 2791 | C |
| 23 | BA | 2802 | G |
| 23 | BA | 2803 | C |
| 23 | BA | 2808 | U |
| 23 | BA | 2820 | A |
| 23 | BA | 2821 | A |
| 23 | BA | 2833 | G |
| 23 | BA | 2834 | G |
| 23 | BA | 2835 | A |
| 23 | BA | 2847 | U |
| 23 | BA | 2872 | G |
| 23 | BA | 2873 | A |
| 23 | BA | 2880 | C |
| 23 | BA | 2892 | A |
| 23 | BA | 2893 | G |
| 23 | BA | 2894 | G |
| 23 | BA | 2895 | U |
| 23 | BA | 2897 | U |
| 24 | BB | 2 | C |
| 24 | BB | 8 | U |
| 24 | BB | 9 | G |
| 24 | BB | 12 | C |
| 24 | BB | 13 | A |
| 24 | BB | 15 | A |
| 24 | BB | 19 | G |
| 24 | BB | 21 | G |
| 24 | BB | 24 | G |
| 24 | BB | 25 | A |
| 24 | BB | 28 | C |
| 24 | BB | 33 | G |
| 24 | BB | 40 | U |
| 24 | BB | 53 | A |
| 24 | BB | 54 | G |
| 24 | BB | 56 | G |
| 24 | BB | 73 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 24 | BB | 74 | U |
| 24 | BB | 75 | G |
| 24 | BB | 84 | C |
| 24 | BB | 85 | G |
| 24 | BB | 88 | C |
| 24 | BB | 89 | G |
| 24 | BB | 106 | G |
| 24 | BB | 110 | G |
| 1 | CA | 5 | U |
| 1 | CA | 6 | G |
| 1 | CA | 7 | G |
| 1 | CA | 9 | G |
| 1 | CA | 32 | A |
| 1 | CA | 39 | G |
| 1 | CA | 47 | C |
| 1 | CA | 48 | C |
| 1 | CA | 50 | A |
| 1 | CA | 51 | A |
| 1 | CA | 53 | A |
| 1 | CA | 60 | A |
| 1 | CA | 61 | G |
| 1 | CA | 62 | U |
| 1 | CA | 65 | U |
| 1 | CA | 66 | G |
| 1 | CA | 67 | C |
| 1 | CA | 77 | G |
| 1 | CA | 78 | G |
| 1 | CA | 79 | G |
| 1 | CA | 91 | C |
| 1 | CA | 93 | G |
| 1 | CA | 96 | U |
| 1 | CA | 97 | G |
| 1 | CA | 115 | G |
| 1 | CA | 116 | A |
| 1 | CA | 121 | C |
| 1 | CA | 131 | C |
| 1 | CA | 142 | G |
| 1 | CA | 150 | C |
| 1 | CA | 163 | C |
| 1 | CA | 173 | U |
| 1 | CA | 182 | U |
| 1 | CA | 189(G) | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 189(H) | G |
| 1 | CA | 195 | A |
| 1 | CA | 197 | A |
| 1 | CA | 201 | C |
| 1 | CA | 203 | U |
| 1 | CA | 204 | U |
| 1 | CA | 216 | G |
| 1 | CA | 227 | G |
| 1 | CA | 243 | A |
| 1 | CA | 244 | U |
| 1 | CA | 247 | G |
| 1 | CA | 251 | G |
| 1 | CA | 266 | G |
| 1 | CA | 267 | C |
| 1 | CA | 289 | G |
| 1 | CA | 321 | A |
| 1 | CA | 328 | C |
| 1 | CA | 332 | G |
| 1 | CA | 342 | C |
| 1 | CA | 343 | U |
| 1 | CA | 344 | A |
| 1 | CA | 345 | C |
| 1 | CA | 351 | G |
| 1 | CA | 352 | C |
| 1 | CA | 353 | A |
| 1 | CA | 354 | G |
| 1 | CA | 365 | U |
| 1 | CA | 367 | U |
| 1 | CA | 372 | C |
| 1 | CA | 373 | A |
| 1 | CA | 388 | G |
| 1 | CA | 392 | G |
| 1 | CA | 397 | A |
| 1 | CA | 398 | C |
| 1 | CA | 406 | G |
| 1 | CA | 409 | G |
| 1 | CA | 412 | A |
| 1 | CA | 413 | G |
| 1 | CA | 414 | A |
| 1 | CA | 422 | C |
| 1 | CA | 423 | G |
| 1 | CA | 424 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 429 | U |
| 1 | CA | 430 | A |
| 1 | CA | 435 | C |
| 1 | CA | 437 | U |
| 1 | CA | 439 | A |
| 1 | CA | 442 | C |
| 1 | CA | 445 | G |
| 1 | CA | 452 | A |
| 1 | CA | 457 | C |
| 1 | CA | 461 | A |
| 1 | CA | 484 | G |
| 1 | CA | 485 | G |
| 1 | CA | 493 | G |
| 1 | CA | 496 | A |
| 1 | CA | 498 | U |
| 1 | CA | 505 | G |
| 1 | CA | 509 | A |
| 1 | CA | 510 | A |
| 1 | CA | 511 | C |
| 1 | CA | 518 | C |
| 1 | CA | 520 | A |
| 1 | CA | 521 | G |
| 1 | CA | 524 | G |
| 1 | CA | 525 | C |
| 1 | CA | 527 | G |
| 1 | CA | 531 | U |
| 1 | CA | 532 | A |
| 1 | CA | 533 | A |
| 1 | CA | 547 | A |
| 1 | CA | 559 | A |
| 1 | CA | 560 | U |
| 1 | CA | 561 | U |
| 1 | CA | 562 | C |
| 1 | CA | 563 | A |
| 1 | CA | 564 | C |
| 1 | CA | 570 | G |
| 1 | CA | 572 | A |
| 1 | CA | 573 | A |
| 1 | CA | 575 | G |
| 1 | CA | 576 | G |
| 1 | CA | 577 | G |
| 1 | CA | 588 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 596 | C |
| 1 | CA | 607 | A |
| 1 | CA | 618 | C |
| 1 | CA | 623 | C |
| 1 | CA | 629 | G |
| 1 | CA | 630 | G |
| 1 | CA | 631 | G |
| 1 | CA | 632 | A |
| 1 | CA | 633 | G |
| 1 | CA | 634 | C |
| 1 | CA | 653 | A |
| 1 | CA | 661 | G |
| 1 | CA | 665 | A |
| 1 | CA | 666 | G |
| 1 | CA | 680 | C |
| 1 | CA | 687 | A |
| 1 | CA | 688 | G |
| 1 | CA | 690 | G |
| 1 | CA | 724 | G |
| 1 | CA | 731 | G |
| 1 | CA | 749 | C |
| 1 | CA | 755 | G |
| 1 | CA | 766 | A |
| 1 | CA | 774 | G |
| 1 | CA | 777 | A |
| 1 | CA | 786 | G |
| 1 | CA | 787 | A |
| 1 | CA | 793 | U |
| 1 | CA | 794 | A |
| 1 | CA | 796 | C |
| 1 | CA | 802 | A |
| 1 | CA | 816 | A |
| 1 | CA | 817 | C |
| 1 | CA | 818 | G |
| 1 | CA | 821 | G |
| 1 | CA | 827 | U |
| 1 | CA | 828 | A |
| 1 | CA | 833 | U |
| 1 | CA | 836 | G |
| 1 | CA | 839 | U |
| 1 | CA | 840 | C |
| 1 | CA | 841 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 848 | C |
| 1 | CA | 859 | A |
| 1 | CA | 870 | U |
| 1 | CA | 873 | A |
| 1 | CA | 875 | C |
| 1 | CA | 876 | G |
| 1 | CA | 902 | G |
| 1 | CA | 914 | A |
| 1 | CA | 926 | G |
| 1 | CA | 927 | G |
| 1 | CA | 932 | C |
| 1 | CA | 933 | G |
| 1 | CA | 934 | C |
| 1 | CA | 935 | A |
| 1 | CA | 936 | C |
| 1 | CA | 937 | A |
| 1 | CA | 940 | C |
| 1 | CA | 942 | G |
| 1 | CA | 945 | G |
| 1 | CA | 950 | U |
| 1 | CA | 953 | G |
| 1 | CA | 954 | G |
| 1 | CA | 958 | A |
| 1 | CA | 960 | U |
| 1 | CA | 961 | U |
| 1 | CA | 964 | A |
| 1 | CA | 966 | G |
| 1 | CA | 969 | A |
| 1 | CA | 971 | G |
| 1 | CA | 972 | C |
| 1 | CA | 974 | A |
| 1 | CA | 975 | A |
| 1 | CA | 976 | G |
| 1 | CA | 977 | A |
| 1 | CA | 978 | A |
| 1 | CA | 982 | U |
| 1 | CA | 984 | C |
| 1 | CA | 985 | C |
| 1 | CA | 989 | C |
| 1 | CA | 990 | C |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 993 | G |
| 1 | CA | 996 | A |
| 1 | CA | 1001(A) | G |
| 1 | CA | 1004 | A |
| 1 | CA | 1005 | A |
| 1 | CA | 1006 | C |
| 1 | CA | 1009 | G |
| 1 | CA | 1012 | U |
| 1 | CA | 1016 | A |
| 1 | CA | 1019 | C |
| 1 | CA | 1023 | G |
| 1 | CA | 1024 | G |
| 1 | CA | 1026 | G |
| 1 | CA | 1027 | C |
| 1 | CA | 1028 | C |
| 1 | CA | 1029 | C |
| 1 | CA | 1030 | C |
| 1 | CA | 1031 | G |
| 1 | CA | 1035 | A |
| 1 | CA | 1036 | G |
| 1 | CA | 1037 | C |
| 1 | CA | 1039 | C |
| 1 | CA | 1042 | G |
| 1 | CA | 1043 | C |
| 1 | CA | 1044 | A |
| 1 | CA | 1045 | C |
| 1 | CA | 1046 | A |
| 1 | CA | 1053 | G |
| 1 | CA | 1054 | C |
| 1 | CA | 1055 | A |
| 1 | CA | 1063 | C |
| 1 | CA | 1064 | G |
| 1 | CA | 1065 | U |
| 1 | CA | 1066 | C |
| 1 | CA | 1068 | G |
| 1 | CA | 1081 | G |
| 1 | CA | 1084 | G |
| 1 | CA | 1085 | U |
| 1 | CA | 1086 | U |
| 1 | CA | 1088 | G |
| 1 | CA | 1089 | G |
| 1 | CA | 1094 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1096 | C |
| 1 | CA | 1101 | A |
| 1 | CA | 1107 | C |
| 1 | CA | 1109 | C |
| 1 | CA | 1112 | C |
| 1 | CA | 1114 | C |
| 1 | CA | 1115 | C |
| 1 | CA | 1117 | G |
| 1 | CA | 1118 | C |
| 1 | CA | 1119 | C |
| 1 | CA | 1124 | G |
| 1 | CA | 1125 | U |
| 1 | CA | 1126 | U |
| 1 | CA | 1127 | G |
| 1 | CA | 1129 | C |
| 1 | CA | 1131 | G |
| 1 | CA | 1134 | G |
| 1 | CA | 1136 | U |
| 1 | CA | 1137 | C |
| 1 | CA | 1138 | G |
| 1 | CA | 1139 | G |
| 1 | CA | 1140 | C |
| 1 | CA | 1144 | G |
| 1 | CA | 1145 | C |
| 1 | CA | 1149 | C |
| 1 | CA | 1150 | U |
| 1 | CA | 1151 | A |
| 1 | CA | 1152 | A |
| 1 | CA | 1155 | G |
| 1 | CA | 1159 | U |
| 1 | CA | 1160 | G |
| 1 | CA | 1161 | C |
| 1 | CA | 1162 | C |
| 1 | CA | 1166 | G |
| 1 | CA | 1170 | A |
| 1 | CA | 1182 | G |
| 1 | CA | 1183 | A |
| 1 | CA | 1184 | G |
| 1 | CA | 1185 | G |
| 1 | CA | 1186 | G |
| 1 | CA | 1187 | G |
| 1 | CA | 1188 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1190 | G |
| 1 | CA | 1196 | U |
| 1 | CA | 1197 | G |
| 1 | CA | 1201 | A |
| 1 | CA | 1202 | G |
| 1 | CA | 1206 | G |
| 1 | CA | 1207 | G |
| 1 | CA | 1210 | C |
| 1 | CA | 1211 | U |
| 1 | CA | 1212 | U |
| 1 | CA | 1213 | A |
| 1 | CA | 1214 | C |
| 1 | CA | 1220 | G |
| 1 | CA | 1224 | G |
| 1 | CA | 1225 | A |
| 1 | CA | 1226 | C |
| 1 | CA | 1227 | A |
| 1 | CA | 1228 | C |
| 1 | CA | 1233 | G |
| 1 | CA | 1236 | A |
| 1 | CA | 1238 | A |
| 1 | CA | 1240 | U |
| 1 | CA | 1241 | G |
| 1 | CA | 1242 | C |
| 1 | CA | 1244 | C |
| 1 | CA | 1245 | A |
| 1 | CA | 1250 | A |
| 1 | CA | 1252 | A |
| 1 | CA | 1256 | A |
| 1 | CA | 1257 | U |
| 1 | CA | 1258 | G |
| 1 | CA | 1260 | C |
| 1 | CA | 1264 | C |
| 1 | CA | 1265 | G |
| 1 | CA | 1266 | G |
| 1 | CA | 1267 | C |
| 1 | CA | 1270 | C |
| 1 | CA | 1271 | G |
| 1 | CA | 1272 | G |
| 1 | CA | 1275 | A |
| 1 | CA | 1278 | U |
| 1 | CA | 1279 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1280 | A |
| 1 | CA | 1282 | C |
| 1 | CA | 1284 | C |
| 1 | CA | 1286 | A |
| 1 | CA | 1287 | A |
| 1 | CA | 1288 | A |
| 1 | CA | 1293 | G |
| 1 | CA | 1294 | G |
| 1 | CA | 1295 | G |
| 1 | CA | 1297 | C |
| 1 | CA | 1298 | C |
| 1 | CA | 1299 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1301 | U |
| 1 | CA | 1302 | U |
| 1 | CA | 1304 | G |
| 1 | CA | 1305 | G |
| 1 | CA | 1307 | U |
| 1 | CA | 1319 | A |
| 1 | CA | 1322 | C |
| 1 | CA | 1323 | G |
| 1 | CA | 1331 | G |
| 1 | CA | 1333 | A |
| 1 | CA | 1335 | C |
| 1 | CA | 1336 | C |
| 1 | CA | 1338 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1347 | G |
| 1 | CA | 1348 | U |
| 1 | CA | 1357 | A |
| 1 | CA | 1359 | C |
| 1 | CA | 1362 | C |
| 1 | CA | 1363 | C |
| 1 | CA | 1363(A) | A |
| 1 | CA | 1364 | U |
| 1 | CA | 1369 | C |
| 1 | CA | 1372 | U |
| 1 | CA | 1373 | G |
| 1 | CA | 1379 | G |
| 1 | CA | 1381 | U |
| 1 | CA | 1394 | A |
| 1 | CA | 1397 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1398 | A |
| 1 | CA | 1401 | G |
| 1 | CA | 1419 | G |
| 1 | CA | 1441 | G |
| 1 | CA | 1442 | G |
| 1 | CA | 1442(B) | A |
| 1 | CA | 1446 | U |
| 1 | CA | 1447 | A |
| 1 | CA | 1452 | C |
| 1 | CA | 1456 | G |
| 1 | CA | 1457 | G |
| 1 | CA | 1459 | C |
| 1 | CA | 1460 | A |
| 1 | CA | 1487 | G |
| 1 | CA | 1492 | A |
| 1 | CA | 1493 | A |
| 1 | CA | 1494 | G |
| 1 | CA | 1495 | U |
| 1 | CA | 1497 | G |
| 1 | CA | 1504 | G |
| 1 | CA | 1505 | G |
| 1 | CA | 1506 | U |
| 1 | CA | 1517 | G |
| 1 | CA | 1520 | G |
| 1 | CA | 1529 | G |
| 1 | CA | 1530 | G |
| 23 | DA | 10 | G |
| 23 | DA | 12 | U |
| 23 | DA | 14 | A |
| 23 | DA | 15 | G |
| 23 | DA | 34 | C |
| 23 | DA | 36 | G |
| 23 | DA | 45 | C |
| 23 | DA | 55 | G |
| 23 | DA | 69 | C |
| 23 | DA | 71 | A |
| 23 | DA | 72 | U |
| 23 | DA | 74 | A |
| 23 | DA | 75 | G |
| 23 | DA | 82 | G |
| 23 | DA | 84 | A |
| 23 | DA | 90 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 94 | C |
| 23 | DA | 95 | G |
| 23 | DA | 96 | G |
| 23 | DA | 100 | G |
| 23 | DA | 102 | G |
| 23 | DA | 103 | A |
| 23 | DA | 118 | A |
| 23 | DA | 119 | A |
| 23 | DA | 120 | U |
| 23 | DA | 131 | G |
| 23 | DA | 141 | A |
| 23 | DA | 154 | G |
| 23 | DA | 154(A) | C |
| 23 | DA | 157 | U |
| 23 | DA | 181 | A |
| 23 | DA | 182 | A |
| 23 | DA | 188 | G |
| 23 | DA | 196 | A |
| 23 | DA | 199 | A |
| 23 | DA | 200 | U |
| 23 | DA | 201 | C |
| 23 | DA | 204 | A |
| 23 | DA | 205 | G |
| 23 | DA | 214 | G |
| 23 | DA | 215 | G |
| 23 | DA | 216 | A |
| 23 | DA | 221 | A |
| 23 | DA | 222 | A |
| 23 | DA | 225 | A |
| 23 | DA | 229 | A |
| 23 | DA | 233 | A |
| 23 | DA | 248 | G |
| 23 | DA | 250 | G |
| 23 | DA | 269 | U |
| 23 | DA | 271(I) | G |
| 23 | DA | 271(K) | U |
| 23 | DA | 271(L) | U |
| 23 | DA | 271(M) | G |
| 23 | DA | 271(N) | U |
| 23 | DA | 271(Y) | U |
| 23 | DA | 272(B) | G |
| 23 | DA | 272(H) | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 272(I) | U |
| 23 | DA | 272(J) | C |
| 23 | DA | 275 | G |
| 23 | DA | 276 | A |
| 23 | DA | 277 | C |
| 23 | DA | 278 | A |
| 23 | DA | 279 | C |
| 23 | DA | 280 | C |
| 23 | DA | 286 | C |
| 23 | DA | 311 | A |
| 23 | DA | 315 | G |
| 23 | DA | 316 | C |
| 23 | DA | 324 | A |
| 23 | DA | 329 | G |
| 23 | DA | 330 | A |
| 23 | DA | 331 | A |
| 23 | DA | 332 | A |
| 23 | DA | 333 | G |
| 23 | DA | 335 | C |
| 23 | DA | 338 | G |
| 23 | DA | 342 | G |
| 23 | DA | 352 | G |
| 23 | DA | 353 | G |
| 23 | DA | 363 | G |
| 23 | DA | 363(C) | G |
| 23 | DA | 363(F) | A |
| 23 | DA | 386 | G |
| 23 | DA | 404 | C |
| 23 | DA | 405 | U |
| 23 | DA | 407 | G |
| 23 | DA | 411 | G |
| 23 | DA | 412 | A |
| 23 | DA | 428 | A |
| 23 | DA | 444 | C |
| 23 | DA | 448 | U |
| 23 | DA | 455 | C |
| 23 | DA | 457 | A |
| 23 | DA | 459 | U |
| 23 | DA | 460 | A |
| 23 | DA | 470 | A |
| 23 | DA | 471 | A |
| 23 | DA | 481 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 482 | A |
| 23 | DA | 505 | A |
| 23 | DA | 509 | C |
| 23 | DA | 512 | G |
| 23 | DA | 529 | A |
| 23 | DA | 530 | G |
| 23 | DA | 531 | C |
| 23 | DA | 532 | A |
| 23 | DA | 533 | G |
| 23 | DA | 543 | C |
| 23 | DA | 545 | G |
| 23 | DA | 546 | C |
| 23 | DA | 547 | A |
| 23 | DA | 548 | A |
| 23 | DA | 563 | G |
| 23 | DA | 573 | G |
| 23 | DA | 575 | A |
| 23 | DA | 587 | C |
| 23 | DA | 588 | U |
| 23 | DA | 602 | G |
| 23 | DA | 603 | A |
| 23 | DA | 604 | G |
| 23 | DA | 607 | U |
| 23 | DA | 614(A) | U |
| 23 | DA | 614(B) | G |
| 23 | DA | 614(C) | A |
| 23 | DA | 615 | G |
| 23 | DA | 620 | G |
| 23 | DA | 627 | A |
| 23 | DA | 632 | A |
| 23 | DA | 637 | A |
| 23 | DA | 645 | C |
| 23 | DA | 646 | A |
| 23 | DA | 647 | G |
| 23 | DA | 652(B) | A |
| 23 | DA | 652(C) | G |
| 23 | DA | 652(E) | G |
| 23 | DA | 652(F) | G |
| 23 | DA | 652(J) | G |
| 23 | DA | 652(Q) | G |
| 23 | DA | 652(R) | C |
| 23 | DA | 652(T) | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 652(U) | G |
| 23 | DA | 668 | G |
| 23 | DA | 669 | G |
| 23 | DA | 686 | G |
| 23 | DA | 701 | G |
| 23 | DA | 702 | G |
| 23 | DA | 707 | G |
| 23 | DA | 708 | C |
| 23 | DA | 709 | U |
| 23 | DA | 715 | G |
| 23 | DA | 717 | G |
| 23 | DA | 730 | C |
| 23 | DA | 752 | A |
| 23 | DA | 753 | C |
| 23 | DA | 762 | U |
| 23 | DA | 764 | A |
| 23 | DA | 765 | G |
| 23 | DA | 771 | G |
| 23 | DA | 775 | G |
| 23 | DA | 776 | G |
| 23 | DA | 782 | A |
| 23 | DA | 784 | A |
| 23 | DA | 785 | G |
| 23 | DA | 790 | C |
| 23 | DA | 792 | G |
| 23 | DA | 805 | G |
| 23 | DA | 810 | U |
| 23 | DA | 811 | U |
| 23 | DA | 812 | C |
| 23 | DA | 819 | A |
| 23 | DA | 827 | U |
| 23 | DA | 828 | U |
| 23 | DA | 830 | G |
| 23 | DA | 857 | C |
| 23 | DA | 859 | G |
| 23 | DA | 879 | G |
| 23 | DA | 882 | G |
| 23 | DA | 895 | U |
| 23 | DA | 896 | A |
| 23 | DA | 897 | C |
| 23 | DA | 900 | A |
| 23 | DA | 901 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 23 | DA | 908 | C |
| 23 | DA | 910 | A |
| 23 | DA | 914 | C |
| 23 | DA | 917 | A |
| 23 | DA | 932 | G |
| 23 | DA | 938 | G |
| 23 | DA | 941 | A |
| 23 | DA | 945 | A |
| 23 | DA | 946 | G |
| 23 | DA | 953 | A |
| 23 | DA | 958 | U |
| 23 | DA | 959 | A |
| 23 | DA | 961 | C |
| 23 | DA | 965 | C |
| 23 | DA | 974 | G |
| 23 | DA | 975 | C |
| 23 | DA | 975(A) | G |
| 23 | DA | 983 | A |
| 23 | DA | 990 | A |
| 23 | DA | 991 | C |
| 23 | DA | 996 | A |
| 23 | DA | 1005 | C |
| 23 | DA | 1012 | U |
| 23 | DA | 1013 | C |
| 23 | DA | 1020 | A |
| 23 | DA | 1022 | G |
| 23 | DA | 1023 | U |
| 23 | DA | 1025 | G |
| 23 | DA | 1026 | U |
| 23 | DA | 1027 | A |
| 23 | DA | 1033 | U |
| 23 | DA | 1038 | C |
| 23 | DA | 1039 | G |
| 23 | DA | 1040 | C |
| 23 | DA | 1041 | C |
| 23 | DA | 1042 | G |
| 23 | DA | 1043 | C |
| 23 | DA | 1045 | A |
| 23 | DA | 1046 | A |
| 23 | DA | 1047 | G |
| 23 | DA | 1048 | A |
| 23 | DA | 1049 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 1050 | A |
| 23 | DA | 1052 | C |
| 23 | DA | 1107 | G |
| 23 | DA | 1109 | C |
| 23 | DA | 1110 | G |
| 23 | DA | 1112 | G |
| 23 | DA | 1115 | G |
| 23 | DA | 1128 | A |
| 23 | DA | 1129 | A |
| 23 | DA | 1130 | U |
| 23 | DA | 1135 | C |
| 23 | DA | 1136 | G |
| 23 | DA | 1139 | G |
| 23 | DA | 1141 | U |
| 23 | DA | 1155 | A |
| 23 | DA | 1170 | G |
| 23 | DA | 1171 | G |
| 23 | DA | 1188 | U |
| 23 | DA | 1210 | A |
| 23 | DA | 1211 | U |
| 23 | DA | 1224 | C |
| 23 | DA | 1244 | G |
| 23 | DA | 1250 | G |
| 23 | DA | 1252 | G |
| 23 | DA | 1253 | A |
| 23 | DA | 1256 | G |
| 23 | DA | 1267 | U |
| 23 | DA | 1271 | G |
| 23 | DA | 1272 | A |
| 23 | DA | 1273 | U |
| 23 | DA | 1300 | U |
| 23 | DA | 1301 | A |
| 23 | DA | 1305 | C |
| 23 | DA | 1314 | C |
| 23 | DA | 1320 | C |
| 23 | DA | 1321 | A |
| 23 | DA | 1329 | U |
| 23 | DA | 1345 | C |
| 23 | DA | 1352 | U |
| 23 | DA | 1359 | A |
| 23 | DA | 1360 | A |
| 23 | DA | 1365 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 23 | DA | 1368 | G |
| 23 | DA | 1370 | C |
| 23 | DA | 1373 | A |
| 23 | DA | 1374 | G |
| 23 | DA | 1378 | A |
| 23 | DA | 1379 | A |
| 23 | DA | 1383 | C |
| 23 | DA | 1384 | A |
| 23 | DA | 1385 | G |
| 23 | DA | 1386 | C |
| 23 | DA | 1395 | A |
| 23 | DA | 1405 | U |
| 23 | DA | 1416 | G |
| 23 | DA | 1417 | C |
| 23 | DA | 1419 | A |
| 23 | DA | 1420 | U |
| 23 | DA | 1421 | G |
| 23 | DA | 1427 | A |
| 23 | DA | 1428 | C |
| 23 | DA | 1437 | C |
| 23 | DA | 1445 | A |
| 23 | DA | 1449 | A |
| 23 | DA | 1455 | G |
| 23 | DA | 1459 | G |
| 23 | DA | 1467 | C |
| 23 | DA | 1471 | A |
| 23 | DA | 1472 | A |
| 23 | DA | 1482 | G |
| 23 | DA | 1488 | G |
| 23 | DA | 1490 | A |
| 23 | DA | 1493 | C |
| 23 | DA | 1497 | U |
| 23 | DA | 1507 | A |
| 23 | DA | 1508 | A |
| 23 | DA | 1509 | C |
| 23 | DA | 1509(A) | A |
| 23 | DA | 1510 | G |
| 23 | DA | 1520 | G |
| 23 | DA | 1531 | C |
| 23 | DA | 1539 | G |
| 23 | DA | 1542 | A |
| 23 | DA | 1543 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 1545 | A |
| 23 | DA | 1548 | C |
| 23 | DA | 1554 | A |
| 23 | DA | 1558 | A |
| 23 | DA | 1559 | G |
| 23 | DA | 1560 | G |
| 23 | DA | 1566 | A |
| 23 | DA | 1569 | A |
| 23 | DA | 1578 | U |
| 23 | DA | 1579 | A |
| 23 | DA | 1580 | A |
| 23 | DA | 1581 | G |
| 23 | DA | 1584 | C |
| 23 | DA | 1586 | A |
| 23 | DA | 1598 | C |
| 23 | DA | 1608 | A |
| 23 | DA | 1609 | A |
| 23 | DA | 1610 | A |
| 23 | DA | 1617 | C |
| 23 | DA | 1640 | C |
| 23 | DA | 1647 | G |
| 23 | DA | 1648 | C |
| 23 | DA | 1652 | A |
| 23 | DA | 1654 | A |
| 23 | DA | 1655 | A |
| 23 | DA | 1674 | G |
| 23 | DA | 1675 | C |
| 23 | DA | 1696 | G |
| 23 | DA | 1698 | A |
| 23 | DA | 1700 | A |
| 23 | DA | 1701 | A |
| 23 | DA | 1703 | G |
| 23 | DA | 1721 | G |
| 23 | DA | 1722 | A |
| 23 | DA | 1746 | G |
| 23 | DA | 1750 | G |
| 23 | DA | 1763 | G |
| 23 | DA | 1764 | G |
| 23 | DA | 1773 | A |
| 23 | DA | 1777 | U |
| 23 | DA | 1780 | A |
| 23 | DA | 1782 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 1791 | A |
| 23 | DA | 1799 | G |
| 23 | DA | 1800 | C |
| 23 | DA | 1801 | G |
| 23 | DA | 1812 | A |
| 23 | DA | 1816 | G |
| 23 | DA | 1819 | A |
| 23 | DA | 1820 | U |
| 23 | DA | 1829 | A |
| 23 | DA | 1835 | G |
| 23 | DA | 1838 | C |
| 23 | DA | 1840 | G |
| 23 | DA | 1847 | A |
| 23 | DA | 1848 | A |
| 23 | DA | 1858 | G |
| 23 | DA | 1865 | G |
| 23 | DA | 1866 | C |
| 23 | DA | 1877 | A |
| 23 | DA | 1878 | G |
| 23 | DA | 1881 | C |
| 23 | DA | 1882 | C |
| 23 | DA | 1896 | G |
| 23 | DA | 1900 | A |
| 23 | DA | 1905 | C |
| 23 | DA | 1906 | G |
| 23 | DA | 1912 | A |
| 23 | DA | 1913 | A |
| 23 | DA | 1914 | C |
| 23 | DA | 1929 | G |
| 23 | DA | 1930 | G |
| 23 | DA | 1931 | U |
| 23 | DA | 1936 | A |
| 23 | DA | 1937 | A |
| 23 | DA | 1938 | A |
| 23 | DA | 1939 | U |
| 23 | DA | 1952 | A |
| 23 | DA | 1955 | U |
| 23 | DA | 1963 | U |
| 23 | DA | 1964 | G |
| 23 | DA | 1966 | A |
| 23 | DA | 1967 | C |
| 23 | DA | 1969 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 1970 | A |
| 23 | DA | 1971 | A |
| 23 | DA | 1972 | A |
| 23 | DA | 1982 | C |
| 23 | DA | 1991 | U |
| 23 | DA | 1993 | U |
| 23 | DA | 1997 | G |
| 23 | DA | 2005 | A |
| 23 | DA | 2018 | G |
| 23 | DA | 2023 | G |
| 23 | DA | 2031 | A |
| 23 | DA | 2032 | G |
| 23 | DA | 2033 | A |
| 23 | DA | 2036 | C |
| 23 | DA | 2043 | C |
| 23 | DA | 2049 | G |
| 23 | DA | 2055 | C |
| 23 | DA | 2056 | G |
| 23 | DA | 2060 | A |
| 23 | DA | 2061 | G |
| 23 | DA | 2062 | A |
| 23 | DA | 2063 | C |
| 23 | DA | 2069 | G |
| 23 | DA | 2099 | U |
| 23 | DA | 2100 | G |
| 23 | DA | 2103 | C |
| 23 | DA | 2104 | G |
| 23 | DA | 2108 | C |
| 23 | DA | 2110 | G |
| 23 | DA | 2111 | C |
| 23 | DA | 2112 | G |
| 23 | DA | 2115 | G |
| 23 | DA | 2116 | G |
| 23 | DA | 2117 | A |
| 23 | DA | 2119 | A |
| 23 | DA | 2123 | G |
| 23 | DA | 2126 | A |
| 23 | DA | 2127 | G |
| 23 | DA | 2128 | C |
| 23 | DA | 2131 | G |
| 23 | DA | 2133 | G |
| 23 | DA | 2134 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 2135 | A |
| 23 | DA | 2136 | C |
| 23 | DA | 2146 | C |
| 23 | DA | 2147 | G |
| 23 | DA | 2150 | U |
| 23 | DA | 2159 | G |
| 23 | DA | 2160 | G |
| 23 | DA | 2161 | C |
| 23 | DA | 2162 | G |
| 23 | DA | 2164 | C |
| 23 | DA | 2169 | A |
| 23 | DA | 2170 | A |
| 23 | DA | 2172 | U |
| 23 | DA | 2173 | A |
| 23 | DA | 2174 | C |
| 23 | DA | 2176 | A |
| 23 | DA | 2179 | C |
| 23 | DA | 2180 | U |
| 23 | DA | 2183 | C |
| 23 | DA | 2185 | C |
| 23 | DA | 2186 | G |
| 23 | DA | 2187 | G |
| 23 | DA | 2188 | C |
| 23 | DA | 2191 | G |
| 23 | DA | 2192 | G |
| 23 | DA | 2193 | G |
| 23 | DA | 2198 | A |
| 23 | DA | 2199 | A |
| 23 | DA | 2200 | C |
| 23 | DA | 2206 | G |
| 23 | DA | 2207 | G |
| 23 | DA | 2208 | A |
| 23 | DA | 2225 | A |
| 23 | DA | 2234 | G |
| 23 | DA | 2238 | G |
| 23 | DA | 2239 | G |
| 23 | DA | 2248 | C |
| 23 | DA | 2252 | G |
| 23 | DA | 2268 | A |
| 23 | DA | 2273 | A |
| 23 | DA | 2275 | C |
| 23 | DA | 2278 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 2283 | C |
| 23 | DA | 2287 | A |
| 23 | DA | 2288 | A |
| 23 | DA | 2289 | G |
| 23 | DA | 2291 | U |
| 23 | DA | 2294 | C |
| 23 | DA | 2305 | A |
| 23 | DA | 2306 | C |
| 23 | DA | 2307 | G |
| 23 | DA | 2308 | G |
| 23 | DA | 2309 | A |
| 23 | DA | 2311 | A |
| 23 | DA | 2316 | C |
| 23 | DA | 2319 | G |
| 23 | DA | 2320 | A |
| 23 | DA | 2321 | G |
| 23 | DA | 2325 | G |
| 23 | DA | 2327 | A |
| 23 | DA | 2334 | G |
| 23 | DA | 2336 | A |
| 23 | DA | 2343 | C |
| 23 | DA | 2347 | C |
| 23 | DA | 2350 | C |
| 23 | DA | 2354 | G |
| 23 | DA | 2379 | G |
| 23 | DA | 2383 | G |
| 23 | DA | 2385 | C |
| 23 | DA | 2388 | A |
| 23 | DA | 2391 | G |
| 23 | DA | 2400 | G |
| 23 | DA | 2406 | U |
| 23 | DA | 2407 | G |
| 23 | DA | 2410 | G |
| 23 | DA | 2414 | G |
| 23 | DA | 2418 | A |
| 23 | DA | 2422 | A |
| 23 | DA | 2425 | A |
| 23 | DA | 2429 | G |
| 23 | DA | 2430 | A |
| 23 | DA | 2435 | A |
| 23 | DA | 2439 | A |
| 23 | DA | 2440 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | DA | 2441 | C |
| 23 | DA | 2448 | A |
| 23 | DA | 2465 | C |
| 23 | DA | 2469 | A |
| 23 | DA | 2470 | G |
| 23 | DA | 2472 | G |
| 23 | DA | 2474 | C |
| 23 | DA | 2476 | A |
| 23 | DA | 2477 | C |
| 23 | DA | 2486 | G |
| 23 | DA | 2487 | G |
| 23 | DA | 2502 | G |
| 23 | DA | 2504 | U |
| 23 | DA | 2505 | G |
| 23 | DA | 2506 | U |
| 23 | DA | 2518 | A |
| 23 | DA | 2520 | C |
| 23 | DA | 2525 | G |
| 23 | DA | 2529 | G |
| 23 | DA | 2535 | G |
| 23 | DA | 2554 | U |
| 23 | DA | 2564 | A |
| 23 | DA | 2566 | A |
| 23 | DA | 2567 | G |
| 23 | DA | 2573 | C |
| 23 | DA | 2582 | G |
| 23 | DA | 2585 | U |
| 23 | DA | 2586 | C |
| 23 | DA | 2602 | A |
| 23 | DA | 2603 | G |
| 23 | DA | 2604 | U |
| 23 | DA | 2608 | G |
| 23 | DA | 2609 | U |
| 23 | DA | 2610 | C |
| 23 | DA | 2611 | U |
| 23 | DA | 2612 | C |
| 23 | DA | 2615 | U |
| 23 | DA | 2628 | C |
| 23 | DA | 2629 | A |
| 23 | DA | 2630 | G |
| 23 | DA | 2654 | A |
| 23 | DA | 2663 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 23 | DA | 2672 | G |
| 23 | DA | 2674 | G |
| 23 | DA | 2686 | G |
| 23 | DA | 2690 | C |
| 23 | DA | 2691 | C |
| 23 | DA | 2702 | U |
| 23 | DA | 2703 | C |
| 23 | DA | 2707 | G |
| 23 | DA | 2712(A) | A |
| 23 | DA | 2713 | A |
| 23 | DA | 2714 | G |
| 23 | DA | 2718 | G |
| 23 | DA | 2726 | U |
| 23 | DA | 2733 | A |
| 23 | DA | 2739 | U |
| 23 | DA | 2744 | G |
