



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:52 PM GMT

PDB ID : 4WPO
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G in the pre-translocational state
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-20
Resolution : 2.80 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

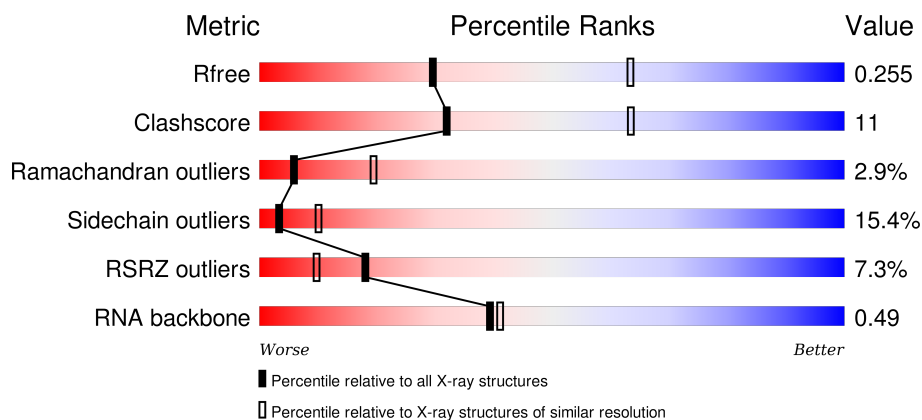
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 | 2393 (2.80-2.80) |
| Clashscore | 102246 | 2827 (2.80-2.80) |
| Ramachandran outliers | 100387 | 2782 (2.80-2.80) |
| Sidechain outliers | 100360 | 2784 (2.80-2.80) |
| RSRZ outliers | 91569 | 2404 (2.80-2.80) |
| RNA backbone | 2183 | 1091 (3.20-2.40) |

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 | 2915 | <div> <div>2%</div> <div>39% 41% 16%</div> </div> |
| 1 | CA | 2915 | <div> <div>4%</div> <div>48% 37% 12%</div> </div> |
| 2 | AB | 121 | <div> <div>56% 35% 8%</div> </div> |
| 2 | CB | 121 | <div> <div>58% 31% 10%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 228 | |
| 3 | CC | 228 | |
| 4 | AD | 276 | |
| 4 | CD | 276 | |
| 5 | AE | 206 | |
| 5 | CE | 206 | |
| 6 | AF | 210 | |
| 6 | CF | 210 | |
| 7 | AG | 182 | |
| 7 | CG | 182 | |
| 8 | AH | 180 | |
| 8 | CH | 180 | |
| 9 | AK | 173 | |
| 9 | CK | 173 | |
| 10 | AL | 147 | |
| 10 | CL | 147 | |
| 11 | AN | 140 | |
| 11 | CN | 140 | |
| 12 | AO | 122 | |
| 12 | CO | 122 | |
| 13 | AP | 150 | |
| 13 | CP | 150 | |
| 14 | AQ | 141 | |
| 14 | CQ | 141 | |
| 15 | AR | 118 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CR | 118 | |
| 16 | AS | 112 | |
| 16 | CS | 112 | |
| 17 | AT | 146 | |
| 17 | CT | 146 | |
| 18 | AU | 118 | |
| 18 | CU | 118 | |
| 19 | AV | 101 | |
| 19 | CV | 101 | |
| 20 | AW | 113 | |
| 20 | CW | 113 | |
| 21 | AX | 96 | |
| 21 | CX | 96 | |
| 22 | AY | 110 | |
| 22 | CY | 110 | |
| 23 | AZ | 206 | |
| 23 | CZ | 206 | |
| 24 | A0 | 85 | |
| 24 | C0 | 85 | |
| 25 | A1 | 98 | |
| 25 | C1 | 98 | |
| 26 | A2 | 72 | |
| 26 | C2 | 72 | |
| 27 | A3 | 60 | |
| 27 | C3 | 60 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | A4 | 71 | |
| 28 | C4 | 71 | |
| 29 | A5 | 60 | |
| 29 | C5 | 60 | |
| 30 | A6 | 54 | |
| 30 | C6 | 54 | |
| 31 | A7 | 49 | |
| 31 | C7 | 49 | |
| 32 | A8 | 65 | |
| 32 | C8 | 65 | |
| 33 | A9 | 37 | |
| 33 | C9 | 37 | |
| 34 | BA | 1521 | |
| 34 | DA | 1521 | |
| 35 | BB | 256 | |
| 35 | DB | 256 | |
| 36 | BC | 239 | |
| 36 | DC | 239 | |
| 37 | BD | 209 | |
| 37 | DD | 209 | |
| 38 | BE | 162 | |
| 38 | DE | 162 | |
| 39 | BF | 101 | |
| 39 | DF | 101 | |
| 40 | BG | 156 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | DG | 156 | |
| 41 | BH | 138 | |
| 41 | DH | 138 | |
| 42 | BI | 128 | |
| 42 | DI | 128 | |
| 43 | BJ | 105 | |
| 43 | DJ | 105 | |
| 44 | BK | 129 | |
| 44 | DK | 129 | |
| 45 | BL | 132 | |
| 45 | DL | 132 | |
| 46 | BM | 126 | |
| 46 | DM | 126 | |
| 47 | BN | 61 | |
| 47 | DN | 61 | |
| 48 | BO | 89 | |
| 48 | DO | 89 | |
| 49 | BP | 88 | |
| 49 | DP | 88 | |
| 50 | BQ | 105 | |
| 50 | DQ | 105 | |
| 51 | BR | 88 | |
| 51 | DR | 88 | |
| 52 | BS | 93 | |
| 52 | DS | 93 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | BT | 106 | |
| 53 | DT | 106 | |
| 54 | BU | 27 | |
| 54 | DU | 27 | |
| 55 | BV | 24 | |
| 55 | DV | 24 | |
| 56 | BW | 76 | |
| 56 | DW | 76 | |
| 57 | BX | 77 | |
| 57 | DX | 77 | |
| 58 | BY | 76 | |
| 58 | DY | 76 | |
| 59 | BZ | 758 | |
| 59 | DZ | 758 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | A0 | 101 | - | - | - | X |
| 60 | MG | AA | 3001 | - | - | - | X |
| 60 | MG | AA | 3008 | - | - | - | X |
| 60 | MG | AA | 3018 | - | - | - | X |
| 60 | MG | AA | 3019 | - | - | - | X |
| 60 | MG | AA | 3020 | - | - | - | X |
| 60 | MG | AA | 3021 | - | - | - | X |
| 60 | MG | AA | 3023 | - | - | - | X |
| 60 | MG | AA | 3033 | - | - | - | X |
| 60 | MG | AA | 3034 | - | - | - | X |
| 60 | MG | AA | 3035 | - | - | - | X |
| 60 | MG | AA | 3036 | - | - | - | X |
| 60 | MG | AA | 3038 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | AA | 3039 | - | - | - | X |
| 60 | MG | AA | 3042 | - | - | - | X |
| 60 | MG | AA | 3043 | - | - | - | X |
| 60 | MG | AA | 3044 | - | - | - | X |
| 60 | MG | AA | 3045 | - | - | - | X |
| 60 | MG | AA | 3047 | - | - | - | X |
| 60 | MG | AA | 3050 | - | - | - | X |
| 60 | MG | AA | 3052 | - | - | - | X |
| 60 | MG | AA | 3060 | - | - | - | X |
| 60 | MG | AA | 3082 | - | - | - | X |
| 60 | MG | AA | 3101 | - | - | - | X |
| 60 | MG | AA | 3102 | - | - | - | X |
| 60 | MG | AA | 3109 | - | - | - | X |
| 60 | MG | AA | 3110 | - | - | - | X |
| 60 | MG | AA | 3112 | - | - | - | X |
| 60 | MG | AA | 3115 | - | - | - | X |
| 60 | MG | AA | 3116 | - | - | - | X |
| 60 | MG | AA | 3119 | - | - | - | X |
| 60 | MG | AA | 3120 | - | - | - | X |
| 60 | MG | AA | 3121 | - | - | - | X |
| 60 | MG | AA | 3127 | - | - | - | X |
| 60 | MG | AA | 3129 | - | - | - | X |
| 60 | MG | AA | 3131 | - | - | - | X |
| 60 | MG | AA | 3133 | - | - | - | X |
| 60 | MG | AA | 3134 | - | - | - | X |
| 60 | MG | AA | 3137 | - | - | - | X |
| 60 | MG | AA | 3141 | - | - | - | X |
| 60 | MG | AA | 3144 | - | - | - | X |
| 60 | MG | AA | 3149 | - | - | - | X |
| 60 | MG | AA | 3160 | - | - | - | X |
| 60 | MG | AA | 3167 | - | - | - | X |
| 60 | MG | AA | 3168 | - | - | - | X |
| 60 | MG | AA | 3170 | - | - | - | X |
| 60 | MG | AA | 3172 | - | - | - | X |
| 60 | MG | AA | 3173 | - | - | - | X |
| 60 | MG | AA | 3178 | - | - | - | X |
| 60 | MG | AA | 3180 | - | - | - | X |
| 60 | MG | AA | 3181 | - | - | - | X |
| 60 | MG | AA | 3183 | - | - | - | X |
| 60 | MG | AA | 3184 | - | - | - | X |
| 60 | MG | AA | 3185 | - | - | - | X |
| 60 | MG | AA | 3187 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | AA | 3190 | - | - | - | X |
| 60 | MG | AA | 3196 | - | - | - | X |
| 60 | MG | AA | 3200 | - | - | - | X |
| 60 | MG | AA | 3206 | - | - | - | X |
| 60 | MG | AA | 3210 | - | - | - | X |
| 60 | MG | AA | 3211 | - | - | - | X |
| 60 | MG | AA | 3212 | - | - | - | X |
| 60 | MG | AA | 3213 | - | - | - | X |
| 60 | MG | AA | 3217 | - | - | - | X |
| 60 | MG | AA | 3218 | - | - | - | X |
| 60 | MG | AA | 3220 | - | - | - | X |
| 60 | MG | AA | 3222 | - | - | - | X |
| 60 | MG | AA | 3228 | - | - | - | X |
| 60 | MG | AA | 3231 | - | - | - | X |
| 60 | MG | AA | 3240 | - | - | - | X |
| 60 | MG | AA | 3241 | - | - | - | X |
| 60 | MG | AA | 3248 | - | - | - | X |
| 60 | MG | AA | 3250 | - | - | - | X |
| 60 | MG | AA | 3251 | - | - | - | X |
| 60 | MG | AA | 3253 | - | - | - | X |
| 60 | MG | AA | 3257 | - | - | - | X |
| 60 | MG | AA | 3258 | - | - | - | X |
| 60 | MG | AA | 3272 | - | - | - | X |
| 60 | MG | AA | 3274 | - | - | - | X |
| 60 | MG | AA | 3277 | - | - | - | X |
| 60 | MG | AA | 3281 | - | - | - | X |
| 60 | MG | AA | 3289 | - | - | - | X |
| 60 | MG | AA | 3294 | - | - | - | X |
| 60 | MG | AA | 3296 | - | - | - | X |
| 60 | MG | AA | 3300 | - | - | - | X |
| 60 | MG | AA | 3302 | - | - | - | X |
| 60 | MG | AA | 3309 | - | - | - | X |
| 60 | MG | AA | 3310 | - | - | - | X |
| 60 | MG | AA | 3313 | - | - | - | X |
| 60 | MG | AA | 3315 | - | - | - | X |
| 60 | MG | AA | 3323 | - | - | - | X |
| 60 | MG | AA | 3330 | - | - | - | X |
| 60 | MG | AA | 3339 | - | - | - | X |
| 60 | MG | AA | 3347 | - | - | - | X |
| 60 | MG | AA | 3352 | - | - | - | X |
| 60 | MG | AA | 3354 | - | - | - | X |
| 60 | MG | AA | 3357 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | AA | 3369 | - | - | - | X |
| 60 | MG | AA | 3376 | - | - | - | X |
| 60 | MG | AA | 3378 | - | - | - | X |
| 60 | MG | AA | 3384 | - | - | - | X |
| 60 | MG | AA | 3385 | - | - | - | X |
| 60 | MG | AA | 3386 | - | - | - | X |
| 60 | MG | AA | 3387 | - | - | - | X |
| 60 | MG | AA | 3398 | - | - | - | X |
| 60 | MG | AA | 3401 | - | - | - | X |
| 60 | MG | AA | 3408 | - | - | - | X |
| 60 | MG | AA | 3415 | - | - | - | X |
| 60 | MG | AA | 3417 | - | - | - | X |
| 60 | MG | AA | 3430 | - | - | - | X |
| 60 | MG | AA | 3437 | - | - | - | X |
| 60 | MG | AA | 3438 | - | - | - | X |
| 60 | MG | AA | 3451 | - | - | - | X |
| 60 | MG | AA | 3454 | - | - | - | X |
| 60 | MG | AA | 3460 | - | - | - | X |
| 60 | MG | AA | 3461 | - | - | - | X |
| 60 | MG | AA | 3471 | - | - | - | X |
| 60 | MG | AA | 3486 | - | - | - | X |
| 60 | MG | AA | 3505 | - | - | - | X |
| 60 | MG | AA | 3506 | - | - | - | X |
| 60 | MG | AA | 3507 | - | - | - | X |
| 60 | MG | AA | 3510 | - | - | - | X |
| 60 | MG | AA | 3513 | - | - | - | X |
| 60 | MG | AA | 3514 | - | - | - | X |
| 60 | MG | AA | 3516 | - | - | - | X |
| 60 | MG | AA | 3517 | - | - | - | X |
| 60 | MG | AA | 3518 | - | - | - | X |
| 60 | MG | AA | 3523 | - | - | - | X |
| 60 | MG | AA | 3524 | - | - | - | X |
| 60 | MG | AA | 3525 | - | - | - | X |
| 60 | MG | AA | 3528 | - | - | - | X |
| 60 | MG | AA | 3529 | - | - | - | X |
| 60 | MG | AA | 3532 | - | - | - | X |
| 60 | MG | AA | 3535 | - | - | - | X |
| 60 | MG | AA | 3539 | - | - | - | X |
| 60 | MG | AA | 3540 | - | - | - | X |
| 60 | MG | AA | 3541 | - | - | - | X |
| 60 | MG | AA | 3551 | - | - | - | X |
| 60 | MG | AA | 3556 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | AA | 3559 | - | - | - | X |
| 60 | MG | AA | 3564 | - | - | - | X |
| 60 | MG | AA | 3565 | - | - | - | X |
| 60 | MG | AA | 3572 | - | - | - | X |
| 60 | MG | AA | 3581 | - | - | - | X |
| 60 | MG | AA | 3582 | - | - | - | X |
| 60 | MG | AA | 3589 | - | - | - | X |
| 60 | MG | AA | 3596 | - | - | - | X |
| 60 | MG | AA | 3602 | - | - | - | X |
| 60 | MG | AA | 3604 | - | - | - | X |
| 60 | MG | AA | 3654 | - | - | - | X |
| 60 | MG | AA | 3662 | - | - | - | X |
| 60 | MG | AA | 3669 | - | - | - | X |
| 60 | MG | AA | 3671 | - | - | - | X |
| 60 | MG | AA | 3686 | - | - | - | X |
| 60 | MG | AA | 3692 | - | - | - | X |
| 60 | MG | AA | 3698 | - | - | - | X |
| 60 | MG | AA | 3702 | - | - | - | X |
| 60 | MG | AA | 3705 | - | - | - | X |
| 60 | MG | AA | 3706 | - | - | - | X |
| 60 | MG | AA | 3708 | - | - | - | X |
| 60 | MG | AA | 3711 | - | - | - | X |
| 60 | MG | AA | 3712 | - | - | - | X |
| 60 | MG | AA | 3714 | - | - | - | X |
| 60 | MG | AA | 3717 | - | - | - | X |
| 60 | MG | AA | 3721 | - | - | - | X |
| 60 | MG | AA | 3735 | - | - | - | X |
| 60 | MG | AA | 3739 | - | - | - | X |
| 60 | MG | AA | 3740 | - | - | - | X |
| 60 | MG | AA | 3741 | - | - | - | X |
| 60 | MG | AA | 3767 | - | - | - | X |
| 60 | MG | AA | 3769 | - | - | - | X |
| 60 | MG | AA | 3770 | - | - | - | X |
| 60 | MG | AA | 3772 | - | - | - | X |
| 60 | MG | AA | 3790 | - | - | - | X |
| 60 | MG | AA | 3792 | - | - | - | X |
| 60 | MG | AA | 3796 | - | - | - | X |
| 60 | MG | AA | 3797 | - | - | - | X |
| 60 | MG | AA | 3803 | - | - | - | X |
| 60 | MG | AA | 3806 | - | - | - | X |
| 60 | MG | AA | 3810 | - | - | - | X |
| 60 | MG | AA | 3816 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | AA | 3817 | - | - | - | X |
| 60 | MG | AA | 3818 | - | - | - | X |
| 60 | MG | AA | 3819 | - | - | - | X |
| 60 | MG | AA | 3822 | - | - | - | X |
| 60 | MG | AA | 3823 | - | - | - | X |
| 60 | MG | AA | 3824 | - | - | - | X |
| 60 | MG | AA | 3825 | - | - | - | X |
| 60 | MG | AA | 3826 | - | - | - | X |
| 60 | MG | AA | 3827 | - | - | - | X |
| 60 | MG | AA | 3828 | - | - | - | X |
| 60 | MG | AA | 3829 | - | - | - | X |
| 60 | MG | AA | 3830 | - | - | - | X |
| 60 | MG | AA | 3832 | - | - | - | X |
| 60 | MG | AA | 3833 | - | - | - | X |
| 60 | MG | AA | 3834 | - | - | - | X |
| 60 | MG | AB | 3008 | - | - | - | X |
| 60 | MG | AB | 3014 | - | - | - | X |
| 60 | MG | AB | 3016 | - | - | - | X |
| 60 | MG | AD | 301 | - | - | - | X |
| 60 | MG | AD | 302 | - | - | - | X |
| 60 | MG | AD | 304 | - | - | - | X |
| 60 | MG | AD | 305 | - | - | - | X |
| 60 | MG | AD | 308 | - | - | - | X |
| 60 | MG | AD | 309 | - | - | - | X |
| 60 | MG | AD | 310 | - | - | - | X |
| 60 | MG | AE | 305 | - | - | - | X |
| 60 | MG | AF | 301 | - | - | - | X |
| 60 | MG | AF | 303 | - | - | - | X |
| 60 | MG | AH | 201 | - | - | - | X |
| 60 | MG | AN | 3001 | - | - | - | X |
| 60 | MG | AN | 3002 | - | - | - | X |
| 60 | MG | AP | 201 | - | - | - | X |
| 60 | MG | AQ | 3001 | - | - | - | X |
| 60 | MG | AU | 201 | - | - | - | X |
| 60 | MG | AU | 202 | - | - | - | X |
| 60 | MG | AU | 203 | - | - | - | X |
| 60 | MG | AU | 204 | - | - | - | X |
| 60 | MG | AW | 3003 | - | - | - | X |
| 60 | MG | AX | 102 | - | - | - | X |
| 60 | MG | BA | 1601 | - | - | - | X |
| 60 | MG | BA | 1615 | - | - | - | X |
| 60 | MG | BA | 1626 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | BA | 1629 | - | - | - | X |
| 60 | MG | BA | 1630 | - | - | - | X |
| 60 | MG | BA | 1648 | - | - | - | X |
| 60 | MG | BA | 1655 | - | - | - | X |
| 60 | MG | BA | 1658 | - | - | - | X |
| 60 | MG | BA | 1662 | - | - | - | X |
| 60 | MG | BA | 1671 | - | - | - | X |
| 60 | MG | BA | 1675 | - | - | - | X |
| 60 | MG | BA | 1679 | - | - | - | X |
| 60 | MG | BA | 1683 | - | - | - | X |
| 60 | MG | BA | 1686 | - | - | - | X |
| 60 | MG | BA | 1687 | - | - | - | X |
| 60 | MG | BA | 1701 | - | - | - | X |
| 60 | MG | BA | 1705 | - | - | - | X |
| 60 | MG | BA | 1724 | - | - | - | X |
| 60 | MG | BA | 1749 | - | - | - | X |
| 60 | MG | BA | 1757 | - | - | - | X |
| 60 | MG | BA | 1765 | - | - | - | X |
| 60 | MG | BA | 1778 | - | - | - | X |
| 60 | MG | BA | 1785 | - | - | - | X |
| 60 | MG | BA | 1804 | - | - | - | X |
| 60 | MG | BB | 3001 | - | - | - | X |
| 60 | MG | C3 | 101 | - | - | - | X |
| 60 | MG | C5 | 101 | - | - | - | X |
| 60 | MG | C7 | 101 | - | - | - | X |
| 60 | MG | CA | 3002 | - | - | - | X |
| 60 | MG | CA | 3004 | - | - | - | X |
| 60 | MG | CA | 3013 | - | - | - | X |
| 60 | MG | CA | 3018 | - | - | - | X |
| 60 | MG | CA | 3022 | - | - | - | X |
| 60 | MG | CA | 3026 | - | - | - | X |
| 60 | MG | CA | 3028 | - | - | - | X |
| 60 | MG | CA | 3032 | - | - | - | X |
| 60 | MG | CA | 3035 | - | - | - | X |
| 60 | MG | CA | 3038 | - | - | - | X |
| 60 | MG | CA | 3068 | - | - | - | X |
| 60 | MG | CA | 3082 | - | - | - | X |
| 60 | MG | CA | 3083 | - | - | - | X |
| 60 | MG | CA | 3084 | - | - | - | X |
| 60 | MG | CA | 3087 | - | - | - | X |
| 60 | MG | CA | 3099 | - | - | - | X |
| 60 | MG | CA | 3100 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | CA | 3102 | - | - | - | X |
| 60 | MG | CA | 3103 | - | - | - | X |
| 60 | MG | CA | 3106 | - | - | - | X |
| 60 | MG | CA | 3110 | - | - | - | X |
| 60 | MG | CA | 3114 | - | - | - | X |
| 60 | MG | CA | 3115 | - | - | - | X |
| 60 | MG | CA | 3121 | - | - | - | X |
| 60 | MG | CA | 3122 | - | - | - | X |
| 60 | MG | CA | 3129 | - | - | - | X |
| 60 | MG | CA | 3143 | - | - | - | X |
| 60 | MG | CA | 3154 | - | - | - | X |
| 60 | MG | CA | 3156 | - | - | - | X |
| 60 | MG | CA | 3157 | - | - | - | X |
| 60 | MG | CA | 3160 | - | - | - | X |
| 60 | MG | CA | 3163 | - | - | - | X |
| 60 | MG | CA | 3165 | - | - | - | X |
| 60 | MG | CA | 3166 | - | - | - | X |
| 60 | MG | CA | 3179 | - | - | - | X |
| 60 | MG | CA | 3181 | - | - | - | X |
| 60 | MG | CA | 3182 | - | - | - | X |
| 60 | MG | CA | 3184 | - | - | - | X |
| 60 | MG | CA | 3187 | - | - | - | X |
| 60 | MG | CA | 3198 | - | - | - | X |
| 60 | MG | CA | 3209 | - | - | - | X |
| 60 | MG | CA | 3210 | - | - | - | X |
| 60 | MG | CA | 3214 | - | - | - | X |
| 60 | MG | CA | 3215 | - | - | - | X |
| 60 | MG | CA | 3218 | - | - | - | X |
| 60 | MG | CA | 3220 | - | - | - | X |
| 60 | MG | CA | 3226 | - | - | - | X |
| 60 | MG | CA | 3227 | - | - | - | X |
| 60 | MG | CA | 3233 | - | - | - | X |
| 60 | MG | CA | 3236 | - | - | - | X |
| 60 | MG | CA | 3249 | - | - | - | X |
| 60 | MG | CA | 3264 | - | - | - | X |
| 60 | MG | CA | 3265 | - | - | - | X |
| 60 | MG | CA | 3274 | - | - | - | X |
| 60 | MG | CA | 3279 | - | - | - | X |
| 60 | MG | CA | 3282 | - | - | - | X |
| 60 | MG | CA | 3288 | - | - | - | X |
| 60 | MG | CA | 3293 | - | - | - | X |
| 60 | MG | CA | 3307 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | CA | 3311 | - | - | - | X |
| 60 | MG | CA | 3312 | - | - | - | X |
| 60 | MG | CA | 3315 | - | - | - | X |
| 60 | MG | CA | 3320 | - | - | - | X |
| 60 | MG | CA | 3324 | - | - | - | X |
| 60 | MG | CA | 3330 | - | - | - | X |
| 60 | MG | CA | 3346 | - | - | - | X |
| 60 | MG | CA | 3356 | - | - | - | X |
| 60 | MG | CA | 3359 | - | - | - | X |
| 60 | MG | CA | 3366 | - | - | - | X |
| 60 | MG | CA | 3381 | - | - | - | X |
| 60 | MG | CA | 3407 | - | - | - | X |
| 60 | MG | CA | 3408 | - | - | - | X |
| 60 | MG | CA | 3411 | - | - | - | X |
| 60 | MG | CA | 3413 | - | - | - | X |
| 60 | MG | CA | 3418 | - | - | - | X |
| 60 | MG | CA | 3423 | - | - | - | X |
| 60 | MG | CA | 3430 | - | - | - | X |
| 60 | MG | CA | 3431 | - | - | - | X |
| 60 | MG | CA | 3438 | - | - | - | X |
| 60 | MG | CA | 3439 | - | - | - | X |
| 60 | MG | CA | 3446 | - | - | - | X |
| 60 | MG | CA | 3449 | - | - | - | X |
| 60 | MG | CA | 3450 | - | - | - | X |
| 60 | MG | CA | 3454 | - | - | - | X |
| 60 | MG | CA | 3455 | - | - | - | X |
| 60 | MG | CA | 3460 | - | - | - | X |
| 60 | MG | CA | 3463 | - | - | - | X |
| 60 | MG | CA | 3464 | - | - | - | X |
| 60 | MG | CA | 3473 | - | - | - | X |
| 60 | MG | CA | 3488 | - | - | - | X |
| 60 | MG | CA | 3496 | - | - | - | X |
| 60 | MG | CA | 3500 | - | - | - | X |
| 60 | MG | CA | 3529 | - | - | - | X |
| 60 | MG | CA | 3541 | - | - | - | X |
| 60 | MG | CA | 3549 | - | - | - | X |
| 60 | MG | CA | 3558 | - | - | - | X |
| 60 | MG | CA | 3576 | - | - | - | X |
| 60 | MG | CA | 3595 | - | - | - | X |
| 60 | MG | CA | 3598 | - | - | - | X |
| 60 | MG | CA | 3601 | - | - | - | X |
| 60 | MG | CA | 3617 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 60 | MG | CA | 3619 | - | - | - | X |
| 60 | MG | CA | 3625 | - | - | - | X |
| 60 | MG | CA | 3641 | - | - | - | X |
| 60 | MG | CA | 3652 | - | - | - | X |
| 60 | MG | CA | 3653 | - | - | - | X |
| 60 | MG | CA | 3655 | - | - | - | X |
| 60 | MG | CA | 3656 | - | - | - | X |
| 60 | MG | CA | 3659 | - | - | - | X |
| 60 | MG | CA | 3662 | - | - | - | X |
| 60 | MG | CD | 301 | - | - | - | X |
| 60 | MG | CE | 301 | - | - | - | X |
| 60 | MG | CE | 303 | - | - | - | X |
| 60 | MG | CE | 304 | - | - | - | X |
| 60 | MG | CF | 301 | - | - | - | X |
| 60 | MG | CF | 302 | - | - | - | X |
| 60 | MG | CF | 306 | - | - | - | X |
| 60 | MG | CQ | 201 | - | - | - | X |
| 60 | MG | CQ | 202 | - | - | - | X |
| 60 | MG | CU | 201 | - | - | - | X |
| 60 | MG | CV | 201 | - | - | - | X |
| 60 | MG | CV | 202 | - | - | - | X |
| 60 | MG | DA | 1602 | - | - | - | X |
| 60 | MG | DA | 1611 | - | - | - | X |
| 60 | MG | DA | 1619 | - | - | - | X |
| 60 | MG | DA | 1631 | - | - | - | X |
| 60 | MG | DA | 1637 | - | - | - | X |
| 60 | MG | DA | 1638 | - | - | - | X |
| 60 | MG | DA | 1646 | - | - | - | X |
| 60 | MG | DA | 1650 | - | - | - | X |
| 60 | MG | DA | 1651 | - | - | - | X |
| 60 | MG | DA | 1667 | - | - | - | X |
| 60 | MG | DA | 1674 | - | - | - | X |
| 60 | MG | DA | 1679 | - | - | - | X |
| 60 | MG | DA | 1686 | - | - | - | X |
| 60 | MG | DA | 1688 | - | - | - | X |
| 60 | MG | DA | 1694 | - | - | - | X |
| 60 | MG | DA | 1696 | - | - | - | X |
| 60 | MG | DA | 1706 | - | - | - | X |
| 60 | MG | DA | 1714 | - | - | - | X |
| 60 | MG | DA | 1719 | - | - | - | X |
| 60 | MG | DA | 1742 | - | - | - | X |
| 60 | MG | DA | 1767 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 60 | MG | DE | 201 | - | - | - | X |

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 313372 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 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | AA | 2872 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61861 | 27532 | 11574 | 19884 | 2871 | | | |
| 1 | CA | 2868 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61771 | 27492 | 11554 | 19858 | 2867 | | | |

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | AB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |
| 2 | CB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2573 | 1146 | 476 | 832 | 119 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | AC | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1063 | 669 | 201 | 192 | 1 | | | |
| 3 | CC | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1063 | 669 | 201 | 192 | 1 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | AD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |
| 4 | CD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2142 | 1352 | 426 | 361 | 3 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |
| 5 | CE | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1559 | 985 | 298 | 270 | 6 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | AF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1584 | 1009 | 298 | 275 | 2 | | | |
| 6 | CF | 203 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1580 | 1007 | 297 | 274 | 2 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1425 | 914 | 256 | 251 | 4 | | | |
| 7 | CG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1424 | 911 | 258 | 251 | 4 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |
| 8 | CH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9 | AK | 130 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 641 | 381 | 130 | 130 | | | | |
| 9 | CK | 130 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 641 | 381 | 130 | 130 | | | | |

- Molecule 10 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | AL | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 498 | 310 | 93 | 92 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10 | CL | 66 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 498 | 310 | 93 | 92 | 3 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |
| 11 | CN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 12 | CO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1139 | 709 | 231 | 196 | 3 | | | |
| 13 | CP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 14 | CQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 15 | CR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 16 | AS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | |
| 16 | CS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 870 | 549 | 173 | 148 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 680 | 225 | 185 | 1 | | | |
| 17 | CT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1083 | 675 | 224 | 183 | 1 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | AU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 18 | CU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |
| 19 | CV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |
| 20 | CW | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 886 | 557 | 174 | 153 | 2 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | AX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |
| 21 | CX | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | AY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |
| 22 | CY | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | AZ | 171 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1349 | 862 | 243 | 242 | 2 | | | |
| 23 | CZ | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1360 | 870 | 243 | 245 | 2 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | A0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 404 | 139 | 109 | 1 | | | |
| 24 | C0 | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 653 | 404 | 139 | 109 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | A1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |
| 25 | C1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | A2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | C2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 27 | A3 | 59 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | | |
| 27 | C3 | 59 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 464 | 296 | 90 | 78 | | | | |

- Molecule 28 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 28 | A4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 558 | 352 | 102 | 99 | 5 | | | |
| 28 | C4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 97 | 91 | 5 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | A5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |
| 29 | C5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | A6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 30 | C6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 279 | 91 | 75 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31 | A7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 31 | C7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32 | A8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 32 | C8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 33 | A9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 33 | C9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 34 | BA | 1497 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32185 | 14324 | 5968 | 10396 | 1497 | | | |
| 34 | DA | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32312 | 14381 | 5990 | 10438 | 1503 | | | |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35 | BB | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1846 | 1179 | 331 | 331 | 5 | | | |
| 35 | DB | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1825 | 1167 | 326 | 327 | 5 | | | |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 976 | 302 | 273 | 1 | | | |
| 36 | DC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1544 | 970 | 300 | 273 | 1 | | | |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 37 | BD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1659 | 1040 | 326 | 286 | 7 | | | |
| 37 | DD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1678 | 1052 | 333 | 286 | 7 | | | |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 213 | 198 | 4 | | | |
| 38 | DE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 716 | 214 | 199 | 4 | | | |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 812 | 514 | 146 | 149 | 3 | | | |
| 39 | DF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 820 | 518 | 147 | 152 | 3 | | | |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1231 | 766 | 243 | 216 | 6 | | | |
| 40 | DG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1235 | 769 | 244 | 216 | 6 | | | |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |
| 41 | DH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 42 | BI | 127 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 986 | 626 | 193 | 167 | | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42 | DI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 978 | 619 | 190 | 169 | | | |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43 | BJ | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 709 | 440 | 138 | 131 | | | |
| 43 | DJ | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 714 | 445 | 138 | 131 | | | |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BK | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 833 | 519 | 156 | 155 | 3 | | | |
| 44 | DK | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 833 | 519 | 156 | 155 | 3 | | | |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 585 | 185 | 159 | 1 | | | |
| 45 | DL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 585 | 185 | 159 | 1 | | | |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BM | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 966 | 598 | 200 | 166 | 2 | | | |
| 46 | DM | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 586 | 197 | 165 | 2 | | | |

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 47 | BN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 47 | DN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 456 | 144 | 126 | 2 | | | |
| 48 | DO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 456 | 144 | 126 | 2 | | | |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | BP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 433 | 134 | 113 | 1 | | | |
| 49 | DP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 677 | 430 | 133 | 113 | 1 | | | |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | BQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |
| 50 | DQ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 151 | 142 | 2 | | | |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 51 | BR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | |
| 51 | DR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BS | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 661 | 423 | 122 | 114 | 2 | | | |
| 52 | DS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 646 | 412 | 119 | 113 | 2 | | | |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53 | BT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 446 | 156 | 124 | 2 | | | |
| 53 | DT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 731 | 449 | 156 | 124 | 2 | | | |

- Molecule 54 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 54 | BU | 23 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | | |
| 54 | DU | 23 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 199 | 122 | 48 | 29 | | | | |

- Molecule 55 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 55 | BV | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 125 | 51 | 88 | 13 | | | |
| 55 | DV | 12 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 252 | 115 | 46 | 80 | 11 | | | |

- Molecule 56 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56 | BW | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1599 | 722 | 287 | 515 | 73 | | | |
| 56 | DW | 72 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1552 | 697 | 280 | 502 | 72 | | | |

- Molecule 57 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 57 | BX | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | | | |
| 57 | DX | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | | | |

- Molecule 58 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 58 | BY | 74 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1581 | 707 | 285 | 515 | 73 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 58 | DY | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1561 | 698 | 283 | 507 | 72 | 1 | | | |

- Molecule 59 is a protein called 50S ribosomal protein L9,Elongation factor G.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 59 | BZ | 728 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5663 | 3599 | 973 | 1072 | 19 | | | |
| 59 | DZ | 730 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5682 | 3611 | 978 | 1074 | 19 | | | |

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 60 | AP | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 60 | CR | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 60 | BA | 213 | Total | Mg | 0 | 0 |
| | | | 213 | 213 | | |
| 60 | CA | 664 | Total | Mg | 0 | 0 |
| | | | 664 | 664 | | |
| 60 | C8 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | C5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | AB | 23 | Total | Mg | 0 | 0 |
| | | | 23 | 23 | | |
| 60 | BL | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 60 | CV | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 60 | A6 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | BE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | AW | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 60 | AN | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 60 | DZ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 60 | AX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | CN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | A2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | DX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | DD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | AE | 5 | Total 5 | Mg 5 | 0 | 0 |
| 60 | BM | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | AV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BX | 15 | Total 15 | Mg 15 | 0 | 0 |
| 60 | DA | 168 | Total 168 | Mg 168 | 0 | 0 |
| 60 | CB | 13 | Total 13 | Mg 13 | 0 | 0 |
| 60 | C0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | AA | 834 | Total 834 | Mg 834 | 0 | 0 |
| 60 | DF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CQ | 4 | Total 4 | Mg 4 | 0 | 0 |
| 60 | A5 | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 60 | AR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | DK | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | A1 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | AD | 10 | Total 10 | Mg 10 | 0 | 0 |
| 60 | BN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | DJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BY | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | C7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | C3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | AZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | A4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | AU | 4 | Total 4 | Mg 4 | 0 | 0 |
| 60 | DW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | A9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CF | 6 | Total 6 | Mg 6 | 0 | 0 |
| 60 | BV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | A0 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 60 | AG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | DE | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 60 | AQ | 3 | Total 3 | Mg 3 | 0 | 0 |
| 60 | CE | 6 | Total 6 | Mg 6 | 0 | 0 |
| 60 | AH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | CP | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | A7 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | CD | 4 | Total 4 | Mg 4 | 0 | 0 |
| 60 | BD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | DT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | A8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | AO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | BW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 60 | AY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 60 | AF | 5 | Total 5 | Mg 5 | 0 | 0 |