| 23 | DA | 2748 | A |
| 23 | DA | 2758 | A |
| 23 | DA | 2761 | G |
| 23 | DA | 2765 | A |
| 23 | DA | 2766 | G |
| 23 | DA | 2775 | A |
| 23 | DA | 2778 | A |
| 23 | DA | 2790 | A |
| 23 | DA | 2791 | C |
| 23 | DA | 2802 | G |
| 23 | DA | 2803 | C |
| 23 | DA | 2808 | U |
| 23 | DA | 2820 | A |
| 23 | DA | 2821 | A |
| 23 | DA | 2833 | G |
| 23 | DA | 2834 | G |
| 23 | DA | 2835 | A |
| 23 | DA | 2847 | U |
| 23 | DA | 2872 | G |
| 23 | DA | 2873 | A |
| 23 | DA | 2880 | C |
| 23 | DA | 2892 | A |
| 24 | DB | 2 | C |
| 24 | DB | 8 | U |
| 24 | DB | 9 | G |
| 24 | DB | 12 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | DB | 13 | A |
| 24 | DB | 15 | A |
| 24 | DB | 19 | G |
| 24 | DB | 21 | G |
| 24 | DB | 24 | G |
| 24 | DB | 25 | A |
| 24 | DB | 26 | A |
| 24 | DB | 28 | C |
| 24 | DB | 33 | G |
| 24 | DB | 34 | U |
| 24 | DB | 40 | U |
| 24 | DB | 53 | A |
| 24 | DB | 54 | G |
| 24 | DB | 56 | G |
| 24 | DB | 73 | A |
| 24 | DB | 74 | U |
| 24 | DB | 75 | G |
| 24 | DB | 85 | G |
| 24 | DB | 88 | C |
| 24 | DB | 89 | G |
| 24 | DB | 106 | G |
| 24 | DB | 110 | G |

All (183) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 60 | A |
| 1 | AA | 115 | G |
| 1 | AA | 173 | U |
| 1 | AA | 243 | A |
| 1 | AA | 266 | G |
| 1 | AA | 344 | A |
| 1 | AA | 428 | G |
| 1 | AA | 484 | G |
| 1 | AA | 495 | A |
| 1 | AA | 509 | A |
| 1 | AA | 532 | A |
| 1 | AA | 560 | U |
| 1 | AA | 687 | A |
| 1 | AA | 748 | C |
| 1 | AA | 793 | U |
| 1 | AA | 913 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 934 | C |
| 1 | AA | 968 | A |
| 1 | AA | 992 | U |
| 1 | AA | 1064 | G |
| 1 | AA | 1065 | U |
| 1 | AA | 1067 | A |
| 1 | AA | 1156 | G |
| 1 | AA | 1201 | A |
| 1 | AA | 1285 | A |
| 1 | AA | 1299 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1346 | A |
| 1 | AA | 1378 | C |
| 1 | AA | 1442 | G |
| 1 | AA | 1452 | C |
| 1 | AA | 1493 | A |
| 1 | AA | 1504 | G |
| 23 | BA | 71 | A |
| 23 | BA | 102 | G |
| 23 | BA | 196 | A |
| 23 | BA | 249 | C |
| 23 | BA | 271(K) | U |
| 23 | BA | 271(L) | U |
| 23 | BA | 271(M) | G |
| 23 | BA | 278 | A |
| 23 | BA | 363(E) | U |
| 23 | BA | 481 | G |
| 23 | BA | 542 | C |
| 23 | BA | 547 | A |
| 23 | BA | 587 | C |
| 23 | BA | 669 | G |
| 23 | BA | 685 | A |
| 23 | BA | 746 | A |
| 23 | BA | 752 | A |
| 23 | BA | 764 | A |
| 23 | BA | 827 | U |
| 23 | BA | 856 | C |
| 23 | BA | 900 | A |
| 23 | BA | 945 | A |
| 23 | BA | 974 | G |
| 23 | BA | 1026 | U |
| 23 | BA | 1047 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | BA | 1049 | C |
| 23 | BA | 1106 | G |
| 23 | BA | 1108 | U |
| 23 | BA | 1110 | G |
| 23 | BA | 1155 | A |
| 23 | BA | 1174 | A |
| 23 | BA | 1175 | U |
| 23 | BA | 1176 | G |
| 23 | BA | 1210 | A |
| 23 | BA | 1300 | U |
| 23 | BA | 1378 | A |
| 23 | BA | 1419 | A |
| 23 | BA | 1427 | A |
| 23 | BA | 1507 | A |
| 23 | BA | 1530 | C |
| 23 | BA | 1536 | C |
| 23 | BA | 1538 | G |
| 23 | BA | 1558 | A |
| 23 | BA | 1608 | A |
| 23 | BA | 1653 | G |
| 23 | BA | 1799 | G |
| 23 | BA | 1819 | A |
| 23 | BA | 1992 | G |
| 23 | BA | 2116 | G |
| 23 | BA | 2126 | A |
| 23 | BA | 2172 | U |
| 23 | BA | 2308 | G |
| 23 | BA | 2318 | G |
| 23 | BA | 2406 | U |
| 23 | BA | 2439 | A |
| 23 | BA | 2602 | A |
| 23 | BA | 2610 | C |
| 23 | BA | 2689 | U |
| 23 | BA | 2778 | A |
| 23 | BA | 2802 | G |
| 1 | CA | 60 | A |
| 1 | CA | 115 | G |
| 1 | CA | 173 | U |
| 1 | CA | 243 | A |
| 1 | CA | 266 | G |
| 1 | CA | 344 | A |
| 1 | CA | 428 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 429 | U |
| 1 | CA | 484 | G |
| 1 | CA | 495 | A |
| 1 | CA | 509 | A |
| 1 | CA | 560 | U |
| 1 | CA | 561 | U |
| 1 | CA | 687 | A |
| 1 | CA | 748 | C |
| 1 | CA | 793 | U |
| 1 | CA | 913 | A |
| 1 | CA | 991 | U |
| 1 | CA | 992 | U |
| 1 | CA | 1064 | G |
| 1 | CA | 1065 | U |
| 1 | CA | 1067 | A |
| 1 | CA | 1201 | A |
| 1 | CA | 1211 | U |
| 1 | CA | 1227 | A |
| 1 | CA | 1256 | A |
| 1 | CA | 1280 | A |
| 1 | CA | 1285 | A |
| 1 | CA | 1299 | A |
| 1 | CA | 1300 | G |
| 1 | CA | 1346 | A |
| 1 | CA | 1442 | G |
| 1 | CA | 1493 | A |
| 1 | CA | 1504 | G |
| 23 | DA | 71 | A |
| 23 | DA | 102 | G |
| 23 | DA | 196 | A |
| 23 | DA | 249 | C |
| 23 | DA | 271(K) | U |
| 23 | DA | 271(L) | U |
| 23 | DA | 271(M) | G |
| 23 | DA | 278 | A |
| 23 | DA | 363(E) | U |
| 23 | DA | 481 | G |
| 23 | DA | 542 | C |
| 23 | DA | 547 | A |
| 23 | DA | 587 | C |
| 23 | DA | 669 | G |
| 23 | DA | 685 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 23 | DA | 752 | A |
| 23 | DA | 764 | A |
| 23 | DA | 827 | U |
| 23 | DA | 856 | C |
| 23 | DA | 900 | A |
| 23 | DA | 945 | A |
| 23 | DA | 1026 | U |
| 23 | DA | 1047 | G |
| 23 | DA | 1049 | C |
| 23 | DA | 1106 | G |
| 23 | DA | 1108 | U |
| 23 | DA | 1110 | G |
| 23 | DA | 1155 | A |
| 23 | DA | 1210 | A |
| 23 | DA | 1300 | U |
| 23 | DA | 1301 | A |
| 23 | DA | 1378 | A |
| 23 | DA | 1396 | U |
| 23 | DA | 1419 | A |
| 23 | DA | 1427 | A |
| 23 | DA | 1507 | A |
| 23 | DA | 1530 | C |
| 23 | DA | 1538 | G |
| 23 | DA | 1558 | A |
| 23 | DA | 1608 | A |
| 23 | DA | 1653 | G |
| 23 | DA | 1799 | G |
| 23 | DA | 1819 | A |
| 23 | DA | 1992 | G |
| 23 | DA | 2116 | G |
| 23 | DA | 2126 | A |
| 23 | DA | 2172 | U |
| 23 | DA | 2308 | G |
| 23 | DA | 2318 | G |
| 23 | DA | 2406 | U |
| 23 | DA | 2439 | A |
| 23 | DA | 2602 | A |
| 23 | DA | 2610 | C |
| 23 | DA | 2689 | U |
| 23 | DA | 2778 | A |
| 23 | DA | 2802 | G |

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1662 ligands modelled in this entry, 1662 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1501/1522 (98%) | 0.04 | 61 (4%) 41 19 | 47, 95, 155, 169 | 0 |
| 1 | CA | 1497/1522 (98%) | 0.02 | 68 (4%) 37 17 | 50, 96, 158, 171 | 0 |
| 2 | AB | 230/256 (89%) | -0.06 | 9 (3%) 43 21 | 87, 114, 134, 148 | 0 |
| 2 | CB | 229/256 (89%) | 0.34 | 13 (5%) 27 11 | 92, 116, 136, 149 | 0 |
| 3 | AC | 206/239 (86%) | 0.09 | 5 (2%) 62 39 | 85, 109, 127, 136 | 0 |
| 3 | CC | 206/239 (86%) | 0.37 | 16 (7%) 16 5 | 94, 120, 143, 158 | 0 |
| 4 | AD | 208/209 (99%) | -0.02 | 7 (3%) 49 24 | 75, 94, 114, 125 | 0 |
| 4 | CD | 208/209 (99%) | 0.06 | 4 (1%) 70 48 | 76, 93, 114, 124 | 0 |
| 5 | AE | 148/162 (91%) | -0.19 | 0 100 100 | 66, 86, 103, 125 | 0 |
| 5 | CE | 148/162 (91%) | -0.04 | 3 (2%) 68 46 | 69, 88, 104, 127 | 0 |
| 6 | AF | 100/101 (99%) | -0.29 | 1 (1%) 84 69 | 67, 82, 100, 116 | 0 |
| 6 | CF | 100/101 (99%) | -0.29 | 1 (1%) 84 69 | 70, 86, 103, 117 | 0 |
| 7 | AG | 155/156 (99%) | 2.02 | 69 (44%) 0 0 | 113, 139, 153, 159 | 0 |
| 7 | CG | 155/156 (99%) | 2.00 | 71 (45%) 0 0 | 122, 137, 149, 159 | 0 |
| 8 | AH | 138/138 (100%) | 0.12 | 2 (1%) 78 60 | 71, 90, 100, 110 | 0 |
| 8 | CH | 138/138 (100%) | -0.02 | 6 (4%) 39 18 | 71, 92, 103, 113 | 0 |
| 9 | AI | 125/128 (97%) | 1.22 | 35 (28%) 1 0 | 110, 137, 149, 154 | 0 |
| 9 | CI | 125/128 (97%) | 2.67 | 67 (53%) 0 0 | 115, 139, 152, 163 | 0 |
| 10 | AJ | 96/105 (91%) | 1.61 | 34 (35%) 0 0 | 92, 126, 141, 147 | 0 |
| 10 | CJ | 96/105 (91%) | 2.00 | 42 (43%) 0 0 | 108, 134, 150, 160 | 0 |
| 11 | AK | 114/129 (88%) | -0.03 | 1 (0%) 85 72 | 60, 86, 108, 120 | 0 |
| 11 | CK | 114/129 (88%) | 0.10 | 5 (4%) 38 17 | 63, 89, 107, 126 | 0 |
| 12 | AL | 122/132 (92%) | -0.10 | 1 (0%) 87 75 | 62, 77, 95, 112 | 0 |
| 12 | CL | 122/132 (92%) | -0.01 | 0 100 100 | 63, 77, 96, 109 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 114/126 (90%) | 1.53 | 35 (30%) 1 0 | 112, 139, 150, 153 | 0 |
| 13 | CM | 114/126 (90%) | 1.93 | 44 (38%) 0 0 | 116, 140, 151, 160 | 0 |
| 14 | AN | 60/61 (98%) | 0.75 | 8 (13%) 4 2 | 93, 118, 131, 144 | 0 |
| 14 | CN | 60/61 (98%) | 0.85 | 9 (15%) 3 1 | 103, 122, 134, 139 | 0 |
| 15 | AO | 88/89 (98%) | -0.09 | 0 100 100 | 63, 85, 103, 113 | 0 |
| 15 | CO | 88/89 (98%) | 0.04 | 1 (1%) 82 66 | 63, 85, 105, 111 | 0 |
| 16 | AP | 82/88 (93%) | 0.60 | 10 (12%) 5 2 | 76, 88, 110, 120 | 0 |
| 16 | CP | 82/88 (93%) | 0.37 | 4 (4%) 33 14 | 73, 85, 105, 117 | 0 |
| 17 | AQ | 99/105 (94%) | 0.01 | 1 (1%) 84 69 | 68, 82, 102, 106 | 0 |
| 17 | CQ | 99/105 (94%) | 0.11 | 1 (1%) 84 69 | 69, 83, 101, 108 | 0 |
| 18 | AR | 68/88 (77%) | -0.08 | 2 (2%) 55 31 | 71, 82, 105, 112 | 0 |
| 18 | CR | 68/88 (77%) | 0.20 | 1 (1%) 76 58 | 75, 85, 105, 117 | 0 |
| 19 | AS | 81/93 (87%) | 2.43 | 37 (45%) 0 0 | 113, 138, 147, 152 | 0 |
| 19 | CS | 81/93 (87%) | 2.91 | 45 (55%) 0 0 | 114, 140, 150, 153 | 0 |
| 20 | AT | 87/106 (82%) | 0.34 | 0 100 100 | 75, 88, 103, 111 | 0 |
| 20 | CT | 97/106 (91%) | 0.09 | 0 100 100 | 72, 86, 105, 115 | 0 |
| 21 | AU | 23/27 (85%) | 3.40 | 15 (65%) 0 0 | 128, 136, 145, 154 | 0 |
| 21 | CU | 23/27 (85%) | 4.34 | 18 (78%) 0 0 | 129, 137, 148, 150 | 0 |
| 22 | AX | 95/101 (94%) | 0.22 | 5 (5%) 30 13 | 69, 94, 115, 123 | 0 |
| 22 | CX | 95/101 (94%) | 1.14 | 19 (20%) 1 0 | 88, 106, 129, 145 | 0 |
| 23 | BA | 2837/2913 (97%) | -0.24 | 51 (1%) 71 50 | 26, 47, 132, 176 | 0 |
| 23 | DA | 2814/2913 (96%) | -0.40 | 81 (2%) 55 31 | 28, 50, 133, 176 | 0 |
| 24 | BB | 120/122 (98%) | -0.36 | 0 100 100 | 43, 72, 93, 110 | 0 |
| 24 | DB | 120/122 (98%) | -0.12 | 1 (0%) 87 75 | 48, 81, 106, 117 | 0 |
| 25 | BD | 275/276 (99%) | -0.43 | 0 100 100 | 29, 45, 63, 113 | 0 |
| 25 | DD | 275/276 (99%) | -0.43 | 1 (0%) 93 85 | 30, 47, 66, 116 | 0 |
| 26 | BE | 204/206 (99%) | -0.38 | 1 (0%) 91 83 | 28, 49, 72, 95 | 0 |
| 26 | DE | 204/206 (99%) | -0.41 | 0 100 100 | 29, 50, 76, 95 | 0 |
| 27 | BF | 203/210 (96%) | -0.39 | 0 100 100 | 29, 54, 88, 111 | 0 |
| 27 | DF | 203/210 (96%) | -0.34 | 0 100 100 | 31, 59, 90, 112 | 0 |
| 28 | BG | 181/182 (99%) | -0.00 | 8 (4%) 38 17 | 76, 110, 133, 144 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DG | 181/182 (99%) | 0.86 | 27 (14%) 3 1 | 86, 117, 138, 148 | 0 |
| 29 | BH | 174/180 (96%) | -0.28 | 0 100 100 | 54, 73, 94, 110 | 0 |
| 29 | DH | 174/180 (96%) | 0.35 | 9 (5%) 31 13 | 65, 82, 101, 119 | 0 |
| 30 | BI | 146/148 (98%) | -0.37 | 1 (0%) 89 78 | 54, 81, 99, 115 | 0 |
| 30 | DI | 146/148 (98%) | -0.02 | 2 (1%) 78 60 | 56, 89, 108, 120 | 0 |
| 31 | BN | 140/140 (100%) | -0.36 | 0 100 100 | 38, 49, 78, 92 | 0 |
| 31 | DN | 140/140 (100%) | -0.26 | 1 (0%) 89 78 | 40, 54, 82, 96 | 0 |
| 32 | BO | 122/122 (100%) | -0.40 | 0 100 100 | 35, 50, 69, 77 | 0 |
| 32 | DO | 122/122 (100%) | -0.56 | 0 100 100 | 36, 52, 69, 77 | 0 |
| 33 | BP | 149/150 (99%) | -0.29 | 0 100 100 | 30, 58, 89, 105 | 0 |
| 33 | DP | 149/150 (99%) | -0.16 | 3 (2%) 68 46 | 31, 62, 92, 112 | 0 |
| 34 | BQ | 141/141 (100%) | -0.31 | 0 100 100 | 39, 54, 71, 83 | 0 |
| 34 | DQ | 141/141 (100%) | -0.34 | 0 100 100 | 41, 58, 77, 88 | 0 |
| 35 | BR | 118/118 (100%) | -0.30 | 0 100 100 | 34, 44, 58, 77 | 0 |
| 35 | DR | 118/118 (100%) | -0.31 | 0 100 100 | 36, 47, 62, 78 | 0 |
| 36 | BS | 110/112 (98%) | -0.08 | 0 100 100 | 50, 69, 89, 96 | 0 |
| 36 | DS | 110/112 (98%) | 0.34 | 5 (4%) 37 17 | 55, 74, 94, 102 | 0 |
| 37 | BT | 131/146 (89%) | -0.43 | 0 100 100 | 43, 55, 92, 119 | 0 |
| 37 | DT | 131/146 (89%) | -0.35 | 1 (0%) 87 75 | 46, 57, 93, 128 | 0 |
| 38 | BU | 116/118 (98%) | -0.41 | 0 100 100 | 32, 44, 62, 71 | 0 |
| 38 | DU | 116/118 (98%) | -0.49 | 0 100 100 | 34, 48, 66, 73 | 0 |
| 39 | BV | 101/101 (100%) | -0.33 | 1 (0%) 84 69 | 29, 56, 79, 103 | 0 |
| 39 | DV | 101/101 (100%) | -0.21 | 0 100 100 | 32, 62, 85, 103 | 0 |
| 40 | BW | 112/113 (99%) | -0.41 | 0 100 100 | 33, 40, 62, 103 | 0 |
| 40 | DW | 112/113 (99%) | -0.48 | 0 100 100 | 35, 42, 67, 105 | 0 |
| 41 | BX | 95/96 (98%) | -0.26 | 0 100 100 | 38, 49, 72, 88 | 0 |
| 41 | DX | 95/96 (98%) | -0.29 | 1 (1%) 82 66 | 41, 52, 77, 90 | 0 |
| 42 | BY | 107/110 (97%) | -0.27 | 0 100 100 | 47, 61, 85, 108 | 0 |
| 42 | DY | 107/110 (97%) | 0.20 | 6 (5%) 28 11 | 52, 65, 89, 113 | 0 |
| 43 | BZ | 201/206 (97%) | -0.41 | 0 100 100 | 53, 76, 99, 122 | 0 |
| 43 | DZ | 198/206 (96%) | 0.05 | 5 (2%) 61 37 | 62, 81, 102, 121 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | B0 | 76/85 (89%) | -0.28 | 0 100 100 | 39, 48, 64, 91 | 0 |
| 44 | D0 | 76/85 (89%) | 0.07 | 2 (2%) 59 35 | 43, 52, 66, 92 | 0 |
| 45 | B1 | 97/98 (98%) | -0.21 | 0 100 100 | 36, 48, 82, 97 | 0 |
| 45 | D1 | 97/98 (98%) | -0.16 | 2 (2%) 67 44 | 36, 51, 83, 98 | 0 |
| 46 | B2 | 70/72 (97%) | -0.24 | 0 100 100 | 46, 60, 76, 107 | 0 |
| 46 | D2 | 70/72 (97%) | -0.20 | 0 100 100 | 50, 64, 81, 103 | 0 |
| 47 | B3 | 59/60 (98%) | -0.22 | 0 100 100 | 38, 49, 86, 97 | 0 |
| 47 | D3 | 59/60 (98%) | 0.17 | 1 (1%) 73 52 | 41, 53, 93, 102 | 0 |
| 48 | B4 | 46/71 (64%) | -0.29 | 2 (4%) 39 18 | 101, 129, 144, 148 | 0 |
| 48 | D4 | 46/71 (64%) | 0.49 | 7 (15%) 3 1 | 113, 133, 144, 152 | 0 |
| 49 | B5 | 59/60 (98%) | -0.53 | 0 100 100 | 30, 45, 66, 80 | 0 |
| 49 | D5 | 59/60 (98%) | -0.53 | 0 100 100 | 32, 47, 68, 81 | 0 |
| 50 | B6 | 53/54 (98%) | -0.54 | 0 100 100 | 42, 51, 70, 79 | 0 |
| 50 | D6 | 53/54 (98%) | -0.25 | 2 (3%) 44 21 | 43, 54, 72, 82 | 0 |
| 51 | B7 | 48/49 (97%) | -0.29 | 0 100 100 | 30, 34, 55, 80 | 0 |
| 51 | D7 | 48/49 (97%) | -0.19 | 0 100 100 | 32, 35, 58, 84 | 0 |
| 52 | B8 | 64/65 (98%) | -0.25 | 0 100 100 | 38, 43, 52, 70 | 0 |
| 52 | D8 | 64/65 (98%) | -0.19 | 0 100 100 | 40, 45, 55, 70 | 0 |
| 53 | B9 | 36/37 (97%) | 0.28 | 0 100 100 | 44, 55, 62, 73 | 0 |
| 53 | D9 | 36/37 (97%) | 0.45 | 2 (5%) 28 11 | 47, 59, 68, 75 | 0 |
| All | All | 20641/21444 (96%) | -0.02 | 999 (4%) 34 15 | 26, 71, 144, 176 | 0 |

All (999) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 21 | CU | 11 | GLY | 12.2 |
| 19 | CS | 69 | HIS | 11.1 |
| 21 | CU | 12 | LYS | 10.6 |
| 19 | CS | 4 | SER | 10.1 |
| 19 | AS | 33 | THR | 9.7 |
| 19 | CS | 39 | THR | 9.7 |
| 1 | CA | 1030(B) | C | 8.8 |
| 23 | BA | 888 | C | 8.8 |
| 19 | AS | 50 | ALA | 8.6 |
| 19 | AS | 39 | THR | 8.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | CI | 13 | ALA | 8.3 |
| 10 | AJ | 10 | GLY | 8.2 |
| 21 | CU | 16 | GLY | 8.2 |
| 11 | CK | 13 | GLN | 8.1 |
| 9 | CI | 65 | VAL | 8.0 |
| 9 | CI | 10 | ARG | 8.0 |
| 9 | CI | 63 | ILE | 7.9 |
| 19 | CS | 68 | GLY | 7.9 |
| 13 | AM | 89 | GLY | 7.9 |
| 10 | CJ | 26 | ALA | 7.8 |
| 21 | AU | 14 | TRP | 7.8 |
| 13 | CM | 85 | GLY | 7.7 |
| 7 | CG | 83 | ALA | 7.5 |
| 9 | CI | 29 | ASN | 7.5 |
| 21 | AU | 12 | LYS | 7.4 |
| 19 | CS | 33 | THR | 7.3 |
| 19 | AS | 59 | PRO | 7.3 |
| 9 | CI | 15 | ALA | 7.3 |
| 23 | DA | 2125 | G | 7.2 |
| 28 | DG | 2 | PRO | 7.2 |
| 10 | CJ | 72 | VAL | 7.2 |
| 7 | AG | 108 | ALA | 7.1 |
| 21 | AU | 5 | ASP | 7.1 |
| 21 | CU | 17 | THR | 7.1 |
| 13 | CM | 93 | ARG | 7.0 |
| 19 | AS | 35 | SER | 6.8 |
| 13 | AM | 86 | CYS | 6.8 |
| 19 | CS | 74 | PHE | 6.8 |
| 13 | CM | 89 | GLY | 6.8 |
| 19 | CS | 62 | ILE | 6.6 |
| 7 | CG | 28 | ASN | 6.6 |
| 21 | AU | 16 | GLY | 6.5 |
| 7 | CG | 37 | ASN | 6.5 |
| 1 | CA | 1036 | G | 6.5 |
| 19 | CS | 76 | PRO | 6.4 |
| 21 | CU | 22 | ARG | 6.4 |
| 21 | AU | 4 | GLY | 6.3 |
| 7 | CG | 154 | TYR | 6.3 |
| 19 | AS | 32 | LYS | 6.3 |
| 10 | CJ | 65 | LEU | 6.3 |
| 13 | CM | 87 | TYR | 6.3 |
| 7 | AG | 75 | VAL | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | AJ | 72 | VAL | 6.3 |
| 7 | CG | 80 | VAL | 6.2 |
| 7 | CG | 40 | ALA | 6.2 |
| 7 | CG | 33 | ASP | 6.2 |
| 23 | DA | 2146 | C | 6.2 |
| 19 | CS | 31 | ILE | 6.1 |
| 13 | CM | 98 | VAL | 6.1 |
| 7 | AG | 156 | TRP | 6.1 |
| 7 | CG | 84 | ASN | 6.1 |
| 19 | AS | 57 | HIS | 6.1 |
| 7 | AG | 76 | ARG | 6.1 |
| 9 | CI | 9 | ARG | 6.1 |
| 19 | CS | 40 | ILE | 6.1 |
| 13 | AM | 68 | GLY | 6.0 |
| 13 | CM | 40 | ASN | 6.0 |
| 10 | AJ | 23 | ILE | 6.0 |
| 28 | DG | 155 | MET | 6.0 |
| 7 | AG | 83 | ALA | 5.9 |
| 9 | CI | 71 | SER | 5.9 |
| 9 | AI | 64 | THR | 5.9 |
| 9 | CI | 30 | GLY | 5.9 |
| 1 | CA | 1286 | A | 5.9 |
| 9 | CI | 106 | ALA | 5.8 |
| 21 | CU | 10 | ARG | 5.8 |
| 23 | DA | 2107 | C | 5.8 |
| 19 | AS | 31 | ILE | 5.8 |
| 13 | AM | 71 | ARG | 5.8 |
| 19 | CS | 38 | SER | 5.8 |
| 13 | CM | 68 | GLY | 5.7 |
| 23 | DA | 2152 | G | 5.7 |
| 1 | CA | 1287 | A | 5.7 |
| 19 | CS | 49 | ILE | 5.7 |
| 19 | AS | 49 | ILE | 5.7 |
| 10 | AJ | 20 | ALA | 5.7 |
| 9 | CI | 73 | GLN | 5.7 |
| 7 | CG | 146 | GLU | 5.6 |
| 1 | AA | 1226 | C | 5.6 |
| 7 | CG | 17 | VAL | 5.6 |
| 9 | CI | 14 | VAL | 5.6 |
| 23 | DA | 2147 | G | 5.5 |
| 28 | DG | 45 | GLU | 5.5 |
| 13 | CM | 91 | ARG | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 21 | AU | 18 | TYR | 5.5 |
| 1 | CA | 1035 | A | 5.5 |
| 13 | CM | 92 | HIS | 5.5 |
| 7 | AG | 12 | LEU | 5.5 |
| 7 | AG | 62 | PHE | 5.5 |
| 19 | CS | 75 | ALA | 5.5 |
| 1 | CA | 1030(A) | G | 5.5 |
| 19 | CS | 50 | ALA | 5.4 |
| 19 | AS | 41 | VAL | 5.4 |
| 10 | CJ | 45 | ARG | 5.4 |
| 7 | AG | 43 | PHE | 5.4 |
| 23 | BA | 887 | A | 5.3 |
| 19 | CS | 82 | GLY | 5.3 |
| 1 | CA | 1030(C) | G | 5.3 |
| 7 | CG | 39 | ALA | 5.3 |
| 23 | DA | 2162 | G | 5.3 |
| 19 | AS | 77 | THR | 5.3 |
| 21 | CU | 14 | TRP | 5.2 |
| 1 | AA | 204 | U | 5.2 |
| 10 | AJ | 24 | VAL | 5.2 |
| 13 | CM | 13 | LYS | 5.2 |
| 10 | AJ | 34 | VAL | 5.2 |
| 13 | CM | 88 | ARG | 5.2 |
| 13 | CM | 86 | CYS | 5.2 |
| 13 | CM | 43 | THR | 5.2 |
| 7 | AG | 40 | ALA | 5.2 |
| 9 | CI | 7 | THR | 5.2 |
| 9 | CI | 70 | LYS | 5.1 |
| 13 | AM | 96 | LEU | 5.1 |
| 9 | CI | 75 | ASP | 5.1 |
| 7 | AG | 105 | VAL | 5.1 |
| 1 | CA | 1026 | G | 5.1 |
| 9 | CI | 36 | TYR | 5.1 |
| 1 | AA | 1035 | A | 5.0 |
| 21 | CU | 15 | ARG | 5.0 |
| 7 | CG | 36 | LYS | 5.0 |
| 19 | AS | 40 | ILE | 5.0 |
| 9 | CI | 19 | LEU | 5.0 |
| 1 | CA | 956 | U | 4.9 |
| 7 | CG | 79 | ARG | 4.9 |
| 19 | AS | 38 | SER | 4.9 |
| 1 | CA | 1001 | A | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 14 | AN | 32 | SER | 4.9 |
| 28 | DG | 88 | ILE | 4.9 |
| 19 | AS | 76 | PRO | 4.8 |
| 7 | AG | 109 | ASN | 4.8 |
| 7 | CG | 32 | ARG | 4.8 |
| 10 | AJ | 76 | ASN | 4.8 |
| 13 | AM | 34 | LEU | 4.8 |
| 23 | DA | 652(H) | C | 4.7 |
| 3 | CC | 206 | GLU | 4.7 |
| 7 | AG | 37 | ASN | 4.7 |
| 7 | CG | 29 | LYS | 4.7 |
| 23 | DA | 652(I) | C | 4.7 |
| 13 | AM | 94 | ARG | 4.7 |
| 21 | AU | 21 | TYR | 4.7 |
| 10 | CJ | 21 | GLN | 4.7 |
| 1 | AA | 1030(B) | C | 4.7 |
| 14 | AN | 13 | THR | 4.7 |
| 7 | CG | 19 | GLY | 4.7 |
| 19 | AS | 81 | ARG | 4.6 |
| 9 | CI | 74 | ILE | 4.6 |
| 7 | AG | 11 | GLN | 4.6 |
| 9 | CI | 50 | LEU | 4.6 |
| 21 | CU | 18 | TYR | 4.6 |
| 9 | CI | 77 | ILE | 4.6 |
| 1 | CA | 1001(A) | G | 4.6 |
| 13 | AM | 87 | TYR | 4.5 |
| 13 | CM | 112 | GLY | 4.5 |
| 7 | CG | 10 | ARG | 4.5 |
| 23 | DA | 2169 | A | 4.5 |
| 1 | CA | 1353 | G | 4.5 |
| 10 | CJ | 23 | ILE | 4.5 |
| 21 | CU | 8 | THR | 4.5 |
| 7 | AG | 73 | MET | 4.5 |
| 13 | CM | 12 | ASN | 4.5 |
| 1 | AA | 1026 | G | 4.5 |
| 9 | CI | 37 | PHE | 4.5 |
| 9 | CI | 88 | TYR | 4.4 |
| 1 | AA | 1002 | G | 4.4 |
| 1 | AA | 1287 | A | 4.4 |
| 39 | BV | 101 | GLY | 4.4 |
| 7 | AG | 134 | ALA | 4.4 |
| 13 | CM | 69 | GLU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 13 | CM | 24 | GLY | 4.4 |
| 7 | CG | 109 | ASN | 4.4 |
| 7 | AG | 85 | TYR | 4.4 |
| 7 | CG | 141 | VAL | 4.4 |
| 23 | DA | 229 | A | 4.4 |
| 9 | CI | 31 | GLN | 4.4 |
| 19 | AS | 70 | LYS | 4.4 |
| 14 | AN | 14 | PRO | 4.4 |
| 10 | CJ | 5 | ARG | 4.4 |
| 7 | CG | 81 | GLY | 4.3 |
| 23 | DA | 2108 | C | 4.3 |
| 7 | AG | 154 | TYR | 4.3 |
| 9 | CI | 32 | ASP | 4.3 |
| 19 | CS | 53 | ASN | 4.3 |
| 19 | CS | 11 | VAL | 4.3 |
| 23 | BA | 2116 | G | 4.3 |
| 10 | CJ | 27 | ALA | 4.3 |
| 7 | AG | 141 | VAL | 4.2 |
| 19 | AS | 74 | PHE | 4.2 |
| 7 | CG | 16 | LEU | 4.2 |
| 1 | AA | 1137 | C | 4.2 |
| 9 | AI | 65 | VAL | 4.2 |
| 23 | DA | 2124 | G | 4.2 |
| 7 | CG | 86 | GLN | 4.2 |
| 1 | AA | 1001(A) | G | 4.2 |
| 9 | CI | 110 | GLU | 4.2 |
| 23 | DA | 2155 | G | 4.2 |
| 9 | CI | 72 | GLY | 4.2 |
| 1 | CA | 1002 | G | 4.2 |
| 23 | DA | 652(G) | G | 4.2 |
| 10 | CJ | 6 | ILE | 4.1 |
| 23 | DA | 2126 | A | 4.1 |
| 1 | AA | 1030 | C | 4.1 |
| 13 | CM | 95 | GLY | 4.1 |
| 23 | DA | 2139 | C | 4.1 |
| 2 | CB | 99 | GLY | 4.1 |
| 19 | AS | 56 | GLN | 4.1 |
| 7 | AG | 50 | ILE | 4.1 |
| 9 | CI | 34 | ASN | 4.1 |
| 9 | CI | 115 | GLY | 4.1 |
| 10 | CJ | 22 | LYS | 4.1 |
| 7 | CG | 62 | PHE | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 28 | BG | 87 | PRO | 4.1 |
| 7 | AG | 77 | SER | 4.1 |
| 21 | AU | 17 | THR | 4.1 |
| 19 | CS | 80 | TYR | 4.1 |
| 36 | DS | 55 | ALA | 4.0 |
| 10 | AJ | 35 | SER | 4.0 |
| 9 | CI | 66 | ARG | 4.0 |
| 19 | CS | 60 | VAL | 4.0 |
| 7 | AG | 152 | ALA | 4.0 |
| 7 | AG | 147 | ALA | 4.0 |
| 23 | DA | 2144 | U | 4.0 |
| 7 | AG | 87 | VAL | 4.0 |
| 13 | AM | 90 | LEU | 4.0 |
| 19 | CS | 61 | TYR | 4.0 |
| 9 | CI | 42 | ARG | 4.0 |
| 19 | AS | 60 | VAL | 4.0 |
| 9 | CI | 18 | PHE | 4.0 |
| 45 | D1 | 2 | SER | 4.0 |
| 10 | CJ | 10 | GLY | 4.0 |
| 1 | CA | 1312 | G | 3.9 |
| 7 | CG | 52 | GLU | 3.9 |
| 13 | AM | 85 | GLY | 3.9 |
| 47 | D3 | 60 | GLU | 3.9 |
| 3 | CC | 65 | ALA | 3.9 |
| 1 | AA | 1288 | A | 3.9 |
| 1 | AA | 1447 | A | 3.9 |
| 23 | DA | 2801(A) | A | 3.9 |
| 9 | AI | 9 | ARG | 3.9 |
| 14 | CN | 2 | ALA | 3.9 |
| 1 | AA | 1030(A) | G | 3.9 |
| 23 | DA | 2165 | G | 3.9 |
| 13 | AM | 49 | THR | 3.9 |
| 19 | AS | 53 | ASN | 3.9 |
| 7 | AG | 31 | MET | 3.9 |
| 9 | AI | 101 | PHE | 3.9 |
| 28 | BG | 75 | LYS | 3.9 |
| 9 | AI | 98 | PRO | 3.9 |
| 10 | AJ | 73 | ASP | 3.9 |
| 1 | CA | 1285 | A | 3.8 |
| 19 | CS | 52 | TYR | 3.8 |
| 19 | CS | 63 | THR | 3.8 |
| 1 | AA | 1332 | A | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 42 | DY | 93 | GLY | 3.8 |
| 21 | AU | 15 | ARG | 3.8 |
| 10 | CJ | 20 | ALA | 3.8 |
| 8 | CH | 131 | GLY | 3.8 |
| 21 | CU | 5 | ASP | 3.8 |
| 13 | AM | 24 | GLY | 3.8 |
| 22 | CX | 94 | GLN | 3.8 |
| 7 | CG | 112 | PRO | 3.8 |
| 10 | CJ | 69 | ASN | 3.8 |
| 9 | CI | 105 | ASP | 3.8 |
| 7 | AG | 120 | ILE | 3.8 |
| 19 | CS | 8 | GLY | 3.8 |
| 10 | AJ | 65 | LEU | 3.8 |
| 23 | DA | 2166 | G | 3.7 |
| 22 | CX | 66 | GLU | 3.7 |
| 19 | AS | 69 | HIS | 3.7 |
| 19 | CS | 77 | THR | 3.7 |
| 10 | AJ | 33 | GLN | 3.7 |
| 9 | CI | 55 | ALA | 3.7 |
| 7 | AG | 49 | ILE | 3.7 |
| 13 | CM | 84 | ILE | 3.7 |
| 3 | CC | 23 | TYR | 3.7 |
| 23 | BA | 2793 | G | 3.7 |
| 1 | AA | 1138 | G | 3.7 |
| 23 | DA | 652(F) | G | 3.7 |
| 9 | CI | 27 | THR | 3.7 |
| 9 | CI | 89 | ASN | 3.7 |
| 1 | CA | 1240 | U | 3.7 |
| 7 | AG | 28 | ASN | 3.7 |
| 13 | CM | 42 | ALA | 3.7 |
| 23 | BA | 2108 | C | 3.7 |
| 7 | AG | 78 | ARG | 3.7 |
| 13 | AM | 91 | ARG | 3.7 |
| 7 | CG | 18 | TYR | 3.7 |
| 13 | AM | 64 | TRP | 3.7 |
| 23 | DA | 275 | G | 3.7 |
| 19 | AS | 71 | LEU | 3.6 |
| 1 | AA | 1001 | A | 3.6 |
| 9 | CI | 4 | TYR | 3.6 |
| 19 | CS | 48 | THR | 3.6 |
| 1 | AA | 1257 | U | 3.6 |
| 7 | AG | 20 | ASP | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | CI | 28 | VAL | 3.6 |
| 10 | CJ | 25 | GLU | 3.6 |
| 13 | AM | 98 | VAL | 3.6 |
| 29 | DH | 159 | GLU | 3.6 |
| 1 | AA | 1028 | C | 3.6 |
| 10 | CJ | 64 | GLU | 3.6 |
| 9 | CI | 23 | ASN | 3.6 |
| 23 | DA | 2173 | A | 3.6 |
| 22 | CX | 95 | HIS | 3.6 |
| 7 | AG | 116 | ALA | 3.6 |
| 9 | AI | 63 | ILE | 3.6 |
| 19 | AS | 58 | VAL | 3.6 |
| 13 | CM | 96 | LEU | 3.6 |
| 10 | CJ | 100 | THR | 3.6 |
| 28 | DG | 87 | PRO | 3.6 |
| 19 | CS | 81 | ARG | 3.6 |
| 23 | DA | 2153 | G | 3.6 |
| 10 | AJ | 27 | ALA | 3.6 |
| 19 | CS | 59 | PRO | 3.6 |
| 7 | AG | 42 | ILE | 3.5 |
| 7 | CG | 35 | LYS | 3.5 |
| 7 | AG | 143 | ARG | 3.5 |
| 13 | CM | 90 | LEU | 3.5 |
| 23 | DA | 2110 | G | 3.5 |
| 23 | DA | 2154 | G | 3.5 |
| 1 | CA | 1030 | C | 3.5 |
| 29 | DH | 97 | ARG | 3.5 |
| 13 | AM | 70 | LEU | 3.5 |
| 23 | DA | 2151 | G | 3.5 |
| 23 | DA | 2803 | C | 3.5 |
| 19 | AS | 61 | TYR | 3.5 |
| 1 | CA | 958 | A | 3.5 |
| 9 | AI | 4 | TYR | 3.5 |
| 13 | AM | 5 | ALA | 3.5 |
| 19 | AS | 79 | THR | 3.5 |
| 41 | DX | 92 | LEU | 3.5 |
| 1 | CA | 1116 | C | 3.5 |