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 61 | AA | 1 | Total 1 | K 1 | 0 | 0 |

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

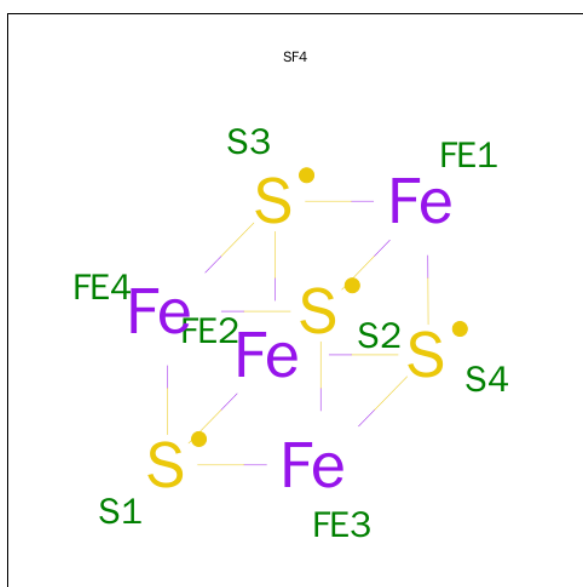
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 62 | AY | 1 | Total 1 | Zn 1 | 0 | 0 |

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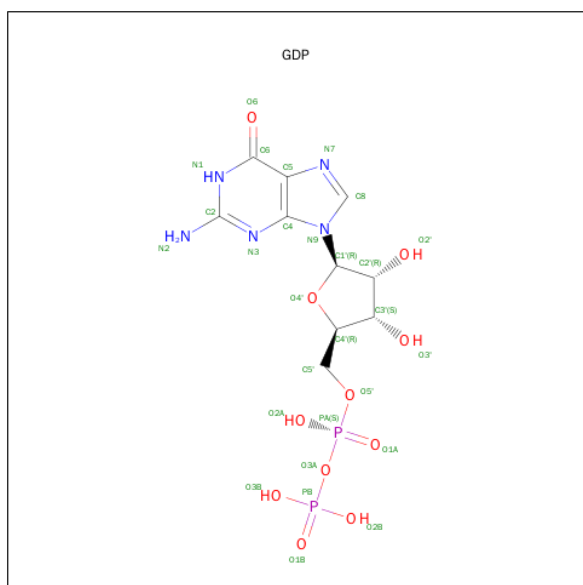
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 62 | BN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | C4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | C5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | C6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | A6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | C9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | DN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | A4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | A5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | A9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | CY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 63 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 63 | BD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 63 | DD | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 65 | AG | 3 | Total 3 | O 3 | 0 | 0 |
| 65 | AH | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | AN | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | AO | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | AP | 15 | Total 15 | O 15 | 0 | 0 |
| 65 | AQ | 4 | Total 4 | O 4 | 0 | 0 |
| 65 | AR | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | AS | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | AT | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | AU | 5 | Total 5 | O 5 | 0 | 0 |
| 65 | AV | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | AW | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | AX | 3 | Total 3 | O 3 | 0 | 0 |
| 65 | AZ | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | A0 | 6 | Total 6 | O 6 | 0 | 0 |
| 65 | A1 | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | A3 | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | A5 | 3 | Total 3 | O 3 | 0 | 0 |
| 65 | A6 | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | A7 | 4 | Total 4 | O 4 | 0 | 0 |
| 65 | A8 | 10 | Total 10 | O 10 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 65 | BA | 212 | Total 212 | O 212 | 0 | 0 |
| 65 | BD | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | BE | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | BL | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | BM | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | BV | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | BW | 3 | Total 3 | O 3 | 0 | 0 |
| 65 | BX | 8 | Total 8 | O 8 | 0 | 0 |
| 65 | BY | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | BZ | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | CA | 985 | Total 985 | O 985 | 0 | 0 |
| 65 | CB | 9 | Total 9 | O 9 | 0 | 0 |
| 65 | CD | 14 | Total 14 | O 14 | 0 | 0 |
| 65 | CE | 13 | Total 13 | O 13 | 0 | 0 |
| 65 | CF | 7 | Total 7 | O 7 | 0 | 0 |
| 65 | CN | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | CP | 10 | Total 10 | O 10 | 0 | 0 |
| 65 | CQ | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | CR | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | CT | 3 | Total 3 | O 3 | 0 | 0 |
| 65 | CU | 2 | Total 2 | O 2 | 0 | 0 |

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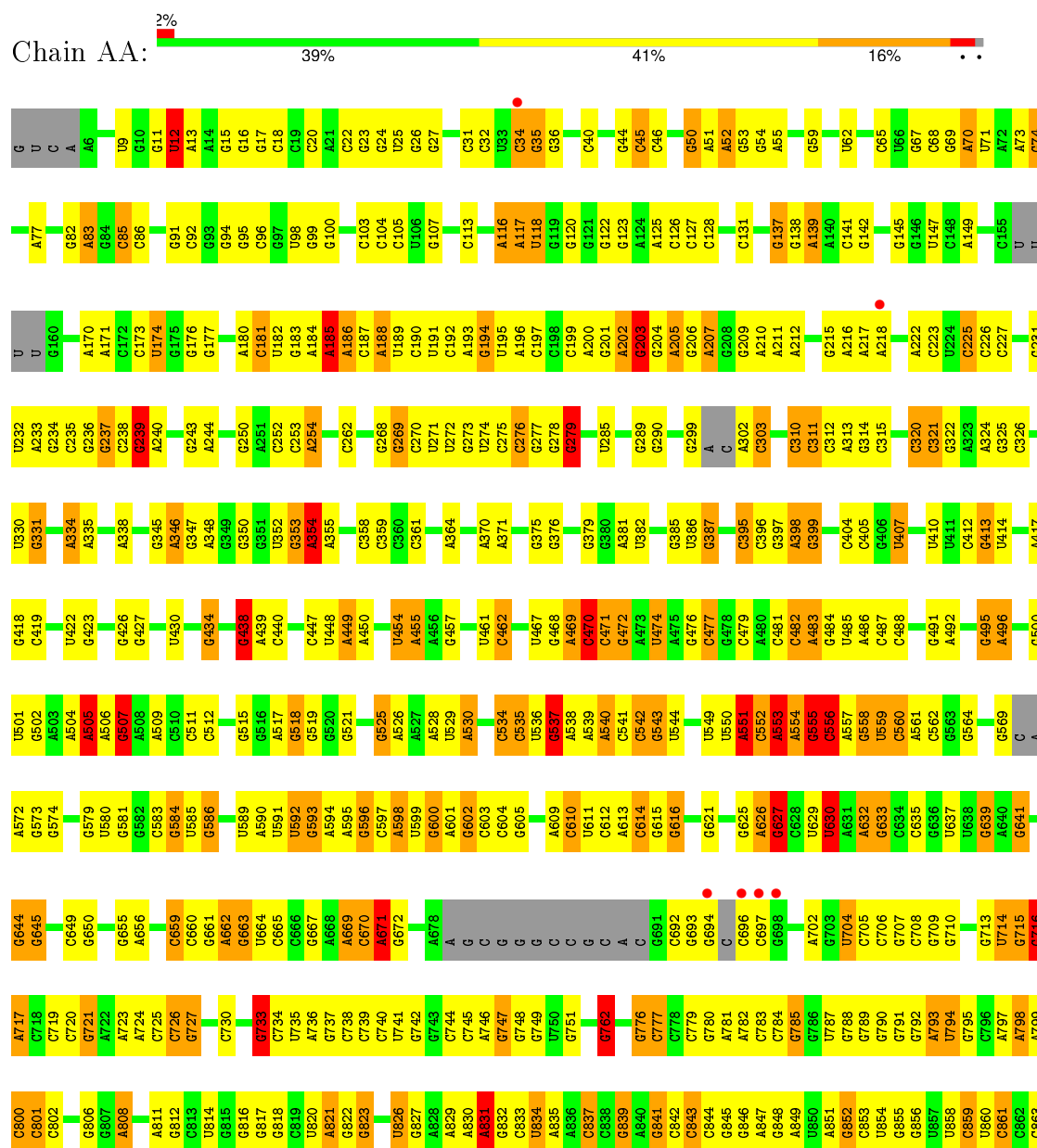
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 65 | CV | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | CY | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | C0 | 6 | Total 6 | O 6 | 0 | 0 |
| 65 | C1 | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | C3 | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | C6 | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | C7 | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | C8 | 3 | Total 3 | O 3 | 0 | 0 |
| 65 | DA | 155 | Total 155 | O 155 | 0 | 0 |
| 65 | DE | 4 | Total 4 | O 4 | 0 | 0 |
| 65 | DJ | 1 | Total 1 | O 1 | 0 | 0 |
| 65 | DK | 2 | Total 2 | O 2 | 0 | 0 |
| 65 | DL | 1 | Total 1 | O 1 | 0 | 0 |
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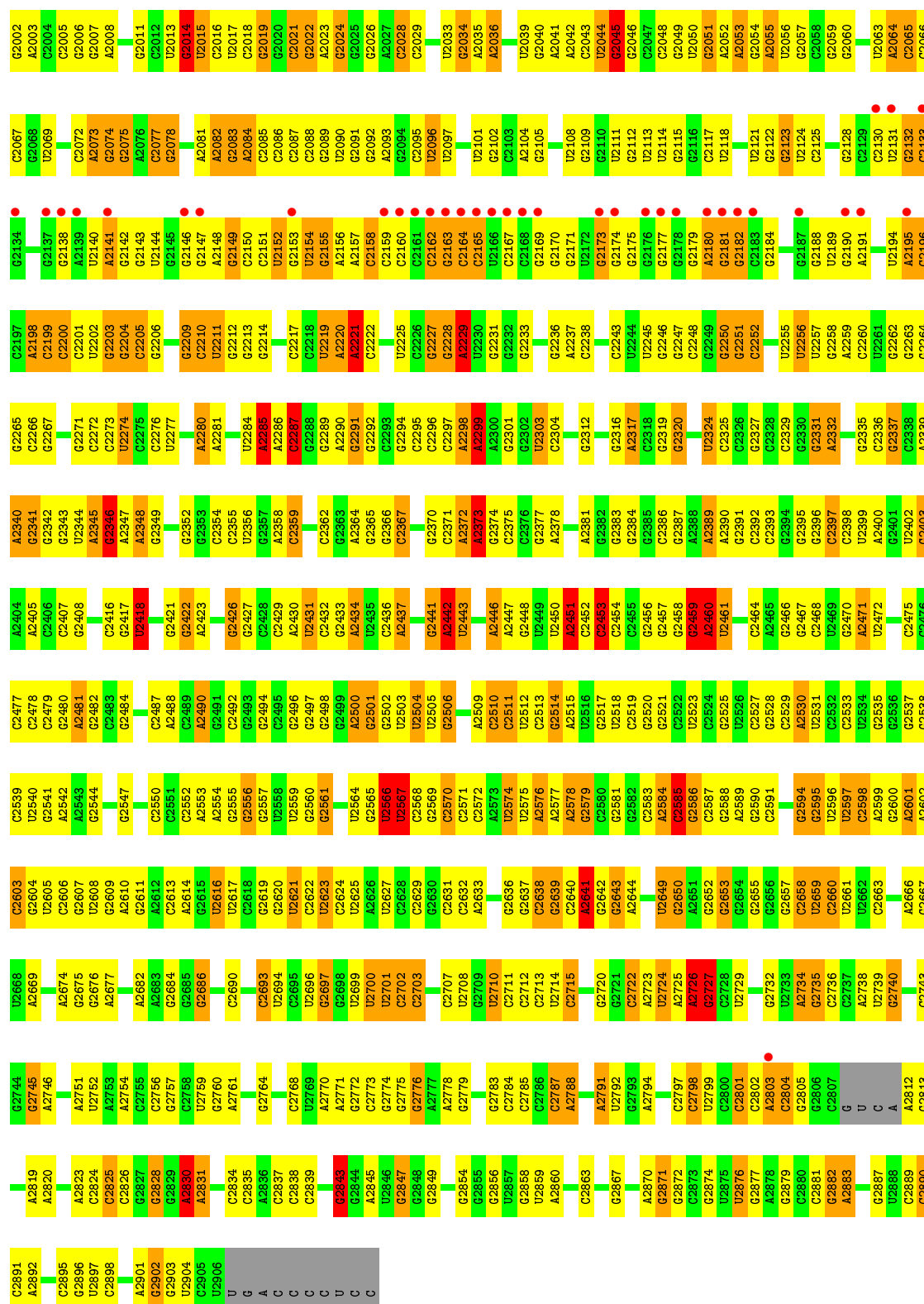
3 Residue-property plots

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: 23S Ribosomal RNA



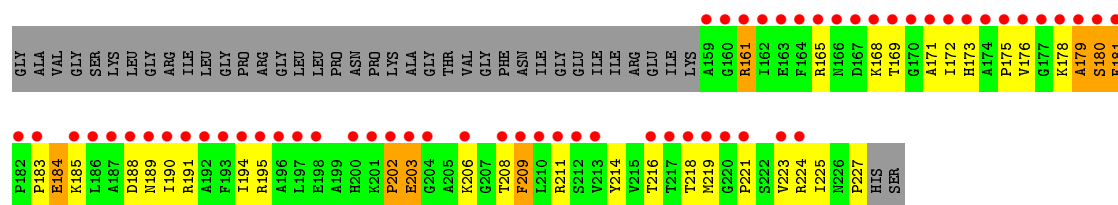
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| G1921 | A1834 | C1755 | A1679 | C1596 | C1514 | U1438 | A1367 | G1291 | G1217 | U1140 | A1074 | U1008 | C936 | G865 |
| A1922 | C1835 | U1756 | C1683 | C1597 | C1515 | A1368 | U1369 | A1292 | G1218 | A1141 | A1075 | C1009 | A937 | A866 |
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| C1924 | U1837 | G1764 | U1686 | C1604 | A1518 | U1440 | G1371 | G1294 | U1220 | U1143 | A1077 | G1011 | C939 | A868 |
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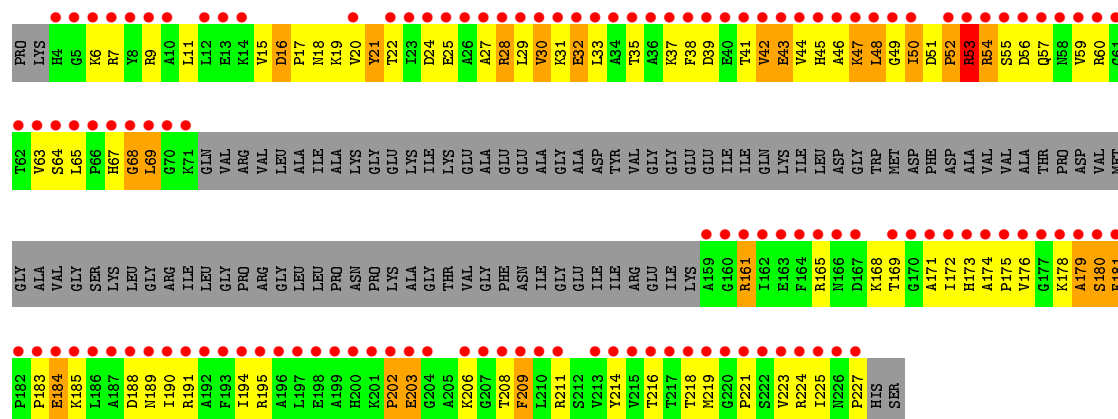
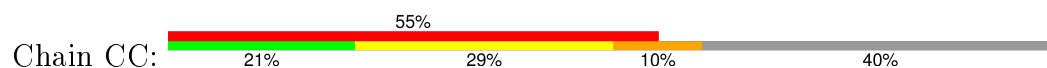
● Molecule 1: 23S Ribosomal RNA



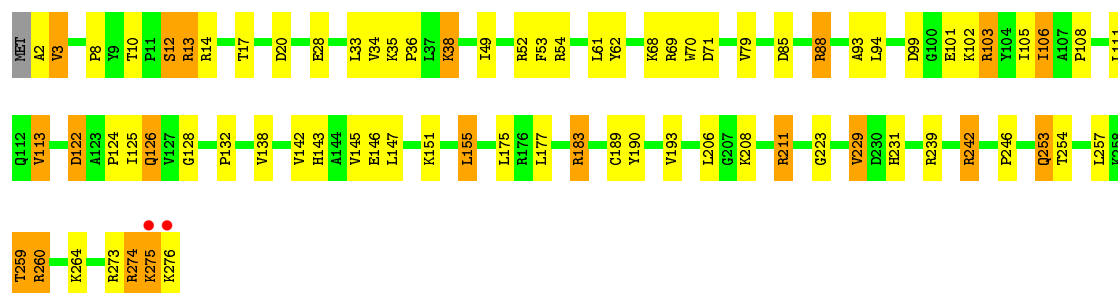
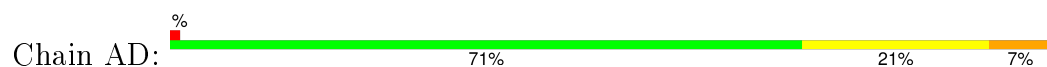
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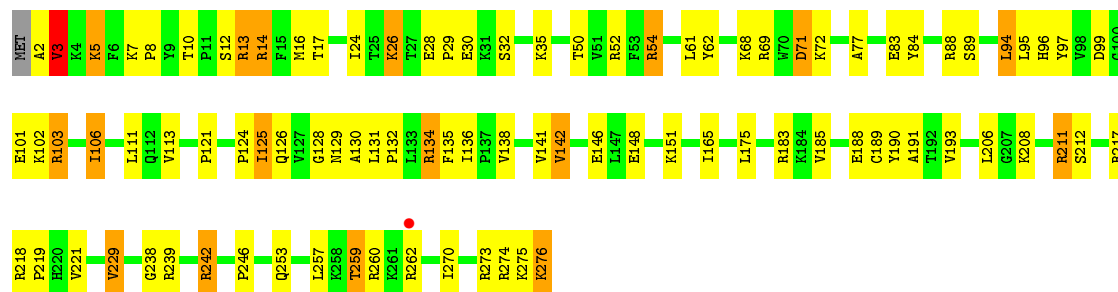
• Molecule 3: 50S ribosomal protein L1



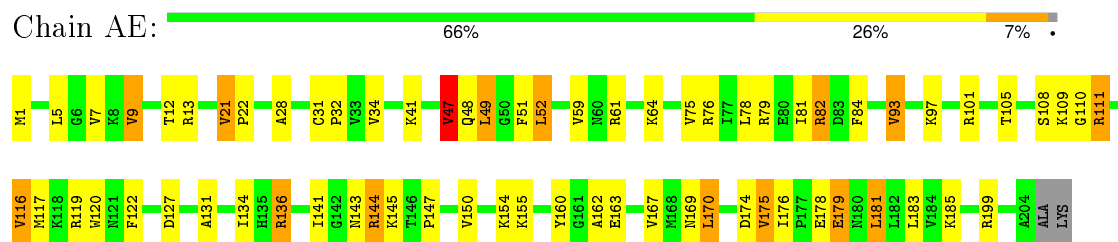
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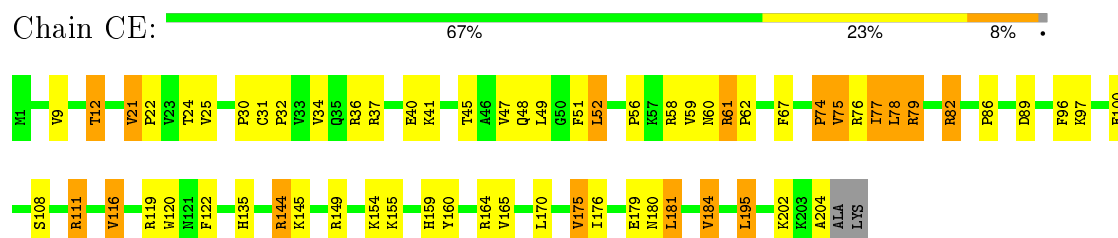
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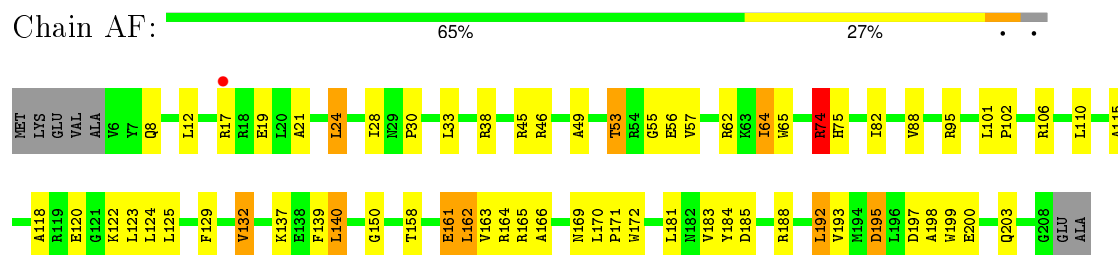
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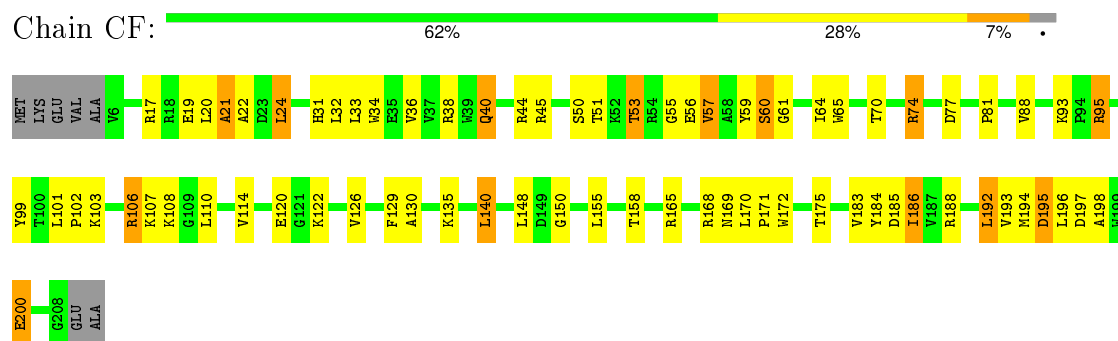
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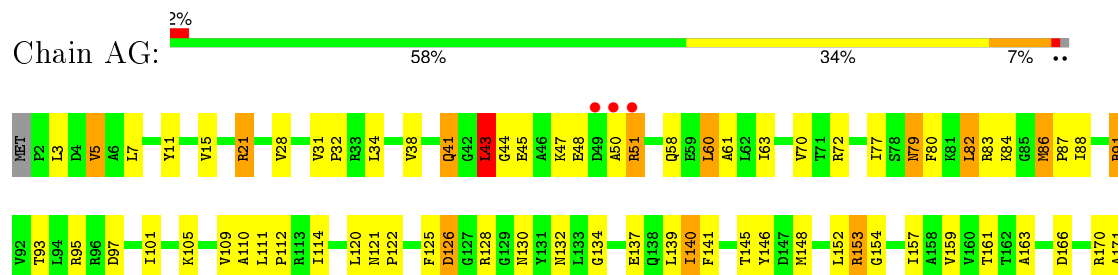
• Molecule 6: 50S ribosomal protein L4

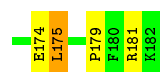


• Molecule 6: 50S ribosomal protein L4

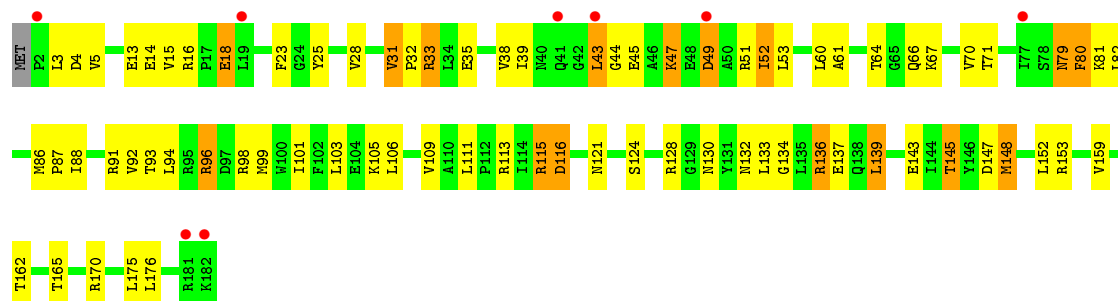


• Molecule 7: 50S ribosomal protein L5

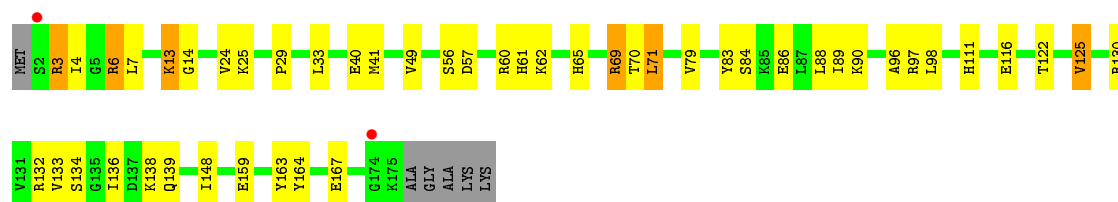
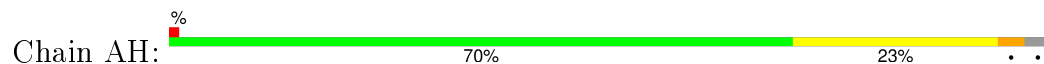




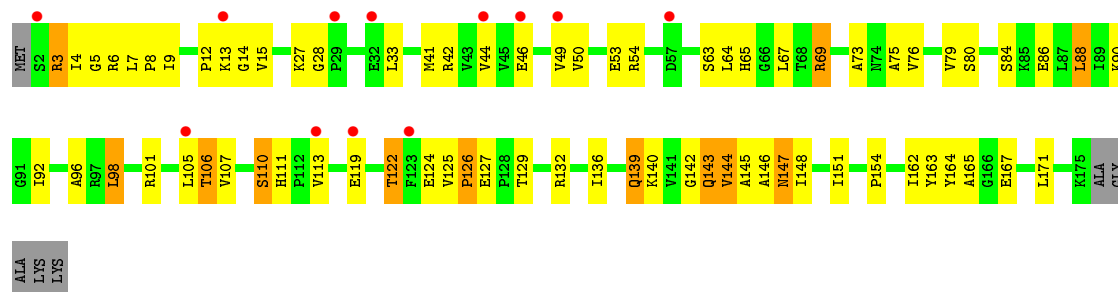
• Molecule 7: 50S ribosomal protein L5



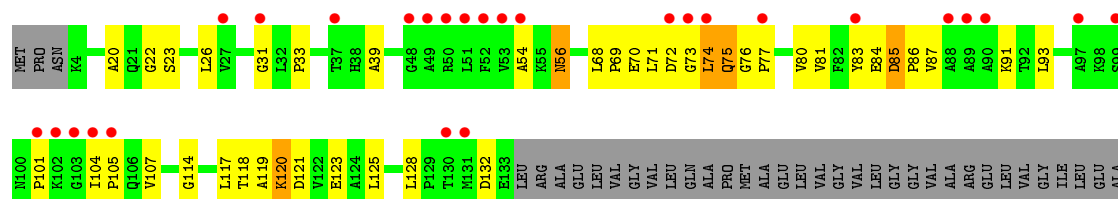
• Molecule 8: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L6

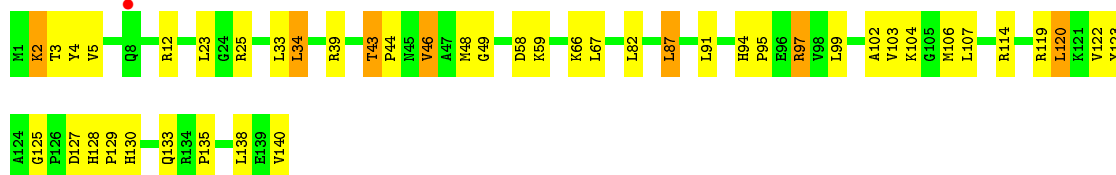


• Molecule 9: 50S ribosomal protein L10

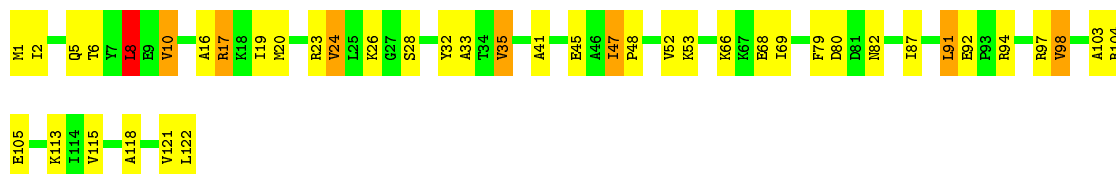




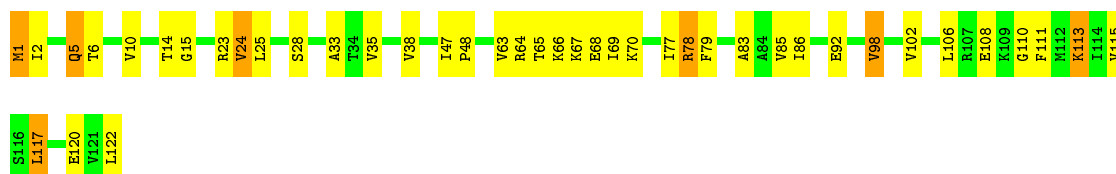
- Molecule 11: 50S ribosomal protein L13



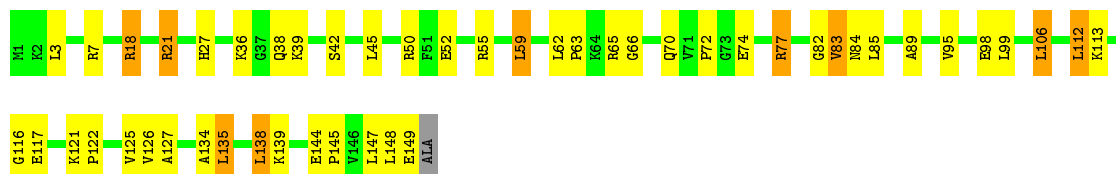
- Molecule 12: 50S ribosomal protein L14



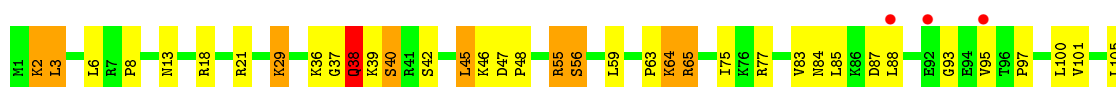
- Molecule 12: 50S ribosomal protein L14

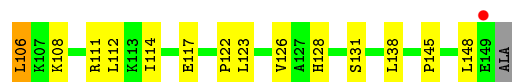


- Molecule 13: 50S ribosomal protein L15



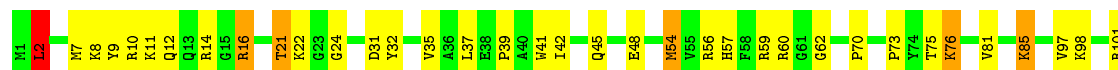
- Molecule 13: 50S ribosomal protein L15





- Molecule 14: 50S ribosomal protein L16

Chain AQ: 65% 28% 6%



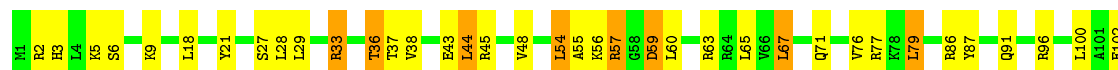
- Molecule 14: 50S ribosomal protein L16

Chain CQ: 66% 28% 6%



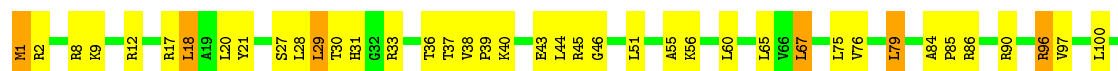
- Molecule 15: 50S ribosomal protein L17

Chain AR: 64% 29% 7%



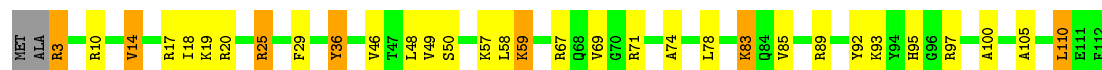
- Molecule 15: 50S ribosomal protein L17

Chain CR: 60% 34% 6%

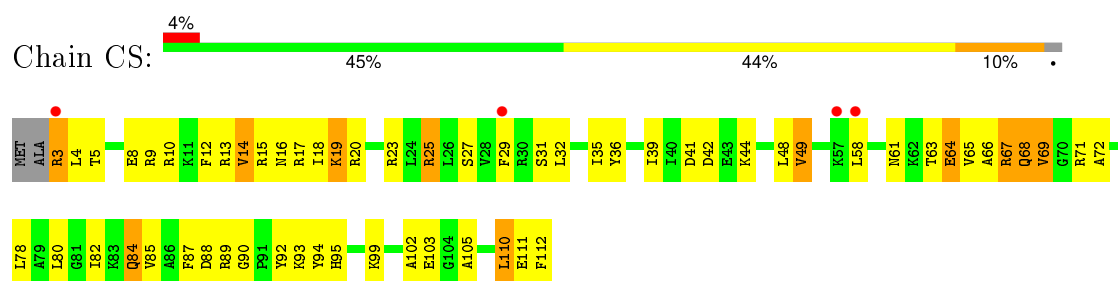


- Molecule 16: 50S ribosomal protein L18

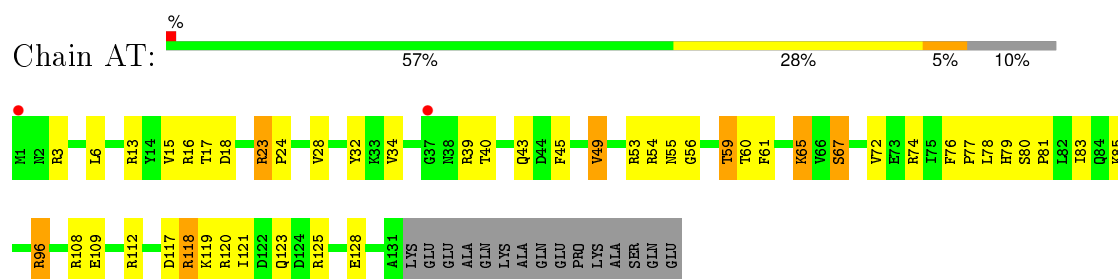
Chain AS: 70% 22% 6%



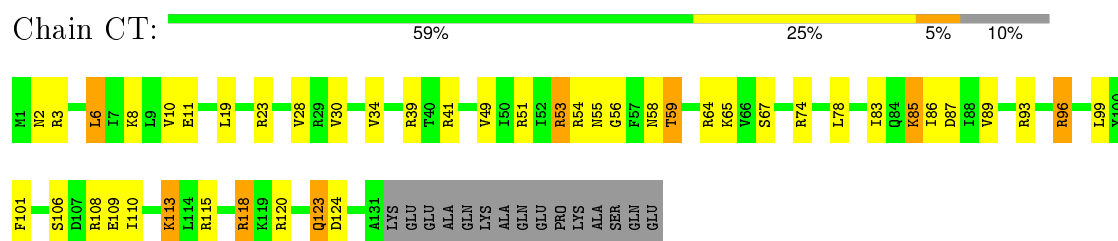
- Molecule 16: 50S ribosomal protein L18



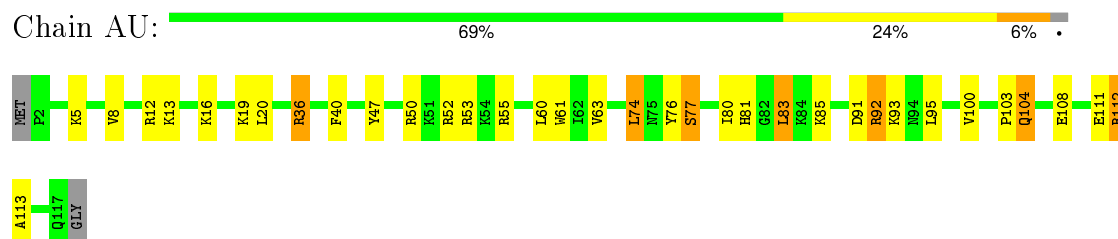
- Molecule 17: 50S ribosomal protein L19



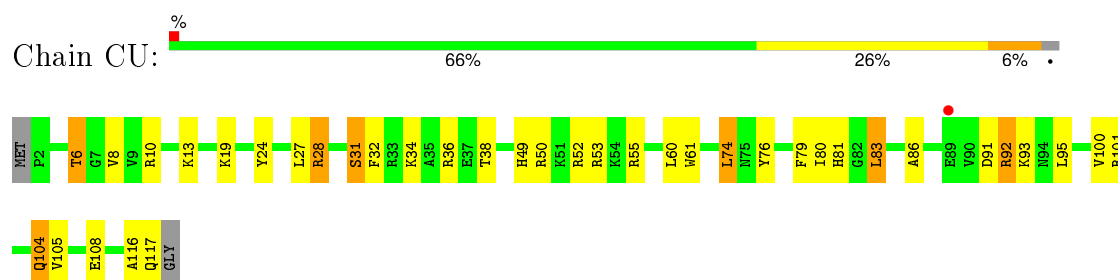
- Molecule 17: 50S ribosomal protein L19



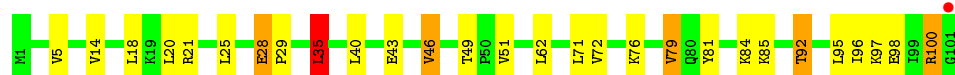
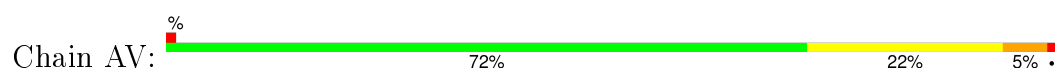
- Molecule 18: 50S ribosomal protein L20



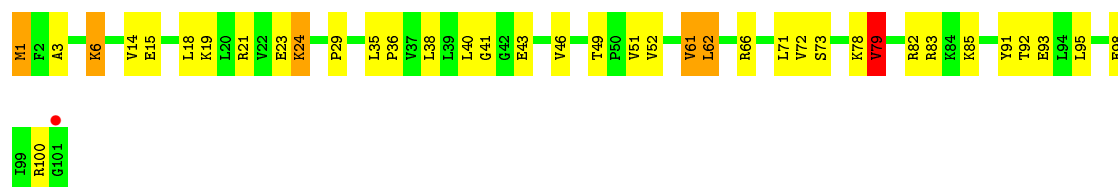
- Molecule 18: 50S ribosomal protein L20



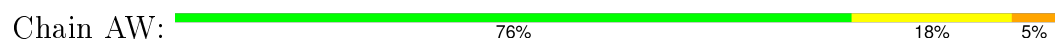
- Molecule 19: 50S ribosomal protein L21



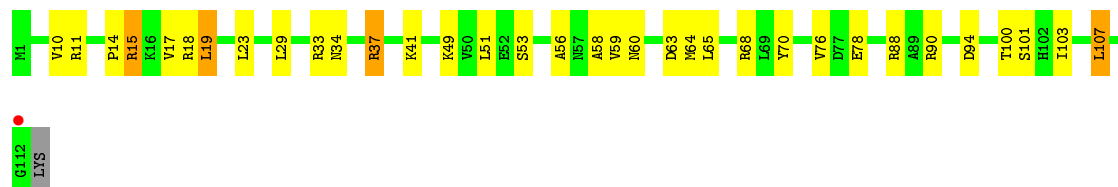
- Molecule 19: 50S ribosomal protein L21



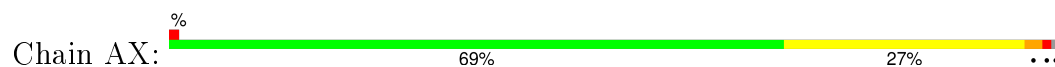
- Molecule 20: 50S ribosomal protein L22



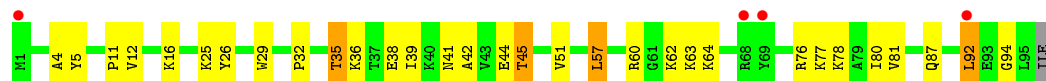
- Molecule 20: 50S ribosomal protein L22



- Molecule 21: 50S ribosomal protein L23

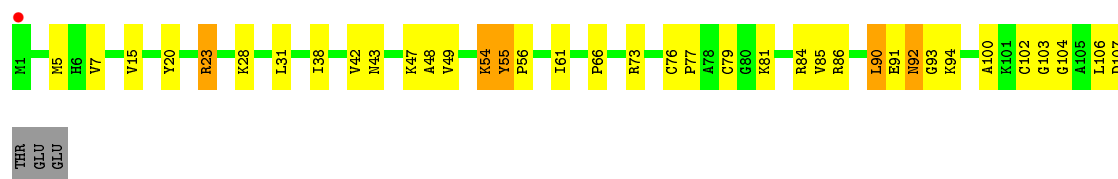


- Molecule 21: 50S ribosomal protein L23

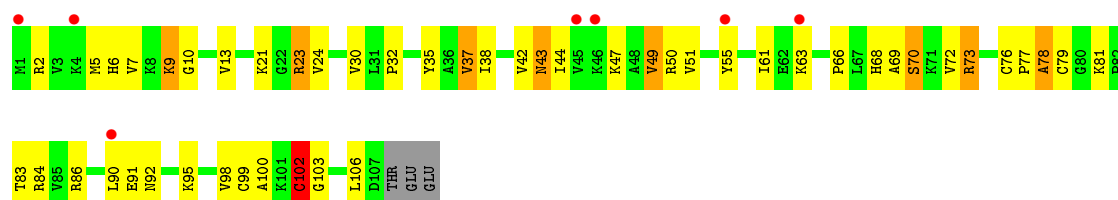


- Molecule 22: 50S ribosomal protein L24

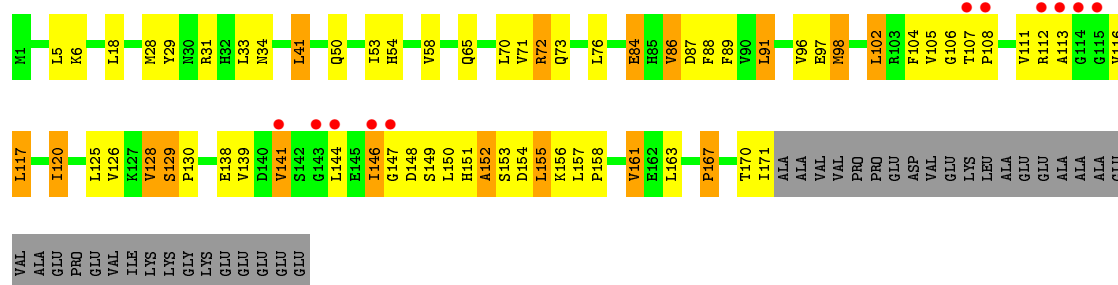




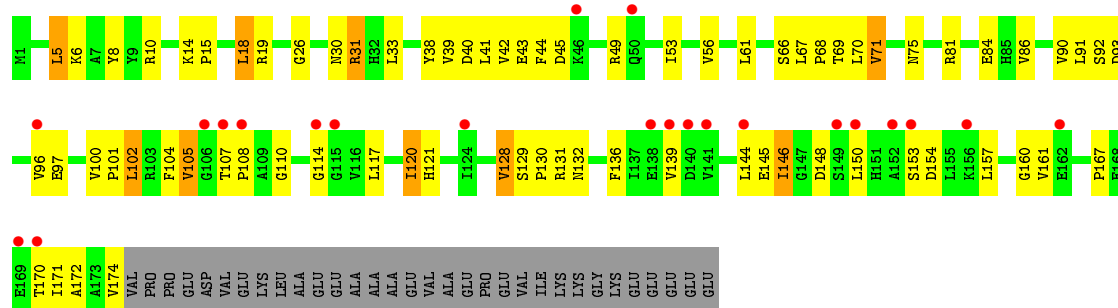
- Molecule 22: 50S ribosomal protein L24



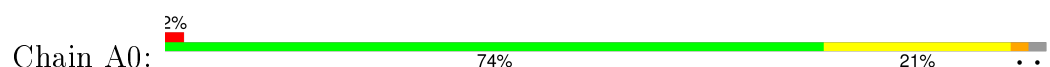
- Molecule 23: 50S ribosomal protein L25



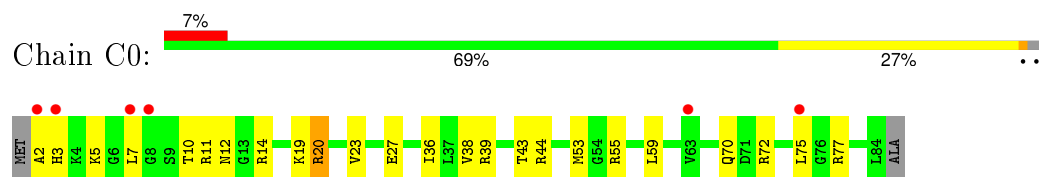
- Molecule 23: 50S ribosomal protein L25



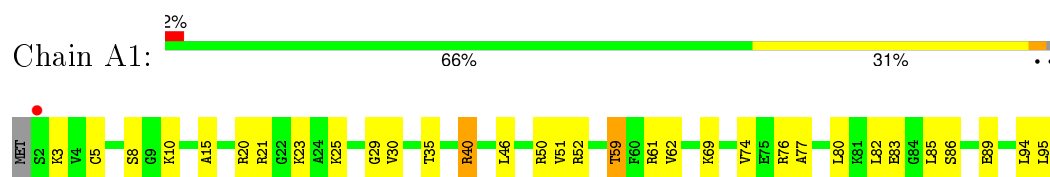
- Molecule 24: 50S ribosomal protein L27



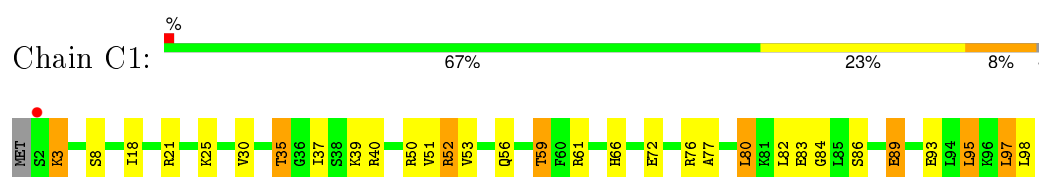
- Molecule 24: 50S ribosomal protein L27



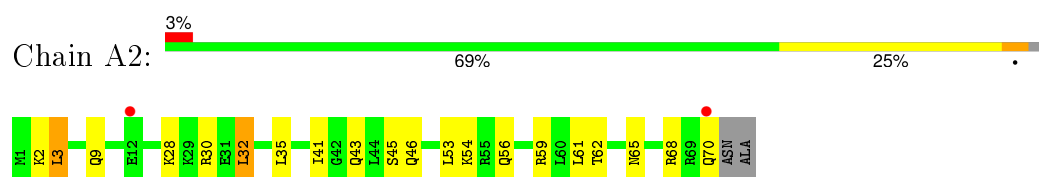
- Molecule 25: 50S ribosomal protein L28



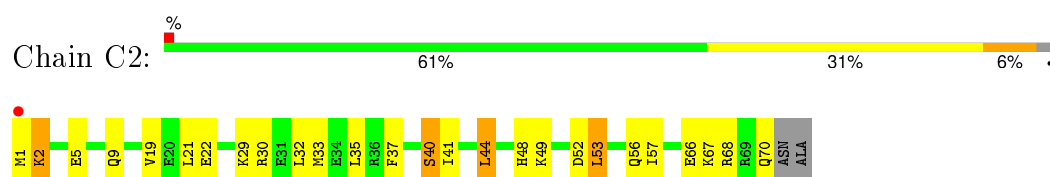
- Molecule 25: 50S ribosomal protein L28



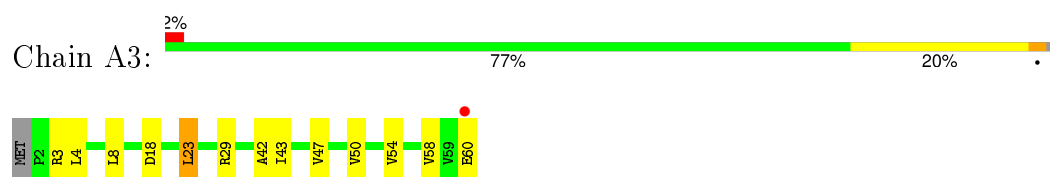
- Molecule 26: 50S ribosomal protein L29



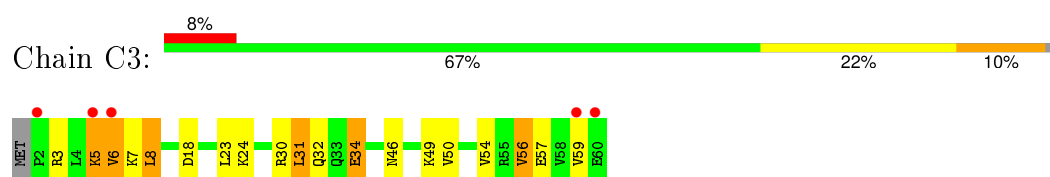
- Molecule 26: 50S ribosomal protein L29



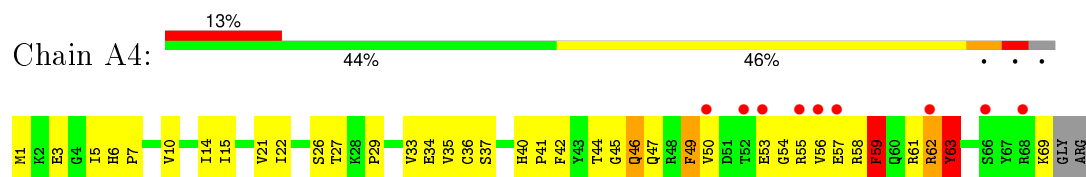
- Molecule 27: 50S ribosomal protein L30



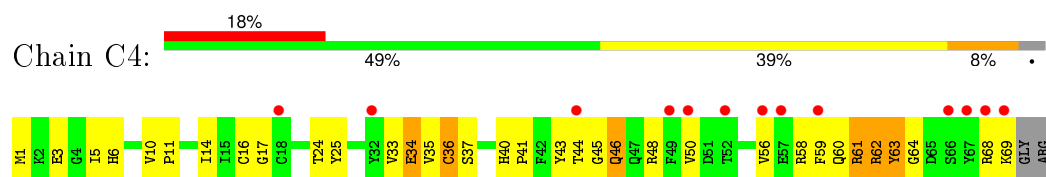
- Molecule 27: 50S ribosomal protein L30



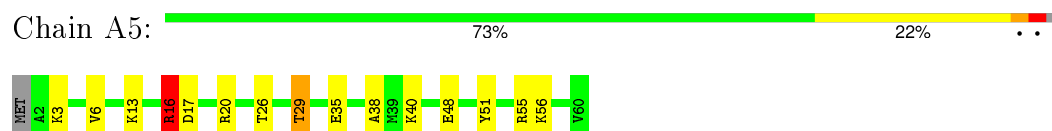
- Molecule 28: 50S ribosomal protein L31



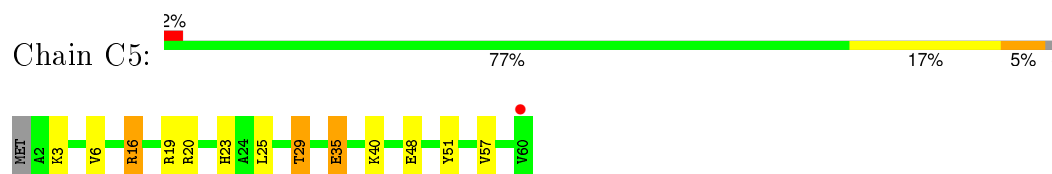
- Molecule 28: 50S ribosomal protein L31



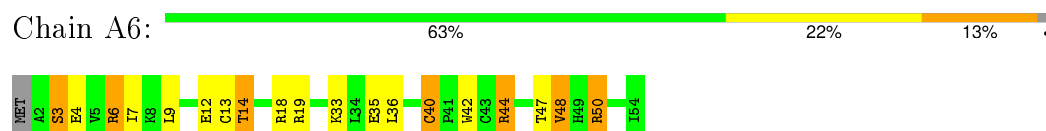
- Molecule 29: 50S ribosomal protein L32



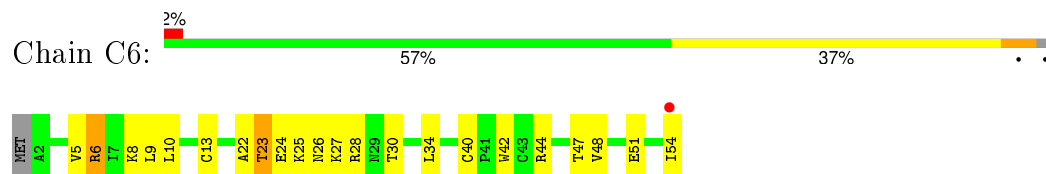
- Molecule 29: 50S ribosomal protein L32



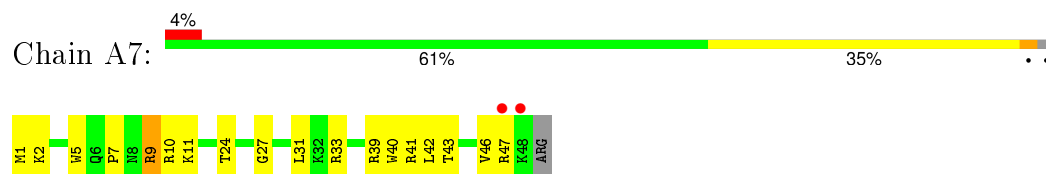
- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33



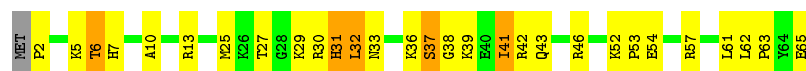
- Molecule 31: 50S ribosomal protein L34



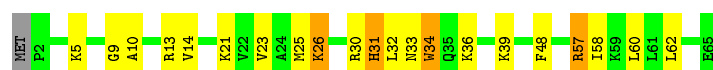
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



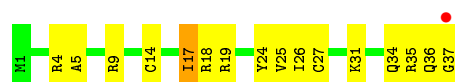
- Molecule 32: 50S ribosomal protein L35



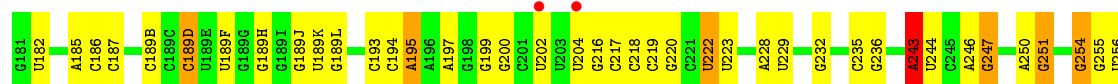
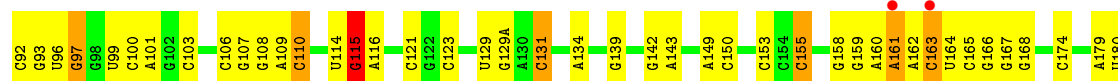
- Molecule 33: 50S ribosomal protein L36

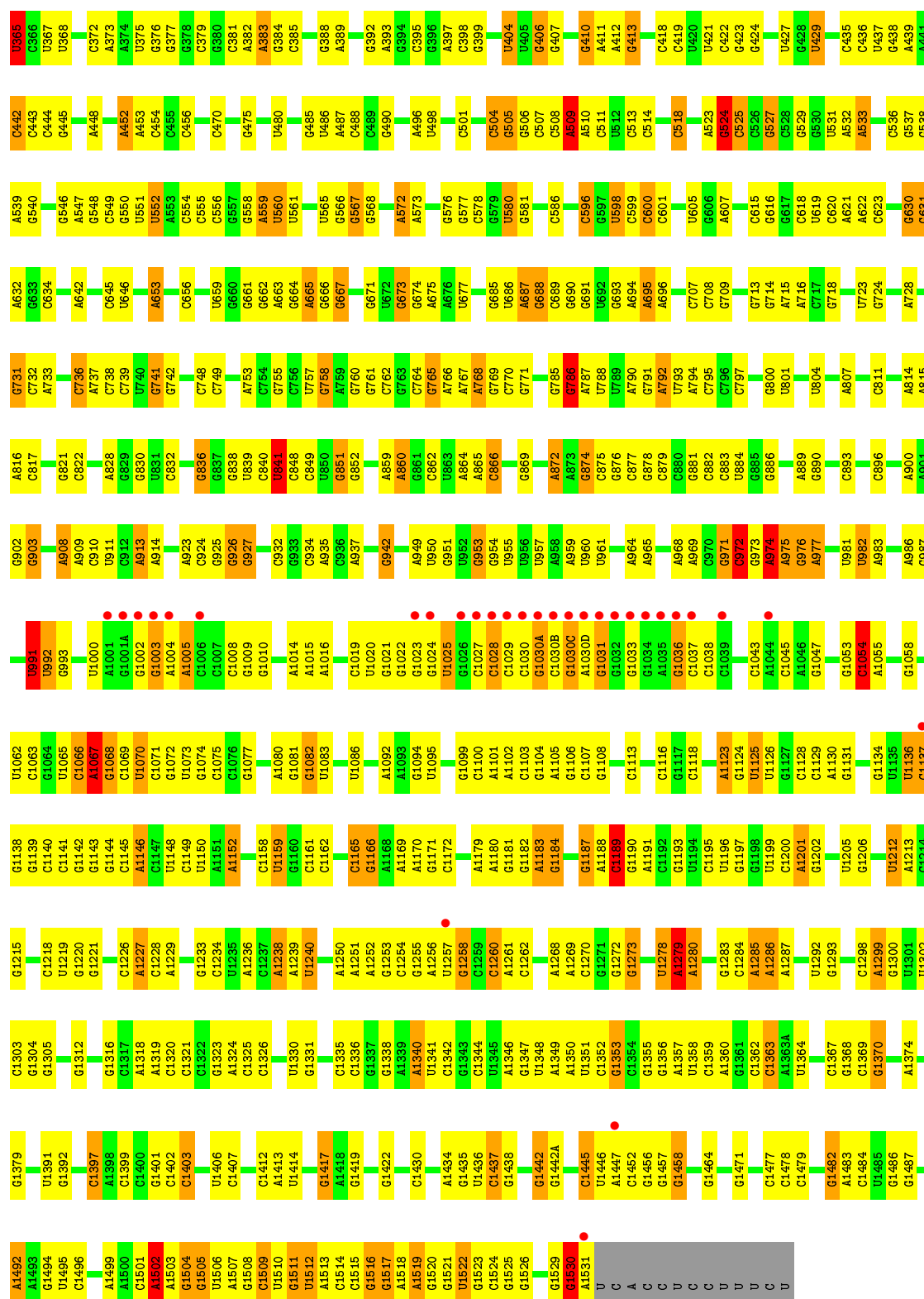


- Molecule 33: 50S ribosomal protein L36



- Molecule 34: 16S Ribosomal RNA

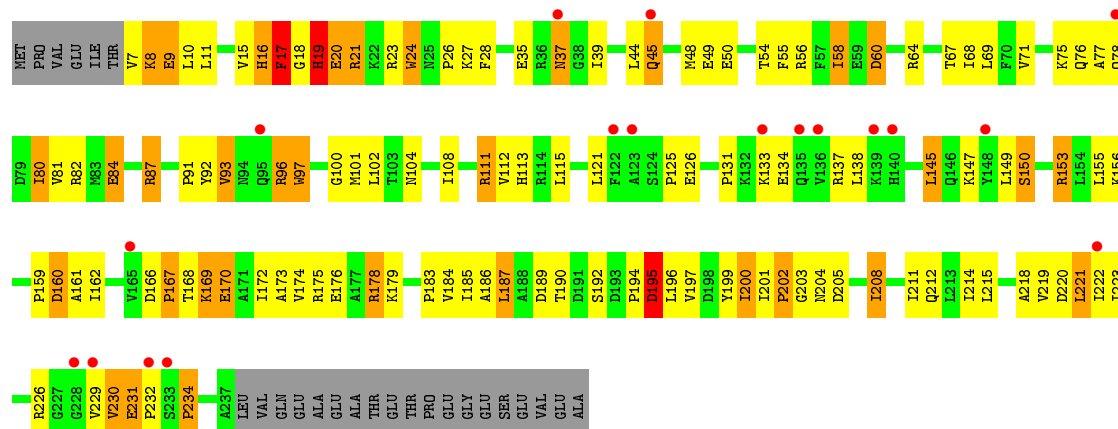
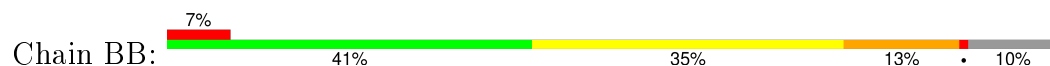




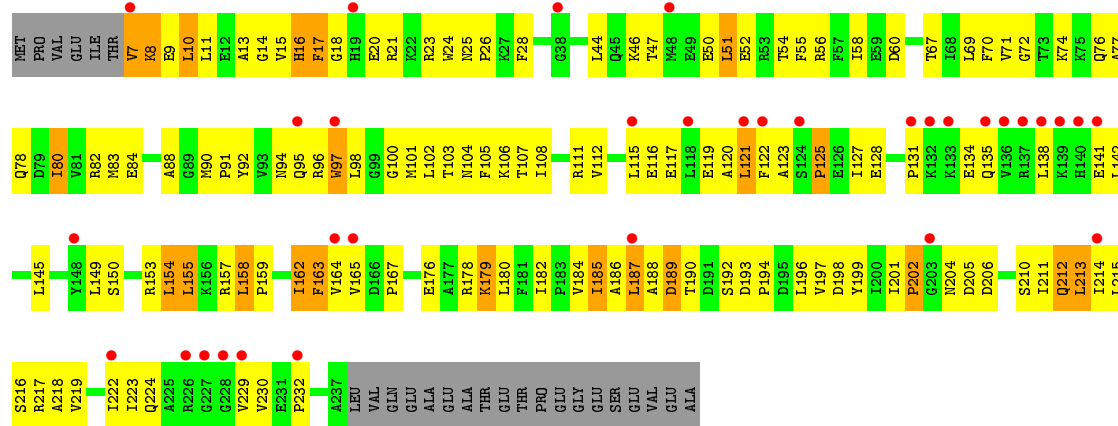
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| A1300 | G1217 | G1134 | U1062 | C1006 | G926 | C848 | G742 | U652 | G557 | G481 | C366 | G260 | G181 | U |
| U1301 | G1218 | U1135 | C1063 | C1007 | G927 | G851 | G748 | A653 | U571 | G481 | U367 | U261 | U182 | G |
| A1302 | G1219 | U1136 | G1064 | C1008 | G934 | G852 | G749 | A655 | A572 | G485 | U368 | A262 | C186 | U4 |
| C1303 | G1220 | G1137 | U1065 | G1009 | A935 | G853 | G750 | A656 | A573 | G489 | C369 | G267 | C187 | U5 |
| G1304 | G1221 | G1138 | C1066 | G1010 | G936 | G857 | G752 | G662 | A574 | G496 | C372 | C267 | C188 | G6 |
| G1305 | G1222 | G1139 | U1070 | U1012 | A937 | G858 | G753 | G663 | G575 | A498 | A373 | C268 | C189 | G7 |
| | G1223 | G1144 | C1071 | G1013 | A938 | G859 | G754 | A663 | G576 | U499 | A374 | C269 | C189A | A8 |
| | G1224 | A1146 | U1072 | A1014 | G939 | A860 | G755 | A665 | G577 | U499 | G376 | G278 | U189E | G9 |
| A1227 | A1227 | C1147 | G1074 | A1015 | C940 | G861 | G756 | A666 | C578 | A499 | U375 | G278 | U189F | A10 |
| A1228 | A1228 | U1148 | G1075 | G1016 | G953 | G865 | G758 | G671 | G579 | G500 | G384 | C280 | U189F | G15 |
| A1230 | A1230 | U1150 | C1076 | C1018 | G954 | C966 | G759 | G672 | G580 | G501 | A101 | G281 | U189K | A16 |
| | | A1152 | U1078 | C1019 | U955 | C966 | A766 | G673 | U582 | G502 | G388 | G289 | U189L | U17 |
| C1237 | C1237 | C1153 | G1079 | U1020 | U956 | C967 | A767 | G674 | A583 | C503 | A389 | G289 | C189L | C18 |
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| U1240 | U1240 | C1158 | G1082 | G1024 | U960 | A873 | A777 | A684 | C596 | A510 | A393 | A298 | U195 | G22 |
| C1241 | C1241 | U1159 | G1083 | U1025 | C962 | G874 | A777 | U686 | C596 | C511 | G394 | G299 | A196 | C23 |
| C1242 | C1242 | | U1084 | G1026 | C962 | G878 | G784 | A887 | C600 | C513 | C395 | A300 | A197 | U24 |
| | | | U1085 | C1027 | A965 | G881 | G785 | A688 | C600 | C513 | G396 | G301 | C201 | C25 |
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| G1258 | G1258 | C1172 | C1096 | G1032 | A974 | A893 | A796 | G703 | C612 | G527 | G425 | G332 | C221 | U37 |
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| C1263 | C1263 | G1181 | C1100 | G1036 | A978 | G899 | U804 | C708 | A621 | U534 | A412 | A338 | C243 | G47 |
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| A1286 | A1286 | C1208 | U1125 | A1055 | U1000 | A919 | G829 | G729 | U641 | G551 | U437 | A344 | C261 | G73 |
| A1287 | A1287 | C1209 | U1126 | U1056 | A1001 | U920 | G830 | G730 | U642 | G552 | U437 | A344 | C262 | G74 |
| | | | C1129 | G1057 | G1001A | U921 | G831 | G731 | U643 | G553 | U437 | A344 | C263 | G75 |
| A1288 | A1288 | U1211 | A1130 | G1058 | G1002 | A922 | G832 | G732 | U644 | G554 | U437 | A344 | C264 | G76 |
| A1289 | A1289 | C1212 | G1131 | C1059 | G1003 | A923 | G833 | G733 | U645 | G555 | U437 | A344 | C265 | G77 |
| G1290 | G1290 | A1213 | G1132 | C1060 | A1004 | C924 | G834 | G734 | U646 | G556 | U437 | A344 | C266 | G78 |
| G1291 | G1291 | | | | | | | | U647 | G557 | U437 | A344 | C267 | G79 |
| | | | | | | | | | C647 | G558 | U437 | A344 | C268 | G80 |
| | | | | | | | | | | G559 | U437 | A344 | C269 | U |
| | | | | | | | | | | G560 | U437 | A344 | C270 | G |