| 9 | AI | 30 | GLY | 3.5 |
| 13 | CM | 107 | ALA | 3.5 |
| 7 | AG | 45 | ASP | 3.5 |
| 23 | BA | 2160 | G | 3.5 |
| 7 | AG | 41 | ARG | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | CB | 90 | MET | 3.5 |
| 13 | AM | 43 | THR | 3.4 |
| 43 | DZ | 198 | LYS | 3.4 |
| 2 | AB | 188 | ALA | 3.4 |
| 23 | DA | 2156 | G | 3.4 |
| 28 | DG | 26 | GLN | 3.4 |
| 7 | CG | 134 | ALA | 3.4 |
| 1 | CA | 1447 | A | 3.4 |
| 7 | AG | 153 | HIS | 3.4 |
| 13 | AM | 95 | GLY | 3.4 |
| 13 | CM | 97 | PRO | 3.4 |
| 1 | AA | 1240 | U | 3.4 |
| 7 | AG | 112 | PRO | 3.4 |
| 21 | AU | 11 | GLY | 3.4 |
| 21 | CU | 24 | ARG | 3.4 |
| 19 | AS | 82 | GLY | 3.4 |
| 23 | DA | 2802 | G | 3.4 |
| 23 | DA | 2174 | C | 3.4 |
| 9 | CI | 126 | SER | 3.4 |
| 1 | AA | 1291 | G | 3.4 |
| 10 | AJ | 11 | PHE | 3.4 |
| 23 | DA | 2159 | G | 3.4 |
| 3 | AC | 13 | GLY | 3.4 |
| 7 | AG | 102 | ARG | 3.4 |
| 10 | CJ | 32 | ALA | 3.4 |
| 13 | AM | 4 | ILE | 3.4 |
| 1 | AA | 1025 | U | 3.4 |
| 23 | BA | 2132 | U | 3.4 |
| 1 | AA | 1290 | G | 3.4 |
| 23 | DA | 2148 | G | 3.4 |
| 22 | CX | 37 | VAL | 3.4 |
| 9 | CI | 62 | TYR | 3.4 |
| 7 | CG | 92 | SER | 3.3 |
| 4 | CD | 110 | PHE | 3.3 |
| 22 | CX | 84 | GLN | 3.3 |
| 10 | CJ | 89 | ASP | 3.3 |
| 7 | CG | 2 | ALA | 3.3 |
| 28 | DG | 64 | THR | 3.3 |
| 21 | CU | 13 | ILE | 3.3 |
| 23 | DA | 2132 | U | 3.3 |
| 4 | AD | 134 | ASP | 3.3 |
| 7 | AG | 39 | ALA | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 10 | AJ | 36 | GLY | 3.3 |
| 10 | CJ | 39 | PRO | 3.3 |
| 13 | CM | 76 | ALA | 3.3 |
| 13 | CM | 94 | ARG | 3.3 |
| 7 | AG | 35 | LYS | 3.3 |
| 10 | CJ | 81 | THR | 3.3 |
| 28 | DG | 73 | ALA | 3.3 |
| 1 | AA | 1286 | A | 3.3 |
| 1 | CA | 1149 | C | 3.3 |
| 3 | AC | 196 | LEU | 3.3 |
| 28 | DG | 142 | PRO | 3.3 |
| 9 | CI | 86 | VAL | 3.3 |
| 2 | AB | 121 | LEU | 3.3 |
| 14 | CN | 13 | THR | 3.3 |
| 23 | DA | 2170 | A | 3.3 |
| 9 | CI | 96 | LEU | 3.3 |
| 23 | BA | 2118 | U | 3.3 |
| 23 | DA | 277 | C | 3.3 |
| 28 | DG | 135 | LEU | 3.3 |
| 1 | AA | 1036 | G | 3.2 |
| 7 | CG | 77 | SER | 3.3 |
| 7 | CG | 156 | TRP | 3.2 |
| 10 | CJ | 29 | ARG | 3.2 |
| 9 | AI | 105 | ASP | 3.2 |
| 3 | AC | 100 | ALA | 3.2 |
| 10 | CJ | 66 | ARG | 3.2 |
| 16 | AP | 47 | ASP | 3.2 |
| 9 | AI | 14 | VAL | 3.2 |
| 10 | CJ | 11 | PHE | 3.2 |
| 21 | AU | 6 | ARG | 3.2 |
| 19 | CS | 45 | VAL | 3.2 |
| 9 | AI | 102 | LEU | 3.2 |
| 23 | DA | 652(O) | C | 3.2 |
| 18 | AR | 29 | PHE | 3.2 |
| 13 | AM | 48 | LEU | 3.2 |
| 23 | DA | 2141 | G | 3.2 |
| 7 | AG | 107 | ALA | 3.2 |
| 22 | CX | 73 | ALA | 3.2 |
| 23 | DA | 652(J) | G | 3.2 |
| 9 | CI | 43 | ALA | 3.2 |
| 13 | CM | 9 | ILE | 3.2 |
| 7 | CG | 95 | ARG | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 9 | CI | 44 | VAL | 3.2 |
| 23 | BA | 2125 | G | 3.2 |
| 1 | CA | 1326 | C | 3.2 |
| 23 | DA | 2790 | A | 3.2 |
| 23 | DA | 2804 | C | 3.2 |
| 9 | CI | 64 | THR | 3.2 |
| 23 | DA | 652(P) | G | 3.2 |
| 7 | AG | 19 | GLY | 3.2 |
| 7 | CG | 9 | VAL | 3.2 |
| 2 | CB | 135 | GLN | 3.2 |
| 36 | DS | 59 | LYS | 3.2 |
| 9 | AI | 17 | VAL | 3.2 |
| 7 | AG | 133 | GLY | 3.1 |
| 14 | AN | 18 | VAL | 3.1 |
| 23 | BA | 2152 | G | 3.1 |
| 4 | AD | 135 | LEU | 3.1 |
| 9 | AI | 88 | TYR | 3.1 |
| 28 | BG | 88 | ILE | 3.1 |
| 8 | CH | 57 | PRO | 3.1 |
| 1 | CA | 1129 | C | 3.1 |
| 19 | AS | 44 | MET | 3.1 |
| 7 | CG | 94 | ARG | 3.1 |
| 1 | AA | 1248 | A | 3.1 |
| 1 | CA | 1280 | A | 3.1 |
| 9 | CI | 49 | PRO | 3.1 |
| 1 | CA | 1459 | C | 3.1 |
| 3 | AC | 193 | TYR | 3.1 |
| 3 | CC | 205 | GLY | 3.1 |
| 10 | AJ | 100 | THR | 3.1 |
| 7 | CG | 153 | HIS | 3.1 |
| 36 | DS | 58 | LEU | 3.1 |
| 23 | DA | 2145 | C | 3.1 |
| 9 | CI | 12 | GLU | 3.1 |
| 1 | CA | 1313 | U | 3.1 |
| 13 | CM | 66 | LEU | 3.1 |
| 13 | CM | 81 | LEU | 3.1 |
| 2 | AB | 135 | GLN | 3.1 |
| 8 | AH | 25 | ASP | 3.1 |
| 29 | DH | 29 | PRO | 3.1 |
| 23 | DA | 1509 | C | 3.0 |
| 19 | AS | 80 | TYR | 3.0 |
| 22 | CX | 20 | VAL | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 10 | CJ | 83 | GLU | 3.0 |
| 23 | BA | 2173 | A | 3.0 |
| 3 | CC | 179 | ARG | 3.0 |
| 1 | CA | 1034 | G | 3.0 |
| 13 | CM | 60 | VAL | 3.0 |
| 7 | CG | 41 | ARG | 3.0 |
| 1 | CA | 1025 | U | 3.0 |
| 7 | AG | 80 | VAL | 3.0 |
| 1 | CA | 1030(D) | A | 3.0 |
| 1 | AA | 1031 | G | 3.0 |
| 36 | DS | 56 | LEU | 3.0 |
| 33 | DP | 92 | GLU | 3.0 |
| 9 | CI | 76 | ALA | 3.0 |
| 29 | DH | 43 | VAL | 3.0 |
| 1 | CA | 1249 | C | 3.0 |
| 23 | BA | 652(H) | C | 3.0 |
| 10 | AJ | 5 | ARG | 3.0 |
| 10 | CJ | 41 | PRO | 3.0 |
| 7 | AG | 15 | ASP | 3.0 |
| 13 | CM | 6 | GLY | 3.0 |
| 1 | AA | 999 | C | 3.0 |
| 7 | CG | 82 | GLY | 3.0 |
| 9 | CI | 17 | VAL | 3.0 |
| 7 | CG | 130 | GLY | 3.0 |
| 1 | CA | 1373 | G | 3.0 |
| 23 | BA | 2794 | C | 3.0 |
| 2 | CB | 70 | PHE | 2.9 |
| 21 | CU | 7 | ARG | 2.9 |
| 23 | BA | 2130 | U | 2.9 |
| 28 | BG | 25 | TYR | 2.9 |
| 10 | CJ | 62 | HIS | 2.9 |
| 19 | AS | 48 | THR | 2.9 |
| 23 | DA | 10 | G | 2.9 |
| 21 | AU | 3 | LYS | 2.9 |
| 7 | CG | 8 | GLU | 2.9 |
| 19 | AS | 68 | GLY | 2.9 |
| 22 | CX | 24 | PHE | 2.9 |
| 7 | AG | 58 | PRO | 2.9 |
| 9 | CI | 84 | ALA | 2.9 |
| 13 | CM | 102 | ARG | 2.9 |
| 23 | DA | 2163 | C | 2.9 |
| 14 | CN | 14 | PRO | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 21 | CU | 4 | GLY | 2.9 |
| 21 | CU | 21 | TYR | 2.9 |
| 23 | BA | 1509 | C | 2.9 |
| 23 | BA | 2161 | C | 2.9 |
| 7 | AG | 149 | ARG | 2.9 |
| 7 | CG | 11 | GLN | 2.9 |
| 9 | CI | 22 | GLY | 2.9 |
| 10 | CJ | 98 | ILE | 2.9 |
| 22 | CX | 5 | ILE | 2.9 |
| 9 | AI | 5 | TYR | 2.9 |
| 9 | AI | 19 | LEU | 2.9 |
| 23 | BA | 2131 | G | 2.9 |
| 5 | CE | 120 | THR | 2.9 |
| 28 | DG | 134 | GLY | 2.9 |
| 13 | CM | 82 | MET | 2.9 |
| 7 | CG | 5 | ARG | 2.9 |
| 7 | CG | 105 | VAL | 2.9 |
| 23 | BA | 1535 | A | 2.9 |
| 1 | CA | 1297 | C | 2.9 |
| 1 | CA | 1314 | C | 2.9 |
| 9 | AI | 103 | THR | 2.9 |
| 23 | DA | 2140 | C | 2.9 |
| 23 | DA | 2157 | G | 2.9 |
| 2 | AB | 165 | VAL | 2.9 |
| 16 | AP | 4 | ILE | 2.9 |
| 7 | AG | 100 | ALA | 2.9 |
| 23 | BA | 2124 | G | 2.9 |
| 23 | BA | 2166 | G | 2.9 |
| 48 | D4 | 43 | TYR | 2.9 |
| 7 | CG | 31 | MET | 2.9 |
| 10 | AJ | 47 | PHE | 2.9 |
| 7 | AG | 5 | ARG | 2.9 |
| 23 | BA | 2804 | C | 2.9 |
| 10 | CJ | 71 | LEU | 2.8 |
| 23 | BA | 652(G) | G | 2.8 |
| 3 | CC | 170 | GLN | 2.8 |
| 7 | CG | 103 | TRP | 2.8 |
| 14 | CN | 8 | GLU | 2.8 |
| 1 | CA | 1031 | G | 2.8 |
| 23 | BA | 2133 | G | 2.8 |
| 23 | DA | 2792 | G | 2.8 |
| 7 | AG | 125 | MET | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | CA | 1296 | C | 2.8 |
| 10 | CJ | 87 | THR | 2.8 |
| 23 | BA | 2168 | G | 2.8 |
| 13 | CM | 99 | ARG | 2.8 |
| 21 | CU | 3 | LYS | 2.8 |
| 18 | AR | 31 | LEU | 2.8 |
| 19 | CS | 51 | VAL | 2.8 |
| 1 | AA | 1331 | G | 2.8 |
| 16 | CP | 19 | ILE | 2.8 |
| 10 | AJ | 67 | THR | 2.8 |
| 10 | CJ | 68 | HIS | 2.8 |
| 42 | DY | 2 | ARG | 2.8 |
| 23 | BA | 272(A) | U | 2.8 |
| 23 | BA | 277 | C | 2.8 |
| 23 | DA | 652(R) | C | 2.8 |
| 1 | AA | 1241 | G | 2.8 |
| 23 | BA | 2167 | U | 2.8 |
| 19 | CS | 35 | SER | 2.8 |
| 23 | DA | 1044 | G | 2.8 |
| 3 | CC | 164 | ARG | 2.8 |
| 7 | AG | 14 | PRO | 2.8 |
| 7 | AG | 18 | TYR | 2.8 |
| 7 | CG | 27 | ILE | 2.8 |
| 9 | AI | 39 | GLY | 2.8 |
| 13 | AM | 39 | ILE | 2.8 |
| 13 | CM | 11 | ARG | 2.8 |
| 19 | CS | 46 | GLY | 2.8 |
| 10 | CJ | 63 | PHE | 2.8 |
| 23 | BA | 2153 | G | 2.8 |
| 9 | CI | 78 | LYS | 2.8 |
| 1 | CA | 1140 | C | 2.8 |
| 23 | BA | 889 | C | 2.8 |
| 3 | CC | 202 | ILE | 2.7 |
| 9 | CI | 91 | ASP | 2.7 |
| 53 | D9 | 10 | ILE | 2.7 |
| 1 | AA | 1113 | C | 2.7 |
| 24 | DB | 52 | A | 2.7 |
| 23 | DA | 2793 | G | 2.7 |
| 28 | DG | 17 | PRO | 2.7 |
| 1 | AA | 1459 | C | 2.7 |
| 9 | AI | 91 | ASP | 2.7 |
| 16 | CP | 39 | TYR | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | AG | 88 | PRO | 2.7 |
| 19 | CS | 41 | VAL | 2.7 |
| 1 | CA | 1379 | G | 2.7 |
| 14 | AN | 8 | GLU | 2.7 |
| 7 | CG | 26 | PHE | 2.7 |
| 2 | CB | 143 | GLU | 2.7 |
| 7 | CG | 76 | ARG | 2.7 |
| 7 | CG | 149 | ARG | 2.7 |
| 16 | AP | 19 | ILE | 2.7 |
| 28 | DG | 157 | ILE | 2.7 |
| 4 | AD | 37 | PRO | 2.7 |
| 9 | AI | 66 | ARG | 2.7 |
| 21 | CU | 6 | ARG | 2.7 |
| 1 | AA | 1129 | C | 2.7 |
| 1 | CA | 1029 | C | 2.7 |
| 9 | AI | 31 | GLN | 2.7 |
| 9 | CI | 6 | GLY | 2.7 |
| 3 | CC | 160 | ALA | 2.7 |
| 6 | AF | 55 | ASP | 2.7 |
| 22 | CX | 85 | LEU | 2.7 |
| 10 | AJ | 21 | GLN | 2.7 |
| 28 | DG | 138 | GLN | 2.7 |
| 11 | CK | 126 | ARG | 2.7 |
| 30 | DI | 92 | VAL | 2.7 |
| 1 | AA | 1267 | C | 2.7 |
| 1 | AA | 1354 | C | 2.7 |
| 23 | DA | 2164 | C | 2.7 |
| 19 | CS | 84 | GLY | 2.7 |
| 7 | AG | 144 | MET | 2.7 |
| 21 | AU | 7 | ARG | 2.7 |
| 13 | AM | 30 | ALA | 2.7 |
| 23 | BA | 2144 | U | 2.7 |
| 9 | AI | 15 | ALA | 2.7 |
| 14 | CN | 16 | PHE | 2.7 |
| 7 | AG | 32 | ARG | 2.7 |
| 9 | AI | 3 | GLN | 2.7 |
| 9 | AI | 37 | PHE | 2.6 |
| 9 | AI | 106 | ALA | 2.6 |
| 13 | CM | 4 | ILE | 2.6 |
| 28 | BG | 144 | ILE | 2.6 |
| 13 | AM | 108 | ARG | 2.6 |
| 7 | CG | 66 | VAL | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CX | 42 | LYS | 2.6 |
| 13 | CM | 2 | ALA | 2.6 |
| 37 | DT | 1 | MET | 2.6 |
| 1 | CA | 1005 | A | 2.6 |
| 7 | AG | 10 | ARG | 2.6 |
| 10 | CJ | 67 | THR | 2.6 |
| 1 | AA | 1005 | A | 2.6 |
| 23 | BA | 2172 | U | 2.6 |
| 10 | AJ | 8 | LEU | 2.6 |
| 19 | AS | 72 | GLY | 2.6 |
| 10 | CJ | 19 | SER | 2.6 |
| 13 | CM | 56 | LEU | 2.6 |
| 19 | CS | 32 | LYS | 2.6 |
| 16 | AP | 39 | TYR | 2.6 |
| 30 | DI | 3 | VAL | 2.6 |
| 28 | DG | 152 | LEU | 2.6 |
| 1 | AA | 202 | U | 2.6 |
| 7 | CG | 133 | GLY | 2.6 |
| 28 | DG | 41 | GLN | 2.6 |
| 22 | AX | 16 | LEU | 2.6 |
| 10 | CJ | 33 | GLN | 2.6 |
| 7 | CG | 147 | ALA | 2.6 |
| 9 | AI | 94 | ALA | 2.6 |
| 14 | AN | 11 | LYS | 2.6 |
| 23 | BA | 2159 | G | 2.6 |
| 19 | CS | 30 | LEU | 2.6 |
| 29 | DH | 123 | PHE | 2.6 |
| 3 | CC | 134 | ILE | 2.6 |
| 3 | CC | 177 | THR | 2.6 |
| 11 | CK | 75 | TYR | 2.6 |
| 1 | CA | 1020 | U | 2.6 |
| 9 | CI | 41 | VAL | 2.6 |
| 1 | AA | 1374 | A | 2.6 |
| 1 | CA | 959 | A | 2.6 |
| 2 | AB | 122 | PHE | 2.6 |
| 19 | CS | 10 | PHE | 2.6 |
| 23 | DA | 2158 | A | 2.6 |
| 2 | CB | 33 | TYR | 2.6 |
| 7 | CG | 108 | ALA | 2.6 |
| 9 | AI | 62 | TYR | 2.6 |
| 9 | CI | 11 | LYS | 2.6 |
| 16 | AP | 17 | TYR | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 23 | BA | 2146 | C | 2.6 |
| 7 | CG | 135 | VAL | 2.6 |
| 31 | DN | 140 | VAL | 2.6 |
| 1 | AA | 1330 | U | 2.6 |
| 7 | AG | 30 | ILE | 2.5 |
| 23 | DA | 652(B) | A | 2.5 |
| 1 | AA | 1266 | G | 2.5 |
| 23 | DA | 2116 | G | 2.5 |
| 23 | BA | 652(S) | C | 2.5 |
| 28 | BG | 76 | SER | 2.5 |
| 28 | DG | 72 | ARG | 2.5 |
| 19 | AS | 29 | ARG | 2.5 |
| 7 | AG | 36 | LYS | 2.5 |
| 1 | AA | 218 | C | 2.5 |
| 23 | DA | 2168 | G | 2.5 |
| 10 | AJ | 69 | ASN | 2.5 |
| 19 | AS | 4 | SER | 2.5 |
| 1 | CA | 1311 | G | 2.5 |
| 7 | AG | 66 | VAL | 2.5 |
| 16 | AP | 2 | VAL | 2.5 |
| 14 | AN | 12 | ARG | 2.5 |
| 1 | CA | 1004 | A | 2.5 |
| 16 | AP | 32 | TYR | 2.5 |
| 28 | DG | 3 | LEU | 2.5 |
| 4 | CD | 158 | ILE | 2.5 |
| 5 | CE | 94 | ALA | 2.5 |
| 1 | CA | 1027 | C | 2.5 |
| 13 | AM | 93 | ARG | 2.5 |
| 23 | DA | 2105 | C | 2.5 |
| 23 | DA | 2161 | C | 2.5 |
| 1 | CA | 1024 | G | 2.5 |
| 10 | AJ | 30 | SER | 2.5 |
| 11 | CK | 98 | LEU | 2.5 |
| 13 | AM | 40 | ASN | 2.5 |
| 13 | AM | 110 | ARG | 2.5 |
| 19 | AS | 36 | ARG | 2.5 |
| 1 | CA | 1045 | C | 2.5 |
| 16 | CP | 21 | VAL | 2.5 |
| 33 | DP | 94 | GLU | 2.5 |
| 9 | CI | 94 | ALA | 2.5 |
| 43 | DZ | 112 | ARG | 2.5 |
| 9 | AI | 89 | ASN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 8 | CH | 99 | GLU | 2.5 |
| 22 | AX | 77 | LEU | 2.5 |
| 14 | AN | 60 | SER | 2.5 |
| 1 | CA | 1319 | A | 2.5 |
| 2 | AB | 132 | LYS | 2.5 |
| 10 | CJ | 7 | LYS | 2.5 |
| 7 | CG | 150 | ALA | 2.4 |
| 22 | CX | 62 | HIS | 2.4 |
| 1 | CA | 1288 | A | 2.4 |
| 9 | AI | 104 | ARG | 2.4 |
| 10 | CJ | 34 | VAL | 2.4 |
| 1 | CA | 1243 | C | 2.4 |
| 23 | DA | 1052 | C | 2.4 |
| 7 | AG | 71 | PRO | 2.4 |
| 13 | AM | 23 | TYR | 2.4 |
| 42 | DY | 44 | ILE | 2.4 |
| 16 | CP | 60 | LEU | 2.4 |
| 1 | AA | 1033 | G | 2.4 |
| 1 | CA | 1250 | A | 2.4 |
| 25 | DD | 276 | LYS | 2.4 |
| 28 | DG | 34 | LEU | 2.4 |
| 1 | CA | 1000 | U | 2.4 |
| 42 | DY | 94 | LYS | 2.4 |
| 10 | AJ | 98 | ILE | 2.4 |
| 13 | CM | 10 | PRO | 2.4 |
| 1 | AA | 71 | C | 2.4 |
| 1 | CA | 723 | U | 2.4 |
| 19 | CS | 12 | ASP | 2.4 |
| 11 | CK | 14 | VAL | 2.4 |
| 1 | CA | 1037 | C | 2.4 |
| 23 | DA | 652(S) | C | 2.4 |
| 1 | AA | 1220 | G | 2.4 |
| 7 | CG | 74 | GLU | 2.4 |
| 9 | CI | 67 | GLY | 2.4 |
| 29 | DH | 82 | GLY | 2.4 |
| 2 | AB | 118 | LEU | 2.4 |
| 7 | CG | 43 | PHE | 2.4 |
| 48 | D4 | 20 | ASN | 2.4 |
| 7 | AG | 29 | LYS | 2.4 |
| 10 | AJ | 66 | ARG | 2.4 |
| 1 | CA | 1354 | C | 2.4 |
| 7 | CG | 30 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 23 | DA | 2172 | U | 2.4 |
| 28 | DG | 84 | LYS | 2.4 |
| 1 | AA | 1034 | G | 2.4 |
| 12 | AL | 29 | GLY | 2.4 |
| 2 | CB | 122 | PHE | 2.4 |
| 7 | CG | 151 | TYR | 2.4 |
| 10 | CJ | 44 | VAL | 2.4 |
| 23 | DA | 276 | A | 2.4 |
| 23 | DA | 2892 | A | 2.4 |
| 48 | D4 | 29 | PRO | 2.4 |
| 9 | CI | 35 | GLU | 2.4 |
| 7 | CG | 3 | ARG | 2.4 |
| 10 | CJ | 99 | LYS | 2.4 |
| 10 | CJ | 8 | LEU | 2.4 |
| 13 | CM | 23 | TYR | 2.4 |
| 19 | CS | 5 | LEU | 2.4 |
| 23 | DA | 272(A) | U | 2.4 |
| 7 | CG | 104 | LEU | 2.4 |
| 1 | AA | 1024 | G | 2.3 |
| 1 | CA | 1032 | G | 2.3 |
| 8 | CH | 1 | MET | 2.3 |
| 48 | D4 | 39 | CYS | 2.3 |
| 45 | D1 | 83 | GLU | 2.3 |
| 10 | AJ | 32 | ALA | 2.3 |
| 10 | CJ | 74 | ILE | 2.3 |
| 23 | DA | 2160 | G | 2.3 |
| 9 | CI | 53 | VAL | 2.3 |
| 1 | CA | 1378 | C | 2.3 |
| 9 | CI | 5 | TYR | 2.3 |
| 1 | AA | 996 | A | 2.3 |
| 19 | CS | 73 | GLU | 2.3 |
| 23 | BA | 2171 | A | 2.3 |
| 7 | AG | 103 | TRP | 2.3 |
| 23 | BA | 2162 | G | 2.3 |
| 23 | DA | 2109 | U | 2.3 |
| 30 | BI | 1 | MET | 2.3 |
| 1 | AA | 100 | C | 2.3 |
| 8 | AH | 59 | LEU | 2.3 |
| 9 | CI | 59 | PHE | 2.3 |
| 22 | CX | 3 | LEU | 2.3 |
| 7 | CG | 34 | GLY | 2.3 |
| 14 | CN | 38 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | DG | 154 | GLY | 2.3 |
| 1 | AA | 1029 | C | 2.3 |
| 43 | DZ | 92 | SER | 2.3 |
| 48 | D4 | 44 | THR | 2.3 |
| 15 | CO | 89 | GLY | 2.3 |
| 19 | CS | 72 | GLY | 2.3 |
| 18 | CR | 31 | LEU | 2.3 |
| 28 | BG | 72 | ARG | 2.3 |
| 1 | AA | 1023 | G | 2.3 |
| 1 | CA | 1028 | C | 2.3 |
| 1 | CA | 1210 | C | 2.3 |
| 23 | BA | 2140 | C | 2.3 |
| 7 | CG | 110 | GLN | 2.3 |
| 21 | AU | 22 | ARG | 2.3 |
| 9 | CI | 92 | TYR | 2.3 |
| 23 | BA | 2142 | C | 2.3 |
| 2 | CB | 81 | VAL | 2.3 |
| 7 | CG | 72 | ARG | 2.3 |
| 23 | DA | 11 | G | 2.3 |
| 7 | AG | 82 | GLY | 2.3 |
| 7 | AG | 145 | ALA | 2.3 |
| 19 | AS | 51 | VAL | 2.3 |
| 29 | DH | 30 | LYS | 2.3 |
| 42 | DY | 95 | LYS | 2.3 |
| 23 | BA | 2803 | C | 2.3 |
| 3 | CC | 148 | GLY | 2.3 |
| 7 | CG | 132 | GLY | 2.3 |
| 22 | CX | 7 | GLY | 2.3 |
| 28 | BG | 80 | PHE | 2.3 |
| 23 | BA | 2117 | A | 2.3 |
| 23 | DA | 1048 | A | 2.3 |
| 5 | CE | 14 | ARG | 2.2 |
| 28 | DG | 108 | ASN | 2.2 |
| 1 | AA | 1037 | C | 2.2 |
| 9 | AI | 90 | PRO | 2.2 |
| 17 | CQ | 74 | LEU | 2.2 |
| 48 | B4 | 29 | PRO | 2.2 |
| 7 | CG | 51 | GLN | 2.2 |
| 10 | CJ | 38 | ILE | 2.2 |
| 4 | AD | 66 | ARG | 2.2 |
| 1 | CA | 1289 | A | 2.2 |
| 13 | AM | 67 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 23 | DA | 652(Q) | G | 2.2 |
| 7 | CG | 12 | LEU | 2.2 |
| 28 | DG | 74 | LYS | 2.2 |
| 23 | DA | 2167 | U | 2.2 |
| 1 | AA | 1347 | G | 2.2 |
| 4 | AD | 120 | LEU | 2.2 |
| 19 | CS | 78 | ARG | 2.2 |
| 42 | DY | 43 | ASN | 2.2 |
| 7 | AG | 33 | ASP | 2.2 |
| 19 | CS | 44 | MET | 2.2 |
| 1 | AA | 64 | G | 2.2 |
| 10 | AJ | 99 | LYS | 2.2 |
| 13 | AM | 50 | GLU | 2.2 |
| 14 | CN | 61 | TRP | 2.2 |
| 7 | CG | 155 | ARG | 2.2 |
| 19 | AS | 30 | LEU | 2.2 |
| 1 | CA | 1310 | G | 2.2 |
| 7 | AG | 151 | TYR | 2.2 |
| 13 | CM | 39 | ILE | 2.2 |
| 23 | BA | 2147 | G | 2.2 |
| 23 | BA | 2154 | G | 2.2 |
| 17 | AQ | 78 | GLU | 2.2 |
| 23 | DA | 34 | C | 2.2 |
| 3 | CC | 149 | ALA | 2.2 |
| 9 | AI | 82 | ALA | 2.2 |
| 13 | AM | 72 | ALA | 2.2 |
| 4 | CD | 23 | GLY | 2.2 |
| 1 | AA | 1004 | A | 2.2 |
| 1 | CA | 1183 | A | 2.2 |
| 1 | AA | 1003 | G | 2.2 |
| 23 | DA | 280 | C | 2.2 |
| 9 | CI | 116 | LYS | 2.2 |
| 19 | CS | 9 | VAL | 2.2 |
| 43 | DZ | 197 | ILE | 2.2 |
| 22 | CX | 50 | SER | 2.2 |
| 43 | DZ | 190 | GLU | 2.2 |
| 7 | AG | 86 | GLN | 2.2 |
| 1 | CA | 1235 | U | 2.2 |
| 23 | BA | 2143 | C | 2.2 |
| 9 | AI | 107 | ARG | 2.2 |
| 28 | DG | 11 | TYR | 2.2 |
| 2 | CB | 163 | PHE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 9 | CI | 102 | LEU | 2.2 |
| 22 | AX | 4 | ASN | 2.2 |
| 22 | CX | 67 | GLY | 2.2 |
| 23 | BA | 2801(A) | A | 2.2 |
| 36 | DS | 34 | HIS | 2.2 |
| 48 | B4 | 17 | GLY | 2.2 |
| 50 | D6 | 54 | ILE | 2.2 |
| 1 | CA | 1266 | G | 2.2 |
| 9 | AI | 126 | SER | 2.2 |
| 13 | AM | 27 | LYS | 2.2 |
| 23 | BA | 2151 | G | 2.2 |
| 50 | D6 | 11 | LEU | 2.2 |
| 16 | AP | 1 | MET | 2.1 |
| 23 | DA | 2138 | C | 2.1 |
| 3 | AC | 145 | GLY | 2.1 |
| 13 | AM | 102 | ARG | 2.1 |
| 8 | CH | 129 | VAL | 2.1 |
| 23 | DA | 2106 | G | 2.1 |
| 1 | CA | 1349 | A | 2.1 |
| 33 | DP | 91 | PHE | 2.1 |
| 2 | AB | 133 | LYS | 2.1 |
| 10 | AJ | 74 | ILE | 2.1 |
| 14 | CN | 25 | VAL | 2.1 |
| 19 | AS | 12 | ASP | 2.1 |
| 22 | CX | 79 | ASP | 2.1 |
| 21 | AU | 9 | ARG | 2.1 |
| 23 | BA | 2115 | G | 2.1 |
| 23 | DA | 2121 | G | 2.1 |
| 1 | AA | 1289 | A | 2.1 |
| 7 | AG | 52 | GLU | 2.1 |
| 10 | AJ | 64 | GLU | 2.1 |
| 22 | AX | 23 | LYS | 2.1 |
| 23 | BA | 2897 | U | 2.1 |
| 11 | AK | 126 | ARG | 2.1 |
| 13 | AM | 44 | ARG | 2.1 |
| 44 | D0 | 75 | LEU | 2.1 |
| 23 | BA | 2896 | C | 2.1 |
| 1 | AA | 1353 | G | 2.1 |
| 7 | CG | 85 | TYR | 2.1 |
| 9 | CI | 101 | PHE | 2.1 |
| 48 | D4 | 37 | SER | 2.1 |
| 23 | BA | 2805 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | AM | 12 | ASN | 2.1 |
| 14 | CN | 51 | GLY | 2.1 |
| 1 | AA | 1027 | C | 2.1 |
| 6 | CF | 65 | VAL | 2.1 |
| 19 | CS | 27 | GLU | 2.1 |
| 44 | D0 | 70 | GLN | 2.1 |
| 23 | DA | 2142 | C | 2.1 |
| 1 | AA | 723 | U | 2.1 |
| 10 | AJ | 53 | PRO | 2.1 |
| 10 | AJ | 63 | PHE | 2.1 |
| 3 | CC | 13 | GLY | 2.1 |
| 7 | AG | 38 | LEU | 2.1 |
| 28 | DG | 46 | ALA | 2.1 |
| 9 | AI | 18 | PHE | 2.1 |
| 29 | DH | 171 | LEU | 2.1 |
| 3 | CC | 180 | ALA | 2.1 |
| 7 | CG | 89 | MET | 2.1 |
| 10 | AJ | 31 | GLY | 2.1 |
| 13 | CM | 41 | PRO | 2.1 |
| 48 | D4 | 10 | VAL | 2.1 |
| 1 | CA | 1138 | G | 2.1 |
| 23 | BA | 2137 | C | 2.1 |
| 10 | AJ | 88 | LEU | 2.1 |
| 22 | CX | 77 | LEU | 2.1 |
| 16 | AP | 38 | TYR | 2.1 |
| 10 | AJ | 38 | ILE | 2.0 |
| 23 | DA | 1046 | A | 2.0 |
| 29 | DH | 110 | SER | 2.0 |
| 1 | CA | 1115 | C | 2.0 |
| 22 | CX | 9 | ASN | 2.0 |
| 23 | DA | 2178 | C | 2.0 |
| 28 | DG | 176 | LEU | 2.0 |
| 4 | AD | 23 | GLY | 2.0 |
| 19 | CS | 58 | VAL | 2.0 |
| 2 | CB | 68 | ILE | 2.0 |
| 2 | CB | 57 | PHE | 2.0 |
| 9 | CI | 33 | PHE | 2.0 |
| 16 | AP | 59 | TRP | 2.0 |
| 23 | BA | 276 | A | 2.0 |
| 8 | CH | 95 | VAL | 2.0 |
| 23 | DA | 352 | G | 2.0 |
| 13 | CM | 110 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1209 | C | 2.0 |
| 10 | AJ | 6 | ILE | 2.0 |
| 23 | DA | 2175 | C | 2.0 |
| 2 | CB | 146 | GLN | 2.0 |
| 7 | AG | 122 | HIS | 2.0 |
| 10 | CJ | 47 | PHE | 2.0 |
| 22 | AX | 55 | HIS | 2.0 |
| 26 | BE | 195 | LEU | 2.0 |
| 9 | AI | 12 | GLU | 2.0 |
| 7 | CG | 20 | ASP | 2.0 |
| 1 | AA | 950 | U | 2.0 |
| 1 | CA | 1257 | U | 2.0 |
| 3 | CC | 184 | TYR | 2.0 |
| 9 | AI | 36 | TYR | 2.0 |
| 13 | CM | 15 | VAL | 2.0 |
| 2 | AB | 28 | PHE | 2.0 |
| 4 | CD | 29 | PRO | 2.0 |
| 1 | AA | 1044 | A | 2.0 |
| 53 | D9 | 12 | ASP | 2.0 |
| 1 | CA | 1338 | G | 2.0 |
| 2 | CB | 207 | ALA | 2.0 |
| 28 | DG | 148 | MET | 2.0 |
| 4 | AD | 110 | PHE | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | DA | 3276 | 1/1 | 0.86 | 0.86 | 73.60 | 60,60,60,60 | 0 |
| 54 | MG | DA | 3231 | 1/1 | 0.89 | 0.29 | 42.16 | 36,36,36,36 | 0 |
| 54 | MG | CA | 1645 | 1/1 | 0.85 | 0.93 | 38.10 | 60,60,60,60 | 0 |
| 54 | MG | BA | 3419 | 1/1 | 0.98 | 0.40 | 36.54 | 21,21,21,21 | 0 |
| 54 | MG | AA | 1659 | 1/1 | 0.73 | 0.86 | 34.62 | 70,70,70,70 | 0 |
| 54 | MG | BA | 3248 | 1/1 | 0.97 | 0.41 | 33.56 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3162 | 1/1 | 0.92 | 0.36 | 32.54 | 35,35,35,35 | 0 |
| 54 | MG | BE | 301 | 1/1 | 0.91 | 0.43 | 32.35 | 34,34,34,34 | 0 |
| 54 | MG | BA | 3061 | 1/1 | 0.83 | 0.47 | 29.24 | 54,54,54,54 | 0 |
| 54 | MG | DA | 3224 | 1/1 | 0.94 | 0.37 | 25.92 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3257 | 1/1 | 0.93 | 0.41 | 24.73 | 23,23,23,23 | 0 |
| 54 | MG | DA | 3302 | 1/1 | 0.96 | 0.51 | 24.51 | 21,21,21,21 | 0 |
| 54 | MG | DA | 3242 | 1/1 | 0.98 | 0.56 | 24.45 | 34,34,34,34 | 0 |
| 54 | MG | AA | 1639 | 1/1 | 0.95 | 0.45 | 23.79 | 67,67,67,67 | 0 |
| 54 | MG | BA | 3105 | 1/1 | 0.93 | 0.36 | 23.11 | 28,28,28,28 | 0 |
| 54 | MG | DA | 3244 | 1/1 | 0.92 | 0.52 | 22.96 | 33,33,33,33 | 0 |
| 54 | MG | BA | 3270 | 1/1 | 0.99 | 0.45 | 22.93 | 25,25,25,25 | 0 |
| 54 | MG | BA | 3172 | 1/1 | 0.94 | 0.38 | 22.88 | 47,47,47,47 | 0 |
| 54 | MG | DA | 3164 | 1/1 | 0.66 | 0.39 | 22.48 | 56,56,56,56 | 0 |
| 54 | MG | AA | 1668 | 1/1 | 0.94 | 0.57 | 22.20 | 62,62,62,62 | 0 |
| 54 | MG | DA | 3196 | 1/1 | 0.79 | 0.39 | 22.19 | 58,58,58,58 | 0 |
| 54 | MG | DA | 3125 | 1/1 | 0.89 | 0.30 | 22.07 | 50,50,50,50 | 0 |
| 54 | MG | BA | 3129 | 1/1 | 0.94 | 0.37 | 21.26 | 37,37,37,37 | 0 |
| 54 | MG | DA | 3157 | 1/1 | 0.96 | 0.35 | 20.74 | 44,44,44,44 | 0 |
| 54 | MG | BA | 3253 | 1/1 | 0.95 | 0.44 | 20.69 | 19,19,19,19 | 0 |
| 54 | MG | DA | 3096 | 1/1 | 0.78 | 0.53 | 20.46 | 59,59,59,59 | 0 |
| 54 | MG | DA | 3266 | 1/1 | 0.92 | 0.32 | 20.04 | 47,47,47,47 | 0 |
| 54 | MG | BA | 3167 | 1/1 | 0.96 | 0.45 | 18.93 | 31,31,31,31 | 0 |
| 54 | MG | DA | 3008 | 1/1 | 0.91 | 0.45 | 18.67 | 58,58,58,58 | 0 |
| 54 | MG | DA | 3303 | 1/1 | 0.96 | 0.48 | 18.49 | 34,34,34,34 | 0 |
| 54 | MG | BA | 3246 | 1/1 | 0.95 | 0.47 | 18.15 | 20,20,20,20 | 0 |
| 54 | MG | BA | 3109 | 1/1 | 0.79 | 0.41 | 18.00 | 62,62,62,62 | 0 |
| 54 | MG | DA | 3272 | 1/1 | 0.93 | 0.38 | 17.80 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3183 | 1/1 | 0.96 | 0.46 | 17.16 | 26,26,26,26 | 0 |
| 54 | MG | DA | 3069 | 1/1 | 0.94 | 0.39 | 15.99 | 42,42,42,42 | 0 |
| 54 | MG | BA | 3279 | 1/1 | 0.86 | 0.49 | 15.69 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3373 | 1/1 | 0.97 | 0.27 | 15.67 | 32,32,32,32 | 0 |
| 54 | MG | DA | 3133 | 1/1 | 0.93 | 0.38 | 15.60 | 36,36,36,36 | 0 |
| 54 | MG | BA | 3284 | 1/1 | 0.97 | 0.37 | 15.52 | 24,24,24,24 | 0 |
| 54 | MG | DA | 3221 | 1/1 | 0.87 | 0.47 | 15.47 | 51,51,51,51 | 0 |
| 54 | MG | CA | 1689 | 1/1 | 0.96 | 0.38 | 15.32 | 61,61,61,61 | 0 |
| 54 | MG | AA | 1660 | 1/1 | 0.92 | 0.52 | 14.78 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | BA | 3590 | 1/1 | 0.90 | 0.31 | 14.58 | 31,31,31,31 | 0 |
| 54 | MG | AA | 1650 | 1/1 | 0.98 | 0.55 | 14.34 | 53,53,53,53 | 0 |
| 54 | MG | DA | 3041 | 1/1 | 0.96 | 0.51 | 14.14 | 36,36,36,36 | 0 |
| 54 | MG | AA | 1671 | 1/1 | 0.81 | 0.35 | 14.07 | 67,67,67,67 | 0 |
| 54 | MG | BA | 3069 | 1/1 | 0.96 | 0.36 | 13.83 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3205 | 1/1 | 0.96 | 0.28 | 13.48 | 47,47,47,47 | 0 |
| 54 | MG | BA | 3247 | 1/1 | 0.96 | 0.47 | 12.80 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3250 | 1/1 | 0.93 | 0.40 | 12.73 | 26,26,26,26 | 0 |
| 54 | MG | AA | 1672 | 1/1 | 0.96 | 0.42 | 12.71 | 46,46,46,46 | 0 |
| 54 | MG | DA | 3092 | 1/1 | 0.89 | 0.32 | 12.47 | 41,41,41,41 | 0 |
| 54 | MG | DA | 3311 | 1/1 | 0.95 | 0.36 | 12.29 | 26,26,26,26 | 0 |
| 54 | MG | DA | 3345 | 1/1 | 0.98 | 0.31 | 12.19 | 54,54,54,54 | 0 |
| 54 | MG | BA | 3127 | 1/1 | 0.96 | 0.28 | 12.17 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3157 | 1/1 | 0.95 | 0.30 | 12.13 | 48,48,48,48 | 0 |
| 54 | MG | DA | 3131 | 1/1 | 0.95 | 0.32 | 11.92 | 56,56,56,56 | 0 |
| 54 | MG | BA | 3262 | 1/1 | 0.91 | 0.37 | 11.86 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3309 | 1/1 | 0.84 | 0.40 | 11.84 | 28,28,28,28 | 0 |
| 54 | MG | DA | 3130 | 1/1 | 0.85 | 0.33 | 11.84 | 47,47,47,47 | 0 |
| 54 | MG | BA | 3282 | 1/1 | 0.97 | 0.34 | 11.64 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3150 | 1/1 | 0.96 | 0.33 | 11.48 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3197 | 1/1 | 0.84 | 0.34 | 11.37 | 49,49,49,49 | 0 |
| 54 | MG | DA | 3304 | 1/1 | 0.94 | 0.42 | 11.29 | 29,29,29,29 | 0 |
| 54 | MG | AA | 1610 | 1/1 | 0.96 | 0.41 | 11.17 | 56,56,56,56 | 0 |
| 54 | MG | DA | 3029 | 1/1 | 0.88 | 0.31 | 11.16 | 40,40,40,40 | 0 |
| 54 | MG | DA | 3178 | 1/1 | 0.95 | 0.33 | 10.96 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3249 | 1/1 | 0.94 | 0.35 | 10.93 | 25,25,25,25 | 0 |
| 54 | MG | BA | 3256 | 1/1 | 0.93 | 0.34 | 10.91 | 23,23,23,23 | 0 |
| 54 | MG | DA | 3163 | 1/1 | 0.89 | 0.39 | 10.83 | 30,30,30,30 | 0 |
| 54 | MG | DR | 202 | 1/1 | 0.92 | 0.37 | 10.78 | 34,34,34,34 | 0 |
| 54 | MG | BD | 301 | 1/1 | 0.93 | 0.45 | 10.75 | 49,49,49,49 | 0 |
| 54 | MG | DA | 3321 | 1/1 | 0.90 | 0.42 | 10.70 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3232 | 1/1 | 0.96 | 0.32 | 10.52 | 57,57,57,57 | 0 |
| 54 | MG | BA | 3102 | 1/1 | 0.80 | 0.34 | 10.40 | 44,44,44,44 | 0 |
| 54 | MG | DA | 3305 | 1/1 | 0.92 | 0.23 | 10.25 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3255 | 1/1 | 0.95 | 0.31 | 10.16 | 25,25,25,25 | 0 |
| 54 | MG | DA | 3337 | 1/1 | 0.97 | 0.29 | 10.00 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3257 | 1/1 | 0.84 | 0.32 | 9.76 | 56,56,56,56 | 0 |
| 54 | MG | BA | 3011 | 1/1 | 0.91 | 0.29 | 9.69 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3278 | 1/1 | 0.96 | 0.38 | 9.69 | 30,30,30,30 | 0 |
| 54 | MG | BA | 3188 | 1/1 | 0.99 | 0.27 | 9.66 | 39,39,39,39 | 0 |
| 54 | MG | AA | 1684 | 1/1 | 0.87 | 0.83 | 9.61 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BB | 212 | 1/1 | 0.91 | 0.27 | 9.60 | 60,60,60,60 | 0 |
| 54 | MG | BA | 3259 | 1/1 | 0.97 | 0.34 | 9.42 | 27,27,27,27 | 0 |
| 54 | MG | BA | 3064 | 1/1 | 0.97 | 0.24 | 9.32 | 34,34,34,34 | 0 |
| 54 | MG | CA | 1685 | 1/1 | 0.94 | 0.34 | 9.29 | 71,71,71,71 | 0 |
| 54 | MG | DA | 3293 | 1/1 | 0.94 | 0.25 | 9.22 | 33,33,33,33 | 0 |
| 54 | MG | AA | 1618 | 1/1 | 0.74 | 1.13 | 9.18 | 94,94,94,94 | 0 |
| 54 | MG | BA | 3473 | 1/1 | 0.94 | 0.23 | 9.07 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3006 | 1/1 | 0.96 | 0.29 | 8.83 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3574 | 1/1 | 0.93 | 0.31 | 8.67 | 33,33,33,33 | 0 |
| 54 | MG | DA | 3042 | 1/1 | 0.93 | 0.23 | 8.35 | 33,33,33,33 | 0 |
| 54 | MG | CA | 1749 | 1/1 | 0.97 | 0.23 | 8.32 | 61,61,61,61 | 0 |
| 54 | MG | AA | 1712 | 1/1 | 0.85 | 0.34 | 8.30 | 86,86,86,86 | 0 |
| 54 | MG | CA | 1611 | 1/1 | 0.93 | 0.22 | 8.25 | 43,43,43,43 | 0 |
| 54 | MG | AA | 1711 | 1/1 | 0.96 | 0.24 | 8.06 | 46,46,46,46 | 0 |
| 54 | MG | DA | 3308 | 1/1 | 0.86 | 0.31 | 7.93 | 33,33,33,33 | 0 |
| 54 | MG | AA | 1633 | 1/1 | 0.92 | 0.28 | 7.93 | 62,62,62,62 | 0 |
| 54 | MG | BA | 3189 | 1/1 | 0.94 | 0.32 | 7.92 | 41,41,41,41 | 0 |
| 54 | MG | BA | 3264 | 1/1 | 0.77 | 0.38 | 7.91 | 41,41,41,41 | 0 |
| 54 | MG | CA | 1741 | 1/1 | 0.97 | 0.32 | 7.80 | 79,79,79,79 | 0 |
| 54 | MG | DA | 3307 | 1/1 | 0.96 | 0.22 | 7.64 | 35,35,35,35 | 0 |
| 54 | MG | DR | 203 | 1/1 | 0.86 | 0.51 | 7.57 | 51,51,51,51 | 0 |
| 54 | MG | BA | 3273 | 1/1 | 0.94 | 0.40 | 7.37 | 37,37,37,37 | 0 |
| 54 | MG | DA | 3229 | 1/1 | 0.90 | 0.30 | 7.16 | 44,44,44,44 | 0 |
| 54 | MG | BA | 3245 | 1/1 | 0.95 | 0.34 | 7.08 | 23,23,23,23 | 0 |
| 54 | MG | DA | 3269 | 1/1 | 0.95 | 0.29 | 7.03 | 47,47,47,47 | 0 |
| 54 | MG | DA | 3374 | 1/1 | 0.98 | 0.21 | 7.00 | 37,37,37,37 | 0 |
| 54 | MG | BA | 3042 | 1/1 | 0.96 | 0.28 | 6.81 | 40,40,40,40 | 0 |
| 54 | MG | AA | 1624 | 1/1 | 0.90 | 0.37 | 6.72 | 70,70,70,70 | 0 |
| 54 | MG | DA | 3284 | 1/1 | 0.79 | 0.22 | 6.69 | 55,55,55,55 | 0 |
| 54 | MG | DA | 3203 | 1/1 | 0.98 | 0.41 | 6.52 | 33,33,33,33 | 0 |
| 54 | MG | BA | 3467 | 1/1 | 0.97 | 0.24 | 6.52 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3382 | 1/1 | 0.92 | 0.23 | 6.46 | 53,53,53,53 | 0 |
| 54 | MG | AA | 1612 | 1/1 | 0.88 | 0.31 | 6.44 | 86,86,86,86 | 0 |
| 54 | MG | DD | 302 | 1/1 | 0.96 | 0.41 | 6.40 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3265 | 1/1 | 0.95 | 0.39 | 6.39 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3209 | 1/1 | 0.85 | 0.26 | 6.37 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3011 | 1/1 | 0.94 | 0.27 | 5.95 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3182 | 1/1 | 0.94 | 0.31 | 5.82 | 46,46,46,46 | 0 |
| 54 | MG | BA | 3050 | 1/1 | 0.93 | 0.23 | 5.76 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3154 | 1/1 | 0.91 | 0.38 | 5.71 | 50,50,50,50 | 0 |
| 54 | MG | DA | 3063 | 1/1 | 0.83 | 0.32 | 5.71 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3089 | 1/1 | 0.97 | 0.33 | 5.68 | 41,41,41,41 | 0 |
| 54 | MG | DA | 3338 | 1/1 | 0.97 | 0.22 | 5.65 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3230 | 1/1 | 0.90 | 0.21 | 5.62 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3040 | 1/1 | 0.92 | 0.34 | 5.59 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3420 | 1/1 | 0.97 | 0.22 | 5.55 | 37,37,37,37 | 0 |
| 54 | MG | DA | 3044 | 1/1 | 0.94 | 0.19 | 5.50 | 46,46,46,46 | 0 |
| 54 | MG | BA | 3065 | 1/1 | 0.88 | 0.24 | 5.41 | 41,41,41,41 | 0 |
| 54 | MG | BA | 3194 | 1/1 | 0.87 | 0.20 | 5.38 | 63,63,63,63 | 0 |
| 54 | MG | DA | 3146 | 1/1 | 0.89 | 0.18 | 5.29 | 44,44,44,44 | 0 |
| 54 | MG | DA | 3039 | 1/1 | 0.96 | 0.20 | 5.14 | 28,28,28,28 | 0 |
| 54 | MG | CQ | 201 | 1/1 | 0.91 | 0.35 | 5.13 | 62,62,62,62 | 0 |
| 54 | MG | AA | 1680 | 1/1 | 0.98 | 0.25 | 5.08 | 72,72,72,72 | 0 |
| 54 | MG | BA | 3424 | 1/1 | 0.85 | 0.21 | 5.06 | 72,72,72,72 | 0 |
| 54 | MG | DA | 3128 | 1/1 | 0.90 | 0.24 | 5.06 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3455 | 1/1 | 0.85 | 0.23 | 5.01 | 22,22,22,22 | 0 |
| 54 | MG | DA | 3040 | 1/1 | 0.93 | 0.26 | 4.96 | 48,48,48,48 | 0 |
| 54 | MG | BA | 3397 | 1/1 | 0.88 | 0.17 | 4.92 | 86,86,86,86 | 0 |
| 54 | MG | DA | 3578 | 1/1 | 0.97 | 0.22 | 4.86 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3441 | 1/1 | 0.95 | 0.26 | 4.84 | 48,48,48,48 | 0 |
| 54 | MG | DA | 3573 | 1/1 | 0.97 | 0.24 | 4.84 | 31,31,31,31 | 0 |
| 54 | MG | B3 | 101 | 1/1 | 0.94 | 0.35 | 4.80 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3353 | 1/1 | 0.85 | 0.21 | 4.65 | 61,61,61,61 | 0 |
| 54 | MG | BA | 3252 | 1/1 | 0.93 | 0.33 | 4.64 | 36,36,36,36 | 0 |
| 54 | MG | AA | 1629 | 1/1 | 0.81 | 0.29 | 4.54 | 44,44,44,44 | 0 |
| 54 | MG | AD | 302 | 1/1 | 0.84 | 0.29 | 4.53 | 77,77,77,77 | 0 |
| 54 | MG | DA | 3017 | 1/1 | 0.89 | 0.20 | 4.46 | 50,50,50,50 | 0 |
| 54 | MG | BA | 3103 | 1/1 | 0.92 | 0.20 | 4.45 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3091 | 1/1 | 0.93 | 0.18 | 4.41 | 55,55,55,55 | 0 |
| 54 | MG | DA | 3366 | 1/1 | 0.91 | 0.20 | 4.41 | 31,31,31,31 | 0 |
| 54 | MG | BA | 3026 | 1/1 | 0.89 | 0.19 | 4.38 | 52,52,52,52 | 0 |
| 54 | MG | BA | 3159 | 1/1 | 0.88 | 0.23 | 4.36 | 46,46,46,46 | 0 |
| 54 | MG | DA | 3156 | 1/1 | 0.95 | 0.20 | 4.32 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3484 | 1/1 | 0.97 | 0.18 | 4.29 | 27,27,27,27 | 0 |
| 54 | MG | AA | 1619 | 1/1 | 0.74 | 0.27 | 4.18 | 86,86,86,86 | 0 |
| 54 | MG | CA | 1607 | 1/1 | 0.89 | 0.21 | 4.17 | 50,50,50,50 | 0 |
| 54 | MG | CA | 1751 | 1/1 | 0.88 | 0.26 | 4.04 | 61,61,61,61 | 0 |
| 54 | MG | BA | 3451 | 1/1 | 0.97 | 0.21 | 4.03 | 28,28,28,28 | 0 |
| 54 | MG | BB | 206 | 1/1 | 0.83 | 0.20 | 4.00 | 57,57,57,57 | 0 |
| 54 | MG | DA | 3247 | 1/1 | 0.83 | 0.33 | 3.95 | 67,67,67,67 | 0 |
| 54 | MG | BA | 3492 | 1/1 | 0.93 | 0.21 | 3.89 | 27,27,27,27 | 0 |
| 54 | MG | BA | 3502 | 1/1 | 0.98 | 0.24 | 3.86 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3449 | 1/1 | 0.98 | 0.21 | 3.82 | 42,42,42,42 | 0 |
| 54 | MG | BA | 3337 | 1/1 | 0.60 | 0.21 | 3.76 | 49,49,49,49 | 0 |
| 54 | MG | BA | 3145 | 1/1 | 0.96 | 0.20 | 3.72 | 44,44,44,44 | 0 |
| 54 | MG | DA | 3167 | 1/1 | 0.83 | 0.21 | 3.45 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3549 | 1/1 | 0.98 | 0.20 | 3.41 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3456 | 1/1 | 0.90 | 0.22 | 3.40 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3170 | 1/1 | 0.93 | 0.22 | 3.33 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3514 | 1/1 | 0.94 | 0.19 | 3.33 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3100 | 1/1 | 0.92 | 0.22 | 3.27 | 38,38,38,38 | 0 |
| 54 | MG | DA | 3010 | 1/1 | 0.95 | 0.18 | 3.10 | 42,42,42,42 | 0 |
| 54 | MG | BA | 3031 | 1/1 | 0.94 | 0.17 | 3.10 | 44,44,44,44 | 0 |
| 54 | MG | BA | 3333 | 1/1 | 0.87 | 0.19 | 3.01 | 40,40,40,40 | 0 |
| 54 | MG | DA | 3083 | 1/1 | 0.97 | 0.23 | 2.98 | 37,37,37,37 | 0 |
| 54 | MG | BA | 3037 | 1/1 | 0.86 | 0.20 | 2.97 | 75,75,75,75 | 0 |
| 54 | MG | DA | 3052 | 1/1 | 0.97 | 0.37 | 2.95 | 52,52,52,52 | 0 |
| 54 | MG | BA | 3226 | 1/1 | 0.96 | 0.22 | 2.77 | 50,50,50,50 | 0 |
| 54 | MG | BB | 220 | 1/1 | 0.97 | 0.18 | 2.75 | 60,60,60,60 | 0 |
| 54 | MG | DA | 3570 | 1/1 | 0.98 | 0.18 | 2.71 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1613 | 1/1 | 0.90 | 0.34 | 2.63 | 66,66,66,66 | 0 |
| 54 | MG | CA | 1619 | 1/1 | 0.96 | 0.16 | 2.59 | 50,50,50,50 | 0 |
| 54 | MG | BA | 3006 | 1/1 | 0.97 | 0.19 | 2.57 | 25,25,25,25 | 0 |
| 54 | MG | BA | 3212 | 1/1 | 0.90 | 0.21 | 2.55 | 68,68,68,68 | 0 |
| 54 | MG | DA | 3123 | 1/1 | 0.91 | 0.23 | 2.55 | 53,53,53,53 | 0 |
| 54 | MG | BA | 3595 | 1/1 | 0.97 | 0.29 | 2.52 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3241 | 1/1 | 0.95 | 0.27 | 2.49 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3019 | 1/1 | 0.92 | 0.18 | 2.47 | 34,34,34,34 | 0 |
| 54 | MG | CA | 1690 | 1/1 | 0.96 | 0.25 | 2.46 | 64,64,64,64 | 0 |
| 54 | MG | DB | 201 | 1/1 | 0.98 | 0.14 | 2.41 | 43,43,43,43 | 0 |
| 54 | MG | BA | 3130 | 1/1 | 0.96 | 0.23 | 2.40 | 43,43,43,43 | 0 |
| 54 | MG | BA | 3251 | 1/1 | 0.95 | 0.25 | 2.35 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3014 | 1/1 | 0.97 | 0.19 | 2.33 | 31,31,31,31 | 0 |
| 54 | MG | DA | 3491 | 1/1 | 0.94 | 0.19 | 2.31 | 44,44,44,44 | 0 |
| 54 | MG | DF | 301 | 1/1 | 0.90 | 0.30 | 2.26 | 50,50,50,50 | 0 |
| 54 | MG | BA | 3046 | 1/1 | 0.90 | 0.18 | 2.25 | 36,36,36,36 | 0 |
| 54 | MG | DA | 3219 | 1/1 | 0.95 | 0.16 | 2.14 | 38,38,38,38 | 0 |
| 54 | MG | DA | 3473 | 1/1 | 0.94 | 0.21 | 2.12 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3368 | 1/1 | 0.78 | 0.21 | 2.09 | 53,53,53,53 | 0 |
| 54 | MG | DA | 3414 | 1/1 | 0.94 | 0.17 | 2.08 | 51,51,51,51 | 0 |
| 54 | MG | BA | 3015 | 1/1 | 0.89 | 0.18 | 2.04 | 48,48,48,48 | 0 |
| 54 | MG | DA | 3397 | 1/1 | 0.85 | 0.19 | 1.98 | 34,34,34,34 | 0 |
| 54 | MG | DA | 3243 | 1/1 | 0.97 | 0.22 | 1.98 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3389 | 1/1 | 0.95 | 0.18 | 1.93 | 46,46,46,46 | 0 |
| 54 | MG | DA | 3396 | 1/1 | 0.96 | 0.17 | 1.93 | 52,52,52,52 | 0 |
| 54 | MG | DA | 3496 | 1/1 | 0.97 | 0.20 | 1.90 | 66,66,66,66 | 0 |
| 54 | MG | CA | 1665 | 1/1 | 0.88 | 0.22 | 1.87 | 84,84,84,84 | 0 |
| 54 | MG | BA | 3328 | 1/1 | 0.98 | 0.20 | 1.87 | 30,30,30,30 | 0 |
| 54 | MG | BA | 3482 | 1/1 | 0.90 | 0.19 | 1.85 | 27,27,27,27 | 0 |
| 54 | MG | BA | 3500 | 1/1 | 0.98 | 0.17 | 1.84 | 44,44,44,44 | 0 |
| 54 | MG | DA | 3022 | 1/1 | 0.92 | 0.16 | 1.81 | 34,34,34,34 | 0 |
| 54 | MG | BA | 3001 | 1/1 | 0.91 | 0.21 | 1.79 | 43,43,43,43 | 0 |
| 54 | MG | BA | 3083 | 1/1 | 0.92 | 0.18 | 1.77 | 43,43,43,43 | 0 |
| 54 | MG | DA | 3248 | 1/1 | 0.90 | 0.18 | 1.75 | 42,42,42,42 | 0 |
| 54 | MG | CA | 1680 | 1/1 | 0.90 | 0.23 | 1.74 | 78,78,78,78 | 0 |
| 54 | MG | BA | 3010 | 1/1 | 0.90 | 0.22 | 1.62 | 39,39,39,39 | 0 |
| 54 | MG | BA | 3558 | 1/1 | 0.98 | 0.19 | 1.58 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1729 | 1/1 | 0.90 | 0.17 | 1.56 | 81,81,81,81 | 0 |
| 54 | MG | DA | 3471 | 1/1 | 0.97 | 0.19 | 1.54 | 31,31,31,31 | 0 |
| 54 | MG | BA | 3225 | 1/1 | 0.84 | 0.18 | 1.50 | 44,44,44,44 | 0 |
| 54 | MG | BA | 3161 | 1/1 | 0.93 | 0.18 | 1.50 | 40,40,40,40 | 0 |
| 54 | MG | BA | 3360 | 1/1 | 0.97 | 0.23 | 1.46 | 35,35,35,35 | 0 |
| 54 | MG | DA | 3007 | 1/1 | 0.95 | 0.14 | 1.43 | 48,48,48,48 | 0 |
| 54 | MG | DA | 3223 | 1/1 | 0.86 | 0.18 | 1.37 | 54,54,54,54 | 0 |
| 54 | MG | BA | 3155 | 1/1 | 0.94 | 0.19 | 1.34 | 41,41,41,41 | 0 |
| 54 | MG | DA | 3216 | 1/1 | 0.94 | 0.15 | 1.32 | 51,51,51,51 | 0 |
| 54 | MG | BA | 3384 | 1/1 | 0.95 | 0.14 | 1.32 | 88,88,88,88 | 0 |
| 54 | MG | D1 | 101 | 1/1 | 0.98 | 0.22 | 1.24 | 38,38,38,38 | 0 |
| 54 | MG | DE | 301 | 1/1 | 0.88 | 0.22 | 1.21 | 41,41,41,41 | 0 |
| 54 | MG | CA | 1726 | 1/1 | 0.97 | 0.18 | 1.15 | 52,52,52,52 | 0 |
| 54 | MG | AA | 1607 | 1/1 | 0.76 | 0.18 | 1.14 | 78,78,78,78 | 0 |
| 54 | MG | BA | 3030 | 1/1 | 0.89 | 0.20 | 1.09 | 48,48,48,48 | 0 |
| 54 | MG | BA | 3052 | 1/1 | 0.95 | 0.17 | 1.07 | 52,52,52,52 | 0 |
| 54 | MG | BA | 3039 | 1/1 | 0.91 | 0.20 | 0.97 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3471 | 1/1 | 0.89 | 0.18 | 0.94 | 27,27,27,27 | 0 |
| 54 | MG | AA | 1725 | 1/1 | 0.95 | 0.20 | 0.85 | 56,56,56,56 | 0 |
| 54 | MG | BA | 3200 | 1/1 | 0.98 | 0.18 | 0.80 | 31,31,31,31 | 0 |
| 54 | MG | BA | 3378 | 1/1 | 0.95 | 0.16 | 0.74 | 25,25,25,25 | 0 |
| 54 | MG | DA | 3417 | 1/1 | 0.87 | 0.16 | 0.69 | 31,31,31,31 | 0 |
| 54 | MG | BA | 3583 | 1/1 | 0.93 | 0.15 | 0.58 | 34,34,34,34 | 0 |
| 54 | MG | DA | 3363 | 1/1 | 0.98 | 0.18 | 0.52 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3067 | 1/1 | 0.92 | 0.18 | 0.51 | 43,43,43,43 | 0 |
| 54 | MG | CA | 1703 | 1/1 | 0.94 | 0.18 | 0.50 | 56,56,56,56 | 0 |
| 54 | MG | D8 | 102 | 1/1 | 0.85 | 0.28 | 0.49 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3338 | 1/1 | 0.77 | 0.15 | 0.40 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | DA | 3169 | 1/1 | 0.91 | 0.16 | 0.32 | 45,45,45,45 | 0 |
| 54 | MG | DA | 3487 | 1/1 | 0.89 | 0.17 | 0.31 | 48,48,48,48 | 0 |
| 54 | MG | BA | 3468 | 1/1 | 0.91 | 0.18 | 0.31 | 24,24,24,24 | 0 |
| 54 | MG | CA | 1728 | 1/1 | 0.97 | 0.16 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | BA | 3314 | 1/1 | 0.95 | 0.17 | 0.14 | 37,37,37,37 | 0 |
| 54 | MG | BG | 201 | 1/1 | 0.85 | 0.21 | 0.07 | 60,60,60,60 | 0 |
| 54 | MG | CA | 1612 | 1/1 | 0.88 | 0.14 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | BA | 3385 | 1/1 | 0.85 | 0.15 | 0.03 | 63,63,63,63 | 0 |
| 54 | MG | B8 | 101 | 1/1 | 0.99 | 0.21 | 0.02 | 51,51,51,51 | 0 |
| 54 | MG | BA | 3190 | 1/1 | 0.99 | 0.17 | -0.02 | 27,27,27,27 | 0 |
| 54 | MG | DA | 3555 | 1/1 | 0.93 | 0.14 | -0.03 | 56,56,56,56 | 0 |
| 54 | MG | DA | 3563 | 1/1 | 0.87 | 0.15 | -0.03 | 70,70,70,70 | 0 |
| 54 | MG | BB | 202 | 1/1 | 0.92 | 0.12 | -0.04 | 43,43,43,43 | 0 |
| 54 | MG | DA | 3477 | 1/1 | 0.94 | 0.15 | -0.06 | 53,53,53,53 | 0 |
| 54 | MG | BA | 3457 | 1/1 | 0.95 | 0.19 | -0.06 | 27,27,27,27 | 0 |
| 55 | ZN | AD | 301 | 1/1 | 0.96 | 0.28 | -0.06 | 74,74,74,74 | 0 |
| 54 | MG | BA | 3323 | 1/1 | 0.90 | 0.17 | -0.07 | 23,23,23,23 | 0 |
| 54 | MG | BA | 3027 | 1/1 | 0.93 | 0.15 | -0.08 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3205 | 1/1 | 0.89 | 0.12 | -0.09 | 54,54,54,54 | 0 |
| 54 | MG | DA | 3404 | 1/1 | 0.98 | 0.14 | -0.09 | 36,36,36,36 | 0 |
| 54 | MG | DA | 3562 | 1/1 | 0.97 | 0.14 | -0.12 | 58,58,58,58 | 0 |
| 54 | MG | CA | 1737 | 1/1 | 0.93 | 0.13 | -0.15 | 89,89,89,89 | 0 |
| 54 | MG | DA | 3333 | 1/1 | 0.93 | 0.15 | -0.17 | 37,37,37,37 | 0 |
| 54 | MG | DA | 3568 | 1/1 | 0.94 | 0.11 | -0.18 | 78,78,78,78 | 0 |
| 54 | MG | BA | 3369 | 1/1 | 0.71 | 0.13 | -0.22 | 52,52,52,52 | 0 |
| 54 | MG | DA | 3418 | 1/1 | 0.98 | 0.15 | -0.25 | 31,31,31,31 | 0 |
| 55 | ZN | CD | 301 | 1/1 | 0.93 | 0.26 | -0.29 | 71,71,71,71 | 0 |
| 54 | MG | DA | 3375 | 1/1 | 0.93 | 0.14 | -0.29 | 31,31,31,31 | 0 |
| 54 | MG | BD | 303 | 1/1 | 0.96 | 0.18 | -0.32 | 35,35,35,35 | 0 |
| 54 | MG | DA | 3090 | 1/1 | 0.89 | 0.11 | -0.34 | 53,53,53,53 | 0 |
| 54 | MG | D8 | 101 | 1/1 | 0.94 | 0.15 | -0.35 | 48,48,48,48 | 0 |
| 54 | MG | BA | 3327 | 1/1 | 0.99 | 0.18 | -0.35 | 23,23,23,23 | 0 |
| 54 | MG | BA | 3458 | 1/1 | 0.92 | 0.17 | -0.37 | 35,35,35,35 | 0 |
| 54 | MG | DA | 3434 | 1/1 | 0.85 | 0.14 | -0.39 | 60,60,60,60 | 0 |
| 54 | MG | DA | 3047 | 1/1 | 0.94 | 0.15 | -0.40 | 38,38,38,38 | 0 |
| 54 | MG | CA | 1655 | 1/1 | 0.93 | 0.22 | -0.45 | 98,98,98,98 | 0 |
| 54 | MG | DA | 3015 | 1/1 | 0.93 | 0.13 | -0.47 | 38,38,38,38 | 0 |
| 55 | ZN | BY | 201 | 1/1 | 0.92 | 0.11 | -0.52 | 69,69,69,69 | 0 |
| 54 | MG | DA | 3558 | 1/1 | 0.93 | 0.15 | -0.55 | 36,36,36,36 | 0 |
| 54 | MG | BA | 3599 | 1/1 | 0.97 | 0.17 | -0.55 | 30,30,30,30 | 0 |
| 54 | MG | CA | 1709 | 1/1 | 0.96 | 0.13 | -0.56 | 63,63,63,63 | 0 |
| 54 | MG | BA | 3425 | 1/1 | 0.91 | 0.15 | -0.56 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | DA | 3051 | 1/1 | 0.95 | 0.14 | -0.57 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3445 | 1/1 | 0.96 | 0.17 | -0.59 | 31,31,31,31 | 0 |
| 54 | MG | BB | 215 | 1/1 | 0.90 | 0.17 | -0.62 | 65,65,65,65 | 0 |
| 54 | MG | BA | 3028 | 1/1 | 0.95 | 0.15 | -0.62 | 22,22,22,22 | 0 |
| 54 | MG | BA | 3227 | 1/1 | 0.97 | 0.14 | -0.62 | 32,32,32,32 | 0 |
| 54 | MG | DA | 3550 | 1/1 | 0.93 | 0.13 | -0.67 | 58,58,58,58 | 0 |
| 54 | MG | BA | 3481 | 1/1 | 0.94 | 0.16 | -0.67 | 25,25,25,25 | 0 |
| 54 | MG | DA | 3452 | 1/1 | 0.87 | 0.10 | -0.68 | 90,90,90,90 | 0 |
| 54 | MG | DA | 3393 | 1/1 | 0.95 | 0.14 | -0.77 | 41,41,41,41 | 0 |
| 55 | ZN | B6 | 101 | 1/1 | 0.99 | 0.11 | -0.80 | 48,48,48,48 | 0 |
| 54 | MG | CA | 1718 | 1/1 | 0.91 | 0.15 | -0.84 | 83,83,83,83 | 0 |
| 54 | MG | BA | 3487 | 1/1 | 0.96 | 0.15 | -0.85 | 20,20,20,20 | 0 |
| 54 | MG | BA | 3466 | 1/1 | 0.98 | 0.16 | -0.85 | 39,39,39,39 | 0 |
| 54 | MG | DA | 3450 | 1/1 | 0.93 | 0.10 | -0.95 | 67,67,67,67 | 0 |
| 54 | MG | DA | 3364 | 1/1 | 0.87 | 0.13 | -0.98 | 32,32,32,32 | 0 |
| 54 | MG | AA | 1702 | 1/1 | 0.76 | 0.16 | -0.98 | 68,68,68,68 | 0 |
| 54 | MG | BA | 3358 | 1/1 | 0.81 | 0.12 | -1.00 | 55,55,55,55 | 0 |
| 54 | MG | BA | 3511 | 1/1 | 0.97 | 0.15 | -1.03 | 32,32,32,32 | 0 |
| 54 | MG | DA | 3045 | 1/1 | 0.95 | 0.12 | -1.04 | 38,38,38,38 | 0 |
| 54 | MG | DA | 3444 | 1/1 | 0.92 | 0.14 | -1.07 | 41,41,41,41 | 0 |
| 54 | MG | BA | 3435 | 1/1 | 0.94 | 0.15 | -1.07 | 48,48,48,48 | 0 |
| 54 | MG | AA | 1631 | 1/1 | 0.95 | 0.16 | -1.08 | 41,41,41,41 | 0 |
| 54 | MG | BA | 3366 | 1/1 | 0.84 | 0.15 | -1.12 | 83,83,83,83 | 0 |
| 55 | ZN | B4 | 101 | 1/1 | 0.87 | 0.07 | -1.13 | 199,199,199,199 | 0 |
| 55 | ZN | AN | 101 | 1/1 | 0.85 | 0.12 | -1.13 | 117,117,117,117 | 0 |
| 55 | ZN | D5 | 102 | 1/1 | 0.98 | 0.08 | -1.15 | 69,69,69,69 | 0 |
| 54 | MG | CA | 1750 | 1/1 | 0.91 | 0.11 | -1.15 | 78,78,78,78 | 0 |
| 54 | MG | DA | 3513 | 1/1 | 0.92 | 0.14 | -1.16 | 34,34,34,34 | 0 |
| 55 | ZN | D6 | 101 | 1/1 | 0.98 | 0.07 | -1.17 | 63,63,63,63 | 0 |
| 54 | MG | DA | 3376 | 1/1 | 0.97 | 0.14 | -1.20 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3476 | 1/1 | 0.82 | 0.13 | -1.22 | 66,66,66,66 | 0 |
| 54 | MG | DA | 3043 | 1/1 | 0.96 | 0.10 | -1.23 | 54,54,54,54 | 0 |
| 54 | MG | DA | 3564 | 1/1 | 0.95 | 0.10 | -1.24 | 61,61,61,61 | 0 |
| 54 | MG | BA | 3271 | 1/1 | 0.97 | 0.14 | -1.26 | 30,30,30,30 | 0 |
| 54 | MG | BA | 3218 | 1/1 | 0.90 | 0.15 | -1.29 | 55,55,55,55 | 0 |
| 55 | ZN | B5 | 101 | 1/1 | 0.99 | 0.09 | -1.34 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3475 | 1/1 | 0.98 | 0.14 | -1.34 | 39,39,39,39 | 0 |
| 54 | MG | BA | 3585 | 1/1 | 0.91 | 0.10 | -1.37 | 52,52,52,52 | 0 |
| 54 | MG | BE | 303 | 1/1 | 0.97 | 0.13 | -1.38 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3331 | 1/1 | 0.92 | 0.15 | -1.39 | 48,48,48,48 | 0 |
| 54 | MG | DA | 3053 | 1/1 | 0.95 | 0.14 | -1.45 | 40,40,40,40 | 0 |
| 54 | MG | DA | 3511 | 1/1 | 0.95 | 0.09 | -1.46 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 55 | ZN | D4 | 101 | 1/1 | 0.58 | 0.08 | -1.48 | 214,214,214,214 | 0 |
| 54 | MG | DA | 3352 | 1/1 | 0.92 | 0.11 | -1.48 | 33,33,33,33 | 0 |
| 54 | MG | AA | 1728 | 1/1 | 0.96 | 0.12 | -1.49 | 53,53,53,53 | 0 |
| 54 | MG | BA | 3036 | 1/1 | 0.94 | 0.13 | -1.50 | 36,36,36,36 | 0 |
| 54 | MG | BA | 3631 | 1/1 | 0.99 | 0.16 | -1.50 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3462 | 1/1 | 0.84 | 0.09 | -1.50 | 43,43,43,43 | 0 |
| 55 | ZN | B9 | 101 | 1/1 | 0.99 | 0.08 | -1.53 | 50,50,50,50 | 0 |
| 54 | MG | DA | 3540 | 1/1 | 0.95 | 0.10 | -1.54 | 53,53,53,53 | 0 |
| 54 | MG | DA | 3378 | 1/1 | 0.92 | 0.15 | -1.59 | 33,33,33,33 | 0 |
| 54 | MG | BA | 3380 | 1/1 | 0.98 | 0.14 | -1.61 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3414 | 1/1 | 0.86 | 0.12 | -1.61 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3160 | 1/1 | 0.96 | 0.09 | -1.61 | 42,42,42,42 | 0 |
| 54 | MG | BA | 3514 | 1/1 | 0.87 | 0.12 | -1.62 | 61,61,61,61 | 0 |
| 54 | MG | BB | 201 | 1/1 | 0.95 | 0.12 | -1.63 | 57,57,57,57 | 0 |
| 54 | MG | BA | 3433 | 1/1 | 0.93 | 0.09 | -1.70 | 55,55,55,55 | 0 |
| 54 | MG | DA | 3370 | 1/1 | 0.88 | 0.10 | -1.70 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3231 | 1/1 | 0.90 | 0.11 | -1.75 | 47,47,47,47 | 0 |
| 54 | MG | BA | 3446 | 1/1 | 0.94 | 0.15 | -1.78 | 30,30,30,30 | 0 |
| 54 | MG | BA | 3401 | 1/1 | 0.93 | 0.14 | -1.80 | 58,58,58,58 | 0 |
| 54 | MG | BA | 3332 | 1/1 | 0.90 | 0.09 | -1.88 | 50,50,50,50 | 0 |
| 54 | MG | DA | 3137 | 1/1 | 0.93 | 0.11 | -1.89 | 38,38,38,38 | 0 |
| 54 | MG | BA | 3033 | 1/1 | 0.95 | 0.10 | -1.89 | 36,36,36,36 | 0 |
| 54 | MG | BA | 3132 | 1/1 | 0.92 | 0.12 | -1.92 | 33,33,33,33 | 0 |
| 55 | ZN | D9 | 101 | 1/1 | 0.95 | 0.06 | -1.97 | 65,65,65,65 | 0 |
| 55 | ZN | CN | 101 | 1/1 | 0.97 | 0.08 | -2.00 | 107,107,107,107 | 0 |
| 54 | MG | BA | 3495 | 1/1 | 0.94 | 0.13 | -2.05 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3480 | 1/1 | 0.97 | 0.13 | -2.14 | 31,31,31,31 | 0 |
| 54 | MG | BA | 3444 | 1/1 | 0.93 | 0.11 | -2.20 | 53,53,53,53 | 0 |
| 54 | MG | BA | 3158 | 1/1 | 0.98 | 0.09 | -2.20 | 40,40,40,40 | 0 |
| 54 | MG | BA | 3448 | 1/1 | 0.87 | 0.15 | -2.20 | 38,38,38,38 | 0 |
| 54 | MG | AA | 1709 | 1/1 | 0.72 | 0.15 | -2.23 | 101,101,101,101 | 0 |
| 54 | MG | BA | 3538 | 1/1 | 0.93 | 0.10 | -2.33 | 66,66,66,66 | 0 |
| 54 | MG | B8 | 102 | 1/1 | 0.94 | 0.10 | -2.35 | 61,61,61,61 | 0 |
| 54 | MG | DA | 3358 | 1/1 | 0.84 | 0.12 | -2.37 | 39,39,39,39 | 0 |
| 54 | MG | DA | 3502 | 1/1 | 0.98 | 0.11 | -2.37 | 37,37,37,37 | 0 |
| 54 | MG | CA | 1722 | 1/1 | 0.98 | 0.08 | -2.39 | 71,71,71,71 | 0 |
| 54 | MG | BA | 3508 | 1/1 | 0.96 | 0.14 | -2.39 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3419 | 1/1 | 0.91 | 0.11 | -2.40 | 44,44,44,44 | 0 |
| 54 | MG | AA | 1634 | 1/1 | 0.91 | 0.10 | -2.48 | 56,56,56,56 | 0 |
| 54 | MG | AA | 1691 | 1/1 | 0.96 | 0.12 | -2.48 | 43,43,43,43 | 0 |
| 54 | MG | DA | 3403 | 1/1 | 0.99 | 0.07 | -2.51 | 34,34,34,34 | 0 |
| 54 | MG | B9 | 102 | 1/1 | 0.96 | 0.12 | -2.56 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | AA | 1662 | 1/1 | 0.94 | 0.12 | -2.58 | 58,58,58,58 | 0 |
| 54 | MG | DA | 3362 | 1/1 | 0.96 | 0.10 | -2.62 | 26,26,26,26 | 0 |
| 54 | MG | DA | 3068 | 1/1 | 0.98 | 0.12 | -2.63 | 33,33,33,33 | 0 |
| 54 | MG | DA | 3469 | 1/1 | 0.93 | 0.07 | -2.63 | 56,56,56,56 | 0 |
| 54 | MG | DA | 3421 | 1/1 | 0.90 | 0.10 | -2.64 | 93,93,93,93 | 0 |