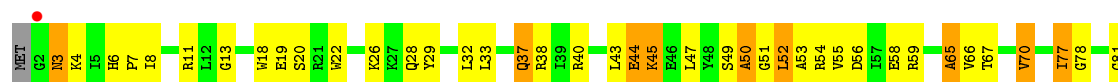
• Molecule 35: 30S ribosomal protein S2



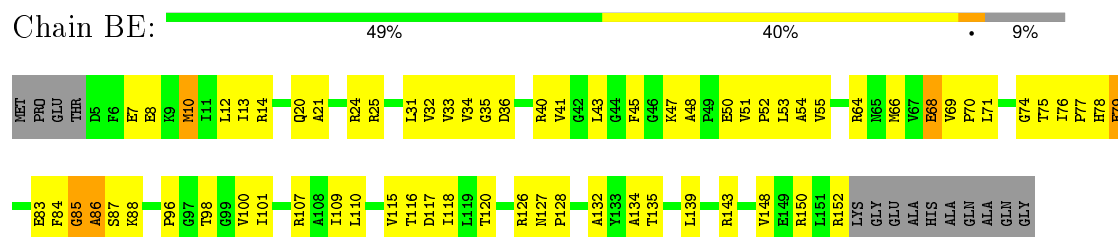
• Molecule 35: 30S ribosomal protein S2



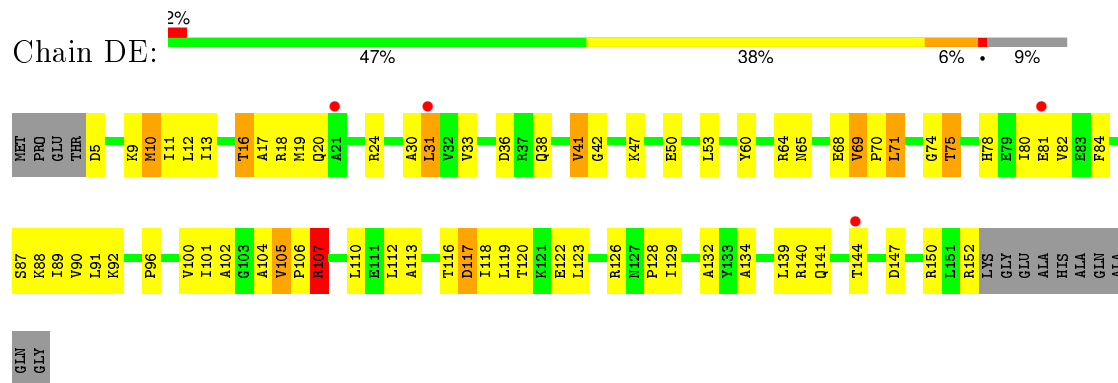
• Molecule 36: 30S ribosomal protein S3



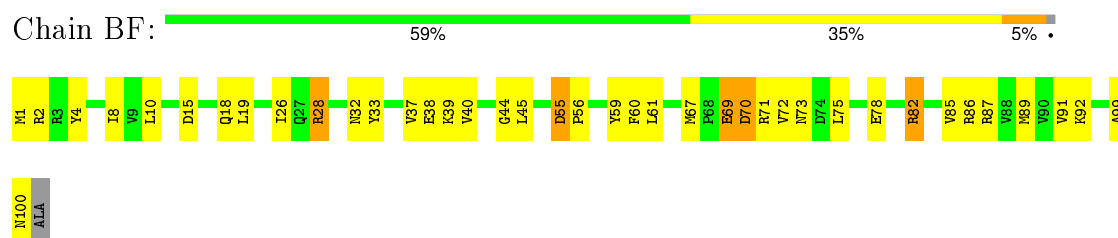
- Molecule 38: 30S ribosomal protein S5



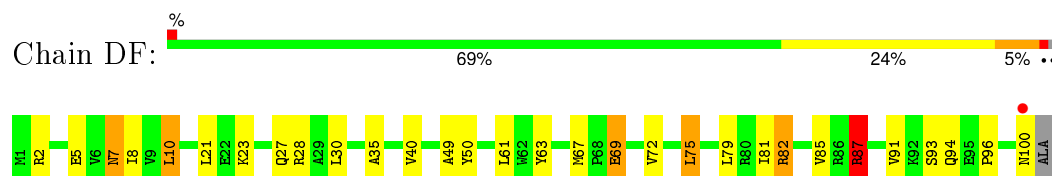
- Molecule 38: 30S ribosomal protein S5



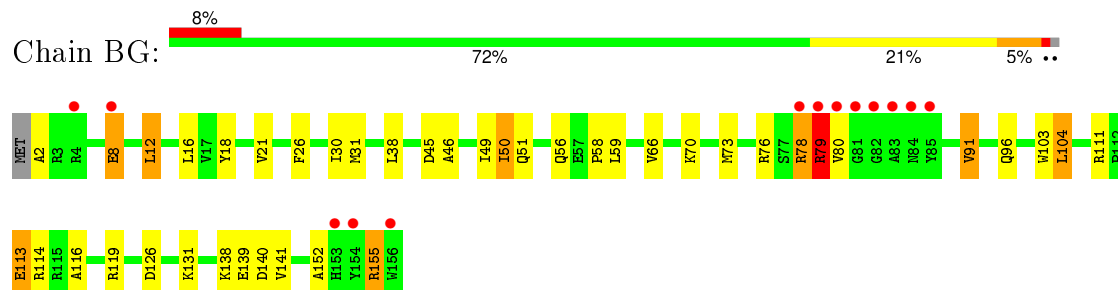
- Molecule 39: 30S ribosomal protein S6



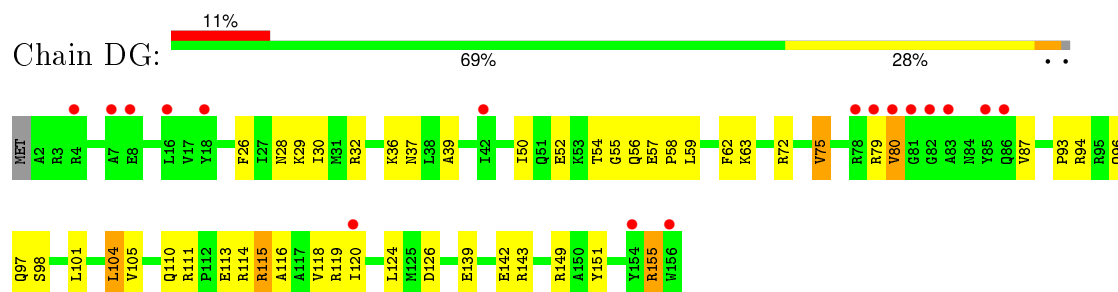
- Molecule 39: 30S ribosomal protein S6



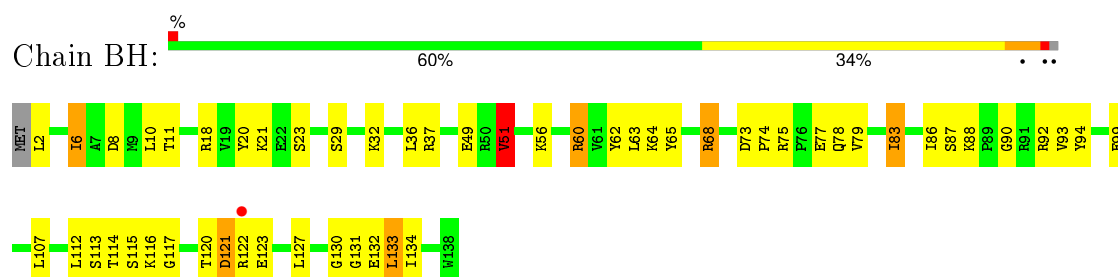
- Molecule 40: 30S ribosomal protein S7



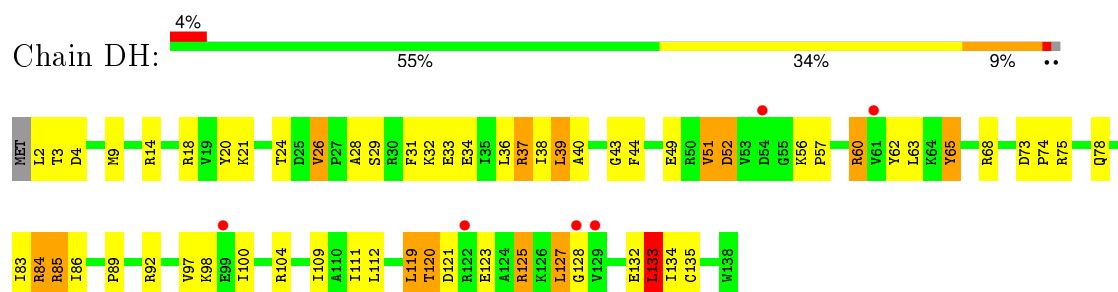
- Molecule 40: 30S ribosomal protein S7



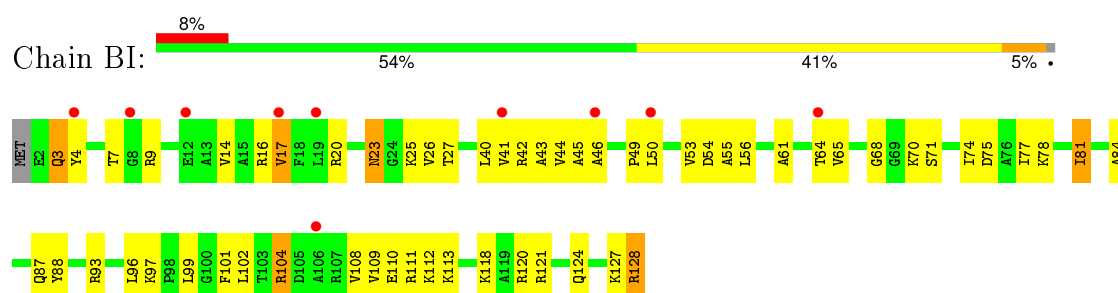
- Molecule 41: 30S ribosomal protein S8



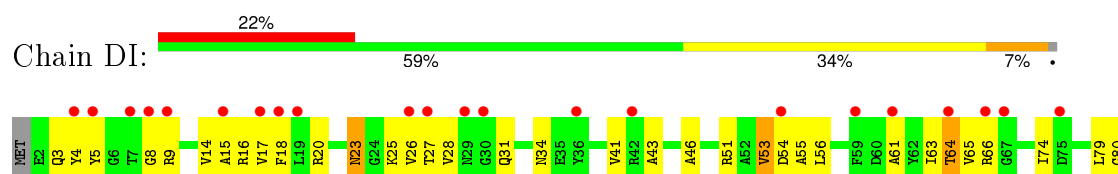
- Molecule 41: 30S ribosomal protein S8

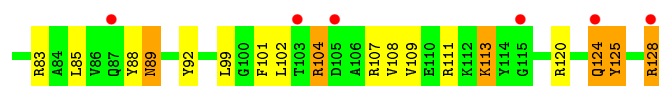


- Molecule 42: 30S ribosomal protein S9

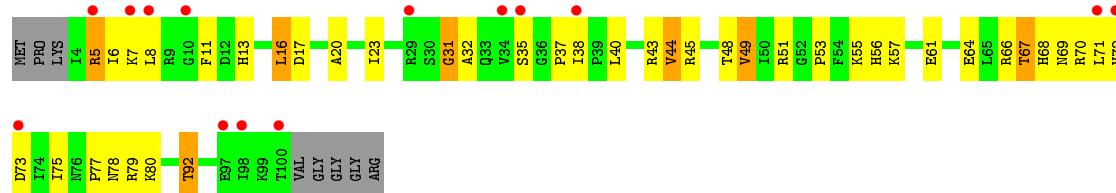


- Molecule 42: 30S ribosomal protein S9

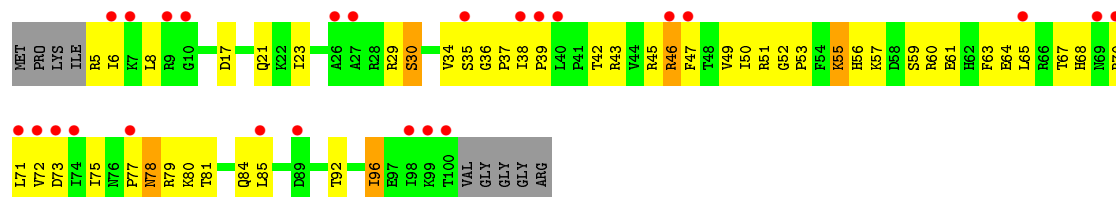




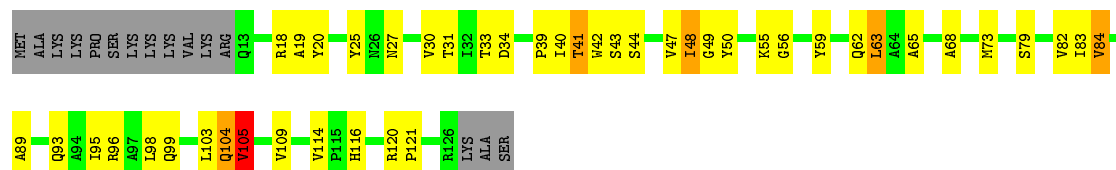
• Molecule 43: 30S ribosomal protein S10



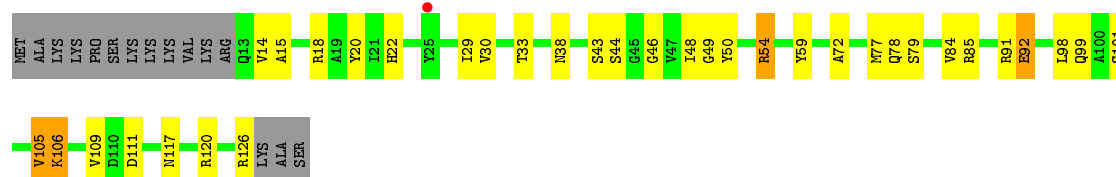
• Molecule 43: 30S ribosomal protein S10



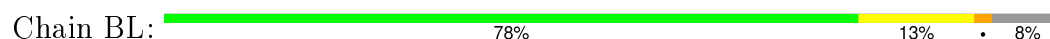
• Molecule 44: 30S ribosomal protein S11



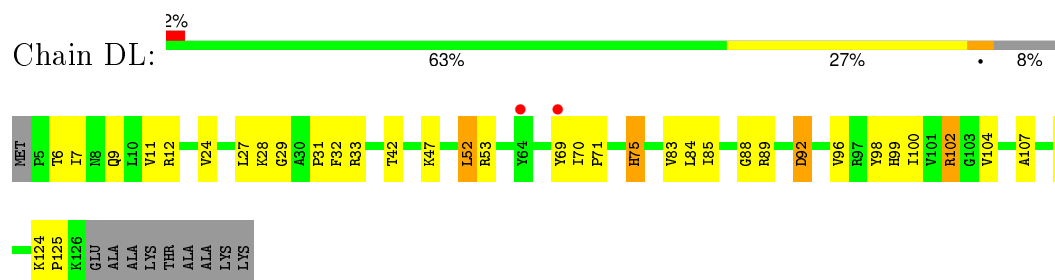
• Molecule 44: 30S ribosomal protein S11



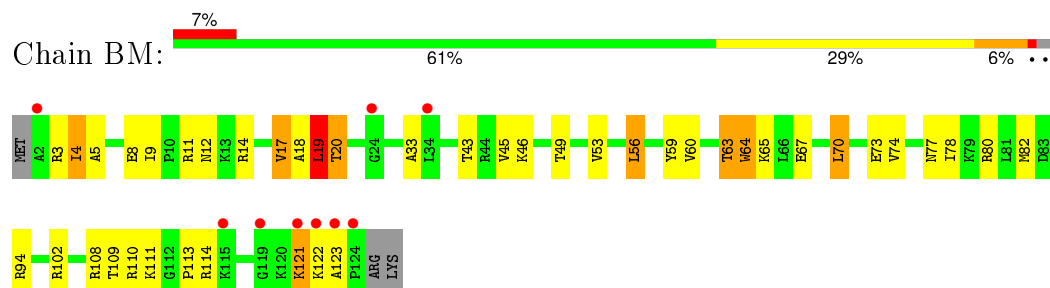
• Molecule 45: 30S ribosomal protein S12



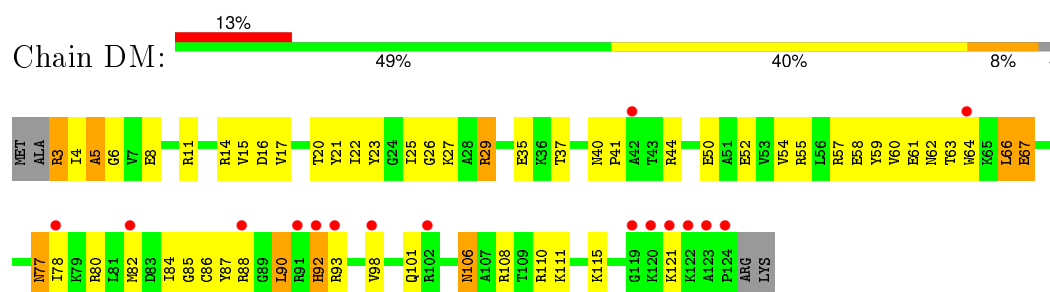
- Molecule 45: 30S ribosomal protein S12



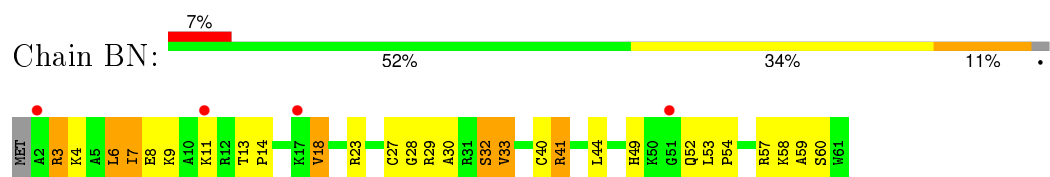
- Molecule 46: 30S ribosomal protein S13



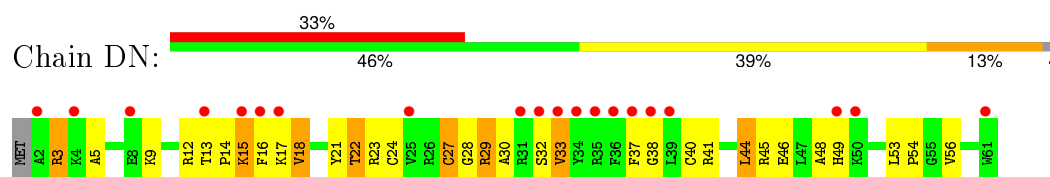
- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14 type Z

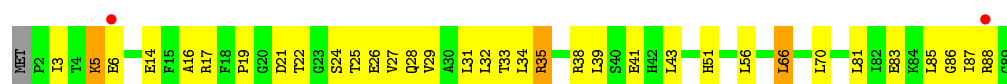


- Molecule 47: 30S ribosomal protein S14 type Z

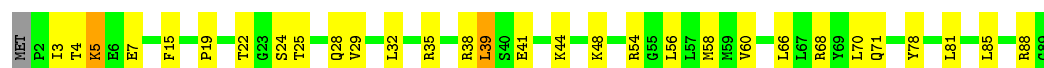


- Molecule 48: 30S ribosomal protein S15

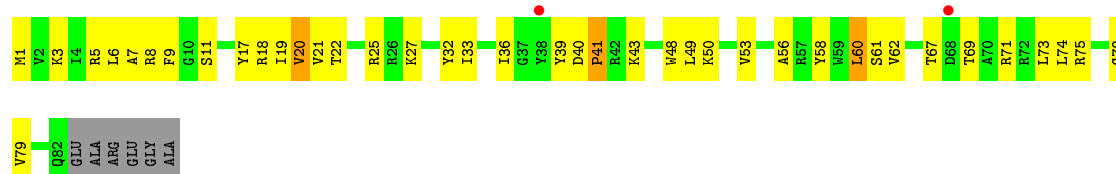




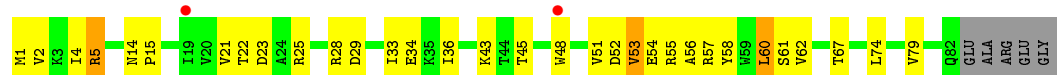
- Molecule 48: 30S ribosomal protein S15



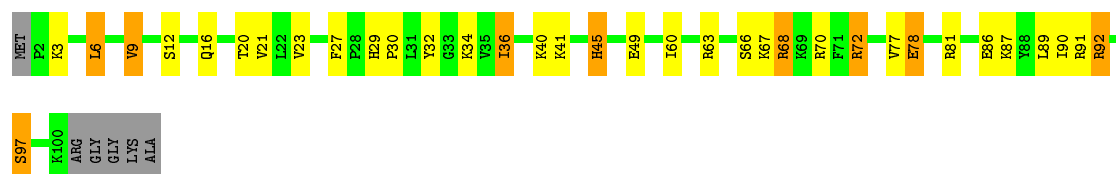
- Molecule 49: 30S ribosomal protein S16



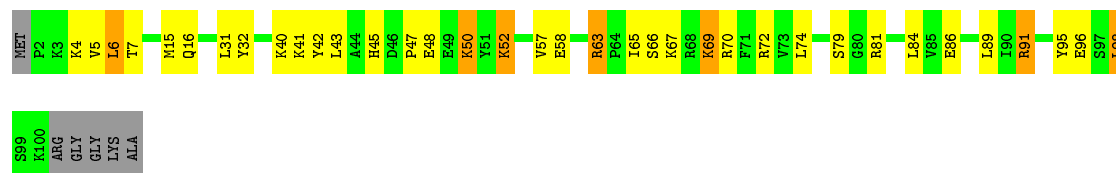
- Molecule 49: 30S ribosomal protein S16



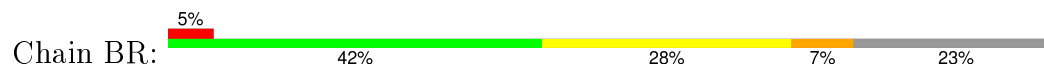
- Molecule 50: 30S ribosomal protein S17

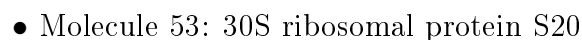
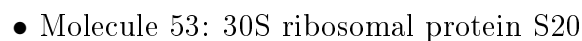
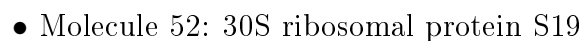
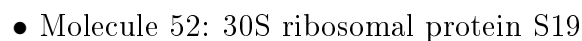
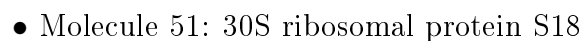


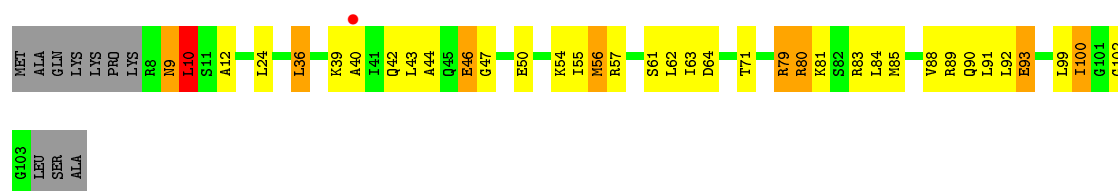
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18







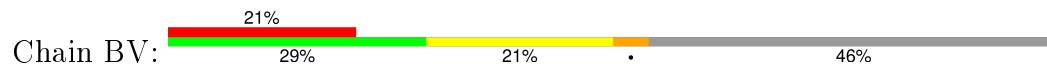
- Molecule 54: 30S ribosomal protein Thx



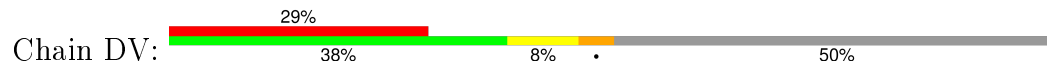
- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: mRNA



- Molecule 55: mRNA

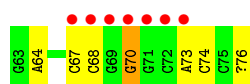


- Molecule 56: A-site tRNA



- Molecule 56: A-site tRNA





• Molecule 57: P-site tRNA

Chain BX: 62% 34%



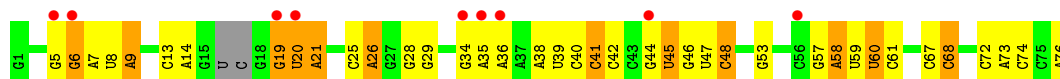
• Molecule 57: P-site tRNA

Chain DX: 3% 52% 35% 12%



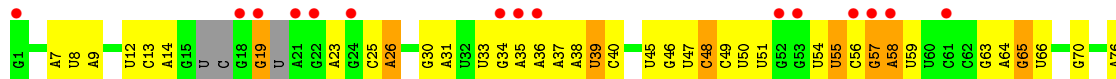
• Molecule 58: E-site tRNA

Chain BY: 12% 46% 36% 16%



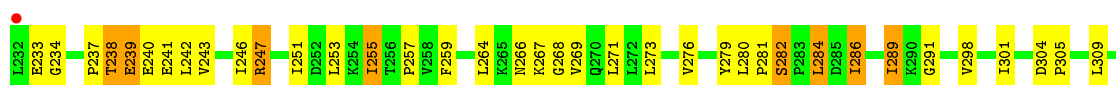
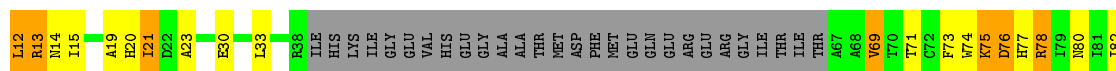
• Molecule 58: E-site tRNA

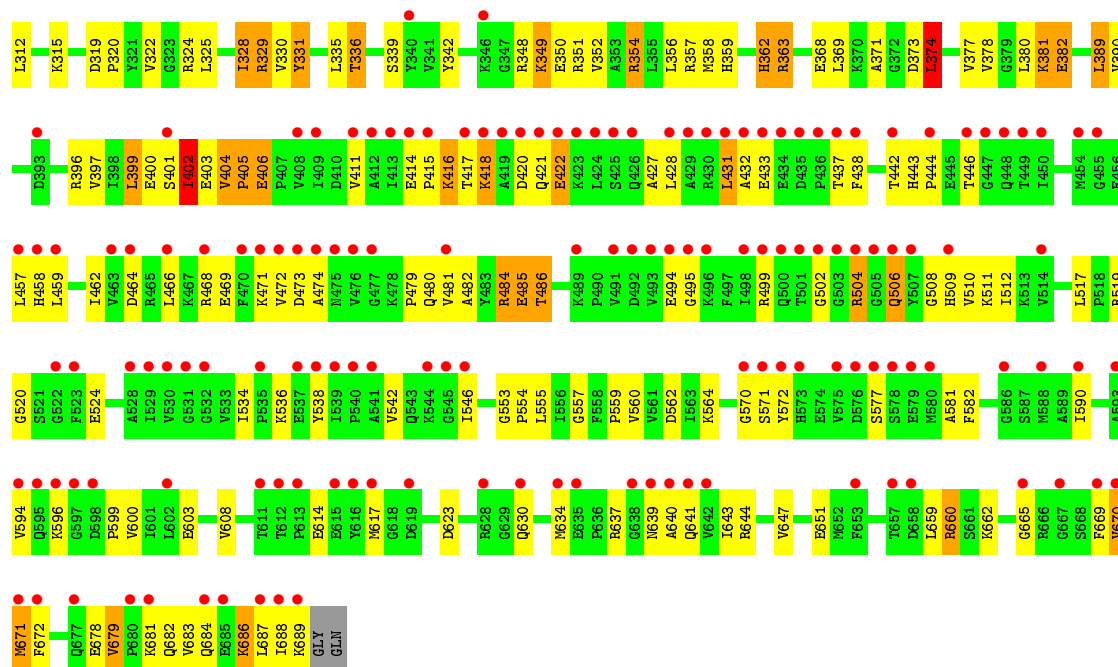
Chain DY: 20% 45% 41% 11%



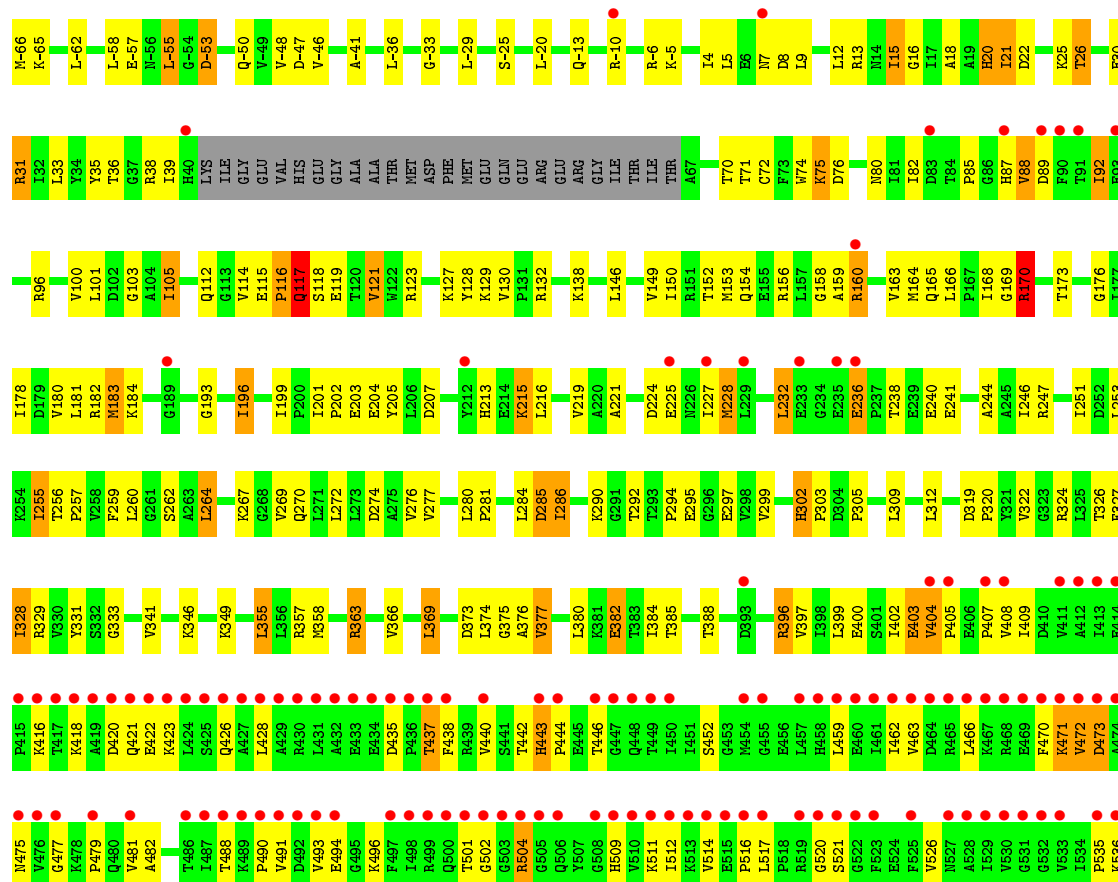
• Molecule 59: 50S ribosomal protein L9, Elongation factor G

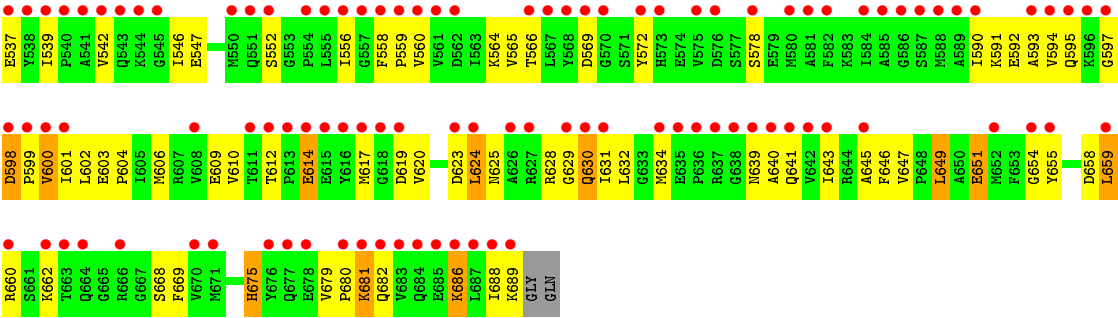
Chain BZ: 21% 51% 35% 9%





- Molecule 59: 50S ribosomal protein L9, Elongation factor G





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.89 Å 449.03 Å 622.90 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.63 – 2.80 49.63 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 99.2 (49.63-2.80) 99.0 (49.63-2.80) | Depositor EDS |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.85 (at 2.81 Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE: 1.8.2_1309) | Depositor |
| R, R_{free} | 0.202 , 0.252 0.208 , 0.255 | Depositor DCC |
| R_{free} test set | 70994 reflections (5.29%) | DCC |
| Wilson B-factor (Å ²) | 54.8 | Xtriage |
| Anisotropy | 0.148 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 67.6 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 1 of 1417809 reflections (0.000%) | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 313372 | wwPDB-VP |
| Average B, all atoms (Å ²) | 76.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: 5MU, GDP, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

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 | 1.20 | 165/69281 (0.2%) | 1.78 | 2173/108144 (2.0%) |
| 1 | CA | 0.89 | 30/69179 (0.0%) | 1.46 | 878/107984 (0.8%) |
| 2 | AB | 0.97 | 0/2878 | 1.65 | 57/4490 (1.3%) |
| 2 | CB | 0.63 | 0/2878 | 1.24 | 15/4490 (0.3%) |
| 3 | AC | 0.34 | 0/1083 | 0.65 | 0/1460 |
| 3 | CC | 0.34 | 0/1083 | 0.65 | 0/1460 |
| 4 | AD | 0.80 | 2/2186 (0.1%) | 0.91 | 2/2944 (0.1%) |
| 4 | CD | 0.65 | 0/2192 | 0.81 | 2/2951 (0.1%) |
| 5 | AE | 0.81 | 0/1592 | 0.89 | 1/2149 (0.0%) |
| 5 | CE | 0.63 | 0/1592 | 0.80 | 0/2149 |
| 6 | AF | 0.75 | 0/1619 | 0.91 | 2/2193 (0.1%) |
| 6 | CF | 0.57 | 0/1615 | 0.74 | 0/2188 |
| 7 | AG | 0.51 | 0/1450 | 0.70 | 0/1959 |
| 7 | CG | 0.39 | 0/1449 | 0.59 | 0/1958 |
| 8 | AH | 0.67 | 0/1356 | 0.79 | 0/1834 |
| 8 | CH | 0.41 | 0/1356 | 0.62 | 0/1834 |
| 9 | AK | 0.33 | 0/640 | 0.63 | 0/889 |
| 9 | CK | 0.26 | 0/640 | 0.58 | 0/889 |
| 10 | AL | 0.31 | 0/503 | 0.53 | 0/673 |
| 10 | CL | 0.34 | 0/503 | 0.54 | 0/673 |
| 11 | AN | 0.81 | 0/1144 | 0.90 | 1/1543 (0.1%) |
| 11 | CN | 0.57 | 0/1144 | 0.71 | 0/1543 |
| 12 | AO | 0.76 | 0/943 | 0.84 | 1/1269 (0.1%) |
| 12 | CO | 0.68 | 0/943 | 0.75 | 0/1269 |
| 13 | AP | 0.70 | 0/1156 | 0.87 | 2/1537 (0.1%) |
| 13 | CP | 0.51 | 0/1152 | 0.80 | 0/1533 |
| 14 | AQ | 0.77 | 0/1143 | 0.86 | 1/1527 (0.1%) |
| 14 | CQ | 0.58 | 0/1143 | 0.69 | 0/1527 |
| 15 | AR | 0.73 | 0/982 | 0.87 | 0/1312 |
| 15 | CR | 0.58 | 0/982 | 0.77 | 0/1312 |
| 16 | AS | 0.58 | 0/887 | 0.76 | 1/1180 (0.1%) |
| 16 | CS | 0.46 | 0/880 | 0.71 | 0/1172 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AT | 0.74 | 0/1105 | 0.88 | 0/1477 |
| 17 | CT | 0.58 | 0/1097 | 0.74 | 0/1468 |
| 18 | AU | 0.89 | 1/977 (0.1%) | 0.92 | 1/1301 (0.1%) |
| 18 | CU | 0.62 | 0/977 | 0.71 | 2/1301 (0.2%) |
| 19 | AV | 0.80 | 0/782 | 0.90 | 1/1049 (0.1%) |
| 19 | CV | 0.52 | 0/782 | 0.74 | 0/1049 |
| 20 | AW | 0.91 | 0/897 | 0.93 | 3/1205 (0.2%) |
| 20 | CW | 0.70 | 0/897 | 0.81 | 0/1205 |
| 21 | AX | 0.82 | 1/764 (0.1%) | 0.80 | 1/1025 (0.1%) |
| 21 | CX | 0.62 | 0/764 | 0.75 | 1/1025 (0.1%) |
| 22 | AY | 0.74 | 0/819 | 0.85 | 0/1095 |
| 22 | CY | 0.54 | 0/819 | 0.69 | 0/1095 |
| 23 | AZ | 0.52 | 0/1379 | 0.70 | 1/1873 (0.1%) |
| 23 | CZ | 0.39 | 0/1390 | 0.58 | 0/1890 |
| 24 | A0 | 0.67 | 0/662 | 0.88 | 1/881 (0.1%) |
| 24 | C0 | 0.56 | 0/662 | 0.68 | 0/881 |
| 25 | A1 | 0.70 | 0/762 | 0.81 | 0/1014 |
| 25 | C1 | 0.61 | 0/762 | 0.77 | 0/1014 |
| 26 | A2 | 0.78 | 0/590 | 0.78 | 0/781 |
| 26 | C2 | 0.53 | 0/590 | 0.63 | 0/781 |
| 27 | A3 | 0.82 | 0/474 | 0.91 | 0/635 |
| 27 | C3 | 0.49 | 0/469 | 0.69 | 0/630 |
| 28 | A4 | 0.43 | 0/571 | 0.70 | 0/768 |
| 28 | C4 | 0.35 | 0/545 | 0.60 | 0/737 |
| 29 | A5 | 0.89 | 1/469 (0.2%) | 1.00 | 2/635 (0.3%) |
| 29 | C5 | 0.66 | 0/469 | 0.82 | 0/635 |
| 30 | A6 | 0.86 | 1/460 (0.2%) | 0.79 | 0/613 |
| 30 | C6 | 0.62 | 0/456 | 0.74 | 0/608 |
| 31 | A7 | 0.84 | 0/426 | 0.99 | 2/561 (0.4%) |
| 31 | C7 | 0.70 | 0/426 | 0.78 | 0/561 |
| 32 | A8 | 0.82 | 0/525 | 0.90 | 0/691 |
| 32 | C8 | 0.61 | 0/525 | 0.78 | 0/691 |
| 33 | A9 | 0.80 | 0/310 | 0.94 | 0/407 |
| 33 | C9 | 0.60 | 0/310 | 0.73 | 0/407 |
| 34 | BA | 0.70 | 4/36027 (0.0%) | 1.28 | 246/56227 (0.4%) |
| 34 | DA | 0.64 | 1/36170 (0.0%) | 1.21 | 131/56452 (0.2%) |
| 35 | BB | 0.40 | 0/1881 | 0.67 | 1/2542 (0.0%) |
| 35 | DB | 0.36 | 0/1860 | 0.61 | 0/2518 |
| 36 | BC | 0.38 | 0/1576 | 0.59 | 0/2130 |
| 36 | DC | 0.35 | 0/1568 | 0.57 | 0/2122 |
| 37 | BD | 0.48 | 0/1689 | 0.67 | 0/2267 |
| 37 | DD | 0.48 | 0/1708 | 0.70 | 1/2289 (0.0%) |
| 38 | BE | 0.51 | 0/1145 | 0.69 | 1/1543 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DE | 0.44 | 0/1149 | 0.67 | 0/1548 |
| 39 | BF | 0.52 | 0/825 | 0.70 | 0/1118 |
| 39 | DF | 0.52 | 0/833 | 0.69 | 1/1128 (0.1%) |
| 40 | BG | 0.43 | 0/1250 | 0.58 | 0/1679 |
| 40 | DG | 0.37 | 0/1254 | 0.56 | 0/1683 |
| 41 | BH | 0.48 | 0/1108 | 0.68 | 0/1494 |
| 41 | DH | 0.42 | 0/1108 | 0.64 | 0/1494 |
| 42 | BI | 0.42 | 0/1005 | 0.62 | 0/1350 |
| 42 | DI | 0.36 | 0/997 | 0.58 | 0/1343 |
| 43 | BJ | 0.38 | 0/722 | 0.58 | 0/982 |
| 43 | DJ | 0.34 | 0/727 | 0.59 | 0/988 |
| 44 | BK | 0.49 | 0/848 | 0.66 | 0/1149 |
| 44 | DK | 0.50 | 0/848 | 0.66 | 0/1149 |
| 45 | BL | 0.56 | 0/946 | 0.70 | 0/1274 |
| 45 | DL | 0.52 | 0/946 | 0.68 | 0/1274 |
| 46 | BM | 0.41 | 0/977 | 0.64 | 0/1310 |
| 46 | DM | 0.35 | 0/961 | 0.56 | 0/1291 |
| 47 | BN | 0.44 | 0/501 | 0.70 | 0/664 |
| 47 | DN | 0.37 | 0/501 | 0.59 | 1/664 (0.2%) |
| 48 | BO | 0.50 | 0/739 | 0.71 | 0/985 |
| 48 | DO | 0.46 | 0/739 | 0.63 | 0/985 |
| 49 | BP | 0.53 | 0/697 | 0.69 | 0/939 |
| 49 | DP | 0.52 | 0/693 | 0.66 | 0/935 |
| 50 | BQ | 0.53 | 0/836 | 0.69 | 1/1117 (0.1%) |
| 50 | DQ | 0.50 | 0/836 | 0.68 | 0/1117 |
| 51 | BR | 0.51 | 0/560 | 0.74 | 0/746 |
| 51 | DR | 0.52 | 0/560 | 0.66 | 0/746 |
| 52 | BS | 0.36 | 0/676 | 0.58 | 0/911 |
| 52 | DS | 0.32 | 0/661 | 0.64 | 0/893 |
| 53 | BT | 0.45 | 0/730 | 0.71 | 0/965 |
| 53 | DT | 0.46 | 0/733 | 0.69 | 0/969 |
| 54 | BU | 0.40 | 0/203 | 0.62 | 0/266 |
| 54 | DU | 0.35 | 0/203 | 0.62 | 0/266 |
| 55 | BV | 0.65 | 0/310 | 1.02 | 1/480 (0.2%) |
| 55 | DV | 0.54 | 0/282 | 0.91 | 0/437 |
| 56 | BW | 0.43 | 0/1577 | 0.96 | 1/2454 (0.0%) |
| 56 | DW | 0.36 | 0/1531 | 0.94 | 0/2379 |
| 57 | BX | 0.71 | 1/1700 (0.1%) | 1.22 | 2/2650 (0.1%) |
| 57 | DX | 0.63 | 1/1700 (0.1%) | 1.12 | 4/2650 (0.2%) |
| 58 | BY | 0.43 | 0/1602 | 0.98 | 1/2493 (0.0%) |
| 58 | DY | 0.36 | 0/1579 | 0.86 | 0/2455 |
| 59 | BZ | 0.44 | 0/5763 | 0.68 | 2/7804 (0.0%) |
| 59 | DZ | 0.41 | 0/5784 | 0.63 | 0/7835 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.82 | 208/333310 (0.1%) | 1.32 | 3545/497173 (0.7%) |