| 54 | MG | AA | 1701 | 1/1 | 0.96 | 0.12 | -2.72 | 48,48,48,48 | 0 |
| 54 | MG | AA | 1694 | 1/1 | 0.94 | 0.08 | -2.73 | 80,80,80,80 | 0 |
| 54 | MG | CA | 1700 | 1/1 | 0.91 | 0.09 | -2.77 | 70,70,70,70 | 0 |
| 54 | MG | BA | 3464 | 1/1 | 0.97 | 0.11 | -2.81 | 39,39,39,39 | 0 |
| 54 | MG | DA | 3474 | 1/1 | 0.97 | 0.10 | -2.83 | 30,30,30,30 | 0 |
| 54 | MG | BA | 3606 | 1/1 | 0.97 | 0.10 | -2.84 | 34,34,34,34 | 0 |
| 54 | MG | BA | 3447 | 1/1 | 0.98 | 0.14 | -2.93 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3350 | 1/1 | 0.97 | 0.11 | -2.99 | 47,47,47,47 | 0 |
| 54 | MG | DA | 3361 | 1/1 | 0.81 | 0.10 | -3.08 | 30,30,30,30 | 0 |
| 54 | MG | DA | 3456 | 1/1 | 0.90 | 0.08 | -3.08 | 42,42,42,42 | 0 |
| 54 | MG | DA | 3105 | 1/1 | 0.98 | 0.09 | -3.13 | 46,46,46,46 | 0 |
| 55 | ZN | DY | 201 | 1/1 | 0.96 | 0.05 | -3.13 | 94,94,94,94 | 0 |
| 54 | MG | DA | 3151 | 1/1 | 0.91 | 0.11 | -3.22 | 43,43,43,43 | 0 |
| 54 | MG | BA | 3469 | 1/1 | 0.91 | 0.15 | -3.28 | 40,40,40,40 | 0 |
| 54 | MG | BQ | 204 | 1/1 | 0.85 | 0.10 | -3.30 | 43,43,43,43 | 0 |
| 54 | MG | DA | 3412 | 1/1 | 0.89 | 0.09 | -3.33 | 58,58,58,58 | 0 |
| 54 | MG | BA | 3490 | 1/1 | 0.94 | 0.10 | -3.39 | 28,28,28,28 | 0 |
| 54 | MG | BA | 3309 | 1/1 | 0.98 | 0.10 | -3.40 | 31,31,31,31 | 0 |
| 54 | MG | CA | 1724 | 1/1 | 0.97 | 0.11 | -3.40 | 49,49,49,49 | 0 |
| 54 | MG | BA | 3483 | 1/1 | 0.98 | 0.13 | -3.42 | 28,28,28,28 | 0 |
| 54 | MG | BA | 3498 | 1/1 | 0.98 | 0.08 | -3.50 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3566 | 1/1 | 0.91 | 0.14 | -3.50 | 44,44,44,44 | 0 |
| 54 | MG | DA | 3454 | 1/1 | 0.85 | 0.08 | -3.54 | 64,64,64,64 | 0 |
| 54 | MG | DA | 3431 | 1/1 | 0.91 | 0.10 | -3.55 | 59,59,59,59 | 0 |
| 54 | MG | BA | 3601 | 1/1 | 0.91 | 0.14 | -3.59 | 76,76,76,76 | 0 |
| 54 | MG | CA | 1732 | 1/1 | 0.87 | 0.12 | -3.61 | 110,110,110,110 | 0 |
| 54 | MG | BA | 3578 | 1/1 | 0.91 | 0.10 | -3.69 | 44,44,44,44 | 0 |
| 54 | MG | DA | 3023 | 1/1 | 0.96 | 0.06 | -3.73 | 43,43,43,43 | 0 |
| 54 | MG | BA | 3355 | 1/1 | 0.93 | 0.14 | -3.74 | 29,29,29,29 | 0 |
| 54 | MG | BA | 3485 | 1/1 | 0.97 | 0.10 | -3.76 | 32,32,32,32 | 0 |
| 54 | MG | BA | 3560 | 1/1 | 0.95 | 0.08 | -3.77 | 74,74,74,74 | 0 |
| 54 | MG | CA | 1754 | 1/1 | 0.91 | 0.05 | -3.83 | 74,74,74,74 | 0 |
| 54 | MG | CA | 1628 | 1/1 | 0.93 | 0.09 | -3.88 | 75,75,75,75 | 0 |
| 54 | MG | BA | 3619 | 1/1 | 0.96 | 0.13 | -3.92 | 64,64,64,64 | 0 |
| 54 | MG | DA | 3377 | 1/1 | 0.99 | 0.07 | -3.95 | 33,33,33,33 | 0 |
| 54 | MG | BA | 3453 | 1/1 | 0.95 | 0.08 | -3.95 | 46,46,46,46 | 0 |
| 54 | MG | DA | 3038 | 1/1 | 0.99 | 0.08 | -4.01 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 54 | MG | BA | 3541 | 1/1 | 0.96 | 0.09 | -4.20 | 42,42,42,42 | 0 |
| 54 | MG | BA | 3517 | 1/1 | 0.95 | 0.11 | -4.21 | 26,26,26,26 | 0 |
| 54 | MG | BA | 3525 | 1/1 | 0.90 | 0.14 | -4.25 | 35,35,35,35 | 0 |
| 54 | MG | BA | 3411 | 1/1 | 0.87 | 0.08 | -4.26 | 63,63,63,63 | 0 |
| 54 | MG | BA | 3603 | 1/1 | 0.98 | 0.08 | -4.48 | 40,40,40,40 | 0 |
| 54 | MG | BA | 3416 | 1/1 | 0.99 | 0.08 | -4.54 | 25,25,25,25 | 0 |
| 54 | MG | AA | 1685 | 1/1 | 0.96 | 0.10 | -4.57 | 71,71,71,71 | 0 |
| 54 | MG | DA | 3579 | 1/1 | 0.94 | 0.08 | -4.64 | 57,57,57,57 | 0 |
| 54 | MG | BA | 3548 | 1/1 | 0.93 | 0.13 | -4.65 | 29,29,29,29 | 0 |
| 54 | MG | DA | 3574 | 1/1 | 0.95 | 0.07 | -4.70 | 41,41,41,41 | 0 |
| 54 | MG | DA | 3359 | 1/1 | 0.95 | 0.10 | -4.72 | 33,33,33,33 | 0 |
| 54 | MG | DA | 3406 | 1/1 | 0.95 | 0.07 | -4.75 | 58,58,58,58 | 0 |
| 54 | MG | BA | 3312 | 1/1 | 0.98 | 0.10 | -4.78 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3501 | 1/1 | 0.96 | 0.08 | -4.81 | 58,58,58,58 | 0 |
| 54 | MG | BA | 3441 | 1/1 | 0.95 | 0.09 | -4.99 | 56,56,56,56 | 0 |
| 54 | MG | BA | 3629 | 1/1 | 0.96 | 0.09 | -5.05 | 24,24,24,24 | 0 |
| 54 | MG | DA | 3389 | 1/1 | 0.96 | 0.07 | -5.08 | 51,51,51,51 | 0 |
| 54 | MG | DA | 3411 | 1/1 | 0.92 | 0.11 | -5.15 | 49,49,49,49 | 0 |
| 54 | MG | BA | 3350 | 1/1 | 0.99 | 0.09 | -5.27 | 40,40,40,40 | 0 |
| 54 | MG | DA | 3539 | 1/1 | 0.94 | 0.09 | -5.39 | 67,67,67,67 | 0 |
| 54 | MG | BA | 3415 | 1/1 | 0.96 | 0.08 | -5.46 | 33,33,33,33 | 0 |
| 54 | MG | DA | 3369 | 1/1 | 0.96 | 0.07 | -5.55 | 50,50,50,50 | 0 |
| 54 | MG | DA | 3519 | 1/1 | 0.98 | 0.07 | -5.68 | 52,52,52,52 | 0 |
| 54 | MG | BA | 3555 | 1/1 | 0.94 | 0.12 | -6.01 | 47,47,47,47 | 0 |
| 54 | MG | DA | 3429 | 1/1 | 0.95 | 0.07 | -6.08 | 56,56,56,56 | 0 |
| 54 | MG | BA | 3463 | 1/1 | 0.99 | 0.09 | -6.12 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1747 | 1/1 | 0.73 | 0.11 | -6.23 | 95,95,95,95 | 0 |
| 54 | MG | BA | 3336 | 1/1 | 0.94 | 0.11 | -6.35 | 45,45,45,45 | 0 |
| 54 | MG | BA | 3635 | 1/1 | 0.98 | 0.08 | -6.89 | 23,23,23,23 | 0 |
| 54 | MG | AA | 1715 | 1/1 | 0.97 | 0.10 | -7.07 | 61,61,61,61 | 0 |
| 54 | MG | BA | 3591 | 1/1 | 0.99 | 0.10 | -8.74 | 34,34,34,34 | 0 |
| 54 | MG | BA | 3348 | 1/1 | 0.93 | 0.08 | -8.76 | 59,59,59,59 | 0 |
| 54 | MG | BA | 3430 | 1/1 | 0.98 | 0.06 | -12.41 | 49,49,49,49 | 0 |
| 54 | MG | CA | 1614 | 1/1 | 0.94 | 0.44 | - | 85,85,85,85 | 0 |
| 54 | MG | BA | 3617 | 1/1 | 0.95 | 0.07 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3298 | 1/1 | 0.79 | 0.26 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3356 | 1/1 | 0.94 | 0.16 | - | 60,60,60,60 | 0 |
| 54 | MG | DP | 201 | 1/1 | 0.91 | 0.18 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3244 | 1/1 | 0.95 | 0.14 | - | 30,30,30,30 | 0 |
| 54 | MG | CA | 1684 | 1/1 | 0.73 | 0.33 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3477 | 1/1 | 0.80 | 0.11 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3234 | 1/1 | 0.97 | 0.18 | - | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | AA | 1641 | 1/1 | 0.98 | 0.17 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3466 | 1/1 | 0.80 | 0.15 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3319 | 1/1 | 0.99 | 0.12 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3016 | 1/1 | 0.82 | 0.22 | - | 47,47,47,47 | 0 |
| 54 | MG | CA | 1735 | 1/1 | 0.94 | 0.28 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3301 | 1/1 | 0.95 | 0.46 | - | 50,50,50,50 | 0 |
| 54 | MG | CA | 1760 | 1/1 | 0.97 | 0.09 | - | 87,87,87,87 | 0 |
| 54 | MG | CA | 1698 | 1/1 | 0.88 | 0.10 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3024 | 1/1 | 0.85 | 0.35 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3387 | 1/1 | 0.89 | 0.11 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3510 | 1/1 | 0.94 | 0.10 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3290 | 1/1 | 0.75 | 0.48 | - | 58,58,58,58 | 0 |
| 54 | MG | CA | 1707 | 1/1 | 0.80 | 0.19 | - | 94,94,94,94 | 0 |
| 54 | MG | BA | 3035 | 1/1 | 0.88 | 0.19 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3516 | 1/1 | 0.92 | 0.25 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3516 | 1/1 | 0.98 | 0.20 | - | 32,32,32,32 | 0 |
| 54 | MG | DA | 3526 | 1/1 | 0.85 | 0.12 | - | 98,98,98,98 | 0 |
| 54 | MG | DA | 3260 | 1/1 | 0.89 | 0.20 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3339 | 1/1 | 0.85 | 0.11 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3527 | 1/1 | 0.98 | 0.18 | - | 29,29,29,29 | 0 |
| 54 | MG | DA | 3073 | 1/1 | 0.89 | 0.52 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3055 | 1/1 | 0.80 | 0.32 | - | 56,56,56,56 | 0 |
| 54 | MG | B0 | 101 | 1/1 | 0.89 | 0.18 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3160 | 1/1 | 0.96 | 0.36 | - | 39,39,39,39 | 0 |
| 54 | MG | AA | 1615 | 1/1 | 0.94 | 0.36 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3115 | 1/1 | 0.93 | 0.12 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3210 | 1/1 | 0.90 | 0.20 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3377 | 1/1 | 0.91 | 0.22 | - | 32,32,32,32 | 0 |
| 54 | MG | DA | 3453 | 1/1 | 0.96 | 0.07 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 3609 | 1/1 | 0.86 | 0.10 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3288 | 1/1 | 0.85 | 0.21 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3224 | 1/1 | 0.94 | 0.28 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3278 | 1/1 | 0.67 | 0.07 | - | 83,83,83,83 | 0 |
| 54 | MG | BA | 3275 | 1/1 | 0.95 | 0.29 | - | 26,26,26,26 | 0 |
| 54 | MG | CA | 1695 | 1/1 | 0.90 | 0.35 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3025 | 1/1 | 0.91 | 0.22 | - | 48,48,48,48 | 0 |
| 54 | MG | AA | 1724 | 1/1 | 0.97 | 0.28 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3580 | 1/1 | 0.87 | 0.15 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3274 | 1/1 | 0.97 | 0.29 | - | 26,26,26,26 | 0 |
| 54 | MG | BA | 3513 | 1/1 | 0.95 | 0.09 | - | 86,86,86,86 | 0 |
| 54 | MG | BA | 3565 | 1/1 | 0.93 | 0.07 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3174 | 1/1 | 0.95 | 0.18 | - | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1649 | 1/1 | 0.86 | 0.41 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3197 | 1/1 | 0.92 | 0.35 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3423 | 1/1 | 0.98 | 0.16 | - | 32,32,32,32 | 0 |
| 54 | MG | BB | 218 | 1/1 | 0.91 | 0.09 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3573 | 1/1 | 0.97 | 0.21 | - | 23,23,23,23 | 0 |
| 54 | MG | BA | 3640 | 1/1 | 0.96 | 0.14 | - | 116,116,116,116 | 0 |
| 54 | MG | BA | 3607 | 1/1 | 0.94 | 0.17 | - | 99,99,99,99 | 0 |
| 54 | MG | CA | 1639 | 1/1 | 0.89 | 0.26 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3632 | 1/1 | 0.95 | 0.05 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1661 | 1/1 | 0.82 | 0.26 | - | 55,55,55,55 | 0 |
| 54 | MG | CA | 1716 | 1/1 | 0.90 | 0.15 | - | 102,102,102,102 | 0 |
| 54 | MG | DA | 3383 | 1/1 | 0.88 | 0.10 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1729 | 1/1 | 0.77 | 0.08 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3150 | 1/1 | 0.92 | 0.12 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3238 | 1/1 | 0.90 | 0.45 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3489 | 1/1 | 0.92 | 0.14 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3495 | 1/1 | 0.90 | 0.06 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3200 | 1/1 | 0.92 | 0.25 | - | 34,34,34,34 | 0 |
| 54 | MG | BB | 211 | 1/1 | 0.90 | 0.21 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3027 | 1/1 | 0.91 | 0.35 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3108 | 1/1 | 0.95 | 0.11 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3056 | 1/1 | 0.89 | 0.16 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3657 | 1/1 | 0.95 | 0.46 | - | 65,65,65,65 | 0 |
| 54 | MG | BB | 207 | 1/1 | 0.86 | 0.20 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3594 | 1/1 | 0.90 | 0.05 | - | 86,86,86,86 | 0 |
| 54 | MG | BA | 3276 | 1/1 | 0.96 | 0.24 | - | 23,23,23,23 | 0 |
| 54 | MG | BA | 3413 | 1/1 | 0.94 | 0.12 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3295 | 1/1 | 0.93 | 0.59 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3289 | 1/1 | 0.85 | 0.58 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3596 | 1/1 | 0.98 | 0.07 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3304 | 1/1 | 0.83 | 0.35 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3336 | 1/1 | 0.99 | 0.17 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3003 | 1/1 | 0.91 | 0.30 | - | 74,74,74,74 | 0 |
| 54 | MG | CA | 1602 | 1/1 | 0.91 | 0.40 | - | 62,62,62,62 | 0 |
| 54 | MG | B5 | 103 | 1/1 | 0.92 | 0.08 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3023 | 1/1 | 0.97 | 0.14 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3341 | 1/1 | 0.94 | 0.05 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3445 | 1/1 | 0.92 | 0.17 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3438 | 1/1 | 0.82 | 0.17 | - | 90,90,90,90 | 0 |
| 54 | MG | AA | 1682 | 1/1 | 0.90 | 0.13 | - | 76,76,76,76 | 0 |
| 54 | MG | CA | 1635 | 1/1 | 0.86 | 0.10 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3365 | 1/1 | 0.97 | 0.07 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | AA | 1718 | 1/1 | 0.86 | 0.05 | - | 96,96,96,96 | 0 |
| 54 | MG | CE | 201 | 1/1 | 0.69 | 0.57 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3572 | 1/1 | 0.98 | 0.10 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 3392 | 1/1 | 0.96 | 0.14 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3179 | 1/1 | 0.89 | 0.27 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3310 | 1/1 | 0.97 | 0.35 | - | 23,23,23,23 | 0 |
| 54 | MG | CA | 1623 | 1/1 | 0.97 | 0.39 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3159 | 1/1 | 0.94 | 0.20 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3387 | 1/1 | 0.94 | 0.06 | - | 63,63,63,63 | 0 |
| 54 | MG | AA | 1681 | 1/1 | 0.87 | 0.24 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3458 | 1/1 | 0.89 | 0.05 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3144 | 1/1 | 0.90 | 0.25 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3334 | 1/1 | 0.97 | 0.10 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3239 | 1/1 | 0.79 | 0.55 | - | 58,58,58,58 | 0 |
| 54 | MG | CA | 1632 | 1/1 | 0.85 | 0.27 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3392 | 1/1 | 0.95 | 0.13 | - | 110,110,110,110 | 0 |
| 54 | MG | DA | 3101 | 1/1 | 0.98 | 0.19 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3047 | 1/1 | 0.97 | 0.31 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3546 | 1/1 | 0.91 | 0.18 | - | 73,73,73,73 | 0 |
| 54 | MG | CA | 1659 | 1/1 | 0.97 | 0.20 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3234 | 1/1 | 0.81 | 0.15 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1727 | 1/1 | 0.91 | 0.09 | - | 61,61,61,61 | 0 |
| 54 | MG | CA | 1673 | 1/1 | 0.91 | 0.60 | - | 57,57,57,57 | 0 |
| 54 | MG | CA | 1605 | 1/1 | 0.92 | 0.34 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1638 | 1/1 | 0.89 | 0.26 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3412 | 1/1 | 0.96 | 0.17 | - | 78,78,78,78 | 0 |
| 54 | MG | DA | 3254 | 1/1 | 0.88 | 0.19 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3170 | 1/1 | 0.83 | 0.13 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3436 | 1/1 | 0.93 | 0.13 | - | 70,70,70,70 | 0 |
| 54 | MG | BV | 201 | 1/1 | 0.79 | 0.22 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3005 | 1/1 | 0.97 | 0.23 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3372 | 1/1 | 0.90 | 0.15 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3075 | 1/1 | 0.85 | 0.19 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3330 | 1/1 | 0.98 | 0.12 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3503 | 1/1 | 0.93 | 0.24 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3630 | 1/1 | 0.98 | 0.08 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3423 | 1/1 | 0.99 | 0.17 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3277 | 1/1 | 0.98 | 0.37 | - | 22,22,22,22 | 0 |
| 54 | MG | AA | 1620 | 1/1 | 0.87 | 0.17 | - | 65,65,65,65 | 0 |
| 54 | MG | AA | 1704 | 1/1 | 0.79 | 0.16 | - | 86,86,86,86 | 0 |
| 54 | MG | BA | 3302 | 1/1 | 0.97 | 0.14 | - | 47,47,47,47 | 0 |
| 54 | MG | DR | 201 | 1/1 | 0.94 | 0.31 | - | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | AA | 1698 | 1/1 | 0.98 | 0.15 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3566 | 1/1 | 0.98 | 0.13 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1655 | 1/1 | 0.90 | 0.47 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3454 | 1/1 | 0.98 | 0.12 | - | 25,25,25,25 | 0 |
| 54 | MG | DA | 3322 | 1/1 | 0.90 | 0.39 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3075 | 1/1 | 0.71 | 0.26 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3410 | 1/1 | 0.91 | 0.09 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3571 | 1/1 | 0.93 | 0.14 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3285 | 1/1 | 0.97 | 0.04 | - | 64,64,64,64 | 0 |
| 54 | MG | DB | 203 | 1/1 | 0.95 | 0.40 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3175 | 1/1 | 0.90 | 0.14 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3581 | 1/1 | 0.79 | 0.11 | - | 86,86,86,86 | 0 |
| 54 | MG | BA | 3216 | 1/1 | 0.79 | 0.30 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3457 | 1/1 | 0.88 | 0.08 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3073 | 1/1 | 0.90 | 0.42 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3086 | 1/1 | 0.90 | 0.95 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3593 | 1/1 | 0.70 | 0.21 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3424 | 1/1 | 0.80 | 0.10 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3353 | 1/1 | 0.89 | 0.20 | - | 91,91,91,91 | 0 |
| 54 | MG | DA | 3118 | 1/1 | 0.94 | 0.24 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3296 | 1/1 | 0.96 | 0.22 | - | 43,43,43,43 | 0 |
| 54 | MG | AA | 1665 | 1/1 | 0.96 | 0.10 | - | 51,51,51,51 | 0 |
| 54 | MG | CA | 1675 | 1/1 | 0.94 | 0.59 | - | 61,61,61,61 | 0 |
| 54 | MG | AA | 1687 | 1/1 | 0.95 | 0.18 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3202 | 1/1 | 0.95 | 0.16 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3647 | 1/1 | 0.96 | 0.15 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1689 | 1/1 | 0.90 | 0.06 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3598 | 1/1 | 0.95 | 0.11 | - | 76,76,76,76 | 0 |
| 54 | MG | BB | 214 | 1/1 | 0.97 | 0.12 | - | 40,40,40,40 | 0 |
| 54 | MG | CA | 1634 | 1/1 | 0.92 | 0.18 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3005 | 1/1 | 0.93 | 0.28 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3018 | 1/1 | 0.85 | 0.60 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3533 | 1/1 | 0.97 | 0.10 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3058 | 1/1 | 0.74 | 0.43 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3152 | 1/1 | 0.89 | 0.44 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3559 | 1/1 | 0.93 | 0.07 | - | 71,71,71,71 | 0 |
| 54 | MG | CA | 1723 | 1/1 | 0.96 | 0.13 | - | 55,55,55,55 | 0 |
| 54 | MG | AA | 1609 | 1/1 | 0.87 | 0.27 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3381 | 1/1 | 0.96 | 0.06 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1686 | 1/1 | 0.81 | 0.21 | - | 61,61,61,61 | 0 |
| 54 | MG | CA | 1748 | 1/1 | 0.97 | 0.06 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3002 | 1/1 | 0.89 | 0.34 | - | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3032 | 1/1 | 0.98 | 0.21 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3472 | 1/1 | 0.95 | 0.33 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3382 | 1/1 | 0.94 | 0.19 | - | 100,100,100,100 | 0 |
| 54 | MG | CA | 1739 | 1/1 | 0.89 | 0.12 | - | 87,87,87,87 | 0 |
| 54 | MG | AA | 1703 | 1/1 | 0.98 | 0.05 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3222 | 1/1 | 0.89 | 0.49 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3351 | 1/1 | 0.95 | 0.08 | - | 60,60,60,60 | 0 |
| 54 | MG | AA | 1720 | 1/1 | 0.97 | 0.07 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3611 | 1/1 | 0.97 | 0.07 | - | 44,44,44,44 | 0 |
| 54 | MG | AA | 1604 | 1/1 | 0.88 | 0.15 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3082 | 1/1 | 0.96 | 0.42 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3486 | 1/1 | 0.85 | 0.17 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3143 | 1/1 | 0.87 | 0.21 | - | 30,30,30,30 | 0 |
| 54 | MG | BA | 3442 | 1/1 | 0.70 | 0.16 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3322 | 1/1 | 0.97 | 0.08 | - | 37,37,37,37 | 0 |
| 54 | MG | CA | 1744 | 1/1 | 0.97 | 0.06 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3116 | 1/1 | 0.92 | 0.20 | - | 43,43,43,43 | 0 |
| 54 | MG | B0 | 103 | 1/1 | 0.94 | 0.12 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3345 | 1/1 | 0.98 | 0.10 | - | 71,71,71,71 | 0 |
| 54 | MG | BP | 201 | 1/1 | 0.84 | 0.13 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3068 | 1/1 | 0.84 | 0.40 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3124 | 1/1 | 0.92 | 0.19 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3022 | 1/1 | 0.92 | 0.26 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3287 | 1/1 | 0.89 | 0.27 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3217 | 1/1 | 0.89 | 0.23 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3044 | 1/1 | 0.99 | 0.08 | - | 33,33,33,33 | 0 |
| 54 | MG | DA | 3326 | 1/1 | 0.90 | 0.21 | - | 46,46,46,46 | 0 |
| 54 | MG | D5 | 101 | 1/1 | 0.85 | 0.35 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3263 | 1/1 | 0.96 | 0.38 | - | 36,36,36,36 | 0 |
| 54 | MG | AA | 1646 | 1/1 | 0.82 | 0.22 | - | 59,59,59,59 | 0 |
| 54 | MG | CA | 1727 | 1/1 | 0.97 | 0.17 | - | 46,46,46,46 | 0 |
| 54 | MG | DE | 302 | 1/1 | 0.94 | 0.35 | - | 21,21,21,21 | 0 |
| 54 | MG | BA | 3652 | 1/1 | 0.96 | 0.06 | - | 97,97,97,97 | 0 |
| 54 | MG | DA | 3355 | 1/1 | 0.99 | 0.13 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3388 | 1/1 | 0.97 | 0.14 | - | 43,43,43,43 | 0 |
| 54 | MG | AA | 1605 | 1/1 | 0.93 | 0.17 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3106 | 1/1 | 0.96 | 0.22 | - | 52,52,52,52 | 0 |
| 54 | MG | CA | 1641 | 1/1 | 0.96 | 0.09 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3128 | 1/1 | 0.86 | 0.18 | - | 49,49,49,49 | 0 |
| 54 | MG | CA | 1647 | 1/1 | 0.97 | 0.15 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3384 | 1/1 | 0.89 | 0.08 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3281 | 1/1 | 0.88 | 0.20 | - | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3646 | 1/1 | 0.76 | 0.18 | - | 142,142,142,142 | 0 |
| 54 | MG | DA | 3470 | 1/1 | 0.90 | 0.10 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3025 | 1/1 | 0.85 | 0.27 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3050 | 1/1 | 0.98 | 0.27 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3119 | 1/1 | 0.88 | 0.34 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3504 | 1/1 | 0.82 | 0.14 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3024 | 1/1 | 0.90 | 0.39 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1644 | 1/1 | 0.90 | 0.33 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3295 | 1/1 | 0.90 | 0.25 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3269 | 1/1 | 0.82 | 0.48 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3562 | 1/1 | 0.82 | 0.13 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3186 | 1/1 | 0.98 | 0.35 | - | 26,26,26,26 | 0 |
| 54 | MG | DA | 3256 | 1/1 | 0.93 | 0.24 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3242 | 1/1 | 0.94 | 0.20 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3560 | 1/1 | 0.95 | 0.14 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3416 | 1/1 | 0.89 | 0.13 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3481 | 1/1 | 0.93 | 0.44 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3492 | 1/1 | 0.89 | 0.07 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3589 | 1/1 | 0.90 | 0.18 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3381 | 1/1 | 0.95 | 0.05 | - | 42,42,42,42 | 0 |
| 54 | MG | CA | 1643 | 1/1 | 0.93 | 0.22 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3507 | 1/1 | 0.98 | 0.12 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3342 | 1/1 | 0.89 | 0.15 | - | 32,32,32,32 | 0 |
| 54 | MG | CA | 1668 | 1/1 | 0.90 | 0.55 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3525 | 1/1 | 0.81 | 0.16 | - | 106,106,106,106 | 0 |
| 54 | MG | AA | 1645 | 1/1 | 0.91 | 0.26 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3362 | 1/1 | 0.96 | 0.11 | - | 43,43,43,43 | 0 |
| 54 | MG | CA | 1637 | 1/1 | 0.69 | 0.42 | - | 73,73,73,73 | 0 |
| 54 | MG | CA | 1617 | 1/1 | 0.88 | 0.13 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3123 | 1/1 | 0.85 | 0.27 | - | 43,43,43,43 | 0 |