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 |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 1 |
| 28 | A4 | 0 | 1 |
| 35 | BB | 0 | 1 |
| 53 | BT | 0 | 1 |
| 53 | DT | 0 | 1 |
| 59 | DZ | 0 | 1 |
| All | All | 0 | 6 |

All (208) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 1 | AA | 1188 | A | N9-C4 | -13.96 | 1.29 | 1.37 |
| 1 | AA | 354 | A | N9-C4 | -13.07 | 1.30 | 1.37 |
| 1 | CA | 528 | A | N9-C4 | -11.34 | 1.31 | 1.37 |
| 57 | DX | 74 | C | O3'-P | -11.14 | 1.47 | 1.61 |
| 1 | AA | 2299 | A | N9-C4 | -10.50 | 1.31 | 1.37 |
| 1 | AA | 1249 | A | N9-C4 | -10.39 | 1.31 | 1.37 |
| 1 | AA | 990 | A | N9-C4 | -10.29 | 1.31 | 1.37 |
| 1 | AA | 1745 | A | N9-C4 | -9.99 | 1.31 | 1.37 |
| 1 | AA | 990 | A | N3-C4 | -9.67 | 1.29 | 1.34 |
| 1 | AA | 1067 | A | N9-C4 | -9.60 | 1.32 | 1.37 |
| 1 | AA | 990 | A | C5-C6 | -9.56 | 1.32 | 1.41 |
| 1 | AA | 978 | A | N9-C4 | -9.49 | 1.32 | 1.37 |
| 1 | CA | 945 | A | N9-C4 | -9.28 | 1.32 | 1.37 |
| 1 | CA | 1142(A) | A | N9-C4 | -9.24 | 1.32 | 1.37 |
| 1 | AA | 254 | A | N7-C5 | -8.38 | 1.34 | 1.39 |
| 4 | AD | 28 | GLU | CG-CD | 8.35 | 1.64 | 1.51 |
| 1 | AA | 555 | G | C2-N3 | -8.30 | 1.26 | 1.32 |
| 1 | AA | 808 | A | N7-C5 | -8.10 | 1.34 | 1.39 |
| 1 | AA | 553 | A | N9-C8 | 8.04 | 1.44 | 1.37 |
| 1 | AA | 254 | A | C5-C6 | -7.96 | 1.33 | 1.41 |
| 1 | CA | 1652 | A | N9-C4 | -7.86 | 1.33 | 1.37 |
| 4 | AD | 28 | GLU | CB-CG | 7.72 | 1.66 | 1.52 |
| 1 | AA | 1249 | A | N3-C4 | -7.68 | 1.30 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|-------|-------------|----------|
| 1 | CA | 1021 | A | N9-C4 | -7.62 | 1.33 | 1.37 |
| 1 | AA | 990 | A | N7-C5 | -7.55 | 1.34 | 1.39 |
| 1 | AA | 555 | G | C6-N1 | -7.52 | 1.34 | 1.39 |
| 1 | AA | 2490 | A | N9-C4 | -7.47 | 1.33 | 1.37 |
| 1 | CA | 945 | A | C5-C6 | -7.45 | 1.34 | 1.41 |
| 1 | AA | 1605 | A | N9-C4 | -7.38 | 1.33 | 1.37 |
| 1 | AA | 553 | A | N9-C4 | -7.30 | 1.33 | 1.37 |
| 1 | AA | 1188 | A | N3-C4 | -7.29 | 1.30 | 1.34 |
| 1 | AA | 1745 | A | N3-C4 | -7.15 | 1.30 | 1.34 |
| 1 | AA | 1157 | A | N9-C4 | -7.11 | 1.33 | 1.37 |
| 1 | AA | 830 | A | N7-C5 | -7.05 | 1.35 | 1.39 |
| 1 | CA | 1698 | A | N3-C4 | -6.99 | 1.30 | 1.34 |
| 18 | AU | 111 | GLU | CG-CD | 6.93 | 1.62 | 1.51 |
| 1 | AA | 808 | A | N3-C4 | -6.90 | 1.30 | 1.34 |
| 1 | AA | 1745 | A | C5-C6 | -6.88 | 1.34 | 1.41 |
| 1 | AA | 2527 | C | N1-C6 | -6.86 | 1.33 | 1.37 |
| 1 | CA | 2287 | A | N9-C4 | -6.76 | 1.33 | 1.37 |
| 1 | AA | 2405 | A | N9-C4 | -6.76 | 1.33 | 1.37 |
| 1 | AA | 139 | A | N9-C4 | -6.64 | 1.33 | 1.37 |
| 1 | AA | 978 | A | N3-C4 | -6.57 | 1.30 | 1.34 |
| 34 | BA | 900 | A | N9-C4 | -6.56 | 1.33 | 1.37 |
| 1 | AA | 851 | A | N9-C4 | -6.54 | 1.33 | 1.37 |
| 1 | CA | 1698 | A | N9-C4 | -6.51 | 1.33 | 1.37 |
| 1 | AA | 2553 | A | N7-C5 | -6.51 | 1.35 | 1.39 |
| 1 | AA | 2072 | C | N1-C6 | -6.50 | 1.33 | 1.37 |
| 1 | CA | 1204 | A | N9-C4 | -6.46 | 1.33 | 1.37 |
| 1 | AA | 1820 | A | N7-C5 | -6.41 | 1.35 | 1.39 |
| 1 | AA | 1829 | U | C2-N3 | -6.38 | 1.33 | 1.37 |
| 1 | AA | 16 | G | C6-N1 | -6.33 | 1.35 | 1.39 |
| 1 | CA | 185 | U | C2-N3 | -6.29 | 1.33 | 1.37 |
| 1 | AA | 2553 | A | C5-C6 | -6.24 | 1.35 | 1.41 |
| 1 | AA | 555 | G | N9-C8 | 6.23 | 1.42 | 1.37 |
| 1 | AA | 2715 | C | N1-C6 | -6.23 | 1.33 | 1.37 |
| 1 | AA | 254 | A | N9-C4 | -6.22 | 1.34 | 1.37 |
| 1 | AA | 127 | C | N1-C6 | -6.21 | 1.33 | 1.37 |
| 1 | AA | 354 | A | C5-C6 | -6.20 | 1.35 | 1.41 |
| 21 | AX | 15 | GLU | CG-CD | 6.19 | 1.61 | 1.51 |
| 1 | AA | 354 | A | N9-C8 | 6.18 | 1.42 | 1.37 |
| 1 | AA | 1249 | A | N9-C8 | 6.17 | 1.42 | 1.37 |
| 1 | AA | 644 | G | C6-N1 | -6.16 | 1.35 | 1.39 |
| 1 | AA | 448 | U | C2-N3 | -6.15 | 1.33 | 1.37 |
| 1 | CA | 1142(A) | A | N3-C4 | -6.15 | 1.31 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | CA | 330 | A | N9-C4 | -6.11 | 1.34 | 1.37 |
| 1 | AA | 2298 | A | N3-C4 | -6.10 | 1.31 | 1.34 |
| 1 | AA | 1188 | A | C5-C6 | -6.09 | 1.35 | 1.41 |
| 1 | AA | 553 | A | N3-C4 | -6.06 | 1.31 | 1.34 |
| 1 | AA | 592 | U | N1-C2 | -6.06 | 1.33 | 1.38 |
| 1 | AA | 2530 | A | N7-C5 | -6.00 | 1.35 | 1.39 |
| 1 | AA | 2515 | A | N9-C4 | 5.99 | 1.41 | 1.37 |
| 1 | AA | 1741 | C | N1-C6 | -5.96 | 1.33 | 1.37 |
| 1 | AA | 591 | U | C4-O4 | -5.93 | 1.19 | 1.23 |
| 1 | CA | 1784 | A | N9-C4 | -5.91 | 1.34 | 1.37 |
| 1 | CA | 784 | A | C6-N1 | -5.89 | 1.31 | 1.35 |
| 1 | AA | 2659 | U | C2-N3 | -5.89 | 1.33 | 1.37 |
| 1 | CA | 792 | G | C5-C4 | -5.87 | 1.34 | 1.38 |
| 1 | AA | 538 | A | N3-C4 | -5.84 | 1.31 | 1.34 |
| 1 | AA | 2466 | G | N1-C2 | -5.82 | 1.33 | 1.37 |
| 1 | AA | 2298 | A | N7-C5 | -5.81 | 1.35 | 1.39 |
| 1 | AA | 1048 | G | N1-C2 | -5.78 | 1.33 | 1.37 |
| 1 | CA | 826 | U | C2-N3 | -5.77 | 1.33 | 1.37 |
| 1 | AA | 978 | A | C5-C6 | -5.77 | 1.35 | 1.41 |
| 1 | AA | 591 | U | N3-C4 | -5.75 | 1.33 | 1.38 |
| 1 | AA | 254 | A | N3-C4 | -5.74 | 1.31 | 1.34 |
| 1 | AA | 593 | G | N7-C5 | -5.73 | 1.35 | 1.39 |
| 1 | AA | 2298 | A | C5-C4 | 5.68 | 1.42 | 1.38 |
| 1 | AA | 897 | C | N3-C4 | -5.67 | 1.29 | 1.33 |
| 1 | AA | 600 | G | N7-C5 | -5.66 | 1.35 | 1.39 |
| 1 | AA | 322 | G | N7-C5 | -5.66 | 1.35 | 1.39 |
| 1 | AA | 2299 | A | C5-C6 | -5.65 | 1.35 | 1.41 |
| 1 | CA | 1184 | G | N7-C5 | -5.63 | 1.35 | 1.39 |
| 1 | AA | 719 | C | C4-N4 | -5.63 | 1.28 | 1.33 |
| 1 | AA | 2024 | G | C8-N7 | -5.63 | 1.27 | 1.30 |
| 1 | AA | 2104 | A | N9-C4 | -5.61 | 1.34 | 1.37 |
| 1 | CA | 2593 | U | C4-O4 | -5.60 | 1.19 | 1.23 |
| 1 | AA | 2883 | A | N3-C4 | -5.60 | 1.31 | 1.34 |
| 1 | AA | 831 | A | C5-C4 | -5.58 | 1.34 | 1.38 |
| 1 | AA | 2054 | G | C6-N1 | -5.58 | 1.35 | 1.39 |
| 1 | AA | 553 | A | C5-C4 | 5.55 | 1.42 | 1.38 |
| 1 | AA | 553 | A | C5-C6 | -5.53 | 1.36 | 1.41 |
| 1 | AA | 2854 | G | N9-C4 | -5.52 | 1.33 | 1.38 |
| 1 | AA | 594 | A | N3-C4 | 5.51 | 1.38 | 1.34 |
| 1 | AA | 905 | U | C2-N3 | -5.50 | 1.33 | 1.37 |
| 1 | AA | 2601 | A | N3-C4 | -5.50 | 1.31 | 1.34 |
| 1 | AA | 1292 | A | N3-C4 | -5.50 | 1.31 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | AA | 455 | A | N3-C4 | -5.50 | 1.31 | 1.34 |
| 1 | AA | 2858 | G | C6-N1 | -5.49 | 1.35 | 1.39 |
| 1 | AA | 1234 | A | N9-C4 | -5.48 | 1.34 | 1.37 |
| 1 | AA | 1321 | A | N9-C8 | -5.48 | 1.33 | 1.37 |
| 1 | AA | 2073 | A | N3-C4 | -5.47 | 1.31 | 1.34 |
| 1 | AA | 528 | A | N7-C5 | -5.47 | 1.35 | 1.39 |
| 1 | AA | 808 | A | C5-C6 | -5.47 | 1.36 | 1.41 |
| 1 | AA | 1001 | G | C6-N1 | 5.46 | 1.43 | 1.39 |
| 1 | AA | 1380 | G | N3-C4 | -5.45 | 1.31 | 1.35 |
| 1 | CA | 1815 | A | N3-C4 | -5.45 | 1.31 | 1.34 |
| 1 | AA | 993 | G | N9-C4 | -5.45 | 1.33 | 1.38 |
| 1 | AA | 1067 | A | N7-C5 | -5.43 | 1.35 | 1.39 |
| 30 | A6 | 40 | CYS | CB-SG | -5.43 | 1.73 | 1.81 |
| 1 | AA | 830 | A | C6-N1 | -5.42 | 1.31 | 1.35 |
| 1 | AA | 1281 | G | N3-C4 | -5.42 | 1.31 | 1.35 |
| 34 | BA | 1512 | U | C2-N3 | -5.42 | 1.33 | 1.37 |
| 1 | AA | 2701 | U | C3'-O3' | 5.41 | 1.49 | 1.42 |
| 1 | AA | 199 | C | N3-C4 | -5.41 | 1.30 | 1.33 |
| 1 | AA | 990 | A | N1-C2 | 5.41 | 1.39 | 1.34 |
| 1 | AA | 2496 | G | C5-C4 | -5.40 | 1.34 | 1.38 |
| 1 | AA | 1605 | A | C5-C6 | -5.40 | 1.36 | 1.41 |
| 1 | AA | 1026 | A | N9-C4 | -5.38 | 1.34 | 1.37 |
| 1 | AA | 1679 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 1 | AA | 2602 | A | N3-C4 | -5.37 | 1.31 | 1.34 |
| 1 | AA | 1067 | A | N3-C4 | -5.36 | 1.31 | 1.34 |
| 1 | AA | 2602 | A | N9-C4 | -5.34 | 1.34 | 1.37 |
| 1 | AA | 1001 | G | C6-O6 | 5.33 | 1.28 | 1.24 |
| 1 | AA | 894 | U | N3-C4 | -5.33 | 1.33 | 1.38 |
| 1 | CA | 1890 | A | N9-C4 | -5.33 | 1.34 | 1.37 |
| 1 | AA | 2084 | A | N9-C4 | 5.32 | 1.41 | 1.37 |
| 34 | BA | 317 | G | N7-C5 | -5.32 | 1.36 | 1.39 |
| 1 | CA | 960 | A | N9-C4 | -5.32 | 1.34 | 1.37 |
| 1 | AA | 1306 | G | C6-O6 | 5.31 | 1.28 | 1.24 |
| 1 | AA | 2677 | A | N7-C5 | -5.31 | 1.36 | 1.39 |
| 1 | AA | 2803 | A | N9-C4 | 5.31 | 1.41 | 1.37 |
| 57 | BX | 75 | C | N1-C6 | -5.29 | 1.33 | 1.37 |
| 1 | AA | 1067 | A | C5-C6 | -5.29 | 1.36 | 1.41 |
| 1 | AA | 724 | A | N7-C5 | -5.29 | 1.36 | 1.39 |
| 1 | AA | 2611 | G | N3-C4 | -5.29 | 1.31 | 1.35 |
| 1 | AA | 1259 | A | N7-C5 | -5.28 | 1.36 | 1.39 |
| 1 | AA | 2272 | C | N1-C6 | -5.27 | 1.33 | 1.37 |
| 1 | AA | 2876 | U | N3-C4 | -5.26 | 1.33 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | AA | 719 | C | N3-C4 | -5.26 | 1.30 | 1.33 |
| 1 | AA | 2459 | G | C6-N1 | -5.26 | 1.35 | 1.39 |
| 1 | CA | 2033 | A | N3-C4 | -5.25 | 1.31 | 1.34 |
| 1 | AA | 2081 | A | N7-C5 | -5.25 | 1.36 | 1.39 |
| 1 | AA | 2066 | C | N1-C6 | -5.25 | 1.34 | 1.37 |
| 1 | AA | 1679 | A | C8-N7 | -5.24 | 1.27 | 1.31 |
| 1 | AA | 1315 | A | N9-C4 | -5.24 | 1.34 | 1.37 |
| 1 | AA | 2112 | G | C5-C4 | -5.23 | 1.34 | 1.38 |
| 1 | AA | 1274 | G | C6-N1 | -5.21 | 1.35 | 1.39 |
| 1 | CA | 450 | G | C6-O6 | -5.21 | 1.19 | 1.24 |
| 1 | AA | 2294 | G | C5-C6 | -5.21 | 1.37 | 1.42 |
| 1 | CA | 2676 | C | N1-C6 | -5.20 | 1.34 | 1.37 |
| 1 | CA | 2458 | G | C6-N1 | -5.20 | 1.35 | 1.39 |
| 1 | AA | 2466 | G | C6-N1 | -5.19 | 1.35 | 1.39 |
| 29 | A5 | 13 | LYS | CE-NZ | 5.19 | 1.62 | 1.49 |
| 1 | AA | 2299 | A | N7-C5 | -5.17 | 1.36 | 1.39 |
| 1 | AA | 741 | U | C2-O2 | -5.17 | 1.17 | 1.22 |
| 1 | AA | 591 | U | N1-C2 | -5.17 | 1.33 | 1.38 |
| 1 | AA | 823 | G | C6-N1 | -5.17 | 1.35 | 1.39 |
| 1 | AA | 2609 | G | C5-C4 | -5.17 | 1.34 | 1.38 |
| 1 | AA | 1518 | A | N9-C4 | 5.16 | 1.41 | 1.37 |
| 34 | DA | 250 | A | N9-C4 | 5.15 | 1.41 | 1.37 |
| 1 | CA | 1021 | A | C5-C6 | -5.15 | 1.36 | 1.41 |
| 1 | AA | 1605 | A | N9-C8 | 5.14 | 1.41 | 1.37 |
| 1 | AA | 2331 | G | N9-C4 | -5.14 | 1.33 | 1.38 |
| 1 | AA | 1323 | G | N7-C5 | -5.13 | 1.36 | 1.39 |
| 1 | AA | 847 | A | N3-C4 | -5.12 | 1.31 | 1.34 |
| 1 | AA | 1068 | G | C2-N2 | -5.12 | 1.29 | 1.34 |
| 1 | AA | 2092 | G | C5-C4 | -5.12 | 1.34 | 1.38 |
| 1 | AA | 2571 | C | C2-N3 | -5.12 | 1.31 | 1.35 |
| 1 | AA | 1786 | A | N9-C4 | -5.11 | 1.34 | 1.37 |
| 1 | AA | 1068 | G | N9-C4 | -5.10 | 1.33 | 1.38 |
| 1 | AA | 586 | G | N1-C2 | -5.10 | 1.33 | 1.37 |
| 1 | AA | 2054 | G | C5-C4 | -5.09 | 1.34 | 1.38 |
| 1 | AA | 1299 | A | C5-C4 | -5.09 | 1.35 | 1.38 |
| 1 | CA | 530 | G | N9-C8 | 5.09 | 1.41 | 1.37 |
| 1 | AA | 1068 | G | N1-C2 | -5.07 | 1.33 | 1.37 |
| 1 | AA | 2605 | U | C2-N3 | -5.07 | 1.34 | 1.37 |
| 1 | AA | 808 | A | N9-C4 | -5.07 | 1.34 | 1.37 |
| 1 | AA | 1848 | G | C6-N1 | -5.07 | 1.36 | 1.39 |
| 1 | AA | 990 | A | N9-C8 | 5.06 | 1.41 | 1.37 |
| 34 | BA | 903 | G | C5-C4 | -5.06 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | AA | 1665 | G | C6-N1 | -5.06 | 1.36 | 1.39 |
| 1 | AA | 2520 | G | N9-C8 | -5.06 | 1.34 | 1.37 |
| 1 | CA | 580 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 1 | CA | 2875 | C | N1-C6 | -5.05 | 1.34 | 1.37 |
| 1 | AA | 182 | U | C2-N3 | -5.05 | 1.34 | 1.37 |
| 1 | AA | 2502 | G | C6-N1 | -5.05 | 1.36 | 1.39 |
| 1 | AA | 1709 | C | N3-C4 | -5.04 | 1.30 | 1.33 |
| 1 | AA | 990 | A | C5-C4 | 5.04 | 1.42 | 1.38 |
| 1 | AA | 1249 | A | N7-C5 | -5.04 | 1.36 | 1.39 |
| 1 | AA | 2084 | A | N3-C4 | 5.04 | 1.37 | 1.34 |
| 1 | AA | 2591 | C | N1-C6 | -5.03 | 1.34 | 1.37 |
| 1 | AA | 492 | A | N7-C5 | -5.03 | 1.36 | 1.39 |
| 1 | AA | 2052 | A | C5-C6 | -5.02 | 1.36 | 1.41 |
| 1 | AA | 2584 | A | N3-C4 | -5.02 | 1.31 | 1.34 |
| 1 | AA | 1324 | A | N3-C4 | -5.02 | 1.31 | 1.34 |
| 1 | AA | 2055 | A | C6-N6 | -5.01 | 1.29 | 1.33 |
| 1 | AA | 669 | A | N7-C5 | -5.00 | 1.36 | 1.39 |