| 54 | MG | DB | 202 | 1/1 | 0.92 | 0.21 | - | 50,50,50,50 | 0 |
| 54 | MG | CA | 1752 | 1/1 | 0.94 | 0.13 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 3443 | 1/1 | 0.93 | 0.11 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3094 | 1/1 | 0.90 | 0.21 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1722 | 1/1 | 0.94 | 0.18 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3413 | 1/1 | 0.89 | 0.12 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3109 | 1/1 | 0.89 | 0.17 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3174 | 1/1 | 0.90 | 0.19 | - | 51,51,51,51 | 0 |
| 54 | MG | CA | 1651 | 1/1 | 0.87 | 0.35 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3321 | 1/1 | 0.96 | 0.06 | - | 32,32,32,32 | 0 |
| 54 | MG | DA | 3001 | 1/1 | 0.87 | 0.31 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3088 | 1/1 | 0.94 | 0.19 | - | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3243 | 1/1 | 0.89 | 0.30 | - | 42,42,42,42 | 0 |
| 54 | MG | CA | 1708 | 1/1 | 0.88 | 0.07 | - | 80,80,80,80 | 0 |
| 54 | MG | DA | 3323 | 1/1 | 0.95 | 0.13 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3409 | 1/1 | 0.95 | 0.07 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3098 | 1/1 | 0.90 | 0.19 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3529 | 1/1 | 0.95 | 0.07 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3550 | 1/1 | 0.91 | 0.06 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3547 | 1/1 | 0.80 | 0.25 | - | 105,105,105,105 | 0 |
| 54 | MG | BA | 3588 | 1/1 | 0.95 | 0.12 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3179 | 1/1 | 0.77 | 0.21 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3624 | 1/1 | 0.97 | 0.11 | - | 36,36,36,36 | 0 |
| 54 | MG | CA | 1694 | 1/1 | 0.89 | 0.17 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3053 | 1/1 | 0.93 | 0.44 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3142 | 1/1 | 0.85 | 0.26 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3198 | 1/1 | 0.98 | 0.12 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3043 | 1/1 | 0.86 | 0.12 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3265 | 1/1 | 0.94 | 0.32 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3341 | 1/1 | 0.97 | 0.14 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3582 | 1/1 | 0.80 | 0.23 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3517 | 1/1 | 0.88 | 0.24 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1650 | 1/1 | 0.91 | 0.21 | - | 60,60,60,60 | 0 |
| 54 | MG | CA | 1693 | 1/1 | 0.87 | 0.85 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3621 | 1/1 | 0.88 | 0.30 | - | 52,52,52,52 | 0 |
| 54 | MG | CA | 1629 | 1/1 | 0.90 | 0.20 | - | 87,87,87,87 | 0 |
| 54 | MG | DA | 3049 | 1/1 | 0.88 | 0.19 | - | 49,49,49,49 | 0 |
| 54 | MG | CA | 1626 | 1/1 | 0.82 | 0.39 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3292 | 1/1 | 0.94 | 0.27 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3359 | 1/1 | 0.93 | 0.11 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3270 | 1/1 | 0.91 | 0.17 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3208 | 1/1 | 0.96 | 0.39 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3089 | 1/1 | 0.89 | 0.11 | - | 52,52,52,52 | 0 |
| 54 | MG | CA | 1721 | 1/1 | 0.97 | 0.21 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3049 | 1/1 | 0.95 | 0.37 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3427 | 1/1 | 0.87 | 0.14 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3074 | 1/1 | 0.92 | 0.19 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1601 | 1/1 | 0.96 | 0.21 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3443 | 1/1 | 0.98 | 0.21 | - | 47,47,47,47 | 0 |
| 54 | MG | CA | 1669 | 1/1 | 0.94 | 0.31 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3572 | 1/1 | 0.88 | 0.17 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3148 | 1/1 | 0.96 | 0.23 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3478 | 1/1 | 0.93 | 0.16 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1710 | 1/1 | 0.97 | 0.07 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | B1 | 101 | 1/1 | 0.95 | 0.18 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3339 | 1/1 | 0.93 | 0.07 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3567 | 1/1 | 0.83 | 0.10 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3002 | 1/1 | 0.93 | 0.12 | - | 69,69,69,69 | 0 |
| 54 | MG | BB | 203 | 1/1 | 0.96 | 0.23 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3297 | 1/1 | 0.82 | 0.22 | - | 78,78,78,78 | 0 |
| 54 | MG | BA | 3528 | 1/1 | 0.94 | 0.17 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3526 | 1/1 | 0.92 | 0.13 | - | 22,22,22,22 | 0 |
| 54 | MG | DA | 3175 | 1/1 | 0.92 | 0.37 | - | 44,44,44,44 | 0 |
| 54 | MG | BB | 208 | 1/1 | 0.90 | 0.23 | - | 43,43,43,43 | 0 |
| 54 | MG | AA | 1730 | 1/1 | 0.90 | 0.10 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3136 | 1/1 | 0.94 | 0.36 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3426 | 1/1 | 0.94 | 0.08 | - | 37,37,37,37 | 0 |
| 54 | MG | AA | 1664 | 1/1 | 0.92 | 0.15 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3460 | 1/1 | 0.92 | 0.19 | - | 65,65,65,65 | 0 |
| 54 | MG | AA | 1630 | 1/1 | 0.97 | 0.26 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3406 | 1/1 | 0.94 | 0.06 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3013 | 1/1 | 0.89 | 0.25 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3101 | 1/1 | 0.91 | 0.11 | - | 37,37,37,37 | 0 |
| 54 | MG | CA | 1687 | 1/1 | 0.96 | 0.22 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3418 | 1/1 | 0.91 | 0.12 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3259 | 1/1 | 0.93 | 0.18 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3087 | 1/1 | 0.88 | 0.09 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3394 | 1/1 | 0.98 | 0.06 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3187 | 1/1 | 0.74 | 0.14 | - | 71,71,71,71 | 0 |
| 54 | MG | AA | 1614 | 1/1 | 0.69 | 0.50 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3291 | 1/1 | 0.94 | 0.32 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3099 | 1/1 | 0.98 | 0.16 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3437 | 1/1 | 0.89 | 0.16 | - | 85,85,85,85 | 0 |
| 54 | MG | DA | 3451 | 1/1 | 0.82 | 0.14 | - | 103,103,103,103 | 0 |
| 54 | MG | BA | 3092 | 1/1 | 0.97 | 0.40 | - | 26,26,26,26 | 0 |
| 54 | MG | DA | 3399 | 1/1 | 0.97 | 0.11 | - | 51,51,51,51 | 0 |
| 54 | MG | AA | 1603 | 1/1 | 0.67 | 0.36 | - | 79,79,79,79 | 0 |
| 54 | MG | AA | 1656 | 1/1 | 0.91 | 0.58 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3223 | 1/1 | 0.96 | 0.51 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3228 | 1/1 | 0.95 | 0.40 | - | 37,37,37,37 | 0 |
| 54 | MG | AA | 1617 | 1/1 | 0.91 | 0.17 | - | 45,45,45,45 | 0 |
| 54 | MG | AA | 1678 | 1/1 | 0.74 | 0.53 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3241 | 1/1 | 0.80 | 0.23 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3534 | 1/1 | 0.96 | 0.14 | - | 28,28,28,28 | 0 |
| 54 | MG | BA | 3479 | 1/1 | 0.93 | 0.18 | - | 32,32,32,32 | 0 |
| 54 | MG | CA | 1606 | 1/1 | 0.86 | 0.24 | - | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3180 | 1/1 | 0.93 | 0.29 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3229 | 1/1 | 0.90 | 0.22 | - | 41,41,41,41 | 0 |
| 54 | MG | BD | 302 | 1/1 | 0.90 | 0.21 | - | 28,28,28,28 | 0 |
| 54 | MG | BA | 3165 | 1/1 | 0.94 | 0.28 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3464 | 1/1 | 0.89 | 0.10 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3056 | 1/1 | 0.95 | 0.18 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3235 | 1/1 | 0.88 | 0.37 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3329 | 1/1 | 0.85 | 0.19 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3260 | 1/1 | 0.97 | 0.39 | - | 30,30,30,30 | 0 |
| 54 | MG | BA | 3138 | 1/1 | 0.91 | 0.35 | - | 42,42,42,42 | 0 |
| 54 | MG | AA | 1638 | 1/1 | 0.88 | 0.13 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3117 | 1/1 | 0.93 | 0.17 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3557 | 1/1 | 0.83 | 0.16 | - | 103,103,103,103 | 0 |
| 54 | MG | DA | 3523 | 1/1 | 0.84 | 0.07 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3434 | 1/1 | 0.97 | 0.11 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3446 | 1/1 | 0.98 | 0.24 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3343 | 1/1 | 0.83 | 0.09 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3103 | 1/1 | 0.92 | 0.17 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3536 | 1/1 | 0.92 | 0.08 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3055 | 1/1 | 0.91 | 0.20 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3214 | 1/1 | 0.88 | 0.22 | - | 52,52,52,52 | 0 |
| 54 | MG | CA | 1702 | 1/1 | 0.82 | 0.12 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3409 | 1/1 | 0.92 | 0.09 | - | 73,73,73,73 | 0 |
| 54 | MG | BB | 209 | 1/1 | 0.87 | 0.11 | - | 60,60,60,60 | 0 |
| 54 | MG | BB | 210 | 1/1 | 0.90 | 0.15 | - | 60,60,60,60 | 0 |
| 54 | MG | BQ | 201 | 1/1 | 0.86 | 0.19 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3594 | 1/1 | 0.99 | 0.18 | - | 58,58,58,58 | 0 |
| 54 | MG | CA | 1609 | 1/1 | 0.90 | 0.24 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3597 | 1/1 | 0.90 | 0.11 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3379 | 1/1 | 0.94 | 0.09 | - | 22,22,22,22 | 0 |
| 54 | MG | BA | 3163 | 1/1 | 0.97 | 0.28 | - | 23,23,23,23 | 0 |
| 54 | MG | CA | 1604 | 1/1 | 0.71 | 0.51 | - | 81,81,81,81 | 0 |
| 54 | MG | CA | 1677 | 1/1 | 0.85 | 0.15 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3111 | 1/1 | 0.93 | 0.20 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3102 | 1/1 | 0.97 | 0.47 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3422 | 1/1 | 0.92 | 0.17 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 3589 | 1/1 | 0.87 | 0.12 | - | 75,75,75,75 | 0 |
| 54 | MG | DA | 3546 | 1/1 | 0.95 | 0.11 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3639 | 1/1 | 0.95 | 0.20 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3246 | 1/1 | 0.82 | 0.38 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3465 | 1/1 | 0.98 | 0.15 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3478 | 1/1 | 0.81 | 0.17 | - | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3463 | 1/1 | 0.98 | 0.09 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3264 | 1/1 | 0.93 | 0.46 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3019 | 1/1 | 0.93 | 0.16 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3152 | 1/1 | 0.90 | 0.37 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3041 | 1/1 | 0.93 | 0.26 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3564 | 1/1 | 0.92 | 0.11 | - | 59,59,59,59 | 0 |
| 54 | MG | CA | 1656 | 1/1 | 0.90 | 0.31 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3273 | 1/1 | 0.88 | 0.33 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3090 | 1/1 | 0.84 | 0.12 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3245 | 1/1 | 0.87 | 0.28 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3289 | 1/1 | 0.97 | 0.34 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3334 | 1/1 | 0.98 | 0.12 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3188 | 1/1 | 0.87 | 0.11 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1667 | 1/1 | 0.95 | 0.19 | - | 38,38,38,38 | 0 |
| 54 | MG | CA | 1701 | 1/1 | 0.89 | 0.08 | - | 72,72,72,72 | 0 |
| 54 | MG | CA | 1660 | 1/1 | 0.51 | 0.41 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3303 | 1/1 | 0.88 | 0.11 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1697 | 1/1 | 0.77 | 0.13 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3340 | 1/1 | 0.93 | 0.12 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3470 | 1/1 | 0.88 | 0.27 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3637 | 1/1 | 0.83 | 0.18 | - | 108,108,108,108 | 0 |
| 54 | MG | BA | 3239 | 1/1 | 0.67 | 0.14 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3518 | 1/1 | 0.96 | 0.10 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3483 | 1/1 | 0.98 | 0.26 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3204 | 1/1 | 0.93 | 0.13 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3261 | 1/1 | 0.90 | 0.32 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3475 | 1/1 | 0.96 | 0.11 | - | 30,30,30,30 | 0 |
| 54 | MG | BA | 3489 | 1/1 | 0.97 | 0.15 | - | 23,23,23,23 | 0 |
| 54 | MG | CA | 1664 | 1/1 | 0.83 | 0.08 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3449 | 1/1 | 0.94 | 0.30 | - | 29,29,29,29 | 0 |
| 54 | MG | DA | 3134 | 1/1 | 0.81 | 0.28 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3437 | 1/1 | 0.86 | 0.11 | - | 49,49,49,49 | 0 |
| 54 | MG | AA | 1653 | 1/1 | 0.98 | 0.08 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3561 | 1/1 | 0.94 | 0.19 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3096 | 1/1 | 0.92 | 0.44 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3410 | 1/1 | 0.61 | 0.12 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3368 | 1/1 | 0.86 | 0.16 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3468 | 1/1 | 0.94 | 0.07 | - | 53,53,53,53 | 0 |
| 54 | MG | AA | 1647 | 1/1 | 0.86 | 0.23 | - | 55,55,55,55 | 0 |
| 54 | MG | AA | 1688 | 1/1 | 0.76 | 0.15 | - | 96,96,96,96 | 0 |
| 54 | MG | BA | 3597 | 1/1 | 0.96 | 0.24 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3161 | 1/1 | 0.95 | 0.34 | - | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3575 | 1/1 | 0.98 | 0.08 | - | 41,41,41,41 | 0 |
| 54 | MG | BS | 201 | 1/1 | 0.83 | 0.54 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3435 | 1/1 | 0.88 | 0.45 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3272 | 1/1 | 0.94 | 0.38 | - | 31,31,31,31 | 0 |
| 54 | MG | BA | 3320 | 1/1 | 0.98 | 0.17 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3429 | 1/1 | 0.96 | 0.21 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3142 | 1/1 | 0.92 | 0.21 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3238 | 1/1 | 0.79 | 0.36 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3057 | 1/1 | 0.94 | 0.15 | - | 35,35,35,35 | 0 |
| 54 | MG | CA | 1646 | 1/1 | 0.89 | 0.38 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3354 | 1/1 | 0.94 | 0.09 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3147 | 1/1 | 0.89 | 0.42 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3240 | 1/1 | 0.98 | 0.15 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3644 | 1/1 | 0.97 | 0.08 | - | 88,88,88,88 | 0 |
| 54 | MG | BA | 3232 | 1/1 | 0.53 | 0.18 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1610 | 1/1 | 0.93 | 0.29 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3031 | 1/1 | 0.92 | 0.23 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3331 | 1/1 | 0.76 | 0.13 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3373 | 1/1 | 0.93 | 0.08 | - | 44,44,44,44 | 0 |
| 54 | MG | AA | 1621 | 1/1 | 0.89 | 0.29 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3365 | 1/1 | 0.97 | 0.08 | - | 40,40,40,40 | 0 |
| 54 | MG | CA | 1691 | 1/1 | 0.95 | 0.43 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3521 | 1/1 | 0.86 | 0.12 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3391 | 1/1 | 0.87 | 0.09 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3407 | 1/1 | 0.93 | 0.06 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3233 | 1/1 | 0.95 | 0.14 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3299 | 1/1 | 0.97 | 0.27 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3655 | 1/1 | 0.88 | 0.18 | - | 104,104,104,104 | 0 |
| 54 | MG | BA | 3557 | 1/1 | 0.86 | 0.15 | - | 78,78,78,78 | 0 |
| 54 | MG | AA | 1652 | 1/1 | 0.97 | 0.25 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3460 | 1/1 | 0.95 | 0.30 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3051 | 1/1 | 0.97 | 0.17 | - | 48,48,48,48 | 0 |
| 54 | MG | CA | 1730 | 1/1 | 0.96 | 0.10 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3112 | 1/1 | 0.96 | 0.19 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3140 | 1/1 | 0.95 | 0.33 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3505 | 1/1 | 0.93 | 0.12 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3156 | 1/1 | 0.97 | 0.27 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3519 | 1/1 | 0.94 | 0.05 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3282 | 1/1 | 0.83 | 0.14 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3003 | 1/1 | 0.88 | 0.22 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3316 | 1/1 | 0.93 | 0.73 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3490 | 1/1 | 0.97 | 0.12 | - | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3026 | 1/1 | 0.95 | 0.08 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3417 | 1/1 | 0.93 | 0.08 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3415 | 1/1 | 0.97 | 0.11 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3149 | 1/1 | 0.81 | 0.37 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3551 | 1/1 | 0.94 | 0.19 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3328 | 1/1 | 0.87 | 0.40 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3344 | 1/1 | 0.94 | 0.09 | - | 30,30,30,30 | 0 |
| 54 | MG | DA | 3479 | 1/1 | 0.90 | 0.15 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3461 | 1/1 | 0.93 | 0.15 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3093 | 1/1 | 0.95 | 0.19 | - | 42,42,42,42 | 0 |
| 54 | MG | DQ | 201 | 1/1 | 0.94 | 0.15 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3658 | 1/1 | 0.84 | 0.14 | - | 114,114,114,114 | 0 |
| 54 | MG | DA | 3313 | 1/1 | 0.95 | 0.36 | - | 29,29,29,29 | 0 |
| 54 | MG | BA | 3654 | 1/1 | 0.57 | 0.15 | - | 126,126,126,126 | 0 |
| 54 | MG | BA | 3542 | 1/1 | 0.94 | 0.11 | - | 83,83,83,83 | 0 |
| 54 | MG | CA | 1714 | 1/1 | 0.82 | 0.15 | - | 87,87,87,87 | 0 |
| 54 | MG | DB | 206 | 1/1 | 0.97 | 0.26 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3440 | 1/1 | 0.96 | 0.07 | - | 46,46,46,46 | 0 |
| 54 | MG | AA | 1642 | 1/1 | 0.88 | 0.82 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3476 | 1/1 | 0.95 | 0.18 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3286 | 1/1 | 0.95 | 0.46 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3072 | 1/1 | 0.94 | 0.49 | - | 50,50,50,50 | 0 |
| 54 | MG | BR | 201 | 1/1 | 0.96 | 0.17 | - | 29,29,29,29 | 0 |
| 54 | MG | DA | 3586 | 1/1 | 0.93 | 0.14 | - | 49,49,49,49 | 0 |
| 54 | MG | CA | 1756 | 1/1 | 0.82 | 0.19 | - | 80,80,80,80 | 0 |
| 54 | MG | AA | 1627 | 1/1 | 0.86 | 0.33 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3132 | 1/1 | 0.89 | 0.42 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3121 | 1/1 | 0.97 | 0.13 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3376 | 1/1 | 0.96 | 0.11 | - | 26,26,26,26 | 0 |
| 54 | MG | BB | 223 | 1/1 | 0.75 | 0.14 | - | 133,133,133,133 | 0 |
| 54 | MG | DA | 3085 | 1/1 | 0.93 | 0.22 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3203 | 1/1 | 0.87 | 0.50 | - | 55,55,55,55 | 0 |
| 54 | MG | BQ | 202 | 1/1 | 0.93 | 0.21 | - | 34,34,34,34 | 0 |
| 54 | MG | AA | 1676 | 1/1 | 0.85 | 0.30 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1669 | 1/1 | 0.15 | 0.17 | - | 103,103,103,103 | 0 |
| 54 | MG | BB | 204 | 1/1 | 0.86 | 0.21 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3111 | 1/1 | 0.90 | 0.17 | - | 50,50,50,50 | 0 |
| 54 | MG | DB | 208 | 1/1 | 0.96 | 0.10 | - | 104,104,104,104 | 0 |
| 54 | MG | BA | 3017 | 1/1 | 0.91 | 0.14 | - | 31,31,31,31 | 0 |
| 54 | MG | DA | 3129 | 1/1 | 0.92 | 0.13 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3343 | 1/1 | 0.92 | 0.06 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3194 | 1/1 | 0.93 | 0.23 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1648 | 1/1 | 0.89 | 0.41 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3210 | 1/1 | 0.95 | 0.26 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3656 | 1/1 | 0.92 | 0.16 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3162 | 1/1 | 0.92 | 0.35 | - | 42,42,42,42 | 0 |
| 54 | MG | BE | 302 | 1/1 | 0.93 | 0.20 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3367 | 1/1 | 0.67 | 0.20 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3522 | 1/1 | 0.93 | 0.11 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3181 | 1/1 | 0.98 | 0.28 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3166 | 1/1 | 0.91 | 0.29 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3021 | 1/1 | 0.93 | 0.13 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3501 | 1/1 | 0.99 | 0.10 | - | 29,29,29,29 | 0 |
| 54 | MG | DA | 3018 | 1/1 | 0.96 | 0.20 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3588 | 1/1 | 0.93 | 0.18 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3542 | 1/1 | 0.91 | 0.07 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3158 | 1/1 | 0.96 | 0.30 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3066 | 1/1 | 0.97 | 0.35 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3462 | 1/1 | 0.94 | 0.12 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3307 | 1/1 | 0.97 | 0.11 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3482 | 1/1 | 0.94 | 0.19 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3533 | 1/1 | 0.95 | 0.14 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3626 | 1/1 | 0.91 | 0.09 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3028 | 1/1 | 0.85 | 0.31 | - | 67,67,67,67 | 0 |
| 54 | MG | BB | 216 | 1/1 | 0.89 | 0.10 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3500 | 1/1 | 0.90 | 0.12 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3547 | 1/1 | 0.96 | 0.17 | - | 29,29,29,29 | 0 |
| 54 | MG | BA | 3602 | 1/1 | 0.97 | 0.05 | - | 56,56,56,56 | 0 |
| 54 | MG | AA | 1735 | 1/1 | 0.93 | 0.16 | - | 110,110,110,110 | 0 |
| 54 | MG | BA | 3153 | 1/1 | 0.88 | 0.37 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3201 | 1/1 | 0.93 | 0.33 | - | 31,31,31,31 | 0 |
| 54 | MG | CA | 1743 | 1/1 | 0.97 | 0.08 | - | 61,61,61,61 | 0 |
| 54 | MG | AA | 1733 | 1/1 | 0.94 | 0.07 | - | 78,78,78,78 | 0 |
| 54 | MG | CA | 1753 | 1/1 | 0.81 | 0.14 | - | 86,86,86,86 | 0 |
| 54 | MG | BQ | 203 | 1/1 | 0.96 | 0.12 | - | 73,73,73,73 | 0 |
| 54 | MG | BA | 3133 | 1/1 | 0.78 | 0.26 | - | 53,53,53,53 | 0 |
| 54 | MG | CA | 1653 | 1/1 | 0.94 | 0.81 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3184 | 1/1 | 0.97 | 0.22 | - | 40,40,40,40 | 0 |
| 54 | MG | DB | 205 | 1/1 | 0.97 | 0.16 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3427 | 1/1 | 0.92 | 0.06 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3094 | 1/1 | 0.90 | 0.16 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3297 | 1/1 | 0.89 | 0.26 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3383 | 1/1 | 0.94 | 0.13 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3219 | 1/1 | 0.88 | 0.15 | - | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3201 | 1/1 | 0.88 | 0.30 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3439 | 1/1 | 0.95 | 0.07 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3567 | 1/1 | 0.85 | 0.24 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3038 | 1/1 | 0.76 | 0.26 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3080 | 1/1 | 0.89 | 0.23 | - | 39,39,39,39 | 0 |
| 54 | MG | BW | 202 | 1/1 | 0.95 | 0.12 | - | 33,33,33,33 | 0 |
| 54 | MG | DA | 3271 | 1/1 | 0.84 | 0.38 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3291 | 1/1 | 0.93 | 0.13 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3390 | 1/1 | 0.96 | 0.07 | - | 47,47,47,47 | 0 |
| 54 | MG | AA | 1651 | 1/1 | 0.70 | 0.31 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3518 | 1/1 | 0.97 | 0.09 | - | 69,69,69,69 | 0 |