All (3545) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | AA | 990 | A | N1-C6-N6 | 23.54 | 132.72 | 118.60 |
| 1 | AA | 354 | A | C2-N3-C4 | -21.82 | 99.69 | 110.60 |
| 1 | AA | 990 | A | C6-C5-N7 | -21.49 | 117.25 | 132.30 |
| 1 | AA | 1188 | A | C2-N3-C4 | -21.02 | 100.09 | 110.60 |
| 1 | AA | 990 | A | C5-N7-C8 | -19.83 | 93.98 | 103.90 |
| 1 | AA | 1067 | A | C2-N3-C4 | -19.66 | 100.77 | 110.60 |
| 1 | AA | 990 | A | C2-N3-C4 | -18.70 | 101.25 | 110.60 |
| 1 | AA | 1745 | A | C2-N3-C4 | -18.36 | 101.42 | 110.60 |
| 1 | AA | 1249 | A | C2-N3-C4 | -18.05 | 101.58 | 110.60 |
| 1 | AA | 2045 | G | O5'-P-OP1 | -17.97 | 89.13 | 110.70 |
| 1 | AA | 990 | A | C4-C5-N7 | 16.94 | 119.17 | 110.70 |
| 1 | AA | 1605 | A | C2-N3-C4 | -16.25 | 102.47 | 110.60 |
| 1 | AA | 2299 | A | C2-N3-C4 | -16.18 | 102.51 | 110.60 |
| 1 | AA | 553 | A | C5-N7-C8 | -15.70 | 96.05 | 103.90 |
| 1 | CA | 528 | A | C2-N3-C4 | -15.31 | 102.95 | 110.60 |
| 1 | AA | 990 | A | N1-C2-N3 | 15.24 | 136.92 | 129.30 |
| 1 | CA | 1698 | A | C2-N3-C4 | -15.20 | 103.00 | 110.60 |
| 1 | AA | 2298 | A | N7-C8-N9 | 14.95 | 121.27 | 113.80 |
| 1 | AA | 354 | A | N3-C4-C5 | 14.76 | 137.13 | 126.80 |
| 1 | AA | 990 | A | N7-C8-N9 | 14.24 | 120.92 | 113.80 |
| 1 | AA | 1249 | A | C5-N7-C8 | -14.21 | 96.79 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1 | AA | 553 | A | N7-C8-N9 | 14.12 | 120.86 | 113.80 |
| 1 | AA | 894 | U | C5-C4-O4 | 14.08 | 134.35 | 125.90 |
| 1 | AA | 978 | A | C5-N7-C8 | -13.99 | 96.91 | 103.90 |
| 1 | AA | 553 | A | C2-N3-C4 | -13.88 | 103.66 | 110.60 |
| 1 | AA | 254 | A | C2-N3-C4 | -13.85 | 103.67 | 110.60 |
| 1 | AA | 139 | A | C5-N7-C8 | -13.73 | 97.04 | 103.90 |
| 1 | AA | 354 | A | N3-C4-N9 | -13.65 | 116.48 | 127.40 |
| 1 | CA | 945 | A | C4-C5-N7 | 13.51 | 117.46 | 110.70 |
| 1 | AA | 1188 | A | N3-C4-C5 | 13.18 | 136.03 | 126.80 |
| 1 | AA | 990 | A | C4-C5-C6 | 13.15 | 123.58 | 117.00 |
| 1 | AA | 2298 | A | C8-N9-C4 | -13.14 | 100.55 | 105.80 |
| 1 | CA | 2023 | G | O5'-P-OP1 | -13.14 | 93.88 | 105.70 |
| 1 | AA | 553 | A | C8-N9-C4 | -13.11 | 100.56 | 105.80 |
| 1 | AA | 2298 | A | C2-N3-C4 | -12.90 | 104.15 | 110.60 |
| 1 | CA | 945 | A | C5-N7-C8 | -12.87 | 97.47 | 103.90 |
| 1 | AA | 553 | A | N1-C6-N6 | 12.81 | 126.28 | 118.60 |
| 1 | AA | 2298 | A | N1-C2-N3 | 12.80 | 135.70 | 129.30 |
| 1 | AA | 474 | U | O5'-P-OP2 | -12.58 | 94.38 | 105.70 |
| 1 | AA | 2355 | C | O5'-P-OP1 | -12.50 | 94.45 | 105.70 |
| 1 | AA | 139 | A | N7-C8-N9 | 12.48 | 120.04 | 113.80 |
| 1 | AA | 1188 | A | N3-C4-N9 | -12.37 | 117.51 | 127.40 |
| 1 | AA | 990 | A | C5-C6-N6 | -12.27 | 113.88 | 123.70 |
| 1 | AA | 2298 | A | C5-N7-C8 | -12.26 | 97.77 | 103.90 |
| 1 | AA | 1745 | A | C5-N7-C8 | -12.15 | 97.83 | 103.90 |
| 1 | AA | 537 | G | O4'-C1'-N9 | 12.15 | 117.92 | 108.20 |
| 1 | AA | 555 | G | C5-C6-O6 | 12.11 | 135.87 | 128.60 |
| 1 | AA | 1067 | A | C5-N7-C8 | -12.10 | 97.85 | 103.90 |
| 1 | AA | 726 | C | N3-C4-C5 | 12.06 | 126.72 | 121.90 |
| 1 | CA | 963 | U | O5'-P-OP1 | -12.04 | 94.86 | 105.70 |
| 1 | CA | 1021 | A | C2-N3-C4 | -11.92 | 104.64 | 110.60 |
| 1 | CA | 141 | A | N7-C8-N9 | 11.89 | 119.75 | 113.80 |
| 1 | AA | 254 | A | C6-C5-N7 | -11.82 | 124.02 | 132.30 |
| 1 | AA | 1237 | G | C5-N7-C8 | 11.76 | 110.18 | 104.30 |
| 1 | CA | 945 | A | C2-N3-C4 | -11.75 | 104.73 | 110.60 |
| 1 | CA | 819 | A | O5'-P-OP1 | -11.73 | 95.14 | 105.70 |
| 1 | AA | 978 | A | C2-N3-C4 | -11.70 | 104.75 | 110.60 |
| 1 | CA | 945 | A | N1-C6-N6 | 11.65 | 125.59 | 118.60 |
| 1 | AA | 2442 | A | O5'-P-OP2 | -11.61 | 95.25 | 105.70 |
| 1 | AA | 2298 | A | C6-C5-N7 | -11.59 | 124.19 | 132.30 |
| 1 | AA | 555 | G | N3-C4-N9 | -11.59 | 119.05 | 126.00 |
| 1 | AA | 2694 | U | O5'-P-OP2 | -11.58 | 95.28 | 105.70 |
| 1 | AA | 1249 | A | N7-C8-N9 | 11.49 | 119.54 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|--------|-------------|----------|
| 1 | AA | 1067 | A | N3-C4-N9 | -11.30 | 118.36 | 127.40 |
| 1 | AA | 2834 | C | C5-C4-N4 | -11.30 | 112.29 | 120.20 |
| 1 | CA | 1368 | G | O5'-P-OP2 | -11.27 | 95.56 | 105.70 |
| 1 | AA | 254 | A | N1-C6-N6 | 11.27 | 125.36 | 118.60 |
| 1 | AA | 553 | A | C4-C5-N7 | 11.26 | 116.33 | 110.70 |
| 1 | AA | 1686 | U | O5'-P-OP2 | -11.26 | 95.56 | 105.70 |
| 1 | AA | 1231 | G | C5-C6-N1 | 11.25 | 117.13 | 111.50 |
| 1 | CA | 1142(A) | A | C2-N3-C4 | -11.25 | 104.98 | 110.60 |
| 1 | AA | 978 | A | N7-C8-N9 | 11.24 | 119.42 | 113.80 |
| 1 | AA | 792 | G | C5-C6-O6 | -11.22 | 121.86 | 128.60 |
| 1 | CA | 1698 | A | N1-C2-N3 | 11.22 | 134.91 | 129.30 |
| 1 | AA | 1188 | A | C5-N7-C8 | -11.20 | 98.30 | 103.90 |
| 1 | CA | 141 | A | C5-N7-C8 | -11.17 | 98.31 | 103.90 |
| 1 | CA | 961 | C | O5'-P-OP2 | -11.08 | 95.73 | 105.70 |
| 1 | AA | 2834 | C | N3-C4-N4 | 11.05 | 125.74 | 118.00 |
| 1 | CA | 528 | A | N3-C4-C5 | 10.98 | 134.49 | 126.80 |
| 1 | AA | 235 | C | C6-N1-C2 | 10.96 | 124.68 | 120.30 |
| 1 | AA | 1067 | A | C5-C6-N1 | -10.94 | 112.23 | 117.70 |
| 1 | AA | 354 | A | C5-N7-C8 | -10.92 | 98.44 | 103.90 |
| 1 | CA | 2824 | C | C6-N1-C2 | 10.88 | 124.65 | 120.30 |
| 1 | AA | 1157 | A | O4'-C1'-N9 | 10.87 | 116.89 | 108.20 |
| 1 | AA | 1249 | A | C8-N9-C4 | -10.86 | 101.46 | 105.80 |
| 1 | AA | 1067 | A | C8-N9-C4 | -10.84 | 101.47 | 105.80 |
| 1 | CA | 945 | A | N3-C4-C5 | 10.82 | 134.37 | 126.80 |
| 1 | AA | 1021 | G | O5'-P-OP2 | -10.69 | 96.08 | 105.70 |
| 1 | CA | 2576 | G | O5'-P-OP1 | -10.68 | 96.09 | 105.70 |
| 1 | AA | 555 | G | N3-C4-C5 | 10.67 | 133.93 | 128.60 |
| 1 | CA | 330 | A | C2-N3-C4 | -10.66 | 105.27 | 110.60 |
| 1 | AA | 1188 | A | C5-C6-N1 | -10.64 | 112.38 | 117.70 |
| 1 | CA | 1614 | A | O5'-P-OP1 | -10.63 | 96.13 | 105.70 |
| 1 | AA | 1067 | A | N3-C4-C5 | 10.63 | 134.24 | 126.80 |
| 1 | AA | 2281 | A | O5'-P-OP1 | -10.62 | 96.14 | 105.70 |
| 1 | AA | 1067 | A | N7-C8-N9 | 10.60 | 119.10 | 113.80 |
| 1 | AA | 894 | U | N3-C4-O4 | -10.58 | 112.00 | 119.40 |
| 1 | CA | 512 | G | O4'-C1'-N9 | 10.51 | 116.60 | 108.20 |
| 1 | CA | 2708 | G | C8-N9-C4 | 10.46 | 110.58 | 106.40 |
| 1 | AA | 1874 | C | C6-N1-C2 | 10.43 | 124.47 | 120.30 |
| 1 | AA | 2287 | C | O5'-P-OP2 | -10.42 | 96.32 | 105.70 |
| 34 | BA | 365 | U | C5-C6-N1 | -10.38 | 117.51 | 122.70 |
| 1 | AA | 1347 | A | O5'-P-OP1 | -10.36 | 96.38 | 105.70 |
| 1 | AA | 592 | U | N1-C2-O2 | -10.35 | 115.56 | 122.80 |
| 1 | AA | 1154 | U | N3-C2-O2 | -10.34 | 114.97 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | AA | 2331 | G | N3-C4-N9 | -10.31 | 119.82 | 126.00 |
| 1 | AA | 2641 | A | N1-C2-N3 | 10.30 | 134.45 | 129.30 |
| 1 | AA | 345 | G | C5-C6-O6 | -10.29 | 122.42 | 128.60 |
| 1 | AA | 1237 | G | N7-C8-N9 | -10.28 | 107.96 | 113.10 |
| 1 | AA | 1695 | C | O5'-P-OP1 | -10.27 | 96.46 | 105.70 |
| 1 | AA | 542 | C | C5-C4-N4 | -10.23 | 113.04 | 120.20 |
| 1 | CA | 614 | U | N3-C2-O2 | -10.23 | 115.04 | 122.20 |
| 1 | AA | 1249 | A | N3-C4-N9 | -10.22 | 119.23 | 127.40 |
| 1 | AA | 254 | A | C5-N7-C8 | -10.16 | 98.82 | 103.90 |
| 1 | CA | 847 | U | C2-N1-C1' | -10.16 | 105.51 | 117.70 |
| 1 | AA | 1037 | C | C2-N3-C4 | -10.13 | 114.83 | 119.90 |
| 1 | AA | 555 | G | C6-N1-C2 | 10.12 | 131.17 | 125.10 |
| 1 | CA | 1130 | U | O5'-P-OP1 | -10.11 | 96.60 | 105.70 |
| 1 | AA | 2045 | G | O5'-P-OP2 | 10.00 | 122.70 | 110.70 |
| 1 | AA | 552 | C | N1-C2-N3 | 9.97 | 126.18 | 119.20 |
| 1 | AA | 1605 | A | N3-C4-C5 | 9.97 | 133.78 | 126.80 |
| 1 | AA | 1150 | C | OP1-P-O3' | -9.97 | 83.27 | 105.20 |
| 1 | AA | 978 | A | C4-C5-N7 | 9.95 | 115.68 | 110.70 |
| 1 | AA | 1249 | A | N3-C4-C5 | 9.95 | 133.77 | 126.80 |
| 1 | CA | 141 | A | C8-N9-C4 | -9.92 | 101.83 | 105.80 |
| 1 | AA | 2427 | G | C5-C6-O6 | -9.88 | 122.67 | 128.60 |
| 1 | CA | 2626 | C | C6-N1-C2 | 9.88 | 124.25 | 120.30 |
| 1 | AA | 2298 | A | C4-C5-C6 | 9.86 | 121.93 | 117.00 |
| 1 | AA | 2331 | G | C8-N9-C4 | -9.86 | 102.46 | 106.40 |
| 1 | AA | 2776 | G | C4-C5-N7 | 9.85 | 114.74 | 110.80 |
| 1 | AA | 1611 | C | O5'-P-OP2 | -9.75 | 96.92 | 105.70 |
| 1 | AA | 205 | A | O5'-P-OP1 | -9.75 | 96.93 | 105.70 |
| 2 | CB | 30 | C | C6-N1-C2 | -9.74 | 116.40 | 120.30 |
| 1 | AA | 481 | C | O5'-P-OP2 | -9.73 | 96.94 | 105.70 |
| 1 | AA | 2386 | C | C6-N1-C2 | 9.73 | 124.19 | 120.30 |
| 1 | AA | 2331 | G | C5-N7-C8 | -9.72 | 99.44 | 104.30 |
| 1 | AA | 555 | G | C8-N9-C4 | -9.71 | 102.52 | 106.40 |
| 1 | AA | 798 | A | O5'-P-OP2 | 9.71 | 122.35 | 110.70 |
| 1 | AA | 2876 | U | C5-C6-N1 | -9.68 | 117.86 | 122.70 |
| 1 | AA | 2515 | A | N1-C6-N6 | 9.68 | 124.41 | 118.60 |
| 1 | AA | 1342 | G | N1-C6-O6 | -9.66 | 114.10 | 119.90 |
| 1 | AA | 2475 | C | C6-N1-C2 | 9.65 | 124.16 | 120.30 |
| 1 | AA | 2776 | G | N9-C4-C5 | -9.63 | 101.55 | 105.40 |
| 1 | AA | 1037 | C | C5-C6-N1 | -9.62 | 116.19 | 121.00 |
| 1 | AA | 598 | A | O5'-P-OP1 | -9.60 | 97.06 | 105.70 |
| 1 | AA | 555 | G | C5-N7-C8 | -9.59 | 99.51 | 104.30 |
| 1 | CA | 450 | G | N1-C6-O6 | -9.58 | 114.15 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1837 | C | O5'-P-OP1 | -9.58 | 97.08 | 105.70 |
| 1 | AA | 2287 | C | O5'-P-OP1 | 9.55 | 122.16 | 110.70 |
| 1 | AA | 596 | G | C6-N1-C2 | -9.54 | 119.37 | 125.10 |
| 1 | AA | 2710 | U | O5'-P-OP2 | -9.54 | 97.11 | 105.70 |
| 1 | CA | 1656 | C | N3-C4-C5 | 9.53 | 125.71 | 121.90 |
| 1 | AA | 1856 | A | N1-C6-N6 | -9.51 | 112.90 | 118.60 |
| 1 | AA | 2089 | G | C8-N9-C4 | -9.51 | 102.60 | 106.40 |
| 1 | CA | 856 | C | C6-N1-C2 | -9.50 | 116.50 | 120.30 |
| 1 | AA | 2643 | G | O5'-P-OP1 | -9.47 | 97.17 | 105.70 |
| 1 | AA | 1249 | A | N1-C2-N3 | 9.47 | 134.03 | 129.30 |
| 1 | AA | 1745 | A | C4-C5-N7 | 9.45 | 115.42 | 110.70 |
| 1 | AA | 1745 | A | N3-C4-C5 | 9.43 | 133.40 | 126.80 |
| 1 | AA | 2528 | G | N1-C6-O6 | -9.43 | 114.24 | 119.90 |
| 1 | AA | 2265 | G | C8-N9-C4 | 9.42 | 110.17 | 106.40 |
| 1 | AA | 2631 | C | C5-C6-N1 | -9.41 | 116.29 | 121.00 |
| 1 | AA | 894 | U | N3-C2-O2 | -9.38 | 115.64 | 122.20 |
| 1 | AA | 2299 | A | N3-C4-C5 | 9.37 | 133.36 | 126.80 |
| 1 | AA | 1318 | A | O5'-P-OP2 | -9.37 | 97.27 | 105.70 |
| 1 | AA | 991 | G | O5'-P-OP1 | -9.37 | 97.27 | 105.70 |
| 34 | BA | 365 | U | C5-C4-O4 | 9.37 | 131.52 | 125.90 |
| 1 | AA | 859 | C | N3-C4-C5 | 9.36 | 125.64 | 121.90 |
| 1 | AA | 1006 | C | O5'-P-OP2 | -9.36 | 97.28 | 105.70 |
| 1 | CA | 2287 | A | C2-N3-C4 | -9.36 | 105.92 | 110.60 |
| 1 | AA | 1249 | A | O4'-C1'-N9 | 9.35 | 115.68 | 108.20 |
| 1 | AA | 792 | G | N1-C6-O6 | 9.31 | 125.49 | 119.90 |
| 1 | CA | 1204 | A | C2-N3-C4 | -9.31 | 105.94 | 110.60 |
| 1 | AA | 1001 | G | N1-C6-O6 | 9.30 | 125.48 | 119.90 |
| 1 | CA | 1698 | A | C5-N7-C8 | -9.29 | 99.25 | 103.90 |
| 1 | AA | 555 | G | C2-N3-C4 | -9.29 | 107.26 | 111.90 |
| 1 | AA | 2638 | C | C5-C6-N1 | -9.24 | 116.38 | 121.00 |
| 1 | AA | 1067 | A | N1-C2-N3 | 9.22 | 133.91 | 129.30 |
| 2 | AB | 80 | U | C5-C6-N1 | -9.22 | 118.09 | 122.70 |
| 1 | AA | 1963 | C | N1-C2-O2 | -9.19 | 113.39 | 118.90 |
| 1 | AA | 186 | A | OP1-P-OP2 | -9.18 | 105.83 | 119.60 |
| 1 | AA | 2754 | A | C8-N9-C4 | 9.18 | 109.47 | 105.80 |
| 2 | AB | 91 | C | C5-C4-N4 | -9.16 | 113.79 | 120.20 |
| 1 | AA | 2336 | C | C6-N1-C2 | 9.16 | 123.96 | 120.30 |
| 1 | AA | 542 | C | C6-N1-C2 | 9.14 | 123.96 | 120.30 |
| 1 | CA | 34 | C | N1-C2-O2 | 9.14 | 124.39 | 118.90 |
| 1 | AA | 798 | A | O5'-P-OP1 | -9.13 | 97.48 | 105.70 |
| 1 | CA | 1204 | A | N1-C6-N6 | 9.11 | 124.07 | 118.60 |
| 1 | AA | 1723 | A | C8-N9-C4 | 9.11 | 109.44 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | AA | 851 | A | C8-N9-C4 | 9.11 | 109.44 | 105.80 |
| 1 | AA | 139 | A | C8-N9-C4 | -9.09 | 102.16 | 105.80 |
| 1 | AA | 1150 | C | OP2-P-O3' | -9.08 | 85.23 | 105.20 |
| 2 | AB | 91 | C | C6-N1-C2 | 9.06 | 123.93 | 120.30 |
| 1 | AA | 2641 | A | C6-C5-N7 | -9.06 | 125.96 | 132.30 |
| 1 | CA | 1653 | G | P-O3'-C3' | 9.05 | 130.56 | 119.70 |
| 1 | AA | 856 | G | C5-C6-O6 | 9.04 | 134.03 | 128.60 |
| 1 | AA | 2162 | C | C2-N1-C1' | 9.04 | 128.75 | 118.80 |
| 1 | CA | 141 | A | C4-C5-N7 | 9.04 | 115.22 | 110.70 |
| 1 | AA | 2657 | G | C4-C5-N7 | 9.03 | 114.41 | 110.80 |
| 1 | AA | 354 | A | C5-C6-N1 | -9.02 | 113.19 | 117.70 |
| 1 | AA | 1605 | A | C5-C6-N1 | -9.02 | 113.19 | 117.70 |
| 1 | AA | 2515 | A | C5-C6-N6 | -9.01 | 116.49 | 123.70 |
| 1 | AA | 2776 | G | C5-C6-O6 | -9.01 | 123.19 | 128.60 |
| 1 | AA | 2049 | G | N1-C6-O6 | -9.00 | 114.50 | 119.90 |
| 1 | CA | 141 | A | N1-C6-N6 | 9.00 | 124.00 | 118.60 |
| 1 | AA | 2046 | G | C8-N9-C4 | 9.00 | 110.00 | 106.40 |
| 1 | AA | 2571 | C | N3-C4-C5 | 9.00 | 125.50 | 121.90 |
| 1 | CA | 963 | U | C5-C4-O4 | -8.99 | 120.50 | 125.90 |
| 1 | AA | 553 | A | O4'-C1'-N9 | -8.99 | 101.01 | 108.20 |
| 1 | AA | 1249 | A | C4-C5-N7 | 8.98 | 115.19 | 110.70 |
| 1 | CA | 528 | A | N3-C4-N9 | -8.96 | 120.23 | 127.40 |
| 1 | AA | 2331 | G | N7-C8-N9 | 8.96 | 117.58 | 113.10 |
| 1 | AA | 627 | G | O5'-P-OP2 | -8.96 | 97.64 | 105.70 |
| 1 | AA | 1728 | G | C4-C5-N7 | 8.93 | 114.37 | 110.80 |
| 1 | AA | 2571 | C | N1-C2-O2 | 8.92 | 124.25 | 118.90 |
| 1 | CA | 915 | C | C6-N1-C2 | -8.90 | 116.74 | 120.30 |
| 1 | AA | 254 | A | C4-C5-N7 | 8.89 | 115.15 | 110.70 |
| 1 | AA | 1184 | G | O5'-P-OP2 | -8.88 | 97.70 | 105.70 |
| 1 | CA | 450 | G | C5-C6-N1 | 8.88 | 115.94 | 111.50 |
| 2 | AB | 91 | C | N3-C4-C5 | 8.88 | 125.45 | 121.90 |
| 1 | CA | 1142(A) | A | N3-C4-N9 | -8.88 | 120.30 | 127.40 |
| 1 | CA | 614 | U | C5-C4-O4 | 8.87 | 131.22 | 125.90 |
| 1 | AA | 470 | C | O5'-P-OP1 | 8.86 | 121.34 | 110.70 |
| 1 | AA | 1715 | A | O5'-P-OP2 | -8.87 | 97.72 | 105.70 |
| 1 | CA | 847 | U | N1-C2-O2 | -8.87 | 116.59 | 122.80 |
| 1 | AA | 1745 | A | N1-C2-N3 | 8.85 | 133.73 | 129.30 |
| 1 | AA | 2331 | G | N3-C4-C5 | 8.85 | 133.03 | 128.60 |
| 1 | AA | 552 | C | C4-C5-C6 | 8.85 | 121.83 | 117.40 |
| 1 | AA | 2882 | G | N1-C6-O6 | -8.85 | 114.59 | 119.90 |
| 1 | AA | 2041 | A | N7-C8-N9 | -8.84 | 109.38 | 113.80 |
| 1 | AA | 139 | A | C4-C5-N7 | 8.82 | 115.11 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | AB | 86 | G | C5-C6-O6 | -8.81 | 123.31 | 128.60 |
| 1 | AA | 1232 | G | N1-C6-O6 | -8.80 | 114.62 | 119.90 |
| 1 | AA | 1374 | G | C5-C6-N1 | 8.77 | 115.88 | 111.50 |
| 1 | AA | 1593 | C | C6-N1-C2 | -8.76 | 116.80 | 120.30 |
| 1 | CA | 330 | A | C5-N7-C8 | -8.76 | 99.52 | 103.90 |
| 1 | CA | 2595 | G | O5'-P-OP1 | -8.73 | 97.84 | 105.70 |
| 1 | AA | 2559 | U | N1-C2-N3 | 8.71 | 120.13 | 114.90 |
| 1 | CA | 1698 | A | C6-C5-N7 | -8.72 | 126.20 | 132.30 |
| 1 | AA | 553 | A | C6-C5-N7 | -8.71 | 126.20 | 132.30 |
| 1 | AA | 1718 | U | O5'-P-OP2 | -8.71 | 97.86 | 105.70 |
| 1 | AA | 776 | G | O5'-P-OP2 | -8.70 | 97.87 | 105.70 |
| 1 | AA | 1812 | C | C6-N1-C2 | 8.70 | 123.78 | 120.30 |
| 1 | AA | 1188 | A | N1-C2-N3 | 8.69 | 133.65 | 129.30 |
| 1 | AA | 2631 | C | C6-N1-C2 | 8.69 | 123.78 | 120.30 |
| 1 | AA | 1291 | G | N1-C6-O6 | -8.69 | 114.69 | 119.90 |
| 1 | AA | 553 | A | N1-C2-N3 | 8.68 | 133.64 | 129.30 |
| 1 | AA | 1412 | A | C8-N9-C4 | 8.68 | 109.27 | 105.80 |
| 1 | AA | 792 | G | C8-N9-C4 | 8.67 | 109.87 | 106.40 |
| 1 | AA | 958 | C | C6-N1-C2 | -8.67 | 116.83 | 120.30 |
| 1 | CA | 1673 | U | C5-C6-N1 | -8.67 | 118.37 | 122.70 |
| 34 | BA | 665 | A | O5'-P-OP1 | -8.66 | 97.90 | 105.70 |
| 1 | CA | 1780 | A | O5'-P-OP1 | -8.66 | 97.91 | 105.70 |
| 1 | AA | 555 | G | N7-C8-N9 | 8.65 | 117.43 | 113.10 |
| 1 | AA | 1249 | A | C5-C6-N1 | -8.65 | 113.37 | 117.70 |
| 1 | AA | 2525 | G | O5'-P-OP2 | -8.65 | 97.92 | 105.70 |
| 1 | AA | 2743 | C | N3-C4-N4 | -8.64 | 111.95 | 118.00 |
| 1 | CA | 1993 | U | O5'-P-OP1 | -8.64 | 97.92 | 105.70 |
| 1 | AA | 1030 | A | O5'-P-OP1 | -8.63 | 97.93 | 105.70 |
| 1 | CA | 527 | C | N3-C4-N4 | -8.63 | 111.96 | 118.00 |
| 34 | BA | 1495 | U | O5'-P-OP2 | -8.62 | 97.94 | 105.70 |
| 1 | AA | 410 | U | C5-C6-N1 | -8.62 | 118.39 | 122.70 |
| 1 | AA | 990 | A | C5-C6-N1 | -8.62 | 113.39 | 117.70 |
| 1 | AA | 2312 | G | C8-N9-C4 | -8.60 | 102.96 | 106.40 |
| 1 | AA | 2608 | U | C5-C6-N1 | -8.59 | 118.40 | 122.70 |
| 1 | AA | 1745 | A | C5-C6-N1 | -8.58 | 113.41 | 117.70 |
| 1 | CA | 1658 | C | C6-N1-C2 | -8.57 | 116.87 | 120.30 |
| 1 | AA | 990 | A | O5'-P-OP1 | -8.56 | 98.00 | 105.70 |
| 1 | AA | 1237 | G | C4-C5-N7 | -8.55 | 107.38 | 110.80 |
| 1 | CA | 1626 | G | N1-C6-O6 | -8.55 | 114.77 | 119.90 |
| 1 | CA | 1644 | C | C6-N1-C2 | -8.55 | 116.88 | 120.30 |
| 1 | CA | 2850 | A | O5'-P-OP2 | -8.55 | 98.01 | 105.70 |
| 1 | AA | 552 | C | C2-N3-C4 | -8.54 | 115.63 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2298 | A | N1-C6-N6 | 8.53 | 123.72 | 118.60 |
| 34 | BA | 365 | U | C2-N1-C1' | -8.51 | 107.49 | 117.70 |
| 1 | AA | 2585 | C | C2-N3-C4 | -8.50 | 115.65 | 119.90 |
| 1 | AA | 2638 | C | C6-N1-C2 | 8.50 | 123.70 | 120.30 |
| 1 | AA | 1050 | C | N1-C2-O2 | -8.49 | 113.80 | 118.90 |
| 1 | AA | 2849 | G | C8-N9-C4 | 8.49 | 109.80 | 106.40 |
| 1 | AA | 1860 | A | O5'-P-OP2 | -8.49 | 98.06 | 105.70 |
| 1 | AA | 2876 | U | C5-C4-O4 | 8.49 | 130.99 | 125.90 |
| 1 | AA | 2041 | A | C8-N9-C4 | 8.48 | 109.19 | 105.80 |
| 1 | AA | 978 | A | C8-N9-C4 | -8.48 | 102.41 | 105.80 |
| 1 | CA | 1787 | A | O5'-P-OP1 | -8.48 | 98.07 | 105.70 |
| 1 | AA | 2641 | A | N1-C6-N6 | 8.48 | 123.69 | 118.60 |
| 1 | AA | 831 | A | O4'-C1'-N9 | 8.47 | 114.98 | 108.20 |
| 1 | AA | 2609 | G | C5-C6-O6 | -8.47 | 123.52 | 128.60 |
| 1 | AA | 630 | U | O5'-P-OP1 | -8.45 | 98.09 | 105.70 |
| 1 | AA | 543 | G | O5'-P-OP2 | -8.45 | 98.10 | 105.70 |
| 1 | AA | 1346 | U | C5-C4-O4 | -8.43 | 120.84 | 125.90 |
| 1 | CA | 772 | C | C6-N1-C2 | 8.43 | 123.67 | 120.30 |
| 1 | AA | 1655 | A | C5-C6-N6 | -8.43 | 116.96 | 123.70 |
| 1 | AA | 1664 | A | N1-C6-N6 | -8.43 | 113.55 | 118.60 |
| 1 | AA | 745 | C | O5'-P-OP2 | -8.42 | 98.12 | 105.70 |
| 34 | DA | 34 | C | C6-N1-C2 | 8.41 | 123.67 | 120.30 |
| 1 | AA | 2515 | A | N1-C2-N3 | -8.41 | 125.09 | 129.30 |
| 1 | AA | 359 | C | C6-N1-C2 | 8.40 | 123.66 | 120.30 |
| 1 | AA | 2299 | A | C5-C6-N1 | -8.40 | 113.50 | 117.70 |
| 34 | BA | 1417 | G | N9-C4-C5 | -8.40 | 102.04 | 105.40 |
| 1 | AA | 1418 | U | N3-C4-O4 | 8.40 | 125.28 | 119.40 |
| 34 | DA | 1484 | C | C6-N1-C2 | 8.38 | 123.65 | 120.30 |
| 1 | CA | 1272 | A | O5'-P-OP2 | -8.36 | 98.18 | 105.70 |
| 34 | BA | 1417 | G | C5-C6-O6 | -8.35 | 123.59 | 128.60 |
| 1 | AA | 139 | A | C2-N3-C4 | -8.35 | 106.43 | 110.60 |
| 1 | AA | 595 | A | O5'-P-OP1 | -8.34 | 98.19 | 105.70 |
| 1 | CA | 1673 | U | C2-N3-C4 | -8.34 | 122.00 | 127.00 |
| 1 | CA | 1899 | G | C5-C6-O6 | -8.33 | 123.60 | 128.60 |
| 1 | AA | 45 | C | O5'-P-OP2 | -8.33 | 98.20 | 105.70 |
| 1 | AA | 2033 | U | N1-C2-N3 | 8.32 | 119.89 | 114.90 |
| 34 | BA | 1502 | A | N1-C2-N3 | 8.31 | 133.45 | 129.30 |
| 1 | AA | 1695 | C | O5'-P-OP2 | 8.30 | 120.67 | 110.70 |
| 1 | CA | 2503 | A | N1-C2-N3 | -8.29 | 125.15 | 129.30 |
| 1 | AA | 894 | U | C5-C6-N1 | -8.29 | 118.55 | 122.70 |
| 1 | AA | 1694 | G | O4'-C1'-N9 | -8.29 | 101.57 | 108.20 |
| 1 | AA | 1655 | A | C8-N9-C4 | 8.28 | 109.11 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2383 | G | C4-C5-N7 | 8.28 | 114.11 | 110.80 |
| 1 | AA | 2609 | G | C5-C6-N1 | 8.28 | 115.64 | 111.50 |
| 1 | AA | 195 | U | C5-C6-N1 | -8.27 | 118.56 | 122.70 |
| 1 | AA | 1813 | C | N3-C4-C5 | 8.27 | 125.21 | 121.90 |
| 1 | AA | 2657 | G | C5-C6-O6 | -8.27 | 123.64 | 128.60 |
| 1 | AA | 1812 | C | N3-C4-N4 | 8.25 | 123.78 | 118.00 |
| 1 | AA | 36 | G | O5'-P-OP2 | -8.25 | 98.28 | 105.70 |
| 1 | AA | 2475 | C | N3-C4-C5 | 8.25 | 125.20 | 121.90 |
| 1 | AA | 123 | G | C5-C6-N1 | 8.25 | 115.62 | 111.50 |
| 1 | AA | 1605 | A | N3-C4-N9 | -8.24 | 120.80 | 127.40 |
| 1 | AA | 978 | A | O4'-C1'-N9 | 8.24 | 114.79 | 108.20 |
| 1 | AA | 2054 | G | N7-C8-N9 | -8.23 | 108.99 | 113.10 |
| 34 | BA | 266 | G | C5-N7-C8 | -8.22 | 100.19 | 104.30 |
| 1 | AA | 2466 | G | N1-C2-N2 | -8.22 | 108.80 | 116.20 |
| 1 | AA | 1462 | G | O5'-P-OP2 | -8.21 | 98.31 | 105.70 |
| 1 | AA | 1750 | G | O5'-P-OP2 | -8.20 | 98.32 | 105.70 |
| 1 | AA | 345 | G | C4-C5-N7 | 8.20 | 114.08 | 110.80 |
| 1 | AA | 881 | C | N1-C2-O2 | -8.19 | 113.98 | 118.90 |
| 1 | CA | 510 | C | O5'-P-OP2 | -8.19 | 98.33 | 105.70 |
| 34 | BA | 525 | C | C6-N1-C2 | -8.19 | 117.03 | 120.30 |
| 1 | AA | 990 | A | C8-N9-C4 | -8.18 | 102.53 | 105.80 |
| 1 | AA | 2054 | G | C5-N7-C8 | 8.17 | 108.39 | 104.30 |
| 1 | CA | 949 | C | N1-C2-O2 | -8.17 | 114.00 | 118.90 |
| 1 | AA | 2101 | U | N1-C2-N3 | 8.16 | 119.80 | 114.90 |
| 1 | AA | 2502 | G | N9-C4-C5 | -8.16 | 102.13 | 105.40 |
| 2 | AB | 41 | U | C5-C6-N1 | -8.16 | 118.62 | 122.70 |
| 1 | AA | 2066 | C | C2-N3-C4 | -8.16 | 115.82 | 119.90 |
| 1 | AA | 1011 | G | C5-C6-O6 | 8.16 | 133.50 | 128.60 |
| 1 | AA | 1397 | C | OP1-P-O3' | 8.15 | 123.14 | 105.20 |
| 1 | AA | 893 | C | C5-C6-N1 | -8.15 | 116.93 | 121.00 |
| 34 | DA | 245 | C | C6-N1-C2 | 8.14 | 123.56 | 120.30 |
| 2 | AB | 101 | G | C8-N9-C4 | 8.14 | 109.66 | 106.40 |
| 1 | AA | 194 | G | C8-N9-C4 | 8.14 | 109.66 | 106.40 |
| 1 | AA | 2740 | G | O5'-P-OP2 | -8.13 | 98.38 | 105.70 |
| 1 | AA | 1208 | G | C4-C5-N7 | -8.13 | 107.55 | 110.80 |
| 1 | AA | 1848 | G | C5-C6-O6 | 8.13 | 133.48 | 128.60 |
| 1 | CA | 1500 | G | N1-C6-O6 | 8.12 | 124.77 | 119.90 |
| 1 | AA | 861 | C | C2-N3-C4 | -8.11 | 115.84 | 119.90 |
| 1 | AA | 1605 | A | C5-N7-C8 | -8.11 | 99.84 | 103.90 |
| 34 | BA | 266 | G | C4-C5-N7 | 8.11 | 114.04 | 110.80 |
| 1 | AA | 254 | A | N7-C8-N9 | 8.10 | 117.85 | 113.80 |
| 1 | AA | 1861 | C | N1-C2-O2 | -8.10 | 114.04 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1824 | C | O5'-P-OP1 | -8.09 | 98.42 | 105.70 |
| 1 | CA | 2824 | C | C5-C6-N1 | -8.09 | 116.95 | 121.00 |
| 1 | CA | 2612 | C | O5'-P-OP2 | -8.09 | 98.42 | 105.70 |
| 1 | AA | 1312 | G | C5-C6-N1 | 8.08 | 115.54 | 111.50 |
| 1 | AA | 370 | A | O5'-P-OP2 | -8.08 | 98.43 | 105.70 |
| 1 | AA | 496 | A | O5'-P-OP1 | -8.07 | 98.43 | 105.70 |
| 1 | AA | 1745 | A | N7-C8-N9 | 8.07 | 117.84 | 113.80 |
| 1 | CA | 330 | A | C4-C5-N7 | 8.07 | 114.74 | 110.70 |
| 2 | AB | 86 | G | C5-C6-N1 | 8.07 | 115.54 | 111.50 |
| 1 | AA | 978 | A | C6-C5-N7 | -8.06 | 126.66 | 132.30 |
| 1 | AA | 1655 | A | N9-C4-C5 | -8.06 | 102.58 | 105.80 |
| 1 | AA | 2632 | C | N3-C4-C5 | 8.05 | 125.12 | 121.90 |
| 1 | AA | 2258 | G | C8-N9-C4 | 8.05 | 109.62 | 106.40 |
| 34 | BA | 328 | C | O5'-P-OP1 | -8.05 | 98.46 | 105.70 |
| 2 | AB | 102 | A | O5'-P-OP2 | 8.05 | 120.36 | 110.70 |
| 1 | AA | 345 | G | N1-C6-O6 | 8.05 | 124.73 | 119.90 |
| 1 | CA | 1807 | G | C8-N9-C4 | 8.04 | 109.62 | 106.40 |
| 1 | AA | 2299 | A | C5-N7-C8 | -8.04 | 99.88 | 103.90 |
| 1 | AA | 1744 | G | C5-C6-O6 | -8.04 | 123.78 | 128.60 |
| 1 | AA | 616 | G | O5'-P-OP2 | -8.03 | 98.47 | 105.70 |
| 1 | AA | 55 | A | C2-N3-C4 | -8.03 | 106.59 | 110.60 |
| 1 | AA | 596 | G | C5-C6-N1 | 8.03 | 115.51 | 111.50 |
| 1 | AA | 2603 | C | C6-N1-C2 | 8.03 | 123.51 | 120.30 |
| 1 | AA | 1728 | G | C5-N7-C8 | -8.02 | 100.29 | 104.30 |
| 1 | AA | 978 | A | N3-C4-C5 | 8.02 | 132.41 | 126.80 |
| 34 | BA | 1502 | A | N7-C8-N9 | 8.02 | 117.81 | 113.80 |
| 1 | AA | 1356 | G | O5'-P-OP1 | -8.01 | 98.49 | 105.70 |
| 1 | CA | 945 | A | N9-C4-C5 | -8.01 | 102.60 | 105.80 |
| 1 | CA | 1021 | A | C5-N7-C8 | -8.01 | 99.89 | 103.90 |
| 1 | AA | 22 | C | N3-C4-N4 | -8.00 | 112.40 | 118.00 |
| 1 | CA | 568 | U | C5-C4-O4 | -8.00 | 121.10 | 125.90 |
| 1 | AA | 2697 | G | C5-C6-N1 | 8.00 | 115.50 | 111.50 |
| 1 | AA | 1234 | A | N1-C6-N6 | 7.98 | 123.39 | 118.60 |
| 1 | AA | 2697 | G | C6-N1-C2 | -7.98 | 120.31 | 125.10 |
| 1 | CA | 1966 | A | C8-N9-C4 | 7.98 | 108.99 | 105.80 |
| 34 | BA | 514 | C | N1-C2-O2 | -7.97 | 114.12 | 118.90 |
| 1 | AA | 2299 | A | N1-C6-N6 | 7.96 | 123.38 | 118.60 |
| 1 | CA | 1812 | A | OP1-P-OP2 | 7.96 | 131.54 | 119.60 |
| 1 | AA | 2835 | C | C2-N3-C4 | -7.96 | 115.92 | 119.90 |
| 1 | AA | 2607 | G | C5-C6-O6 | 7.95 | 133.37 | 128.60 |
| 1 | AA | 1745 | A | C6-C5-N7 | -7.95 | 126.74 | 132.30 |
| 1 | CA | 330 | A | N1-C6-N6 | 7.94 | 123.36 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1444 | C | N3-C4-C5 | 7.93 | 125.07 | 121.90 |