| 54 | MG | CA | 1738 | 1/1 | 0.86 | 0.08 | - | 112,112,112,112 | 0 |
| 54 | MG | DA | 3046 | 1/1 | 0.93 | 0.19 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3095 | 1/1 | 0.93 | 0.19 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3583 | 1/1 | 0.88 | 0.10 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3570 | 1/1 | 0.55 | 0.12 | - | 78,78,78,78 | 0 |
| 54 | MG | CA | 1662 | 1/1 | 0.93 | 0.40 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3625 | 1/1 | 0.96 | 0.06 | - | 53,53,53,53 | 0 |
| 54 | MG | CA | 1640 | 1/1 | 0.75 | 0.23 | - | 82,82,82,82 | 0 |
| 54 | MG | CA | 1712 | 1/1 | 0.93 | 0.28 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3540 | 1/1 | 0.97 | 0.14 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3199 | 1/1 | 0.96 | 0.14 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1731 | 1/1 | 0.81 | 0.17 | - | 119,119,119,119 | 0 |
| 54 | MG | AA | 1683 | 1/1 | 0.90 | 0.65 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3218 | 1/1 | 0.90 | 0.65 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3258 | 1/1 | 0.85 | 0.45 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3348 | 1/1 | 0.96 | 0.15 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3137 | 1/1 | 0.92 | 0.23 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3404 | 1/1 | 0.93 | 0.10 | - | 45,45,45,45 | 0 |
| 54 | MG | BW | 201 | 1/1 | 0.98 | 0.12 | - | 32,32,32,32 | 0 |
| 54 | MG | BA | 3181 | 1/1 | 0.93 | 0.20 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3430 | 1/1 | 0.96 | 0.12 | - | 30,30,30,30 | 0 |
| 54 | MG | DA | 3569 | 1/1 | 0.83 | 0.12 | - | 104,104,104,104 | 0 |
| 54 | MG | DA | 3432 | 1/1 | 0.92 | 0.10 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3113 | 1/1 | 0.93 | 0.42 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3520 | 1/1 | 0.94 | 0.14 | - | 95,95,95,95 | 0 |
| 54 | MG | BA | 3613 | 1/1 | 0.94 | 0.07 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3095 | 1/1 | 0.93 | 0.24 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3113 | 1/1 | 0.77 | 0.09 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3508 | 1/1 | 0.89 | 0.10 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3059 | 1/1 | 0.96 | 0.12 | - | 48,48,48,48 | 0 |
| 54 | MG | BT | 202 | 1/1 | 0.89 | 0.28 | - | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3032 | 1/1 | 0.98 | 0.09 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3561 | 1/1 | 0.96 | 0.09 | - | 54,54,54,54 | 0 |
| 54 | MG | DA | 3180 | 1/1 | 0.82 | 0.24 | - | 49,49,49,49 | 0 |
| 54 | MG | B0 | 102 | 1/1 | 0.96 | 0.16 | - | 54,54,54,54 | 0 |
| 54 | MG | DQ | 202 | 1/1 | 0.89 | 0.17 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3120 | 1/1 | 0.87 | 0.13 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3375 | 1/1 | 0.98 | 0.16 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3493 | 1/1 | 0.97 | 0.20 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3173 | 1/1 | 0.98 | 0.40 | - | 32,32,32,32 | 0 |
| 54 | MG | BA | 3118 | 1/1 | 0.97 | 0.22 | - | 44,44,44,44 | 0 |
| 54 | MG | CA | 1745 | 1/1 | 0.91 | 0.34 | - | 116,116,116,116 | 0 |
| 54 | MG | AA | 1690 | 1/1 | 0.80 | 0.09 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3176 | 1/1 | 0.87 | 0.42 | - | 70,70,70,70 | 0 |
| 54 | MG | AA | 1717 | 1/1 | 0.46 | 0.14 | - | 93,93,93,93 | 0 |
| 54 | MG | BA | 3091 | 1/1 | 0.91 | 0.35 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3539 | 1/1 | 0.89 | 0.08 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3258 | 1/1 | 0.92 | 0.38 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3097 | 1/1 | 0.97 | 0.27 | - | 23,23,23,23 | 0 |
| 54 | MG | DA | 3497 | 1/1 | 0.84 | 0.26 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3426 | 1/1 | 0.93 | 0.07 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3330 | 1/1 | 0.92 | 0.13 | - | 34,34,34,34 | 0 |
| 54 | MG | AA | 1719 | 1/1 | 0.78 | 0.17 | - | 144,144,144,144 | 0 |
| 54 | MG | BA | 3183 | 1/1 | 0.91 | 0.34 | - | 29,29,29,29 | 0 |
| 54 | MG | CA | 1670 | 1/1 | 0.77 | 0.64 | - | 73,73,73,73 | 0 |
| 54 | MG | CA | 1663 | 1/1 | 0.93 | 0.34 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3204 | 1/1 | 0.94 | 0.44 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3122 | 1/1 | 0.84 | 0.20 | - | 49,49,49,49 | 0 |
| 54 | MG | CA | 1672 | 1/1 | 0.89 | 0.20 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3538 | 1/1 | 0.92 | 0.13 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3071 | 1/1 | 0.95 | 0.17 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3009 | 1/1 | 0.93 | 0.29 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3433 | 1/1 | 0.86 | 0.12 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3014 | 1/1 | 0.80 | 0.55 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3211 | 1/1 | 0.96 | 0.09 | - | 26,26,26,26 | 0 |
| 54 | MG | AA | 1613 | 1/1 | 0.92 | 0.19 | - | 65,65,65,65 | 0 |
| 54 | MG | AA | 1714 | 1/1 | 0.92 | 0.25 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3196 | 1/1 | 0.93 | 0.17 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3643 | 1/1 | 0.94 | 0.10 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1673 | 1/1 | 0.94 | 0.59 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3149 | 1/1 | 0.84 | 0.28 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3084 | 1/1 | 0.95 | 0.25 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3274 | 1/1 | 0.90 | 0.41 | - | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1761 | 1/1 | 0.98 | 0.18 | - | 65,65,65,65 | 0 |
| 54 | MG | AA | 1632 | 1/1 | 0.92 | 0.21 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3308 | 1/1 | 0.92 | 0.17 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3122 | 1/1 | 0.94 | 0.31 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3226 | 1/1 | 0.94 | 0.50 | - | 55,55,55,55 | 0 |
| 54 | MG | BA | 3114 | 1/1 | 0.85 | 0.32 | - | 63,63,63,63 | 0 |
| 54 | MG | AA | 1734 | 1/1 | 0.87 | 0.11 | - | 96,96,96,96 | 0 |
| 54 | MG | BA | 3494 | 1/1 | 0.97 | 0.13 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3394 | 1/1 | 0.81 | 0.14 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3192 | 1/1 | 0.93 | 0.17 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3317 | 1/1 | 0.76 | 0.17 | - | 34,34,34,34 | 0 |
| 54 | MG | AA | 1716 | 1/1 | 0.89 | 0.08 | - | 116,116,116,116 | 0 |
| 54 | MG | DB | 207 | 1/1 | 0.96 | 0.24 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3554 | 1/1 | 0.69 | 0.10 | - | 88,88,88,88 | 0 |
| 54 | MG | DA | 3065 | 1/1 | 0.84 | 0.14 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3220 | 1/1 | 0.94 | 0.28 | - | 31,31,31,31 | 0 |
| 54 | MG | DA | 3349 | 1/1 | 0.95 | 0.15 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3407 | 1/1 | 0.89 | 0.17 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3512 | 1/1 | 0.89 | 0.13 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3067 | 1/1 | 0.95 | 0.23 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3641 | 1/1 | 0.92 | 0.21 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3199 | 1/1 | 0.93 | 0.18 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3467 | 1/1 | 0.97 | 0.11 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3352 | 1/1 | 0.97 | 0.14 | - | 81,81,81,81 | 0 |
| 54 | MG | DA | 3367 | 1/1 | 0.96 | 0.24 | - | 30,30,30,30 | 0 |
| 54 | MG | AA | 1732 | 1/1 | 0.94 | 0.10 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3250 | 1/1 | 0.94 | 0.17 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3088 | 1/1 | 0.97 | 0.39 | - | 55,55,55,55 | 0 |
| 54 | MG | AA | 1628 | 1/1 | 0.78 | 0.25 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3057 | 1/1 | 0.97 | 0.24 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3361 | 1/1 | 0.98 | 0.04 | - | 59,59,59,59 | 0 |
| 54 | MG | AA | 1637 | 1/1 | 0.69 | 0.24 | - | 84,84,84,84 | 0 |
| 54 | MG | CA | 1717 | 1/1 | 0.82 | 0.14 | - | 110,110,110,110 | 0 |
| 54 | MG | BA | 3532 | 1/1 | 0.74 | 0.23 | - | 79,79,79,79 | 0 |
| 54 | MG | CA | 1734 | 1/1 | 0.95 | 0.23 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3390 | 1/1 | 0.92 | 0.08 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3081 | 1/1 | 0.70 | 0.59 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3553 | 1/1 | 0.95 | 0.08 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3178 | 1/1 | 0.97 | 0.29 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3488 | 1/1 | 0.85 | 0.17 | - | 58,58,58,58 | 0 |
| 54 | MG | CA | 1671 | 1/1 | 0.94 | 0.43 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3357 | 1/1 | 0.99 | 0.16 | - | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3549 | 1/1 | 0.98 | 0.05 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3299 | 1/1 | 0.95 | 0.43 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3212 | 1/1 | 0.72 | 0.27 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3230 | 1/1 | 0.91 | 0.20 | - | 30,30,30,30 | 0 |
| 54 | MG | AA | 1643 | 1/1 | 0.93 | 0.59 | - | 47,47,47,47 | 0 |
| 54 | MG | CA | 1679 | 1/1 | 0.86 | 0.51 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3660 | 1/1 | 0.93 | 0.13 | - | 104,104,104,104 | 0 |
| 54 | MG | DA | 3577 | 1/1 | 0.98 | 0.09 | - | 57,57,57,57 | 0 |
| 54 | MG | AA | 1721 | 1/1 | 0.97 | 0.06 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3436 | 1/1 | 0.85 | 0.14 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3292 | 1/1 | 0.88 | 0.32 | - | 70,70,70,70 | 0 |
| 54 | MG | DA | 3318 | 1/1 | 0.87 | 0.14 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3235 | 1/1 | 0.94 | 0.20 | - | 50,50,50,50 | 0 |
| 54 | MG | DE | 303 | 1/1 | 0.89 | 0.12 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3035 | 1/1 | 0.94 | 0.17 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3121 | 1/1 | 0.98 | 0.33 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3131 | 1/1 | 0.89 | 0.82 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3498 | 1/1 | 0.96 | 0.10 | - | 28,28,28,28 | 0 |
| 54 | MG | BA | 3318 | 1/1 | 0.92 | 0.20 | - | 35,35,35,35 | 0 |
| 54 | MG | CA | 1688 | 1/1 | 0.97 | 0.35 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3125 | 1/1 | 0.95 | 0.31 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3154 | 1/1 | 0.95 | 0.33 | - | 26,26,26,26 | 0 |
| 54 | MG | BA | 3388 | 1/1 | 0.85 | 0.10 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3077 | 1/1 | 0.84 | 0.27 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3191 | 1/1 | 0.92 | 0.27 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3604 | 1/1 | 0.96 | 0.07 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3524 | 1/1 | 0.73 | 0.17 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 3072 | 1/1 | 0.93 | 0.10 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3385 | 1/1 | 0.96 | 0.09 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3012 | 1/1 | 0.91 | 0.34 | - | 27,27,27,27 | 0 |
| 54 | MG | DA | 3576 | 1/1 | 0.89 | 0.10 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3584 | 1/1 | 0.94 | 0.30 | - | 48,48,48,48 | 0 |
| 54 | MG | CA | 1746 | 1/1 | 0.90 | 0.11 | - | 97,97,97,97 | 0 |
| 54 | MG | BA | 3592 | 1/1 | 0.90 | 0.13 | - | 47,47,47,47 | 0 |
| 54 | MG | CA | 1624 | 1/1 | 0.96 | 0.54 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3116 | 1/1 | 0.95 | 0.17 | - | 53,53,53,53 | 0 |
| 54 | MG | DD | 301 | 1/1 | 0.92 | 0.22 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3127 | 1/1 | 0.91 | 0.25 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3325 | 1/1 | 0.96 | 0.11 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3332 | 1/1 | 0.92 | 0.23 | - | 53,53,53,53 | 0 |
| 54 | MG | AA | 1626 | 1/1 | 0.94 | 0.43 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 3455 | 1/1 | 0.95 | 0.05 | - | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3577 | 1/1 | 0.82 | 0.13 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 3240 | 1/1 | 0.64 | 0.28 | - | 71,71,71,71 | 0 |
| 54 | MG | DA | 3033 | 1/1 | 0.91 | 0.16 | - | 66,66,66,66 | 0 |
| 54 | MG | DA | 3136 | 1/1 | 0.91 | 0.33 | - | 62,62,62,62 | 0 |
| 54 | MG | AA | 1666 | 1/1 | 0.94 | 0.13 | - | 74,74,74,74 | 0 |
| 54 | MG | D0 | 101 | 1/1 | 0.95 | 0.09 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3112 | 1/1 | 0.98 | 0.24 | - | 51,51,51,51 | 0 |
| 54 | MG | BB | 219 | 1/1 | 0.91 | 0.06 | - | 105,105,105,105 | 0 |
| 54 | MG | DA | 3402 | 1/1 | 0.87 | 0.13 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3004 | 1/1 | 0.93 | 0.07 | - | 88,88,88,88 | 0 |
| 54 | MG | BF | 302 | 1/1 | 0.87 | 0.24 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3620 | 1/1 | 0.95 | 0.05 | - | 68,68,68,68 | 0 |
| 54 | MG | AA | 1693 | 1/1 | 0.96 | 0.11 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3364 | 1/1 | 0.95 | 0.07 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3459 | 1/1 | 0.87 | 0.17 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3605 | 1/1 | 0.96 | 0.07 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3107 | 1/1 | 0.98 | 0.08 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1642 | 1/1 | 0.89 | 0.17 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3054 | 1/1 | 0.90 | 0.17 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3465 | 1/1 | 0.86 | 0.08 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3534 | 1/1 | 0.84 | 0.19 | - | 25,25,25,25 | 0 |
| 54 | MG | AA | 1705 | 1/1 | 0.55 | 0.39 | - | 97,97,97,97 | 0 |
| 54 | MG | DA | 3190 | 1/1 | 0.94 | 0.10 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3503 | 1/1 | 0.86 | 0.10 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3146 | 1/1 | 0.70 | 0.60 | - | 65,65,65,65 | 0 |
| 54 | MG | AA | 1623 | 1/1 | 0.93 | 0.17 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3488 | 1/1 | 0.94 | 0.17 | - | 24,24,24,24 | 0 |
| 54 | MG | BA | 3420 | 1/1 | 0.97 | 0.19 | - | 61,61,61,61 | 0 |
| 54 | MG | BA | 3324 | 1/1 | 0.96 | 0.10 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3021 | 1/1 | 0.88 | 0.20 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3126 | 1/1 | 0.94 | 0.60 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3386 | 1/1 | 0.96 | 0.09 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3408 | 1/1 | 0.86 | 0.22 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3485 | 1/1 | 0.95 | 0.26 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3399 | 1/1 | 0.83 | 0.13 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3141 | 1/1 | 0.88 | 0.52 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3108 | 1/1 | 0.91 | 0.23 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3335 | 1/1 | 0.88 | 0.10 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3141 | 1/1 | 0.83 | 0.30 | - | 36,36,36,36 | 0 |
| 54 | MG | CA | 1725 | 1/1 | 0.95 | 0.18 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3104 | 1/1 | 0.95 | 0.22 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3236 | 1/1 | 0.92 | 0.30 | - | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1678 | 1/1 | 0.96 | 0.24 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3062 | 1/1 | 0.97 | 0.37 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3106 | 1/1 | 0.96 | 0.41 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3148 | 1/1 | 0.90 | 0.16 | - | 48,48,48,48 | 0 |
| 54 | MG | BB | 222 | 1/1 | 0.95 | 0.18 | - | 80,80,80,80 | 0 |
| 54 | MG | BA | 3098 | 1/1 | 0.94 | 0.24 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3251 | 1/1 | 0.89 | 0.18 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3642 | 1/1 | 0.72 | 0.15 | - | 139,139,139,139 | 0 |
| 54 | MG | BE | 304 | 1/1 | 1.00 | 0.19 | - | 25,25,25,25 | 0 |
| 54 | MG | BA | 3007 | 1/1 | 0.90 | 0.30 | - | 28,28,28,28 | 0 |
| 54 | MG | DA | 3493 | 1/1 | 0.96 | 0.04 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3144 | 1/1 | 0.92 | 0.47 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3013 | 1/1 | 0.95 | 0.12 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3544 | 1/1 | 0.92 | 0.06 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3522 | 1/1 | 0.87 | 0.23 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3173 | 1/1 | 0.95 | 0.13 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3386 | 1/1 | 0.96 | 0.08 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3494 | 1/1 | 0.94 | 0.14 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3587 | 1/1 | 0.84 | 0.24 | - | 95,95,95,95 | 0 |
| 54 | MG | AA | 1707 | 1/1 | 0.86 | 0.17 | - | 102,102,102,102 | 0 |
| 54 | MG | AA | 1654 | 1/1 | 0.86 | 0.52 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3608 | 1/1 | 0.95 | 0.26 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3576 | 1/1 | 0.97 | 0.19 | - | 21,21,21,21 | 0 |
| 54 | MG | AA | 1635 | 1/1 | 0.84 | 0.15 | - | 61,61,61,61 | 0 |
| 54 | MG | BB | 217 | 1/1 | 0.95 | 0.11 | - | 67,67,67,67 | 0 |
| 54 | MG | CA | 1618 | 1/1 | 0.83 | 0.40 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3120 | 1/1 | 0.92 | 0.26 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3140 | 1/1 | 0.96 | 0.56 | - | 36,36,36,36 | 0 |
| 54 | MG | DA | 3405 | 1/1 | 0.96 | 0.15 | - | 32,32,32,32 | 0 |
| 54 | MG | AA | 1723 | 1/1 | 0.65 | 0.12 | - | 112,112,112,112 | 0 |
| 54 | MG | AA | 1726 | 1/1 | 0.97 | 0.14 | - | 86,86,86,86 | 0 |
| 54 | MG | DA | 3145 | 1/1 | 0.89 | 0.23 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3076 | 1/1 | 0.96 | 0.15 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3615 | 1/1 | 0.94 | 0.12 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3215 | 1/1 | 0.88 | 0.09 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3228 | 1/1 | 0.92 | 0.48 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3342 | 1/1 | 0.76 | 0.18 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3061 | 1/1 | 0.93 | 0.17 | - | 32,32,32,32 | 0 |
| 54 | MG | DA | 3115 | 1/1 | 0.78 | 0.42 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3569 | 1/1 | 0.88 | 0.08 | - | 69,69,69,69 | 0 |
| 54 | MG | BA | 3147 | 1/1 | 0.93 | 0.11 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3064 | 1/1 | 0.94 | 0.36 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3283 | 1/1 | 0.97 | 0.45 | - | 21,21,21,21 | 0 |
| 54 | MG | BA | 3087 | 1/1 | 0.98 | 0.20 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3380 | 1/1 | 0.89 | 0.10 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3372 | 1/1 | 0.98 | 0.07 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3486 | 1/1 | 0.89 | 0.21 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3442 | 1/1 | 0.87 | 0.12 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3535 | 1/1 | 0.96 | 0.15 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3221 | 1/1 | 0.89 | 0.34 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3062 | 1/1 | 0.82 | 0.34 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3329 | 1/1 | 0.92 | 0.13 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3266 | 1/1 | 0.98 | 0.46 | - | 22,22,22,22 | 0 |
| 54 | MG | BA | 3209 | 1/1 | 0.95 | 0.21 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3515 | 1/1 | 0.83 | 0.28 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3480 | 1/1 | 0.98 | 0.18 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3253 | 1/1 | 0.96 | 0.09 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3172 | 1/1 | 0.79 | 0.29 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3202 | 1/1 | 0.60 | 0.33 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1740 | 1/1 | 0.93 | 0.40 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3275 | 1/1 | 0.88 | 0.36 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3529 | 1/1 | 0.97 | 0.09 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3189 | 1/1 | 0.83 | 0.19 | - | 84,84,84,84 | 0 |
| 54 | MG | DA | 3171 | 1/1 | 0.93 | 0.17 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3425 | 1/1 | 0.98 | 0.07 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3531 | 1/1 | 0.95 | 0.18 | - | 91,91,91,91 | 0 |
| 54 | MG | DA | 3552 | 1/1 | 0.95 | 0.39 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3268 | 1/1 | 0.94 | 0.37 | - | 27,27,27,27 | 0 |
| 54 | MG | AA | 1677 | 1/1 | 0.92 | 0.32 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3554 | 1/1 | 0.98 | 0.09 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3004 | 1/1 | 0.94 | 0.08 | - | 76,76,76,76 | 0 |
| 54 | MG | DA | 3324 | 1/1 | 0.86 | 0.12 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3030 | 1/1 | 0.90 | 0.28 | - | 55,55,55,55 | 0 |
| 54 | MG | BA | 3078 | 1/1 | 0.96 | 0.27 | - | 30,30,30,30 | 0 |
| 54 | MG | BA | 3505 | 1/1 | 0.97 | 0.20 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3651 | 1/1 | 0.95 | 0.21 | - | 87,87,87,87 | 0 |
| 54 | MG | BA | 3506 | 1/1 | 0.99 | 0.11 | - | 30,30,30,30 | 0 |
| 54 | MG | BA | 3301 | 1/1 | 0.88 | 0.66 | - | 75,75,75,75 | 0 |
| 54 | MG | BA | 3081 | 1/1 | 0.94 | 0.36 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3155 | 1/1 | 0.95 | 0.36 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1625 | 1/1 | 0.89 | 0.36 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3395 | 1/1 | 0.96 | 0.11 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3484 | 1/1 | 0.94 | 0.07 | - | 64,64,64,64 | 0 |
| 54 | MG | DA | 3351 | 1/1 | 0.96 | 0.12 | - | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1715 | 1/1 | 0.95 | 0.05 | - | 103,103,103,103 | 0 |
| 54 | MG | DA | 3288 | 1/1 | 0.91 | 0.25 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3192 | 1/1 | 0.96 | 0.10 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3616 | 1/1 | 0.80 | 0.28 | - | 131,131,131,131 | 0 |
| 54 | MG | DA | 3099 | 1/1 | 0.94 | 0.23 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3315 | 1/1 | 0.97 | 0.15 | - | 31,31,31,31 | 0 |
| 54 | MG | DA | 3306 | 1/1 | 0.92 | 0.35 | - | 29,29,29,29 | 0 |
| 54 | MG | CA | 1759 | 1/1 | 0.92 | 0.22 | - | 69,69,69,69 | 0 |
| 54 | MG | DA | 3509 | 1/1 | 0.91 | 0.19 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3510 | 1/1 | 0.74 | 0.11 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3177 | 1/1 | 0.64 | 0.13 | - | 88,88,88,88 | 0 |
| 54 | MG | DA | 3537 | 1/1 | 0.86 | 0.09 | - | 63,63,63,63 | 0 |
| 54 | MG | AA | 1601 | 1/1 | 0.93 | 0.29 | - | 55,55,55,55 | 0 |
| 54 | MG | CA | 1652 | 1/1 | 0.73 | 0.50 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3117 | 1/1 | 0.89 | 0.28 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3565 | 1/1 | 0.93 | 0.20 | - | 34,34,34,34 | 0 |
| 54 | MG | BA | 3507 | 1/1 | 0.91 | 0.28 | - | 41,41,41,41 | 0 |
| 54 | MG | AA | 1658 | 1/1 | 0.88 | 0.51 | - | 57,57,57,57 | 0 |
| 54 | MG | DA | 3548 | 1/1 | 0.84 | 0.12 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3459 | 1/1 | 0.90 | 0.07 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3124 | 1/1 | 0.97 | 0.38 | - | 37,37,37,37 | 0 |
| 54 | MG | CA | 1733 | 1/1 | 0.97 | 0.14 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3379 | 1/1 | 0.95 | 0.12 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3653 | 1/1 | 0.94 | 0.15 | - | 104,104,104,104 | 0 |
| 54 | MG | BA | 3579 | 1/1 | 0.87 | 0.09 | - | 100,100,100,100 | 0 |
| 54 | MG | DA | 3335 | 1/1 | 0.98 | 0.10 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3509 | 1/1 | 0.96 | 0.15 | - | 50,50,50,50 | 0 |
| 54 | MG | B2 | 101 | 1/1 | 0.95 | 0.17 | - | 45,45,45,45 | 0 |
| 54 | MG | CA | 1667 | 1/1 | 0.80 | 0.33 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3294 | 1/1 | 0.94 | 0.15 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3535 | 1/1 | 0.94 | 0.11 | - | 55,55,55,55 | 0 |
| 54 | MG | CA | 1704 | 1/1 | 0.77 | 0.15 | - | 92,92,92,92 | 0 |
| 54 | MG | DA | 3327 | 1/1 | 0.96 | 0.49 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3506 | 1/1 | 0.67 | 0.11 | - | 96,96,96,96 | 0 |
| 54 | MG | CA | 1720 | 1/1 | 0.80 | 0.14 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3135 | 1/1 | 0.96 | 0.41 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3491 | 1/1 | 0.97 | 0.10 | - | 28,28,28,28 | 0 |
| 54 | MG | CA | 1682 | 1/1 | 0.94 | 0.14 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3461 | 1/1 | 0.88 | 0.17 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3357 | 1/1 | 0.94 | 0.19 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3233 | 1/1 | 0.92 | 0.45 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3497 | 1/1 | 0.97 | 0.26 | - | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3252 | 1/1 | 0.90 | 0.54 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3060 | 1/1 | 0.89 | 0.14 | - | 54,54,54,54 | 0 |
| 54 | MG | BE | 305 | 1/1 | 0.82 | 0.16 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3521 | 1/1 | 0.95 | 0.09 | - | 40,40,40,40 | 0 |
| 54 | MG | BA | 3045 | 1/1 | 0.90 | 0.23 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3544 | 1/1 | 0.81 | 0.15 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3552 | 1/1 | 0.87 | 0.22 | - | 82,82,82,82 | 0 |
| 54 | MG | AQ | 201 | 1/1 | 0.89 | 0.25 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3627 | 1/1 | 0.81 | 0.10 | - | 50,50,50,50 | 0 |
| 54 | MG | CA | 1736 | 1/1 | 0.97 | 0.18 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3598 | 1/1 | 0.88 | 0.11 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3076 | 1/1 | 0.90 | 0.22 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3363 | 1/1 | 0.91 | 0.14 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3298 | 1/1 | 0.90 | 0.55 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1700 | 1/1 | 0.95 | 0.09 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3360 | 1/1 | 0.91 | 0.20 | - | 37,37,37,37 | 0 |
| 54 | MG | DA | 3408 | 1/1 | 0.90 | 0.15 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3474 | 1/1 | 0.93 | 0.08 | - | 37,37,37,37 | 0 |
| 54 | MG | AA | 1674 | 1/1 | 0.86 | 0.32 | - | 63,63,63,63 | 0 |
| 54 | MG | CA | 1658 | 1/1 | 0.93 | 0.34 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3215 | 1/1 | 0.85 | 0.22 | - | 50,50,50,50 | 0 |
| 54 | MG | DA | 3530 | 1/1 | 0.61 | 0.24 | - | 132,132,132,132 | 0 |
| 54 | MG | BA | 3524 | 1/1 | 0.76 | 0.12 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3191 | 1/1 | 0.88 | 0.19 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3344 | 1/1 | 0.95 | 0.31 | - | 61,61,61,61 | 0 |
| 54 | MG | BB | 221 | 1/1 | 0.94 | 0.06 | - | 50,50,50,50 | 0 |
| 54 | MG | CA | 1654 | 1/1 | 0.96 | 0.13 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3438 | 1/1 | 0.91 | 0.20 | - | 65,65,65,65 | 0 |
| 54 | MG | BA | 3371 | 1/1 | 0.96 | 0.12 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3195 | 1/1 | 0.94 | 0.22 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3176 | 1/1 | 0.94 | 0.16 | - | 60,60,60,60 | 0 |
| 54 | MG | CA | 1666 | 1/1 | 0.94 | 0.37 | - | 64,64,64,64 | 0 |
| 54 | MG | BZ | 301 | 1/1 | 0.94 | 0.17 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3354 | 1/1 | 0.90 | 0.09 | - | 49,49,49,49 | 0 |
| 54 | MG | CA | 1705 | 1/1 | 0.80 | 0.14 | - | 96,96,96,96 | 0 |
| 54 | MG | DA | 3448 | 1/1 | 0.96 | 0.10 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3551 | 1/1 | 0.97 | 0.11 | - | 82,82,82,82 | 0 |
| 54 | MG | AA | 1686 | 1/1 | 0.83 | 0.11 | - | 68,68,68,68 | 0 |
| 54 | MG | DA | 3520 | 1/1 | 0.95 | 0.12 | - | 56,56,56,56 | 0 |
| 54 | MG | AA | 1670 | 1/1 | 0.91 | 0.32 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3168 | 1/1 | 0.96 | 0.26 | - | 28,28,28,28 | 0 |
| 54 | MG | DA | 3422 | 1/1 | 0.97 | 0.18 | - | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3400 | 1/1 | 0.92 | 0.22 | - | 47,47,47,47 | 0 |
| 54 | MG | AA | 1616 | 1/1 | 0.88 | 0.14 | - | 92,92,92,92 | 0 |
| 54 | MG | CA | 1742 | 1/1 | 0.95 | 0.07 | - | 113,113,113,113 | 0 |
| 54 | MG | BA | 3636 | 1/1 | 0.97 | 0.06 | - | 28,28,28,28 | 0 |
| 54 | MG | BA | 3628 | 1/1 | 0.96 | 0.15 | - | 35,35,35,35 | 0 |
| 54 | MG | CA | 1657 | 1/1 | 0.79 | 0.41 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3220 | 1/1 | 0.82 | 0.24 | - | 51,51,51,51 | 0 |
| 54 | MG | DA | 3165 | 1/1 | 0.69 | 0.41 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3177 | 1/1 | 0.91 | 0.10 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3070 | 1/1 | 0.95 | 0.20 | - | 37,37,37,37 | 0 |
| 54 | MG | DO | 202 | 1/1 | 0.90 | 0.17 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3263 | 1/1 | 0.93 | 0.20 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3595 | 1/1 | 0.93 | 0.12 | - | 58,58,58,58 | 0 |
| 54 | MG | AA | 1696 | 1/1 | 0.97 | 0.16 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3261 | 1/1 | 0.77 | 0.36 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3237 | 1/1 | 0.87 | 0.29 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3556 | 1/1 | 0.96 | 0.20 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3403 | 1/1 | 0.81 | 0.15 | - | 67,67,67,67 | 0 |
| 54 | MG | DA | 3346 | 1/1 | 0.90 | 0.12 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3586 | 1/1 | 0.90 | 0.10 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3340 | 1/1 | 0.72 | 0.14 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3195 | 1/1 | 0.84 | 0.24 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3623 | 1/1 | 0.94 | 0.12 | - | 73,73,73,73 | 0 |
| 54 | MG | DA | 3268 | 1/1 | 0.82 | 0.58 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3313 | 1/1 | 0.96 | 0.08 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3126 | 1/1 | 0.96 | 0.22 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3581 | 1/1 | 0.96 | 0.09 | - | 52,52,52,52 | 0 |
| 54 | MG | CA | 1683 | 1/1 | 0.84 | 0.21 | - | 100,100,100,100 | 0 |
| 54 | MG | CA | 1731 | 1/1 | 0.89 | 0.12 | - | 74,74,74,74 | 0 |
| 54 | MG | DA | 3079 | 1/1 | 0.96 | 0.18 | - | 47,47,47,47 | 0 |
| 54 | MG | BA | 3166 | 1/1 | 0.96 | 0.29 | - | 36,36,36,36 | 0 |
| 54 | MG | DA | 3080 | 1/1 | 0.96 | 0.17 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3280 | 1/1 | 0.93 | 0.30 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3306 | 1/1 | 0.92 | 0.18 | - | 55,55,55,55 | 0 |
| 54 | MG | BA | 3185 | 1/1 | 0.87 | 0.51 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3622 | 1/1 | 0.93 | 0.11 | - | 45,45,45,45 | 0 |
| 54 | MG | BA | 3356 | 1/1 | 0.92 | 0.17 | - | 29,29,29,29 | 0 |
| 54 | MG | AA | 1622 | 1/1 | 0.68 | 0.19 | - | 81,81,81,81 | 0 |
| 54 | MG | DA | 3277 | 1/1 | 0.86 | 0.17 | - | 77,77,77,77 | 0 |
| 54 | MG | DA | 3066 | 1/1 | 0.91 | 0.20 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3236 | 1/1 | 0.79 | 0.23 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3649 | 1/1 | 0.83 | 0.22 | - | 125,125,125,125 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3592 | 1/1 | 0.93 | 0.06 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3279 | 1/1 | 0.97 | 0.12 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3614 | 1/1 | 0.97 | 0.04 | - | 66,66,66,66 | 0 |
| 54 | MG | AA | 1692 | 1/1 | 0.79 | 0.57 | - | 144,144,144,144 | 0 |
| 54 | MG | DA | 3499 | 1/1 | 0.91 | 0.14 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3063 | 1/1 | 0.93 | 0.13 | - | 54,54,54,54 | 0 |
| 54 | MG | CA | 1631 | 1/1 | 0.88 | 0.45 | - | 48,48,48,48 | 0 |
| 54 | MG | CA | 1696 | 1/1 | 0.95 | 0.43 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3527 | 1/1 | 0.94 | 0.15 | - | 91,91,91,91 | 0 |
| 54 | MG | DA | 3036 | 1/1 | 0.96 | 0.29 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3071 | 1/1 | 0.95 | 0.19 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3645 | 1/1 | 0.81 | 0.08 | - | 102,102,102,102 | 0 |
| 54 | MG | BA | 3346 | 1/1 | 0.90 | 0.12 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3374 | 1/1 | 0.93 | 0.08 | - | 34,34,34,34 | 0 |
| 54 | MG | DA | 3034 | 1/1 | 0.97 | 0.10 | - | 32,32,32,32 | 0 |
| 54 | MG | BA | 3326 | 1/1 | 0.97 | 0.11 | - | 49,49,49,49 | 0 |
| 54 | MG | AF | 201 | 1/1 | 0.88 | 0.20 | - | 62,62,62,62 | 0 |
| 54 | MG | DA | 3398 | 1/1 | 0.84 | 0.26 | - | 88,88,88,88 | 0 |
| 54 | MG | B5 | 102 | 1/1 | 0.97 | 0.10 | - | 52,52,52,52 | 0 |
| 54 | MG | DB | 204 | 1/1 | 0.71 | 0.70 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3421 | 1/1 | 0.90 | 0.07 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3058 | 1/1 | 0.95 | 0.14 | - | 32,32,32,32 | 0 |
| 54 | MG | AA | 1697 | 1/1 | 0.80 | 0.20 | - | 106,106,106,106 | 0 |
| 54 | MG | DA | 3086 | 1/1 | 0.90 | 0.21 | - | 48,48,48,48 | 0 |
| 54 | MG | CA | 1615 | 1/1 | 0.91 | 0.12 | - | 65,65,65,65 | 0 |
| 54 | MG | DA | 3591 | 1/1 | 0.81 | 0.11 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3650 | 1/1 | 0.91 | 0.16 | - | 88,88,88,88 | 0 |
| 54 | MG | BA | 3305 | 1/1 | 0.91 | 0.26 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1602 | 1/1 | 0.97 | 0.29 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3428 | 1/1 | 0.95 | 0.09 | - | 56,56,56,56 | 0 |
| 54 | MG | CA | 1719 | 1/1 | 0.98 | 0.07 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3393 | 1/1 | 0.90 | 0.19 | - | 37,37,37,37 | 0 |
| 54 | MG | CA | 1661 | 1/1 | 0.85 | 0.64 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3472 | 1/1 | 0.97 | 0.27 | - | 26,26,26,26 | 0 |
| 54 | MG | DA | 3310 | 1/1 | 0.96 | 0.37 | - | 28,28,28,28 | 0 |
| 54 | MG | CA | 1706 | 1/1 | 0.80 | 0.10 | - | 103,103,103,103 | 0 |
| 54 | MG | DA | 3395 | 1/1 | 0.96 | 0.11 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3227 | 1/1 | 0.89 | 0.28 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3020 | 1/1 | 0.90 | 0.18 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3590 | 1/1 | 0.82 | 0.24 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 3600 | 1/1 | 0.69 | 0.07 | - | 81,81,81,81 | 0 |
| 54 | MG | BA | 3634 | 1/1 | 0.99 | 0.11 | - | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BB | 205 | 1/1 | 0.92 | 0.38 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3536 | 1/1 | 0.93 | 0.16 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3169 | 1/1 | 0.94 | 0.23 | - | 31,31,31,31 | 0 |
| 54 | MG | AA | 1679 | 1/1 | 0.92 | 0.22 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3593 | 1/1 | 0.90 | 0.15 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3283 | 1/1 | 0.93 | 0.18 | - | 61,61,61,61 | 0 |
| 54 | MG | CA | 1603 | 1/1 | 0.83 | 0.30 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3314 | 1/1 | 0.93 | 0.39 | - | 43,43,43,43 | 0 |
| 54 | MG | DO | 201 | 1/1 | 0.95 | 0.09 | - | 120,120,120,120 | 0 |
| 54 | MG | AA | 1625 | 1/1 | 0.62 | 0.40 | - | 79,79,79,79 | 0 |
| 54 | MG | CA | 1757 | 1/1 | 0.69 | 0.26 | - | 80,80,80,80 | 0 |
| 54 | MG | CA | 1630 | 1/1 | 0.94 | 0.62 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3530 | 1/1 | 0.96 | 0.14 | - | 56,56,56,56 | 0 |
| 54 | MG | BA | 3107 | 1/1 | 0.86 | 0.20 | - | 60,60,60,60 | 0 |
| 54 | MG | DE | 304 | 1/1 | 0.96 | 0.21 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3060 | 1/1 | 0.92 | 0.34 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3016 | 1/1 | 0.84 | 0.22 | - | 62,62,62,62 | 0 |
| 54 | MG | BA | 3207 | 1/1 | 0.94 | 0.13 | - | 33,33,33,33 | 0 |
| 54 | MG | DA | 3153 | 1/1 | 0.86 | 0.42 | - | 58,58,58,58 | 0 |
| 54 | MG | AA | 1699 | 1/1 | 0.80 | 0.20 | - | 99,99,99,99 | 0 |
| 54 | MG | DA | 3198 | 1/1 | 0.82 | 0.79 | - | 57,57,57,57 | 0 |
| 54 | MG | CA | 1620 | 1/1 | 0.89 | 0.12 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3213 | 1/1 | 0.90 | 0.33 | - | 48,48,48,48 | 0 |
| 54 | MG | CA | 1676 | 1/1 | 0.88 | 0.24 | - | 73,73,73,73 | 0 |
| 54 | MG | CA | 1621 | 1/1 | 0.86 | 0.56 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3584 | 1/1 | 0.92 | 0.11 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3139 | 1/1 | 0.87 | 0.50 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3317 | 1/1 | 0.94 | 0.23 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3325 | 1/1 | 0.88 | 0.19 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3034 | 1/1 | 0.99 | 0.10 | - | 41,41,41,41 | 0 |
| 54 | MG | CA | 1674 | 1/1 | 0.88 | 0.11 | - | 74,74,74,74 | 0 |
| 54 | MG | CA | 1633 | 1/1 | 0.64 | 0.57 | - | 77,77,77,77 | 0 |
| 54 | MG | BA | 3208 | 1/1 | 0.95 | 0.29 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3164 | 1/1 | 0.83 | 0.35 | - | 50,50,50,50 | 0 |
| 54 | MG | BA | 3287 | 1/1 | 0.80 | 0.42 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3207 | 1/1 | 0.84 | 0.28 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3648 | 1/1 | 0.81 | 0.12 | - | 91,91,91,91 | 0 |
| 54 | MG | AA | 1648 | 1/1 | 0.96 | 0.44 | - | 44,44,44,44 | 0 |
| 54 | MG | DA | 3596 | 1/1 | 0.89 | 0.19 | - | 125,125,125,125 | 0 |
| 54 | MG | BA | 3347 | 1/1 | 0.76 | 0.16 | - | 94,94,94,94 | 0 |
| 54 | MG | DA | 3347 | 1/1 | 0.96 | 0.17 | - | 35,35,35,35 | 0 |
| 54 | MG | DA | 3312 | 1/1 | 0.86 | 0.52 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1699 | 1/1 | 0.95 | 0.15 | - | 83,83,83,83 | 0 |
| 54 | MG | DA | 3267 | 1/1 | 0.91 | 0.28 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1636 | 1/1 | 0.84 | 0.27 | - | 79,79,79,79 | 0 |
| 54 | MG | BA | 3633 | 1/1 | 0.95 | 0.12 | - | 43,43,43,43 | 0 |
| 54 | MG | AC | 301 | 1/1 | 0.94 | 0.14 | - | 57,57,57,57 | 0 |
| 54 | MG | CA | 1755 | 1/1 | 0.50 | 0.12 | - | 129,129,129,129 | 0 |
| 54 | MG | DA | 3214 | 1/1 | 0.90 | 0.24 | - | 37,37,37,37 | 0 |
| 54 | MG | BA | 3405 | 1/1 | 0.93 | 0.15 | - | 61,61,61,61 | 0 |
| 54 | MG | DA | 3037 | 1/1 | 0.96 | 0.12 | - | 43,43,43,43 | 0 |
| 54 | MG | BA | 3187 | 1/1 | 0.97 | 0.59 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3193 | 1/1 | 0.84 | 0.58 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3528 | 1/1 | 0.85 | 0.17 | - | 124,124,124,124 | 0 |
| 54 | MG | CA | 1622 | 1/1 | 0.94 | 0.28 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3185 | 1/1 | 0.85 | 0.16 | - | 57,57,57,57 | 0 |
| 54 | MG | AA | 1706 | 1/1 | 0.67 | 0.10 | - | 91,91,91,91 | 0 |
| 54 | MG | AA | 1708 | 1/1 | 0.88 | 0.29 | - | 91,91,91,91 | 0 |
| 54 | MG | D0 | 102 | 1/1 | 0.97 | 0.16 | - | 72,72,72,72 | 0 |
| 54 | MG | DA | 3143 | 1/1 | 0.97 | 0.19 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3077 | 1/1 | 0.93 | 0.17 | - | 49,49,49,49 | 0 |
| 54 | MG | DA | 3559 | 1/1 | 0.85 | 0.06 | - | 79,79,79,79 | 0 |
| 54 | MG | DA | 3249 | 1/1 | 0.95 | 0.29 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3085 | 1/1 | 0.89 | 0.49 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3541 | 1/1 | 0.76 | 0.12 | - | 130,130,130,130 | 0 |
| 54 | MG | DA | 3300 | 1/1 | 0.95 | 0.14 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3396 | 1/1 | 0.91 | 0.17 | - | 29,29,29,29 | 0 |
| 54 | MG | BA | 3100 | 1/1 | 0.86 | 0.20 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3186 | 1/1 | 0.93 | 0.13 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3029 | 1/1 | 0.87 | 0.18 | - | 32,32,32,32 | 0 |
| 54 | MG | BA | 3139 | 1/1 | 0.84 | 0.28 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3452 | 1/1 | 0.91 | 0.13 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3316 | 1/1 | 0.97 | 0.13 | - | 45,45,45,45 | 0 |
| 54 | MG | AA | 1649 | 1/1 | 0.89 | 0.31 | - | 43,43,43,43 | 0 |
| 54 | MG | CA | 1644 | 1/1 | 0.97 | 0.26 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3110 | 1/1 | 0.82 | 0.31 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3048 | 1/1 | 0.87 | 0.18 | - | 68,68,68,68 | 0 |
| 54 | MG | CA | 1762 | 1/1 | 0.88 | 0.07 | - | 156,156,156,156 | 0 |
| 54 | MG | CA | 1692 | 1/1 | 0.50 | 0.51 | - | 86,86,86,86 | 0 |
| 54 | MG | BB | 213 | 1/1 | 0.88 | 0.14 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3009 | 1/1 | 0.96 | 0.28 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3070 | 1/1 | 0.89 | 0.36 | - | 57,57,57,57 | 0 |
| 54 | MG | BA | 3537 | 1/1 | 0.98 | 0.17 | - | 31,31,31,31 | 0 |
| 54 | MG | DA | 3401 | 1/1 | 0.71 | 0.29 | - | 108,108,108,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DA | 3225 | 1/1 | 0.92 | 0.50 | - | 51,51,51,51 | 0 |
| 54 | MG | BA | 3431 | 1/1 | 0.92 | 0.08 | - | 71,71,71,71 | 0 |
| 54 | MG | AA | 1675 | 1/1 | 0.90 | 0.23 | - | 76,76,76,76 | 0 |
| 54 | MG | BA | 3097 | 1/1 | 0.68 | 0.54 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3262 | 1/1 | 0.85 | 0.33 | - | 53,53,53,53 | 0 |
| 54 | MG | BT | 201 | 1/1 | 0.92 | 0.15 | - | 53,53,53,53 | 0 |
| 54 | MG | DA | 3315 | 1/1 | 0.96 | 0.11 | - | 31,31,31,31 | 0 |
| 54 | MG | BA | 3349 | 1/1 | 0.94 | 0.10 | - | 36,36,36,36 | 0 |
| 54 | MG | DA | 3320 | 1/1 | 0.95 | 0.14 | - | 38,38,38,38 | 0 |
| 54 | MG | DA | 3545 | 1/1 | 0.92 | 0.08 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3114 | 1/1 | 0.97 | 0.39 | - | 30,30,30,30 | 0 |
| 54 | MG | BA | 3515 | 1/1 | 0.91 | 0.16 | - | 72,72,72,72 | 0 |
| 54 | MG | BA | 3079 | 1/1 | 0.95 | 0.20 | - | 50,50,50,50 | 0 |
| 54 | MG | CA | 1681 | 1/1 | 0.82 | 0.41 | - | 82,82,82,82 | 0 |
| 54 | MG | DA | 3184 | 1/1 | 0.94 | 0.15 | - | 46,46,46,46 | 0 |
| 54 | MG | BA | 3213 | 1/1 | 0.98 | 0.10 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3575 | 1/1 | 0.96 | 0.21 | - | 35,35,35,35 | 0 |
| 54 | MG | DA | 3585 | 1/1 | 0.99 | 0.13 | - | 33,33,33,33 | 0 |
| 54 | MG | CA | 1636 | 1/1 | 0.90 | 0.36 | - | 59,59,59,59 | 0 |
| 54 | MG | BF | 301 | 1/1 | 0.95 | 0.21 | - | 33,33,33,33 | 0 |
| 54 | MG | AA | 1657 | 1/1 | 0.93 | 0.39 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3237 | 1/1 | 0.51 | 0.32 | - | 71,71,71,71 | 0 |
| 54 | MG | BA | 3293 | 1/1 | 0.97 | 0.18 | - | 48,48,48,48 | 0 |
| 54 | MG | BA | 3182 | 1/1 | 0.94 | 0.41 | - | 37,37,37,37 | 0 |
| 54 | MG | CA | 1627 | 1/1 | 0.86 | 0.37 | - | 55,55,55,55 | 0 |
| 54 | MG | DA | 3319 | 1/1 | 0.87 | 0.32 | - | 57,57,57,57 | 0 |
| 54 | MG | AA | 1611 | 1/1 | 0.91 | 0.28 | - | 83,83,83,83 | 0 |
| 54 | MG | CA | 1710 | 1/1 | 0.94 | 0.09 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3532 | 1/1 | 0.54 | 0.23 | - | 116,116,116,116 | 0 |
| 54 | MG | DA | 3504 | 1/1 | 0.89 | 0.07 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3447 | 1/1 | 0.89 | 0.27 | - | 74,74,74,74 | 0 |
| 54 | MG | BA | 3563 | 1/1 | 0.91 | 0.09 | - | 70,70,70,70 | 0 |
| 54 | MG | BA | 3571 | 1/1 | 0.91 | 0.17 | - | 44,44,44,44 | 0 |
| 54 | MG | BA | 3110 | 1/1 | 0.93 | 0.20 | - | 66,66,66,66 | 0 |
| 54 | MG | CA | 1758 | 1/1 | 0.87 | 0.22 | - | 84,84,84,84 | 0 |
| 54 | MG | BA | 3450 | 1/1 | 0.93 | 0.10 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3512 | 1/1 | 0.59 | 0.28 | - | 109,109,109,109 | 0 |
| 54 | MG | AA | 1713 | 1/1 | 0.91 | 0.10 | - | 91,91,91,91 | 0 |
| 54 | MG | BA | 3496 | 1/1 | 0.92 | 0.17 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3281 | 1/1 | 0.94 | 0.25 | - | 24,24,24,24 | 0 |
| 54 | MG | DA | 3206 | 1/1 | 0.96 | 0.60 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3300 | 1/1 | 0.89 | 0.42 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1608 | 1/1 | 0.81 | 0.53 | - | 93,93,93,93 | 0 |
| 54 | MG | DA | 3138 | 1/1 | 0.97 | 0.31 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3082 | 1/1 | 0.99 | 0.12 | - | 36,36,36,36 | 0 |
| 54 | MG | BA | 3553 | 1/1 | 0.87 | 0.11 | - | 89,89,89,89 | 0 |
| 54 | MG | BA | 3267 | 1/1 | 0.90 | 0.33 | - | 36,36,36,36 | 0 |
| 54 | MG | CA | 1713 | 1/1 | 0.89 | 0.14 | - | 73,73,73,73 | 0 |
| 54 | MG | BA | 3612 | 1/1 | 0.91 | 0.07 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3370 | 1/1 | 0.83 | 0.23 | - | 41,41,41,41 | 0 |
| 54 | MG | BA | 3074 | 1/1 | 0.81 | 0.44 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3659 | 1/1 | 0.88 | 0.07 | - | 81,81,81,81 | 0 |
| 54 | MG | AA | 1608 | 1/1 | 0.97 | 0.33 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3391 | 1/1 | 0.96 | 0.11 | - | 39,39,39,39 | 0 |
| 54 | MG | AA | 1663 | 1/1 | 0.84 | 0.52 | - | 64,64,64,64 | 0 |
| 54 | MG | BA | 3398 | 1/1 | 0.93 | 0.14 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3211 | 1/1 | 0.90 | 0.23 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3135 | 1/1 | 0.95 | 0.32 | - | 47,47,47,47 | 0 |
| 54 | MG | DA | 3119 | 1/1 | 0.89 | 0.33 | - | 48,48,48,48 | 0 |
| 54 | MG | DA | 3556 | 1/1 | 0.92 | 0.06 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3255 | 1/1 | 0.88 | 0.20 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3432 | 1/1 | 0.93 | 0.04 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3206 | 1/1 | 0.97 | 0.26 | - | 49,49,49,49 | 0 |
| 54 | MG | BA | 3545 | 1/1 | 0.96 | 0.07 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3168 | 1/1 | 0.96 | 0.20 | - | 42,42,42,42 | 0 |
| 54 | MG | DA | 3428 | 1/1 | 0.98 | 0.05 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3285 | 1/1 | 0.89 | 0.57 | - | 38,38,38,38 | 0 |
| 54 | MG | BA | 3254 | 1/1 | 0.91 | 0.35 | - | 25,25,25,25 | 0 |
| 54 | MG | DA | 3054 | 1/1 | 0.95 | 0.12 | - | 46,46,46,46 | 0 |
| 54 | MG | DA | 3012 | 1/1 | 0.88 | 0.19 | - | 30,30,30,30 | 0 |
| 54 | MG | DA | 3286 | 1/1 | 0.98 | 0.20 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3294 | 1/1 | 0.97 | 0.19 | - | 39,39,39,39 | 0 |
| 54 | MG | BA | 3543 | 1/1 | 0.78 | 0.19 | - | 119,119,119,119 | 0 |
| 54 | MG | BA | 3134 | 1/1 | 0.92 | 0.43 | - | 41,41,41,41 | 0 |
| 54 | MG | DA | 3371 | 1/1 | 0.83 | 0.25 | - | 43,43,43,43 | 0 |
| 54 | MG | DA | 3440 | 1/1 | 0.96 | 0.28 | - | 42,42,42,42 | 0 |
| 54 | MG | BA | 3523 | 1/1 | 0.86 | 0.10 | - | 110,110,110,110 | 0 |
| 54 | MG | BA | 3568 | 1/1 | 0.97 | 0.12 | - | 39,39,39,39 | 0 |
| 54 | MG | DA | 3280 | 1/1 | 0.77 | 0.44 | - | 58,58,58,58 | 0 |
| 54 | MG | CA | 1616 | 1/1 | 0.88 | 0.26 | - | 58,58,58,58 | 0 |
| 54 | MG | DA | 3582 | 1/1 | 0.89 | 0.25 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3311 | 1/1 | 0.93 | 0.17 | - | 24,24,24,24 | 0 |
| 54 | MG | AA | 1695 | 1/1 | 0.95 | 0.11 | - | 74,74,74,74 | 0 |
| 54 | MG | CA | 1711 | 1/1 | 0.66 | 0.11 | - | 103,103,103,103 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | BA | 3638 | 1/1 | 0.75 | 0.13 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3499 | 1/1 | 0.97 | 0.12 | - | 60,60,60,60 | 0 |
| 54 | MG | DA | 3400 | 1/1 | 0.90 | 0.17 | - | 66,66,66,66 | 0 |
| 54 | MG | BA | 3531 | 1/1 | 0.83 | 0.09 | - | 89,89,89,89 | 0 |
| 54 | MG | DA | 3048 | 1/1 | 0.91 | 0.25 | - | 40,40,40,40 | 0 |
| 54 | MG | DA | 3078 | 1/1 | 0.97 | 0.17 | - | 48,48,48,48 | 0 |
| 54 | MG | AA | 1640 | 1/1 | 0.90 | 0.19 | - | 58,58,58,58 | 0 |
| 54 | MG | BA | 3587 | 1/1 | 0.86 | 0.14 | - | 60,60,60,60 | 0 |
| 54 | MG | BA | 3402 | 1/1 | 0.98 | 0.06 | - | 54,54,54,54 | 0 |
| 54 | MG | BA | 3104 | 1/1 | 0.85 | 0.23 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3020 | 1/1 | 0.92 | 0.09 | - | 82,82,82,82 | 0 |
| 54 | MG | BA | 3151 | 1/1 | 0.98 | 0.35 | - | 33,33,33,33 | 0 |
| 54 | MG | BA | 3610 | 1/1 | 0.95 | 0.08 | - | 63,63,63,63 | 0 |
| 54 | MG | DA | 3093 | 1/1 | 0.92 | 0.27 | - | 56,56,56,56 | 0 |
| 54 | MG | DA | 3296 | 1/1 | 0.93 | 0.09 | - | 67,67,67,67 | 0 |
| 54 | MG | BA | 3618 | 1/1 | 0.95 | 0.08 | - | 52,52,52,52 | 0 |
| 54 | MG | DA | 3222 | 1/1 | 0.85 | 0.23 | - | 68,68,68,68 | 0 |
| 54 | MG | BA | 3193 | 1/1 | 0.92 | 0.67 | - | 35,35,35,35 | 0 |
| 54 | MG | BA | 3008 | 1/1 | 0.89 | 0.23 | - | 28,28,28,28 | 0 |
| 54 | MG | DA | 3580 | 1/1 | 0.98 | 0.17 | - | 52,52,52,52 | 0 |
| 54 | MG | BA | 3439 | 1/1 | 0.90 | 0.16 | - | 59,59,59,59 | 0 |
| 54 | MG | BA | 3171 | 1/1 | 0.92 | 0.32 | - | 31,31,31,31 | 0 |
| 54 | MG | DA | 3059 | 1/1 | 0.86 | 0.21 | - | 45,45,45,45 | 0 |
| 54 | MG | DA | 3543 | 1/1 | 0.90 | 0.09 | - | 53,53,53,53 | 0 |
| 54 | MG | BA | 3290 | 1/1 | 0.92 | 0.17 | - | 63,63,63,63 | 0 |
| 54 | MG | BA | 3084 | 1/1 | 0.87 | 0.11 | - | 59,59,59,59 | 0 |
| 54 | MG | DA | 3217 | 1/1 | 0.99 | 0.49 | - | 32,32,32,32 | 0 |
| 54 | MG | AA | 1606 | 1/1 | 0.86 | 0.19 | - | 79,79,79,79 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.