| 1 | AA | 1342 | G | C5-C6-O6 | 7.92 | 133.35 | 128.60 |
| 1 | CA | 1500 | G | C5-C6-O6 | -7.92 | 123.84 | 128.60 |
| 1 | AA | 477 | C | C5-C6-N1 | -7.91 | 117.04 | 121.00 |
| 1 | CA | 2374 | C | C6-N1-C2 | 7.91 | 123.47 | 120.30 |
| 1 | AA | 2631 | C | C2-N3-C4 | -7.91 | 115.94 | 119.90 |
| 1 | AA | 2049 | G | C4-C5-N7 | -7.90 | 107.64 | 110.80 |
| 1 | AA | 1181 | G | C8-N9-C4 | 7.90 | 109.56 | 106.40 |
| 34 | BA | 550 | G | O5'-P-OP1 | -7.90 | 98.59 | 105.70 |
| 1 | AA | 2251 | G | C5-C6-O6 | -7.90 | 123.86 | 128.60 |
| 1 | CA | 494 | G | C5-C6-N1 | -7.89 | 107.55 | 111.50 |
| 1 | CA | 807 | U | C5-C4-O4 | -7.89 | 121.16 | 125.90 |
| 1 | CA | 2589 | A | N1-C2-N3 | 7.89 | 133.25 | 129.30 |
| 1 | CA | 2253 | G | N1-C6-O6 | 7.89 | 124.63 | 119.90 |
| 1 | AA | 2515 | A | C2-N3-C4 | 7.88 | 114.54 | 110.60 |
| 1 | CA | 141 | A | C6-C5-N7 | -7.88 | 126.78 | 132.30 |
| 1 | CA | 1661 | G | C8-N9-C4 | 7.88 | 109.55 | 106.40 |
| 1 | AA | 2290 | A | OP1-P-OP2 | -7.88 | 107.78 | 119.60 |
| 2 | AB | 7 | G | C5-C6-O6 | -7.88 | 123.87 | 128.60 |
| 1 | CA | 494 | G | C2-N3-C4 | -7.88 | 107.96 | 111.90 |
| 1 | AA | 1539 | C | N3-C2-O2 | -7.87 | 116.39 | 121.90 |
| 1 | AA | 1009 | C | N3-C2-O2 | -7.87 | 116.39 | 121.90 |
| 1 | AA | 2052 | A | N1-C6-N6 | 7.87 | 123.32 | 118.60 |
| 1 | CA | 2827 | C | C6-N1-C2 | 7.86 | 123.44 | 120.30 |
| 1 | AA | 1812 | C | C5-C4-N4 | -7.86 | 114.70 | 120.20 |
| 1 | AA | 472 | G | C2-N3-C4 | 7.85 | 115.82 | 111.90 |
| 1 | AA | 2386 | C | C5-C6-N1 | -7.85 | 117.08 | 121.00 |
| 1 | CA | 1698 | A | N7-C8-N9 | 7.83 | 117.72 | 113.80 |
| 1 | AA | 2019 | G | O5'-P-OP2 | -7.83 | 98.65 | 105.70 |
| 1 | AA | 1232 | G | C4-C5-C6 | -7.82 | 114.11 | 118.80 |
| 1 | CA | 1688 | U | O5'-P-OP2 | -7.81 | 98.67 | 105.70 |
| 1 | CA | 847 | U | C6-N1-C1' | 7.80 | 132.13 | 121.20 |
| 2 | AB | 90 | A | C8-N9-C4 | 7.79 | 108.92 | 105.80 |
| 1 | AA | 2788 | A | N1-C6-N6 | -7.79 | 113.93 | 118.60 |
| 34 | BA | 1417 | G | C5-C6-N1 | 7.79 | 115.39 | 111.50 |
| 1 | AA | 194 | G | N1-C6-O6 | 7.79 | 124.57 | 119.90 |
| 34 | BA | 786 | G | C5-C6-O6 | 7.79 | 133.27 | 128.60 |
| 1 | AA | 779 | C | N1-C2-O2 | -7.79 | 114.23 | 118.90 |
| 1 | CA | 806 | C | N3-C4-C5 | 7.78 | 125.01 | 121.90 |
| 34 | BA | 1520 | G | C5-C6-O6 | -7.77 | 123.94 | 128.60 |
| 1 | AA | 1240 | G | C2-N3-C4 | 7.77 | 115.79 | 111.90 |
| 1 | AA | 2838 | C | C6-N1-C2 | 7.77 | 123.41 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 851 | A | C2-N3-C4 | -7.77 | 106.72 | 110.60 |
| 1 | AA | 1743 | G | O5'-P-OP2 | -7.77 | 98.71 | 105.70 |
| 1 | AA | 1625 | U | O5'-P-OP2 | -7.76 | 98.71 | 105.70 |
| 1 | AA | 2802 | C | C2-N1-C1' | -7.76 | 110.26 | 118.80 |
| 34 | DA | 689 | C | C6-N1-C2 | -7.75 | 117.20 | 120.30 |
| 1 | CA | 915 | C | N3-C2-O2 | -7.75 | 116.48 | 121.90 |
| 1 | AA | 742 | G | N1-C6-O6 | -7.74 | 115.26 | 119.90 |
| 1 | AA | 2727 | G | O5'-P-OP2 | -7.73 | 98.74 | 105.70 |
| 1 | CA | 955 | C | N3-C4-C5 | -7.73 | 118.81 | 121.90 |
| 1 | AA | 1667 | U | C6-N1-C2 | 7.71 | 125.63 | 121.00 |
| 1 | AA | 2858 | G | O4'-C1'-N9 | 7.71 | 114.37 | 108.20 |
| 1 | AA | 1418 | U | C5-C4-O4 | -7.70 | 121.28 | 125.90 |
| 1 | CA | 2503 | A | C2-N3-C4 | 7.70 | 114.45 | 110.60 |
| 1 | AA | 2632 | C | C2-N3-C4 | -7.70 | 116.05 | 119.90 |
| 1 | AA | 1053 | C | N3-C4-C5 | 7.69 | 124.98 | 121.90 |
| 1 | CA | 1698 | A | C5-C6-N1 | -7.69 | 113.86 | 117.70 |
| 34 | BA | 1524 | C | N1-C2-O2 | -7.69 | 114.29 | 118.90 |
| 1 | CA | 12 | U | C2-N1-C1' | 7.69 | 126.93 | 117.70 |
| 1 | CA | 2441 | C | O5'-P-OP1 | -7.69 | 98.78 | 105.70 |
| 1 | AA | 176 | G | C6-C5-N7 | -7.68 | 125.79 | 130.40 |
| 56 | BW | 74 | C | N1-C2-O2 | 7.68 | 123.51 | 118.90 |
| 1 | AA | 188 | A | O5'-P-OP2 | -7.68 | 98.79 | 105.70 |
| 1 | AA | 2342 | G | C5-C6-O6 | -7.68 | 123.99 | 128.60 |
| 1 | AA | 856 | G | N1-C6-O6 | -7.67 | 115.30 | 119.90 |
| 1 | CA | 2286 | A | C2-N3-C4 | -7.67 | 106.76 | 110.60 |
| 1 | AA | 724 | A | N1-C2-N3 | 7.67 | 133.13 | 129.30 |
| 34 | BA | 1499 | A | N1-C6-N6 | 7.67 | 123.20 | 118.60 |
| 1 | AA | 866 | A | O5'-P-OP2 | -7.66 | 98.80 | 105.70 |
| 1 | AA | 1299 | A | C8-N9-C4 | 7.66 | 108.86 | 105.80 |
| 1 | AA | 1741 | C | C2-N3-C4 | -7.66 | 116.07 | 119.90 |
| 1 | AA | 254 | A | C4-C5-C6 | 7.66 | 120.83 | 117.00 |
| 1 | AA | 894 | U | N1-C2-N3 | 7.66 | 119.49 | 114.90 |
| 1 | CA | 530 | G | C4-C5-N7 | 7.65 | 113.86 | 110.80 |
| 1 | AA | 2734 | A | C8-N9-C4 | 7.65 | 108.86 | 105.80 |
| 1 | AA | 2162 | C | N1-C2-O2 | 7.64 | 123.49 | 118.90 |
| 1 | AA | 1033 | G | C4-C5-N7 | -7.64 | 107.74 | 110.80 |
| 58 | BY | 74 | C | C6-N1-C2 | 7.64 | 123.36 | 120.30 |
| 1 | AA | 2510 | C | O5'-P-OP1 | 7.63 | 119.86 | 110.70 |
| 1 | AA | 893 | C | C6-N1-C2 | 7.63 | 123.35 | 120.30 |
| 1 | AA | 906 | G | C8-N9-C4 | 7.62 | 109.45 | 106.40 |
| 1 | AA | 2641 | A | O4'-C1'-N9 | 7.62 | 114.29 | 108.20 |
| 1 | AA | 1645 | C | C2-N3-C4 | -7.61 | 116.09 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 176 | G | C5-C6-O6 | -7.60 | 124.04 | 128.60 |
| 1 | AA | 595 | A | C8-N9-C4 | -7.60 | 102.76 | 105.80 |
| 1 | AA | 285 | U | O4'-C1'-N1 | 7.59 | 114.28 | 108.20 |
| 1 | AA | 1816 | A | C8-N9-C4 | -7.59 | 102.76 | 105.80 |
| 1 | AA | 2451 | A | O5'-P-OP2 | -7.59 | 98.87 | 105.70 |
| 1 | AA | 1721 | G | C4-C5-N7 | 7.59 | 113.84 | 110.80 |
| 1 | AA | 2034 | G | C4-C5-N7 | 7.59 | 113.83 | 110.80 |
| 34 | BA | 1113 | C | C6-N1-C2 | -7.57 | 117.27 | 120.30 |
| 1 | CA | 1210 | A | P-O3'-C3' | 7.57 | 128.78 | 119.70 |
| 1 | AA | 254 | A | N1-C2-N3 | 7.56 | 133.08 | 129.30 |
| 1 | CA | 2689 | U | P-O3'-C3' | 7.56 | 128.78 | 119.70 |
| 1 | AA | 1231 | G | C5-C6-O6 | -7.56 | 124.06 | 128.60 |
| 1 | AA | 1243 | U | C2-N3-C4 | -7.56 | 122.46 | 127.00 |
| 1 | AA | 2533 | C | C6-N1-C2 | 7.56 | 123.32 | 120.30 |
| 34 | BA | 764 | C | N1-C2-O2 | 7.56 | 123.43 | 118.90 |
| 1 | AA | 542 | C | N3-C4-C5 | 7.55 | 124.92 | 121.90 |
| 1 | AA | 872 | C | C5-C6-N1 | -7.55 | 117.22 | 121.00 |
| 1 | AA | 2535 | G | C5-C6-O6 | -7.55 | 124.07 | 128.60 |
| 1 | AA | 2238 | C | C5-C6-N1 | -7.55 | 117.22 | 121.00 |
| 1 | AA | 2509 | A | N1-C6-N6 | -7.54 | 114.07 | 118.60 |
| 34 | BA | 1417 | G | C4-C5-N7 | 7.54 | 113.82 | 110.80 |
| 1 | AA | 2392 | C | C2-N3-C4 | -7.53 | 116.14 | 119.90 |
| 1 | CA | 265 | A | C5-N7-C8 | -7.52 | 100.14 | 103.90 |
| 1 | CA | 1692 | U | N1-C2-O2 | -7.52 | 117.54 | 122.80 |
| 1 | AA | 2559 | U | C2-N3-C4 | -7.51 | 122.49 | 127.00 |
| 1 | CA | 1826 | G | C4-C5-N7 | -7.51 | 107.80 | 110.80 |
| 1 | CA | 2289 | G | O5'-P-OP2 | -7.50 | 98.94 | 105.70 |
| 1 | AA | 122 | G | O5'-P-OP2 | -7.50 | 98.95 | 105.70 |
| 1 | AA | 1986 | G | O5'-P-OP1 | -7.50 | 98.95 | 105.70 |
| 34 | BA | 841 | U | C5-C6-N1 | 7.50 | 126.45 | 122.70 |
| 1 | AA | 1683 | C | C5-C6-N1 | -7.50 | 117.25 | 121.00 |
| 1 | AA | 553 | A | N3-C4-C5 | 7.50 | 132.05 | 126.80 |
| 1 | AA | 1151 | U | OP1-P-OP2 | 7.50 | 130.84 | 119.60 |
| 1 | AA | 2001 | C | N1-C2-O2 | -7.49 | 114.40 | 118.90 |
| 1 | AA | 139 | A | O4'-C1'-N9 | 7.48 | 114.18 | 108.20 |
| 1 | AA | 1719 | C | N1-C2-O2 | -7.47 | 114.42 | 118.90 |
| 1 | AA | 1374 | G | C6-N1-C2 | -7.45 | 120.63 | 125.10 |
| 1 | AA | 1255 | A | P-O3'-C3' | 7.45 | 128.64 | 119.70 |
| 1 | AA | 1843 | A | N1-C6-N6 | -7.45 | 114.13 | 118.60 |
| 1 | AA | 2049 | G | N3-C4-C5 | -7.45 | 124.87 | 128.60 |
| 1 | AA | 2561 | G | C4-C5-N7 | 7.45 | 113.78 | 110.80 |
| 1 | AA | 2597 | U | N3-C2-O2 | -7.45 | 116.98 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | AA | 2636 | G | C6-N1-C2 | -7.45 | 120.63 | 125.10 |
| 1 | CA | 1142(A) | A | N3-C4-C5 | 7.45 | 132.01 | 126.80 |
| 1 | AA | 2250 | G | OP1-P-OP2 | 7.45 | 130.77 | 119.60 |
| 1 | AA | 2294 | G | O5'-P-OP1 | -7.44 | 99.00 | 105.70 |
| 1 | AA | 2581 | G | N1-C6-O6 | -7.44 | 115.44 | 119.90 |
| 1 | AA | 1031 | C | C6-N1-C2 | -7.43 | 117.33 | 120.30 |
| 1 | AA | 859 | C | C2-N3-C4 | -7.43 | 116.18 | 119.90 |
| 34 | BA | 1501 | C | N1-C2-O2 | -7.43 | 114.44 | 118.90 |
| 1 | CA | 2585 | U | N3-C4-O4 | -7.43 | 114.20 | 119.40 |
| 1 | AA | 1788 | U | C6-N1-C2 | 7.43 | 125.45 | 121.00 |
| 1 | AA | 1745 | A | O4'-C1'-N9 | 7.42 | 114.14 | 108.20 |
| 1 | AA | 2039 | U | N3-C2-O2 | -7.42 | 117.00 | 122.20 |
| 1 | CA | 588 | U | O5'-P-OP2 | -7.42 | 99.02 | 105.70 |
| 1 | CA | 1901 | A | C2-N3-C4 | 7.42 | 114.31 | 110.60 |
| 1 | AA | 637 | U | N3-C2-O2 | -7.41 | 117.01 | 122.20 |
| 1 | AA | 1299 | A | C5-C6-N1 | 7.41 | 121.41 | 117.70 |
| 1 | AA | 370 | A | C8-N9-C4 | 7.41 | 108.76 | 105.80 |
| 1 | AA | 1920 | U | N3-C4-O4 | -7.41 | 114.22 | 119.40 |
| 1 | AA | 50 | G | N3-C4-C5 | -7.40 | 124.90 | 128.60 |
| 1 | AA | 790 | G | C5-C6-O6 | 7.40 | 133.04 | 128.60 |
| 1 | AA | 1291 | G | C5-C6-O6 | 7.40 | 133.04 | 128.60 |
| 1 | CA | 752 | A | P-O3'-C3' | 7.40 | 128.57 | 119.70 |
| 1 | AA | 1961 | U | C4-C5-C6 | -7.39 | 115.27 | 119.70 |
| 1 | AA | 197 | C | C4-C5-C6 | 7.39 | 121.09 | 117.40 |
| 1 | AA | 1660 | A | O5'-P-OP1 | -7.39 | 99.05 | 105.70 |
| 1 | CA | 34 | C | C2-N1-C1' | 7.38 | 126.92 | 118.80 |
| 1 | AA | 2466 | G | N1-C6-O6 | -7.38 | 115.47 | 119.90 |
| 1 | AA | 1264 | G | C2-N3-C4 | -7.38 | 108.21 | 111.90 |
| 1 | AA | 2451 | A | C5-N7-C8 | -7.38 | 100.21 | 103.90 |
| 1 | AA | 1605 | A | N1-C6-N6 | 7.38 | 123.03 | 118.60 |
| 1 | CA | 2238 | G | OP1-P-OP2 | 7.37 | 130.66 | 119.60 |
| 1 | AA | 872 | C | C6-N1-C2 | 7.37 | 123.25 | 120.30 |
| 1 | AA | 69 | G | N1-C6-O6 | -7.37 | 115.48 | 119.90 |
| 1 | AA | 2377 | G | C5-C6-N1 | 7.37 | 115.19 | 111.50 |
| 1 | AA | 98 | U | C5-C4-O4 | 7.37 | 130.32 | 125.90 |
| 1 | AA | 990 | A | O4'-C1'-N9 | 7.36 | 114.08 | 108.20 |
| 1 | AA | 1344 | C | N3-C4-C5 | 7.35 | 124.84 | 121.90 |
| 1 | AA | 1745 | A | N3-C4-N9 | -7.35 | 121.52 | 127.40 |
| 1 | AA | 1243 | U | N1-C2-N3 | 7.35 | 119.31 | 114.90 |
| 1 | AA | 2657 | G | C5-N7-C8 | -7.35 | 100.63 | 104.30 |
| 1 | AA | 1721 | G | C5-C6-O6 | -7.34 | 124.19 | 128.60 |
| 1 | CA | 1673 | U | C2-N1-C1' | -7.34 | 108.89 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 961 | C | C6-N1-C2 | -7.34 | 117.36 | 120.30 |
| 1 | AA | 207 | A | C2-N3-C4 | -7.33 | 106.93 | 110.60 |
| 1 | AA | 978 | A | C5-C6-N1 | -7.33 | 114.03 | 117.70 |
| 1 | CA | 265 | A | N7-C8-N9 | 7.33 | 117.47 | 113.80 |
| 1 | AA | 2571 | C | N3-C2-O2 | -7.33 | 116.77 | 121.90 |
| 34 | BA | 1502 | A | C2-N3-C4 | -7.32 | 106.94 | 110.60 |
| 34 | BA | 736 | C | N3-C4-C5 | 7.32 | 124.83 | 121.90 |
| 1 | AA | 2831 | A | C2-N3-C4 | -7.32 | 106.94 | 110.60 |
| 1 | AA | 254 | A | C5-C6-N1 | -7.31 | 114.04 | 117.70 |
| 1 | CA | 2229 | C | C6-N1-C2 | 7.31 | 123.22 | 120.30 |
| 1 | AA | 1766 | G | C4-C5-N7 | 7.31 | 113.72 | 110.80 |
| 34 | BA | 365 | U | N1-C2-N3 | 7.30 | 119.28 | 114.90 |
| 1 | AA | 723 | A | C8-N9-C4 | 7.29 | 108.72 | 105.80 |
| 1 | CA | 2085 | C | N1-C2-O2 | -7.29 | 114.52 | 118.90 |
| 1 | AA | 2743 | C | N3-C4-C5 | 7.29 | 124.82 | 121.90 |
| 1 | AA | 1874 | C | N3-C4-C5 | 7.29 | 124.82 | 121.90 |
| 1 | AA | 2620 | G | C5-C6-N1 | 7.29 | 115.14 | 111.50 |
| 2 | AB | 7 | G | C4-C5-N7 | 7.29 | 113.71 | 110.80 |
| 1 | CA | 195 | A | P-O3'-C3' | 7.29 | 128.44 | 119.70 |
| 1 | AA | 1920 | U | N1-C2-O2 | 7.28 | 127.90 | 122.80 |
| 1 | AA | 1298 | G | OP2-P-O3' | 7.28 | 121.22 | 105.20 |
| 1 | AA | 199 | C | N3-C4-N4 | -7.28 | 112.91 | 118.00 |
| 1 | AA | 645 | G | C8-N9-C4 | 7.28 | 109.31 | 106.40 |
| 1 | AA | 1426 | G | C8-N9-C4 | 7.28 | 109.31 | 106.40 |
| 34 | BA | 1502 | A | O5'-P-OP2 | -7.27 | 99.15 | 105.70 |
| 1 | AA | 1155 | C | C5-C6-N1 | 7.27 | 124.63 | 121.00 |
| 1 | CA | 1202 | C | C6-N1-C2 | 7.27 | 123.21 | 120.30 |
| 1 | AA | 906 | G | N3-C4-C5 | 7.26 | 132.23 | 128.60 |
| 1 | AA | 2531 | U | C5-C6-N1 | -7.26 | 119.07 | 122.70 |
| 1 | AA | 2751 | A | C8-N9-C4 | 7.26 | 108.70 | 105.80 |
| 1 | CA | 2207 | G | N1-C6-O6 | 7.25 | 124.25 | 119.90 |
| 1 | AA | 874 | U | C6-N1-C2 | 7.25 | 125.35 | 121.00 |
| 1 | AA | 1009 | C | C6-N1-C2 | -7.25 | 117.40 | 120.30 |
| 1 | AA | 194 | G | N9-C4-C5 | -7.24 | 102.50 | 105.40 |
| 1 | AA | 354 | A | C4-C5-N7 | 7.24 | 114.32 | 110.70 |
| 1 | CA | 2504 | U | O5'-P-OP1 | -7.24 | 99.19 | 105.70 |
| 1 | AA | 893 | C | C2-N3-C4 | -7.23 | 116.28 | 119.90 |
| 1 | CA | 1200 | C | C5-C6-N1 | -7.23 | 117.38 | 121.00 |
| 1 | AA | 2641 | A | N9-C1'-C2' | 7.23 | 123.39 | 114.00 |
| 1 | CA | 1212 | G | N3-C4-N9 | 7.23 | 130.34 | 126.00 |
| 1 | AA | 2464 | C | N3-C4-C5 | 7.22 | 124.79 | 121.90 |
| 1 | AA | 2641 | A | C4-N9-C1' | 7.22 | 139.30 | 126.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1204 | A | C5-N7-C8 | -7.22 | 100.29 | 103.90 |
| 1 | AA | 2732 | G | C5-C6-O6 | -7.22 | 124.27 | 128.60 |
| 1 | CA | 1947 | C | C6-N1-C2 | 7.22 | 123.19 | 120.30 |
| 31 | A7 | 39 | ARG | NE-CZ-NH2 | -7.22 | 116.69 | 120.30 |
| 1 | AA | 1204 | C | C5-C6-N1 | -7.21 | 117.39 | 121.00 |
| 1 | AA | 2468 | C | C6-N1-C2 | 7.21 | 123.19 | 120.30 |
| 1 | AA | 404 | C | C6-N1-C2 | 7.21 | 123.18 | 120.30 |
| 34 | BA | 1195 | C | C6-N1-C2 | -7.21 | 117.42 | 120.30 |
| 1 | AA | 714 | U | C5-C6-N1 | -7.21 | 119.10 | 122.70 |
| 34 | BA | 266 | G | N7-C8-N9 | 7.21 | 116.70 | 113.10 |
| 1 | CA | 1626 | G | N9-C4-C5 | 7.20 | 108.28 | 105.40 |
| 1 | CA | 2685 | G | N1-C6-O6 | -7.20 | 115.58 | 119.90 |
| 1 | AA | 1154 | U | N1-C2-O2 | 7.20 | 127.84 | 122.80 |
| 1 | AA | 128 | C | O5'-P-OP1 | -7.20 | 99.22 | 105.70 |
| 1 | AA | 2506 | G | C5-C6-O6 | 7.20 | 132.92 | 128.60 |
| 1 | CA | 1204 | A | C4-C5-N7 | 7.20 | 114.30 | 110.70 |
| 1 | AA | 907 | U | O5'-P-OP2 | -7.19 | 99.22 | 105.70 |
| 1 | AA | 69 | G | N3-C2-N2 | 7.19 | 124.94 | 119.90 |
| 1 | AA | 1691 | C | N3-C2-O2 | -7.19 | 116.87 | 121.90 |
| 1 | AA | 2451 | A | N7-C8-N9 | 7.19 | 117.39 | 113.80 |
| 1 | AA | 254 | A | O4'-C1'-N9 | 7.19 | 113.95 | 108.20 |
| 1 | AA | 1001 | G | N3-C2-N2 | -7.19 | 114.87 | 119.90 |
| 1 | AA | 1827 | U | OP1-P-OP2 | 7.18 | 130.37 | 119.60 |
| 1 | CA | 2708 | G | N7-C8-N9 | -7.18 | 109.51 | 113.10 |
| 1 | AA | 1821 | C | P-O3'-C3' | 7.18 | 128.31 | 119.70 |
| 1 | CA | 847 | U | C5-C6-N1 | -7.18 | 119.11 | 122.70 |
| 1 | AA | 1723 | A | N7-C8-N9 | -7.17 | 110.21 | 113.80 |
| 1 | AA | 1827 | U | C6-N1-C2 | 7.17 | 125.30 | 121.00 |
| 1 | CA | 945 | A | C6-C5-N7 | -7.17 | 127.28 | 132.30 |
| 2 | AB | 79 | C | C6-N1-C2 | -7.16 | 117.44 | 120.30 |
| 1 | AA | 197 | C | C5-C6-N1 | -7.16 | 117.42 | 121.00 |
| 1 | AA | 2331 | G | C2-N3-C4 | -7.16 | 108.32 | 111.90 |
| 1 | AA | 637 | U | C5-C4-O4 | 7.15 | 130.19 | 125.90 |
| 1 | AA | 123 | G | C6-N1-C2 | -7.15 | 120.81 | 125.10 |
| 1 | AA | 215 | G | O4'-C1'-N9 | 7.15 | 113.92 | 108.20 |
| 1 | AA | 2641 | A | C4-C5-C6 | 7.14 | 120.57 | 117.00 |
| 34 | BA | 365 | U | C4-C5-C6 | 7.14 | 123.99 | 119.70 |
| 1 | AA | 1717 | C | N3-C4-C5 | -7.12 | 119.05 | 121.90 |
| 1 | AA | 2014 | G | C5-C6-N1 | 7.12 | 115.06 | 111.50 |
| 1 | CA | 2523 | G | C6-C5-N7 | -7.12 | 126.13 | 130.40 |
| 1 | AA | 1038 | C | C5-C4-N4 | -7.12 | 115.22 | 120.20 |
| 1 | CA | 1604 | C | N3-C4-C5 | 7.12 | 124.75 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 933 | A | N7-C8-N9 | 7.11 | 117.36 | 113.80 |
| 1 | CA | 527 | C | C5-C4-N4 | 7.11 | 125.18 | 120.20 |
| 1 | AA | 1645 | C | N1-C2-O2 | -7.11 | 114.64 | 118.90 |
| 1 | CA | 784 | A | N1-C6-N6 | -7.11 | 114.33 | 118.60 |
| 1 | AA | 1543 | U | C5-C4-O4 | 7.10 | 130.16 | 125.90 |
| 1 | CA | 1899 | G | N1-C6-O6 | 7.10 | 124.16 | 119.90 |
| 34 | DA | 821 | G | O5'-P-OP1 | -7.10 | 99.31 | 105.70 |
| 1 | AA | 12 | U | C2-N1-C1' | 7.10 | 126.22 | 117.70 |
| 1 | AA | 471 | C | C4-C5-C6 | 7.09 | 120.95 | 117.40 |
| 1 | AA | 1249 | A | C6-C5-N7 | -7.09 | 127.34 | 132.30 |
| 1 | CA | 1781 | C | N3-C4-N4 | -7.09 | 113.04 | 118.00 |
| 1 | AA | 1812 | C | N3-C2-O2 | 7.09 | 126.86 | 121.90 |
| 1 | AA | 2049 | G | C5-C6-O6 | 7.09 | 132.85 | 128.60 |
| 1 | AA | 216 | A | N1-C2-N3 | 7.08 | 132.84 | 129.30 |
| 1 | AA | 1605 | A | C4-C5-N7 | 7.08 | 114.24 | 110.70 |
| 1 | CA | 1658 | C | N3-C4-C5 | -7.08 | 119.07 | 121.90 |
| 1 | CA | 474 | G | O5'-P-OP2 | -7.08 | 99.33 | 105.70 |
| 1 | CA | 393 | C | N1-C2-O2 | -7.08 | 114.65 | 118.90 |
| 1 | AA | 2849 | G | N3-C2-N2 | 7.07 | 124.85 | 119.90 |
| 1 | AA | 354 | A | C6-N1-C2 | 7.07 | 122.84 | 118.60 |
| 1 | AA | 990 | A | C4-N9-C1' | 7.07 | 139.02 | 126.30 |
| 1 | CA | 528 | A | C5-N7-C8 | -7.07 | 100.37 | 103.90 |
| 34 | BA | 365 | U | C6-N1-C1' | 7.06 | 131.08 | 121.20 |
| 1 | AA | 954 | C | N1-C2-O2 | -7.05 | 114.67 | 118.90 |
| 1 | CA | 1204 | A | O4'-C1'-N9 | 7.05 | 113.84 | 108.20 |
| 1 | CA | 2552 | U | N3-C4-O4 | -7.05 | 114.47 | 119.40 |
| 1 | AA | 2072 | C | N3-C4-C5 | -7.04 | 119.08 | 121.90 |
| 1 | CA | 2824 | C | C2-N3-C4 | -7.04 | 116.38 | 119.90 |
| 1 | AA | 2838 | C | N3-C4-C5 | 7.03 | 124.71 | 121.90 |
| 1 | CA | 2683 | C | N3-C4-C5 | -7.03 | 119.09 | 121.90 |
| 1 | AA | 2631 | C | C4-C5-C6 | 7.02 | 120.91 | 117.40 |
| 1 | CA | 1783 | A | OP1-P-OP2 | -7.02 | 109.07 | 119.60 |
| 1 | AA | 720 | C | N1-C2-O2 | 7.02 | 123.11 | 118.90 |
| 1 | AA | 1422 | C | N3-C4-C5 | 7.02 | 124.71 | 121.90 |
| 1 | AA | 2597 | U | N1-C2-O2 | 7.01 | 127.71 | 122.80 |
| 1 | AA | 2608 | U | C2-N3-C4 | -7.01 | 122.79 | 127.00 |
| 1 | AA | 1861 | C | N3-C2-O2 | 7.01 | 126.81 | 121.90 |
| 1 | AA | 980 | C | C5-C6-N1 | -7.01 | 117.50 | 121.00 |
| 1 | AA | 853 | C | N3-C4-C5 | 7.01 | 124.70 | 121.90 |
| 1 | AA | 2331 | G | O4'-C1'-N9 | 7.01 | 113.81 | 108.20 |
| 1 | AA | 2111 | U | C5-C6-N1 | -7.00 | 119.20 | 122.70 |
| 1 | AA | 1456 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 34 | DA | 898 | G | C5-C6-O6 | -7.00 | 124.40 | 128.60 |
| 1 | AA | 851 | A | N1-C6-N6 | 7.00 | 122.80 | 118.60 |
| 1 | AA | 993 | G | O5'-P-OP1 | -7.00 | 99.40 | 105.70 |
| 1 | AA | 2162 | C | C6-N1-C2 | -7.00 | 117.50 | 120.30 |
| 1 | AA | 792 | G | N9-C4-C5 | -6.99 | 102.60 | 105.40 |
| 1 | CA | 1142(A) | A | C5-N7-C8 | -6.99 | 100.40 | 103.90 |
| 34 | BA | 866 | C | N1-C2-O2 | -6.99 | 114.71 | 118.90 |
| 1 | AA | 2641 | A | N7-C8-N9 | 6.98 | 117.29 | 113.80 |
| 1 | AA | 785 | G | C5-N7-C8 | -6.98 | 100.81 | 104.30 |
| 1 | AA | 2515 | A | N9-C4-C5 | -6.98 | 103.01 | 105.80 |
| 1 | AA | 534 | C | C6-N1-C2 | 6.98 | 123.09 | 120.30 |
| 34 | BA | 913 | A | P-O3'-C3' | 6.98 | 128.08 | 119.70 |
| 1 | AA | 139 | A | C6-C5-N7 | -6.98 | 127.42 | 132.30 |
| 1 | AA | 1011 | G | C2-N3-C4 | -6.98 | 108.41 | 111.90 |
| 1 | AA | 2502 | G | C8-N9-C4 | 6.98 | 109.19 | 106.40 |
| 1 | AA | 2722 | C | O5'-P-OP1 | -6.98 | 99.42 | 105.70 |
| 1 | AA | 995 | G | C5-N7-C8 | -6.98 | 100.81 | 104.30 |
| 1 | AA | 1745 | A | N1-C6-N6 | 6.98 | 122.79 | 118.60 |
| 1 | AA | 2684 | G | OP2-P-O3' | 6.98 | 120.55 | 105.20 |
| 1 | AA | 1179 | U | C5-C6-N1 | -6.97 | 119.21 | 122.70 |
| 1 | AA | 354 | A | N1-C2-N3 | 6.97 | 132.79 | 129.30 |
| 1 | AA | 978 | A | N1-C6-N6 | 6.97 | 122.78 | 118.60 |
| 1 | AA | 2632 | C | C5-C6-N1 | -6.97 | 117.52 | 121.00 |
| 1 | AA | 194 | G | C2-N3-C4 | -6.97 | 108.42 | 111.90 |
| 1 | AA | 1788 | U | C5-C6-N1 | -6.97 | 119.22 | 122.70 |
| 1 | AA | 2441 | G | O5'-P-OP1 | 6.97 | 119.06 | 110.70 |
| 2 | AB | 101 | G | N7-C8-N9 | -6.97 | 109.62 | 113.10 |
| 1 | AA | 1237 | G | C8-N9-C4 | 6.96 | 109.19 | 106.40 |
| 1 | AA | 2060 | G | C5-C6-O6 | 6.96 | 132.78 | 128.60 |
| 1 | AA | 176 | G | N3-C4-N9 | 6.96 | 130.18 | 126.00 |
| 1 | AA | 1244 | U | C5-C6-N1 | -6.96 | 119.22 | 122.70 |
| 1 | CA | 1664 | A | C8-N9-C4 | -6.96 | 103.02 | 105.80 |
| 1 | AA | 2605 | U | N3-C4-O4 | -6.95 | 114.53 | 119.40 |
| 1 | AA | 980 | C | C2-N3-C4 | -6.95 | 116.42 | 119.90 |
| 1 | AA | 2298 | A | C5-C6-N1 | -6.95 | 114.22 | 117.70 |
| 1 | AA | 2405 | A | C2-N3-C4 | -6.95 | 107.12 | 110.60 |
| 1 | CA | 1296 | G | N1-C6-O6 | -6.95 | 115.73 | 119.90 |
| 34 | DA | 754 | C | C2-N1-C1' | 6.95 | 126.44 | 118.80 |
| 1 | AA | 2528 | G | C5-C6-O6 | 6.95 | 132.77 | 128.60 |
| 1 | AA | 553 | A | N3-C4-N9 | -6.95 | 121.84 | 127.40 |
| 1 | AA | 724 | A | C4-C5-C6 | 6.95 | 120.47 | 117.00 |
| 1 | AA | 1023 | G | O5'-P-OP2 | -6.94 | 99.45 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 798 | A | N1-C6-N6 | 6.94 | 122.77 | 118.60 |
| 1 | AA | 616 | G | C4-C5-N7 | -6.94 | 108.03 | 110.80 |
| 1 | AA | 2040 | G | C5-C6-N1 | 6.94 | 114.97 | 111.50 |
| 1 | CA | 794 | G | N3-C2-N2 | 6.94 | 124.75 | 119.90 |
| 1 | AA | 912 | C | N1-C2-O2 | -6.93 | 114.74 | 118.90 |
| 1 | AA | 790 | G | N1-C6-O6 | -6.93 | 115.74 | 119.90 |
| 34 | BA | 1442 | G | N7-C8-N9 | 6.93 | 116.56 | 113.10 |
| 1 | CA | 933 | A | C5-N7-C8 | -6.93 | 100.44 | 103.90 |
| 1 | CA | 1947 | C | N3-C4-C5 | 6.93 | 124.67 | 121.90 |
| 1 | AA | 1254 | G | C5-C6-N1 | 6.93 | 114.96 | 111.50 |
| 1 | AA | 1067 | A | C4-C5-N7 | 6.92 | 114.16 | 110.70 |
| 21 | CX | 57 | LEU | CA-CB-CG | 6.92 | 131.23 | 115.30 |
| 1 | AA | 2299 | A | C4-C5-N7 | 6.92 | 114.16 | 110.70 |
| 1 | AA | 477 | C | C6-N1-C2 | 6.92 | 123.07 | 120.30 |
| 1 | AA | 555 | G | C5-C6-N1 | -6.92 | 108.04 | 111.50 |
| 1 | AA | 1966 | U | N3-C4-O4 | -6.91 | 114.56 | 119.40 |
| 1 | AA | 1755 | C | C6-N1-C2 | 6.91 | 123.06 | 120.30 |
| 1 | AA | 1665 | G | N3-C2-N2 | 6.91 | 124.73 | 119.90 |
| 1 | AA | 500 | G | C8-N9-C4 | -6.90 | 103.64 | 106.40 |
| 1 | AA | 1965 | U | C5-C6-N1 | -6.90 | 119.25 | 122.70 |
| 1 | AA | 470 | C | C5-C6-N1 | -6.90 | 117.55 | 121.00 |
| 1 | AA | 511 | C | O5'-P-OP2 | 6.90 | 118.98 | 110.70 |
| 1 | CA | 2286 | A | C6-C5-N7 | -6.89 | 127.47 | 132.30 |
| 1 | AA | 1848 | G | N3-C2-N2 | 6.89 | 124.72 | 119.90 |
| 1 | AA | 2264 | G | N9-C4-C5 | 6.89 | 108.15 | 105.40 |
| 1 | AA | 2329 | C | C6-N1-C2 | -6.89 | 117.55 | 120.30 |
| 1 | AA | 2889 | C | N3-C2-O2 | -6.88 | 117.08 | 121.90 |
| 1 | AA | 649 | C | C2-N3-C4 | -6.88 | 116.46 | 119.90 |
| 1 | AA | 2077 | C | C6-N1-C2 | 6.88 | 123.05 | 120.30 |
| 34 | BA | 345 | C | C6-N1-C2 | -6.88 | 117.55 | 120.30 |
| 34 | DA | 1154 | G | C4-N9-C1' | 6.87 | 135.43 | 126.50 |
| 1 | AA | 2448 | G | N1-C6-O6 | -6.87 | 115.78 | 119.90 |
| 1 | AA | 2460 | A | N9-C4-C5 | 6.87 | 108.55 | 105.80 |
| 1 | AA | 1026 | A | N9-C4-C5 | -6.87 | 103.05 | 105.80 |
| 1 | AA | 2423 | A | C8-N9-C4 | 6.86 | 108.54 | 105.80 |
| 1 | CA | 2536 | G | N1-C6-O6 | 6.86 | 124.01 | 119.90 |
| 2 | CB | 30 | C | N3-C4-C5 | -6.86 | 119.16 | 121.90 |
| 1 | AA | 2571 | C | N3-C4-N4 | -6.85 | 113.20 | 118.00 |
| 1 | AA | 2613 | C | OP2-P-O3' | 6.85 | 120.28 | 105.20 |
| 34 | BA | 247 | G | N3-C4-C5 | -6.85 | 125.17 | 128.60 |
| 1 | AA | 1543 | U | N3-C4-O4 | -6.85 | 114.60 | 119.40 |
| 1 | CA | 334 | C | C6-N1-C2 | 6.85 | 123.04 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1828 | G | O5'-P-OP1 | -6.85 | 99.54 | 105.70 |
| 1 | AA | 720 | C | N3-C2-O2 | -6.85 | 117.11 | 121.90 |
| 1 | AA | 1374 | G | N3-C4-N9 | 6.85 | 130.11 | 126.00 |
| 1 | AA | 2046 | G | N7-C8-N9 | -6.85 | 109.68 | 113.10 |
| 1 | AA | 2667 | G | O4'-C1'-N9 | 6.85 | 113.68 | 108.20 |
| 1 | CA | 1021 | A | N3-C4-C5 | 6.85 | 131.59 | 126.80 |
| 1 | AA | 407 | U | C5-C6-N1 | -6.84 | 119.28 | 122.70 |
| 34 | BA | 910 | C | C6-N1-C2 | 6.84 | 123.04 | 120.30 |
| 1 | AA | 405 | C | N1-C2-O2 | -6.84 | 114.80 | 118.90 |
| 34 | BA | 1401 | G | N3-C2-N2 | -6.84 | 115.11 | 119.90 |
| 1 | AA | 1273 | G | C4-C5-N7 | -6.84 | 108.06 | 110.80 |
| 1 | AA | 1667 | U | C5-C6-N1 | -6.84 | 119.28 | 122.70 |
| 1 | CA | 614 | U | N3-C4-O4 | -6.84 | 114.61 | 119.40 |
| 34 | DA | 770 | C | O5'-P-OP2 | -6.83 | 99.55 | 105.70 |
| 1 | CA | 39 | C | C6-N1-C2 | 6.83 | 123.03 | 120.30 |
| 1 | CA | 1425 | G | C6-C5-N7 | -6.83 | 126.30 | 130.40 |
| 34 | BA | 1502 | A | C5-N7-C8 | -6.83 | 100.48 | 103.90 |
| 1 | AA | 345 | G | N9-C4-C5 | -6.83 | 102.67 | 105.40 |
| 1 | AA | 1190 | G | N1-C6-O6 | -6.83 | 115.80 | 119.90 |
| 1 | AA | 2454 | C | C5-C6-N1 | -6.83 | 117.59 | 121.00 |
| 1 | AA | 2512 | U | C5-C4-O4 | -6.83 | 121.80 | 125.90 |
| 1 | AA | 2745 | G | N9-C4-C5 | 6.83 | 108.13 | 105.40 |
| 1 | AA | 240 | A | C8-N9-C4 | 6.83 | 108.53 | 105.80 |
| 1 | AA | 1643 | A | C8-N9-C4 | 6.83 | 108.53 | 105.80 |
| 1 | AA | 2600 | G | C8-N9-C4 | 6.82 | 109.13 | 106.40 |
| 21 | AX | 57 | LEU | CA-CB-CG | 6.82 | 130.99 | 115.30 |
| 1 | AA | 1369 | U | N3-C4-C5 | 6.82 | 118.69 | 114.60 |
| 34 | BA | 1520 | G | O5'-P-OP2 | -6.82 | 99.56 | 105.70 |
| 34 | DA | 245 | C | C5-C6-N1 | -6.82 | 117.59 | 121.00 |
| 1 | AA | 1184 | G | O5'-P-OP1 | 6.82 | 118.88 | 110.70 |
| 1 | AA | 2801 | C | N1-C2-O2 | -6.82 | 114.81 | 118.90 |
| 1 | CA | 1811 | G | N1-C6-O6 | -6.82 | 115.81 | 119.90 |
| 1 | AA | 1001 | G | C5-C6-N1 | -6.81 | 108.09 | 111.50 |
| 1 | AA | 2492 | C | N3-C4-C5 | -6.81 | 119.17 | 121.90 |
| 1 | CA | 751 | A | C8-N9-C4 | 6.81 | 108.53 | 105.80 |
| 1 | CA | 1669 | A | C4-C5-C6 | 6.81 | 120.41 | 117.00 |
| 1 | CA | 933 | A | O4'-C1'-N9 | 6.81 | 113.65 | 108.20 |
| 34 | DA | 567 | G | O5'-P-OP1 | -6.81 | 99.57 | 105.70 |
| 1 | AA | 616 | G | C5-C6-O6 | 6.81 | 132.68 | 128.60 |
| 1 | CA | 1437 | C | C6-N1-C2 | -6.81 | 117.58 | 120.30 |
| 1 | AA | 993 | G | C8-N9-C4 | 6.80 | 109.12 | 106.40 |
| 1 | AA | 1812 | C | N1-C2-N3 | -6.80 | 114.44 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1199 | C | N1-C2-O2 | -6.80 | 114.82 | 118.90 |
| 1 | AA | 1474 | C | O5'-P-OP1 | -6.80 | 99.58 | 105.70 |
| 1 | AA | 1992 | A | N1-C6-N6 | 6.80 | 122.68 | 118.60 |
| 1 | AA | 860 | U | N3-C4-O4 | -6.80 | 114.64 | 119.40 |
| 1 | CA | 1976 | U | N1-C2-N3 | 6.80 | 118.98 | 114.90 |
| 1 | AA | 500 | G | N7-C8-N9 | 6.80 | 116.50 | 113.10 |
| 1 | AA | 706 | C | C5-C6-N1 | -6.79 | 117.60 | 121.00 |
| 1 | CA | 705 | A | N1-C6-N6 | 6.79 | 122.68 | 118.60 |
| 1 | CA | 1654 | A | O5'-P-OP2 | 6.79 | 118.85 | 110.70 |
| 1 | AA | 1316 | C | C6-N1-C2 | 6.79 | 123.02 | 120.30 |
| 34 | BA | 219 | C | C6-N1-C2 | -6.79 | 117.58 | 120.30 |
| 1 | CA | 1763 | G | C8-N9-C4 | 6.79 | 109.12 | 106.40 |
| 1 | CA | 941 | A | C2-N3-C4 | -6.79 | 107.20 | 110.60 |
| 1 | AA | 2636 | G | C5-C6-O6 | -6.78 | 124.53 | 128.60 |
| 1 | AA | 873 | U | C5-C6-N1 | -6.78 | 119.31 | 122.70 |
| 1 | AA | 1845 | G | N1-C6-O6 | 6.78 | 123.97 | 119.90 |
| 1 | CA | 2818 | G | C8-N9-C4 | 6.78 | 109.11 | 106.40 |
| 37 | DD | 188 | LEU | CA-CB-CG | 6.78 | 130.89 | 115.30 |
| 1 | AA | 1210 | G | C5-C6-O6 | 6.78 | 132.66 | 128.60 |
| 1 | AA | 1232 | G | N3-C2-N2 | 6.78 | 124.64 | 119.90 |
| 1 | AA | 2441 | G | O5'-P-OP2 | -6.77 | 99.60 | 105.70 |
| 1 | CA | 2609 | U | O5'-P-OP2 | -6.77 | 99.60 | 105.70 |
| 34 | DA | 1502 | A | C6-C5-N7 | -6.77 | 127.56 | 132.30 |
| 1 | AA | 585 | U | N3-C4-C5 | 6.77 | 118.66 | 114.60 |
| 1 | AA | 1014 | U | N3-C4-C5 | 6.77 | 118.66 | 114.60 |
| 1 | AA | 1346 | U | N3-C4-O4 | 6.77 | 124.14 | 119.40 |
| 1 | CA | 460 | A | N1-C2-N3 | 6.77 | 132.68 | 129.30 |
| 1 | AA | 1829 | U | N3-C4-C5 | 6.76 | 118.66 | 114.60 |
| 2 | AB | 50 | G | O5'-P-OP2 | -6.76 | 99.61 | 105.70 |
| 1 | AA | 726 | C | N3-C4-N4 | -6.76 | 113.27 | 118.00 |
| 1 | AA | 1232 | G | C5-C6-N1 | 6.76 | 114.88 | 111.50 |
| 1 | AA | 1766 | G | C5-N7-C8 | -6.76 | 100.92 | 104.30 |
| 1 | AA | 2220 | A | OP1-P-O3' | 6.76 | 120.08 | 105.20 |
| 1 | AA | 69 | G | N1-C2-N2 | -6.76 | 110.12 | 116.20 |
| 1 | AA | 2354 | C | N1-C2-O2 | -6.76 | 114.84 | 118.90 |
| 1 | AA | 859 | C | C5-C6-N1 | -6.75 | 117.62 | 121.00 |
| 1 | AA | 1757 | C | C6-N1-C2 | 6.75 | 123.00 | 120.30 |
| 1 | AA | 1261 | G | C5-C6-O6 | -6.75 | 124.55 | 128.60 |
| 1 | AA | 1968 | U | N1-C2-N3 | 6.75 | 118.95 | 114.90 |
| 34 | BA | 1442 | G | C5-N7-C8 | -6.75 | 100.93 | 104.30 |
| 34 | DA | 64 | G | N1-C6-O6 | 6.74 | 123.95 | 119.90 |
| 1 | AA | 555 | G | C4-C5-N7 | 6.74 | 113.50 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 2028 | C | C2-N3-C4 | -6.74 | 116.53 | 119.90 |
| 1 | AA | 2298 | A | C4-N9-C1' | 6.74 | 138.43 | 126.30 |
| 1 | AA | 191 | U | C6-N1-C2 | 6.74 | 125.04 | 121.00 |
| 1 | AA | 2703 | C | C6-N1-C2 | 6.74 | 122.99 | 120.30 |
| 1 | CA | 1652 | A | C8-N9-C4 | 6.74 | 108.49 | 105.80 |
| 1 | CA | 672 | C | C6-N1-C2 | 6.73 | 122.99 | 120.30 |
| 1 | CA | 2490 | G | C4-C5-N7 | 6.73 | 113.49 | 110.80 |
| 1 | AA | 254 | A | C8-N9-C4 | -6.73 | 103.11 | 105.80 |
| 1 | CA | 2626 | C | N3-C2-O2 | 6.73 | 126.61 | 121.90 |
| 1 | AA | 978 | A | N3-C4-N9 | -6.73 | 122.02 | 127.40 |
| 34 | BA | 1201 | A | P-O3'-C3' | 6.72 | 127.77 | 119.70 |
| 1 | AA | 1728 | G | C6-C5-N7 | -6.72 | 126.37 | 130.40 |
| 34 | BA | 1030(B) | C | C2-N1-C1' | 6.71 | 126.19 | 118.80 |
| 1 | AA | 2458 | G | C8-N9-C4 | -6.71 | 103.72 | 106.40 |
| 1 | AA | 2500 | A | C8-N9-C4 | 6.71 | 108.48 | 105.80 |
| 1 | AA | 2760 | G | C5-C6-O6 | -6.71 | 124.57 | 128.60 |
| 1 | CA | 1287 | A | C8-N9-C4 | -6.71 | 103.11 | 105.80 |
| 1 | AA | 122 | G | N1-C6-O6 | 6.71 | 123.93 | 119.90 |
| 1 | AA | 1411 | A | C8-N9-C4 | 6.71 | 108.48 | 105.80 |
| 1 | CA | 82 | G | C8-N9-C4 | 6.71 | 109.08 | 106.40 |
| 34 | BA | 1407 | C | C4-C5-C6 | -6.70 | 114.05 | 117.40 |
| 34 | BA | 792 | A | C8-N9-C4 | 6.70 | 108.48 | 105.80 |
| 1 | CA | 1021 | A | N3-C4-N9 | -6.70 | 122.04 | 127.40 |
| 1 | CA | 1278 | A | C2-N3-C4 | -6.70 | 107.25 | 110.60 |
| 1 | AA | 2641 | A | C5-N7-C8 | -6.70 | 100.55 | 103.90 |
| 1 | AA | 999 | G | C5-C6-O6 | 6.70 | 132.62 | 128.60 |
| 1 | AA | 735 | U | C5-C6-N1 | -6.70 | 119.35 | 122.70 |
| 1 | AA | 2393 | C | C2-N3-C4 | -6.70 | 116.55 | 119.90 |
| 1 | AA | 2471 | A | C2-N3-C4 | 6.70 | 113.95 | 110.60 |
| 1 | CA | 205 | G | OP1-P-OP2 | 6.70 | 129.64 | 119.60 |
| 1 | CA | 2253 | G | C5-C6-O6 | -6.70 | 124.58 | 128.60 |
| 1 | AA | 187 | C | O5'-P-OP2 | -6.69 | 99.68 | 105.70 |
| 1 | AA | 1255 | A | OP2-P-O3' | 6.69 | 119.91 | 105.20 |
| 1 | CA | 962 | G | C2-N3-C4 | -6.69 | 108.56 | 111.90 |
| 1 | CA | 2347 | C | N1-C2-O2 | 6.69 | 122.91 | 118.90 |
| 1 | AA | 792 | G | N7-C8-N9 | -6.68 | 109.76 | 113.10 |
| 1 | AA | 999 | G | N1-C6-O6 | -6.68 | 115.89 | 119.90 |
| 1 | AA | 2265 | G | N9-C4-C5 | -6.68 | 102.73 | 105.40 |
| 1 | AA | 2610 | A | OP2-P-O3' | 6.68 | 119.91 | 105.20 |
| 34 | BA | 365 | U | N3-C4-O4 | -6.68 | 114.72 | 119.40 |
| 11 | AN | 65 | LYS | CD-CE-NZ | 6.68 | 127.06 | 111.70 |
| 34 | DA | 509 | A | C8-N9-C4 | -6.68 | 103.13 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | CA | 1698 | A | C4-C5-N7 | 6.68 | 114.04 | 110.70 |
| 1 | AA | 2096 | U | N3-C4-O4 | 6.68 | 124.07 | 119.40 |
| 1 | CA | 460 | A | N1-C6-N6 | 6.68 | 122.61 | 118.60 |
| 1 | CA | 1253 | A | N1-C6-N6 | -6.68 | 114.59 | 118.60 |
| 1 | AA | 82 | G | C8-N9-C4 | 6.67 | 109.07 | 106.40 |
| 1 | CA | 2546 | U | C4-C5-C6 | 6.67 | 123.70 | 119.70 |
| 1 | AA | 1474 | C | C4-C5-C6 | 6.67 | 120.74 | 117.40 |
| 34 | BA | 900 | A | O5'-P-OP2 | 6.67 | 118.71 | 110.70 |
| 1 | CA | 2424 | C | C6-N1-C2 | 6.67 | 122.97 | 120.30 |
| 1 | AA | 1605 | A | N1-C2-N3 | 6.67 | 132.63 | 129.30 |
| 1 | AA | 2553 | A | C6-C5-N7 | -6.67 | 127.63 | 132.30 |
| 1 | CA | 2221 | G | N9-C4-C5 | 6.67 | 108.07 | 105.40 |
| 1 | AA | 1831 | C | C2-N3-C4 | -6.67 | 116.57 | 119.90 |
| 1 | CA | 669 | G | OP1-P-OP2 | -6.67 | 109.60 | 119.60 |
| 1 | AA | 2876 | U | N3-C4-O4 | -6.66 | 114.74 | 119.40 |
| 1 | AA | 2895 | C | N3-C4-N4 | 6.66 | 122.66 | 118.00 |
| 1 | AA | 2490 | A | C8-N9-C4 | 6.66 | 108.47 | 105.80 |
| 1 | AA | 992 | G | N3-C2-N2 | 6.66 | 124.56 | 119.90 |
| 1 | AA | 1440 | U | C5-C6-N1 | 6.66 | 126.03 | 122.70 |
| 1 | AA | 2054 | G | OP1-P-OP2 | 6.66 | 129.59 | 119.60 |
| 1 | CA | 1337 | G | C8-N9-C4 | 6.66 | 109.06 | 106.40 |
| 1 | CA | 2893 | G | N3-C4-N9 | 6.66 | 130.00 | 126.00 |
| 1 | AA | 2496 | G | C2-N3-C4 | 6.66 | 115.23 | 111.90 |
| 34 | BA | 345 | C | C5-C6-N1 | 6.66 | 124.33 | 121.00 |
| 1 | CA | 195 | A | OP2-P-O3' | 6.65 | 119.83 | 105.20 |
| 1 | AA | 1605 | A | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 1 | AA | 2515 | A | N3-C4-N9 | 6.65 | 132.72 | 127.40 |
| 1 | AA | 1976 | G | N1-C6-O6 | 6.64 | 123.89 | 119.90 |
| 1 | AA | 604 | C | C5-C6-N1 | -6.64 | 117.68 | 121.00 |
| 1 | AA | 1874 | C | C2-N3-C4 | -6.64 | 116.58 | 119.90 |
| 1 | CA | 1142(A) | A | C5-C6-N1 | -6.64 | 114.38 | 117.70 |
| 1 | CA | 2618 | G | N7-C8-N9 | -6.64 | 109.78 | 113.10 |
| 1 | AA | 1232 | G | O5'-P-OP2 | -6.64 | 99.73 | 105.70 |
| 1 | CA | 530 | G | C5-N7-C8 | -6.64 | 100.98 | 104.30 |
| 1 | AA | 85 | C | C6-N1-C2 | 6.63 | 122.95 | 120.30 |
| 1 | AA | 2039 | U | C5-C6-N1 | -6.63 | 119.38 | 122.70 |
| 1 | CA | 933 | A | C8-N9-C4 | -6.63 | 103.15 | 105.80 |
| 1 | CA | 2394 | C | N3-C4-C5 | 6.63 | 124.55 | 121.90 |
| 1 | CA | 2893 | G | C2-N3-C4 | 6.63 | 115.22 | 111.90 |
| 1 | AA | 182 | U | N1-C2-N3 | 6.63 | 118.88 | 114.90 |
| 1 | AA | 1859 | G | C2-N3-C4 | -6.63 | 108.59 | 111.90 |
| 1 | CA | 1558 | A | P-O3'-C3' | 6.63 | 127.65 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1771 | C | C2-N3-C4 | -6.62 | 116.59 | 119.90 |
| 1 | CA | 705 | A | C5-C6-N6 | -6.62 | 118.40 | 123.70 |
| 1 | CA | 442 | G | O5'-P-OP1 | -6.62 | 99.74 | 105.70 |
| 2 | AB | 28 | C | O5'-P-OP2 | -6.62 | 99.74 | 105.70 |
| 34 | DA | 1502 | A | C4-C5-N7 | 6.62 | 114.01 | 110.70 |
| 1 | AA | 552 | C | C5-C6-N1 | -6.62 | 117.69 | 121.00 |
| 2 | CB | 104 | U | O5'-P-OP2 | -6.61 | 99.75 | 105.70 |
| 1 | AA | 834 | U | O5'-P-OP1 | -6.61 | 99.75 | 105.70 |
| 1 | AA | 884 | C | C2-N3-C4 | -6.61 | 116.60 | 119.90 |
| 1 | AA | 345 | G | C6-C5-N7 | -6.61 | 126.44 | 130.40 |
| 1 | AA | 2459 | G | C8-N9-C4 | 6.61 | 109.04 | 106.40 |
| 1 | AA | 2660 | C | C2-N3-C4 | -6.61 | 116.60 | 119.90 |
| 34 | BA | 1499 | A | C8-N9-C4 | 6.60 | 108.44 | 105.80 |
| 34 | BA | 1522 | U | OP1-P-OP2 | 6.60 | 129.51 | 119.60 |
| 1 | AA | 2513 | C | C2-N1-C1' | -6.60 | 111.54 | 118.80 |
| 34 | BA | 687 | A | P-O3'-C3' | 6.60 | 127.62 | 119.70 |
| 1 | CA | 2207 | G | C6-C5-N7 | -6.60 | 126.44 | 130.40 |
| 1 | AA | 196 | A | N1-C6-N6 | 6.59 | 122.56 | 118.60 |
| 1 | AA | 1342 | G | N3-C2-N2 | 6.59 | 124.52 | 119.90 |
| 1 | AA | 182 | U | C5-C6-N1 | -6.59 | 119.41 | 122.70 |
| 1 | AA | 2745 | G | C8-N9-C4 | -6.59 | 103.76 | 106.40 |
| 57 | BX | 75 | C | C5-C4-N4 | -6.59 | 115.59 | 120.20 |
| 1 | CA | 2679 | A | O5'-P-OP2 | -6.59 | 99.77 | 105.70 |
| 1 | AA | 185 | A | N1-C6-N6 | 6.59 | 122.55 | 118.60 |
| 1 | AA | 1059 | C | N3-C4-C5 | 6.58 | 124.53 | 121.90 |
| 1 | CA | 2464 | C | C2-N3-C4 | -6.58 | 116.61 | 119.90 |
| 34 | DA | 1502 | A | N1-C6-N6 | 6.58 | 122.55 | 118.60 |
| 1 | CA | 2247 | A | C8-N9-C4 | 6.58 | 108.43 | 105.80 |
| 1 | AA | 199 | C | C5-C6-N1 | -6.58 | 117.71 | 121.00 |
| 1 | AA | 399 | G | O4'-C1'-N9 | 6.58 | 113.46 | 108.20 |
| 1 | AA | 1822 | A | OP1-P-OP2 | -6.58 | 109.73 | 119.60 |
| 1 | AA | 2375 | C | N3-C4-N4 | -6.58 | 113.40 | 118.00 |
| 1 | AA | 2690 | C | N1-C2-O2 | -6.58 | 114.95 | 118.90 |
| 1 | AA | 2649 | U | N1-C2-N3 | 6.57 | 118.84 | 114.90 |
| 1 | CA | 2026 | C | N1-C2-O2 | -6.57 | 114.95 | 118.90 |
| 34 | DA | 1501 | C | N1-C2-O2 | -6.57 | 114.96 | 118.90 |
| 1 | AA | 2761 | A | C8-N9-C4 | 6.57 | 108.43 | 105.80 |
| 1 | AA | 1311 | A | O5'-P-OP2 | -6.57 | 99.79 | 105.70 |
| 34 | BA | 504 | C | O5'-P-OP1 | -6.57 | 99.79 | 105.70 |
| 1 | AA | 139 | A | N1-C6-N6 | 6.57 | 122.54 | 118.60 |
| 1 | AA | 1438 | A | C5-C6-N6 | -6.57 | 118.45 | 123.70 |
| 1 | AA | 1701 | A | C5-C6-N1 | -6.57 | 114.42 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1291 | G | C6-C5-N7 | 6.56 | 134.34 | 130.40 |
| 1 | AA | 629 | U | OP2-P-O3' | 6.56 | 119.64 | 105.20 |
| 1 | AA | 1281 | G | C2-N3-C4 | -6.56 | 108.62 | 111.90 |
| 1 | CA | 672 | C | C5-C6-N1 | -6.56 | 117.72 | 121.00 |
| 1 | CA | 2447 | G | C8-N9-C4 | 6.56 | 109.02 | 106.40 |
| 57 | BX | 75 | C | N3-C4-N4 | 6.55 | 122.59 | 118.00 |
| 1 | CA | 1692 | U | C5-C6-N1 | -6.55 | 119.42 | 122.70 |
| 1 | AA | 549 | U | N3-C4-C5 | 6.55 | 118.53 | 114.60 |
| 1 | AA | 476 | G | N1-C6-O6 | -6.55 | 115.97 | 119.90 |
| 2 | AB | 86 | G | N3-C4-N9 | 6.55 | 129.93 | 126.00 |
| 1 | CA | 1799 | G | O5'-P-OP2 | -6.55 | 99.80 | 105.70 |
| 1 | AA | 539 | A | OP2-P-O3' | 6.55 | 119.61 | 105.20 |
| 1 | AA | 1458 | A | O5'-P-OP2 | 6.55 | 118.56 | 110.70 |
| 34 | DA | 481 | G | N3-C4-C5 | -6.55 | 125.33 | 128.60 |
| 1 | AA | 530 | A | C8-N9-C4 | -6.55 | 103.18 | 105.80 |
| 1 | AA | 2418 | U | O5'-P-OP2 | 6.55 | 118.56 | 110.70 |
| 1 | AA | 1985 | U | C2-N1-C1' | 6.55 | 125.56 | 117.70 |
| 1 | AA | 992 | G | O5'-P-OP1 | -6.54 | 99.81 | 105.70 |
| 1 | AA | 1029 | A | C5-C6-N6 | 6.54 | 128.94 | 123.70 |
| 1 | AA | 2383 | G | N9-C4-C5 | -6.54 | 102.78 | 105.40 |
| 1 | AA | 1175 | A | OP1-P-OP2 | 6.54 | 129.41 | 119.60 |
| 1 | AA | 23 | G | C4-C5-N7 | -6.54 | 108.19 | 110.80 |
| 1 | CA | 1698 | A | O4'-C1'-N9 | 6.54 | 113.43 | 108.20 |
| 1 | CA | 2500 | U | C5-C6-N1 | -6.54 | 119.43 | 122.70 |
| 1 | AA | 1522 | G | O5'-P-OP1 | -6.54 | 99.82 | 105.70 |
| 1 | CA | 782 | A | N1-C6-N6 | 6.54 | 122.52 | 118.60 |
| 1 | CA | 2221 | G | N1-C6-O6 | -6.54 | 115.98 | 119.90 |
| 34 | DA | 1154 | G | C8-N9-C1' | -6.53 | 118.51 | 127.00 |
| 1 | AA | 1805 | C | N3-C4-C5 | 6.53 | 124.51 | 121.90 |
| 1 | AA | 2641 | A | C6-N1-C2 | -6.53 | 114.68 | 118.60 |
| 1 | CA | 1004 | C | N1-C2-O2 | -6.53 | 114.98 | 118.90 |
| 1 | CA | 2286 | A | C5-N7-C8 | -6.53 | 100.64 | 103.90 |
| 1 | CA | 2875 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 1 | AA | 2882 | G | C5-C6-O6 | 6.53 | 132.52 | 128.60 |
| 1 | AA | 1233 | U | C5-C4-O4 | 6.53 | 129.82 | 125.90 |
| 1 | AA | 1986 | G | C8-N9-C4 | 6.53 | 109.01 | 106.40 |
| 1 | CA | 955 | C | C6-N1-C2 | -6.53 | 117.69 | 120.30 |
| 1 | CA | 1479 | G | O5'-P-OP2 | -6.53 | 99.83 | 105.70 |
| 1 | CA | 2394 | C | C6-N1-C2 | 6.53 | 122.91 | 120.30 |
| 1 | CA | 1968 | G | N3-C2-N2 | -6.52 | 115.33 | 119.90 |
| 1 | AA | 2464 | C | C4-C5-C6 | -6.52 | 114.14 | 117.40 |
| 1 | CA | 1675 | C | N3-C4-C5 | -6.52 | 119.29 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 206 | U | O5'-P-OP2 | -6.52 | 99.83 | 105.70 |
| 1 | AA | 641 | G | O5'-P-OP2 | -6.52 | 99.83 | 105.70 |
| 1 | AA | 1316 | C | C5-C6-N1 | -6.52 | 117.74 | 121.00 |
| 1 | AA | 2471 | A | C5-C6-N1 | 6.52 | 120.96 | 117.70 |
| 1 | AA | 2652 | G | N9-C4-C5 | 6.51 | 108.00 | 105.40 |
| 1 | AA | 749 | G | O5'-P-OP2 | -6.51 | 99.84 | 105.70 |
| 1 | AA | 2605 | U | N3-C4-C5 | 6.51 | 118.50 | 114.60 |
| 1 | AA | 2830 | A | N1-C6-N6 | 6.51 | 122.50 | 118.60 |
| 1 | CA | 476 | G | O5'-P-OP2 | -6.50 | 99.85 | 105.70 |
| 1 | AA | 2383 | G | C8-N9-C4 | 6.50 | 109.00 | 106.40 |
| 1 | AA | 2466 | G | N3-C2-N2 | 6.50 | 124.45 | 119.90 |
| 1 | CA | 2286 | A | C5-C6-N1 | -6.50 | 114.45 | 117.70 |
| 1 | AA | 855 | G | O5'-P-OP2 | -6.50 | 99.85 | 105.70 |
| 1 | AA | 1462 | G | O4'-C1'-N9 | 6.50 | 113.40 | 108.20 |
| 1 | AA | 1647 | G | C8-N9-C4 | 6.50 | 109.00 | 106.40 |
| 1 | AA | 2497 | G | N3-C2-N2 | 6.50 | 124.45 | 119.90 |
| 1 | AA | 1231 | G | O5'-P-OP2 | -6.49 | 99.86 | 105.70 |
| 1 | AA | 1911 | A | N1-C6-N6 | -6.49 | 114.70 | 118.60 |
| 1 | AA | 2083 | G | C5-C6-O6 | -6.49 | 124.70 | 128.60 |
| 1 | AA | 2701 | U | N1-C2-N3 | 6.49 | 118.80 | 114.90 |
| 1 | CA | 1779 | U | O4'-C1'-N1 | 6.49 | 113.39 | 108.20 |
| 1 | AA | 1815 | A | O5'-P-OP2 | -6.49 | 99.86 | 105.70 |
| 2 | AB | 48 | A | C2-N3-C4 | -6.49 | 107.36 | 110.60 |
| 1 | AA | 1247 | C | N1-C2-O2 | -6.49 | 115.01 | 118.90 |
| 1 | CA | 1558 | A | C2-N3-C4 | -6.48 | 107.36 | 110.60 |
| 34 | DA | 713 | G | O5'-P-OP1 | -6.48 | 99.87 | 105.70 |
| 1 | AA | 191 | U | N3-C4-C5 | 6.48 | 118.49 | 114.60 |
| 1 | AA | 708 | C | C2-N3-C4 | -6.48 | 116.66 | 119.90 |
| 59 | BZ | 374 | LEU | CA-CB-CG | 6.48 | 130.20 | 115.30 |
| 1 | AA | 1920 | U | N3-C4-C5 | 6.48 | 118.49 | 114.60 |
| 1 | CA | 2430 | A | O4'-C1'-N9 | 6.48 | 113.38 | 108.20 |
| 2 | AB | 83 | G | C5-C6-O6 | 6.47 | 132.48 | 128.60 |
| 34 | BA | 804 | U | N3-C4-O4 | -6.47 | 114.87 | 119.40 |
| 1 | CA | 2570 | G | N9-C4-C5 | 6.47 | 107.99 | 105.40 |
| 1 | AA | 2238 | C | C6-N1-C2 | 6.47 | 122.89 | 120.30 |
| 34 | BA | 243 | A | O5'-P-OP1 | -6.47 | 99.88 | 105.70 |
| 1 | AA | 279 | G | C5-C6-N1 | -6.47 | 108.27 | 111.50 |
| 1 | AA | 1992 | A | C5-C6-N6 | -6.46 | 118.53 | 123.70 |
| 34 | BA | 1499 | A | N9-C4-C5 | -6.46 | 103.22 | 105.80 |
| 1 | AA | 1423 | G | N1-C6-O6 | -6.46 | 116.02 | 119.90 |
| 1 | CA | 1215 | G | C5-C6-N1 | 6.46 | 114.73 | 111.50 |
| 1 | AA | 1597 | C | N1-C2-O2 | -6.46 | 115.03 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1848 | G | N1-C2-N2 | -6.46 | 110.39 | 116.20 |
| 1 | AA | 604 | C | C2-N3-C4 | -6.46 | 116.67 | 119.90 |
| 1 | CA | 1673 | U | N3-C4-O4 | -6.46 | 114.88 | 119.40 |
| 1 | CA | 2337 | G | N1-C6-O6 | 6.46 | 123.77 | 119.90 |
| 1 | AA | 177 | G | N1-C2-N2 | -6.46 | 110.39 | 116.20 |
| 1 | CA | 90 | U | N3-C2-O2 | -6.45 | 117.68 | 122.20 |
| 1 | CA | 963 | U | O5'-P-OP2 | 6.45 | 118.44 | 110.70 |
| 1 | AA | 35 | G | O5'-P-OP1 | -6.45 | 99.89 | 105.70 |
| 1 | AA | 820 | U | N1-C2-N3 | 6.45 | 118.77 | 114.90 |
| 34 | BA | 509 | A | C8-N9-C4 | -6.45 | 103.22 | 105.80 |
| 1 | AA | 1844 | G | C8-N9-C4 | 6.45 | 108.98 | 106.40 |
| 1 | AA | 2587 | C | N3-C4-C5 | 6.45 | 124.48 | 121.90 |
| 1 | CA | 1656 | C | N3-C4-N4 | -6.45 | 113.49 | 118.00 |
| 1 | AA | 1190 | G | C5-C6-N1 | 6.44 | 114.72 | 111.50 |
| 1 | AA | 1814 | A | O5'-P-OP2 | -6.44 | 99.90 | 105.70 |
| 1 | CA | 1781 | C | C2-N1-C1' | -6.44 | 111.71 | 118.80 |
| 1 | AA | 891 | C | C6-N1-C2 | 6.44 | 122.88 | 120.30 |
| 34 | BA | 1517 | G | N3-C4-N9 | -6.44 | 122.14 | 126.00 |
| 1 | AA | 797 | A | OP2-P-O3' | 6.44 | 119.36 | 105.20 |
| 1 | CA | 1824 | G | N3-C4-N9 | -6.44 | 122.14 | 126.00 |
| 1 | AA | 2501 | G | N3-C4-N9 | 6.44 | 129.86 | 126.00 |
| 1 | AA | 2889 | C | N1-C2-O2 | 6.44 | 122.76 | 118.90 |
| 34 | DA | 1405 | G | N3-C4-C5 | -6.44 | 125.38 | 128.60 |
| 1 | CA | 2682 | U | O5'-P-OP2 | -6.43 | 99.91 | 105.70 |
| 1 | AA | 1980 | C | N1-C2-O2 | -6.43 | 115.04 | 118.90 |
| 1 | AA | 2619 | G | N1-C6-O6 | -6.43 | 116.04 | 119.90 |
| 1 | CA | 1698 | A | N1-C6-N6 | 6.43 | 122.46 | 118.60 |
| 1 | AA | 855 | G | C5-C6-N1 | 6.43 | 114.72 | 111.50 |
| 1 | AA | 2498 | G | C5-C6-N1 | 6.43 | 114.72 | 111.50 |
| 1 | CA | 2046 | G | C2-N3-C4 | -6.43 | 108.69 | 111.90 |
| 1 | CA | 2782 | G | N1-C6-O6 | 6.43 | 123.76 | 119.90 |
| 1 | AA | 477 | C | C2-N3-C4 | -6.42 | 116.69 | 119.90 |
| 1 | AA | 1546 | G | N1-C6-O6 | 6.42 | 123.75 | 119.90 |
| 1 | CA | 312 | G | O5'-P-OP1 | -6.42 | 99.92 | 105.70 |
| 1 | AA | 2041 | A | C5-N7-C8 | 6.42 | 107.11 | 103.90 |
| 1 | AA | 127 | C | C2-N3-C4 | -6.42 | 116.69 | 119.90 |
| 1 | AA | 1090 | G | N1-C6-O6 | -6.42 | 116.05 | 119.90 |
| 1 | AA | 2083 | G | C6-N1-C2 | -6.42 | 121.25 | 125.10 |
| 1 | AA | 2503 | U | C5-C4-O4 | -6.42 | 122.05 | 125.90 |
| 1 | CA | 1692 | U | C5-C4-O4 | -6.42 | 122.05 | 125.90 |
| 1 | AA | 2496 | G | C5-C6-N1 | 6.42 | 114.71 | 111.50 |
| 2 | AB | 33 | G | C8-N9-C4 | 6.41 | 108.97 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | CA | 2286 | A | N1-C6-N6 | 6.41 | 122.45 | 118.60 |
| 1 | AA | 45 | C | O5'-P-OP1 | 6.41 | 118.39 | 110.70 |
| 1 | AA | 1264 | G | N1-C6-O6 | 6.41 | 123.75 | 119.90 |
| 1 | AA | 1479 | U | C5-C6-N1 | -6.41 | 119.49 | 122.70 |
| 34 | DA | 1502 | A | C5-N7-C8 | -6.41 | 100.69 | 103.90 |
| 1 | AA | 2266 | C | N1-C2-O2 | -6.41 | 115.06 | 118.90 |
| 1 | AA | 2291 | G | N1-C6-O6 | 6.41 | 123.74 | 119.90 |
| 1 | AA | 2587 | C | C6-N1-C2 | 6.41 | 122.86 | 120.30 |
| 1 | AA | 2590 | G | N9-C4-C5 | -6.41 | 102.84 | 105.40 |
| 1 | CA | 1425 | G | N9-C4-C5 | -6.41 | 102.84 | 105.40 |
| 1 | AA | 1836 | U | OP1-P-OP2 | -6.40 | 110.00 | 119.60 |
| 1 | AA | 726 | C | C2-N3-C4 | -6.40 | 116.70 | 119.90 |
| 1 | AA | 2443 | U | C2-N3-C4 | -6.40 | 123.16 | 127.00 |
| 1 | AA | 2331 | G | C4-C5-N7 | 6.40 | 113.36 | 110.80 |
| 1 | AA | 2876 | U | N1-C2-N3 | 6.40 | 118.74 | 114.90 |
| 1 | CA | 2252 | G | C8-N9-C4 | 6.40 | 108.96 | 106.40 |
| 1 | AA | 704 | U | C5-C6-N1 | -6.40 | 119.50 | 122.70 |
| 1 | AA | 1278 | G | O5'-P-OP2 | 6.40 | 118.38 | 110.70 |
| 1 | AA | 808 | A | C5-C6-N1 | -6.39 | 114.50 | 117.70 |
| 1 | AA | 2520 | G | N9-C4-C5 | 6.39 | 107.96 | 105.40 |
| 1 | AA | 2036 | A | C8-N9-C4 | 6.39 | 108.36 | 105.80 |
| 1 | CA | 272(F) | C | C6-N1-C2 | 6.39 | 122.86 | 120.30 |
| 1 | CA | 1337 | G | N7-C8-N9 | -6.39 | 109.90 | 113.10 |
| 1 | AA | 2383 | G | C5-C6-N1 | 6.39 | 114.70 | 111.50 |
| 1 | AA | 2594 | G | O5'-P-OP2 | -6.39 | 99.95 | 105.70 |
| 1 | CA | 2626 | C | C5-C4-N4 | -6.39 | 115.73 | 120.20 |
| 1 | AA | 2294 | G | C4-C5-N7 | 6.39 | 113.36 | 110.80 |
| 1 | CA | 807 | U | N3-C4-O4 | 6.38 | 123.87 | 119.40 |
| 1 | AA | 2273 | C | C4-C5-C6 | 6.38 | 120.59 | 117.40 |
| 1 | AA | 1022 | C | C6-N1-C2 | -6.38 | 117.75 | 120.30 |
| 1 | AA | 1318 | A | O4'-C1'-N9 | 6.38 | 113.31 | 108.20 |
| 1 | AA | 2340 | A | C8-N9-C4 | 6.38 | 108.35 | 105.80 |
| 1 | AA | 2590 | G | C8-N9-C4 | 6.38 | 108.95 | 106.40 |
| 1 | AA | 2743 | C | C5-C6-N1 | -6.38 | 117.81 | 121.00 |
| 1 | CA | 848 | G | N3-C4-C5 | -6.38 | 125.41 | 128.60 |
| 1 | CA | 1384 | A | C2-N3-C4 | 6.38 | 113.79 | 110.60 |
| 1 | CA | 1668 | A | O5'-P-OP1 | -6.38 | 99.96 | 105.70 |
| 1 | AA | 92 | C | C6-N1-C2 | -6.38 | 117.75 | 120.30 |
| 1 | AA | 2515 | A | O5'-P-OP1 | -6.38 | 99.96 | 105.70 |
| 1 | AA | 744 | C | O5'-P-OP2 | -6.38 | 99.96 | 105.70 |
| 1 | AA | 1290 | G | N1-C2-N2 | -6.37 | 110.46 | 116.20 |
| 1 | AA | 1518 | A | C8-N9-C4 | -6.37 | 103.25 | 105.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2535 | G | C4-C5-N7 | 6.37 | 113.35 | 110.80 |
| 1 | CA | 961 | C | C6-N1-C2 | 6.37 | 122.85 | 120.30 |
| 1 | AA | 858 | U | O5'-P-OP2 | -6.37 | 99.97 | 105.70 |
| 1 | AA | 85 | C | N3-C4-C5 | 6.37 | 124.45 | 121.90 |
| 1 | AA | 851 | A | N9-C4-C5 | -6.37 | 103.25 | 105.80 |
| 1 | AA | 2298 | A | C4-C5-N7 | 6.37 | 113.88 | 110.70 |
| 1 | CA | 917 | A | O5'-P-OP1 | 6.37 | 118.34 | 110.70 |
| 1 | AA | 581 | G | N1-C6-O6 | -6.37 | 116.08 | 119.90 |
| 1 | AA | 2480 | G | C8-N9-C4 | 6.37 | 108.95 | 106.40 |
| 1 | AA | 2540 | U | O5'-P-OP1 | -6.37 | 99.97 | 105.70 |
| 1 | AA | 25 | U | C5-C4-O4 | -6.36 | 122.08 | 125.90 |
| 1 | AA | 650 | G | C8-N9-C4 | -6.36 | 103.85 | 106.40 |
| 1 | AA | 1422 | C | C2-N3-C4 | -6.36 | 116.72 | 119.90 |
| 1 | AA | 2872 | G | N1-C6-O6 | -6.36 | 116.08 | 119.90 |
| 1 | AA | 2625 | U | N3-C2-O2 | -6.36 | 117.75 | 122.20 |
| 31 | A7 | 39 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 1 | AA | 1402 | G | C5-C6-O6 | -6.36 | 124.78 | 128.60 |
| 12 | AO | 8 | LEU | CA-CB-CG | 6.36 | 129.93 | 115.30 |
| 1 | AA | 176 | G | N1-C6-O6 | 6.36 | 123.72 | 119.90 |
| 1 | AA | 1703 | C | C6-N1-C2 | 6.35 | 122.84 | 120.30 |
| 1 | AA | 555 | G | N1-C6-O6 | -6.35 | 116.09 | 119.90 |
| 1 | AA | 846 | G | N1-C2-N2 | -6.35 | 110.49 | 116.20 |
| 1 | AA | 2014 | G | P-O3'-C3' | 6.35 | 127.32 | 119.70 |
| 1 | AA | 2299 | A | N3-C4-N9 | -6.34 | 122.32 | 127.40 |
| 1 | AA | 2724 | U | C6-N1-C2 | 6.34 | 124.81 | 121.00 |
| 1 | AA | 637 | U | N3-C4-O4 | -6.34 | 114.96 | 119.40 |
| 1 | AA | 1026 | A | N1-C6-N6 | 6.34 | 122.41 | 118.60 |
| 1 | AA | 2520 | G | C4-C5-N7 | -6.34 | 108.26 | 110.80 |
| 1 | AA | 585 | U | O5'-P-OP1 | -6.34 | 100.00 | 105.70 |
| 1 | AA | 1976 | G | C5-C6-O6 | -6.34 | 124.80 | 128.60 |
| 1 | AA | 2251 | G | N1-C6-O6 | 6.34 | 123.70 | 119.90 |
| 34 | BA | 1067 | A | O4'-C1'-N9 | -6.34 | 103.13 | 108.20 |
| 1 | AA | 240 | A | N1-C6-N6 | -6.34 | 114.80 | 118.60 |
| 1 | AA | 235 | C | C5-C6-N1 | -6.33 | 117.83 | 121.00 |
| 34 | BA | 546 | G | C8-N9-C4 | -6.33 | 103.87 | 106.40 |
| 1 | CA | 141 | A | C5-C6-N6 | -6.33 | 118.63 | 123.70 |
| 1 | CA | 2012 | G | C8-N9-C4 | -6.33 | 103.87 | 106.40 |
| 1 | AA | 1347 | A | OP1-P-OP2 | 6.33 | 129.09 | 119.60 |
| 1 | CA | 917 | A | O5'-P-OP2 | -6.33 | 100.00 | 105.70 |
| 1 | CA | 2589 | A | C6-N1-C2 | -6.33 | 114.80 | 118.60 |
| 1 | AA | 2418 | U | O4'-C1'-N1 | -6.33 | 103.14 | 108.20 |
| 1 | CA | 2818 | G | N3-C2-N2 | 6.33 | 124.33 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2585 | C | C4-C5-C6 | 6.33 | 120.56 | 117.40 |
| 1 | AA | 2601 | A | N9-C4-C5 | 6.32 | 108.33 | 105.80 |
| 1 | CA | 330 | A | C6-C5-N7 | -6.32 | 127.87 | 132.30 |
| 1 | CA | 1824 | G | C5-C6-O6 | 6.32 | 132.39 | 128.60 |
| 1 | AA | 2825 | C | N3-C2-O2 | -6.32 | 117.48 | 121.90 |
| 1 | CA | 1696 | G | C2-N3-C4 | 6.32 | 115.06 | 111.90 |
| 1 | CA | 2582 | G | O5'-P-OP2 | -6.32 | 100.01 | 105.70 |
| 1 | AA | 2502 | G | C5-C6-N1 | 6.32 | 114.66 | 111.50 |
| 1 | AA | 1304 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 1 | AA | 1354 | A | C5-C6-N6 | 6.32 | 128.75 | 123.70 |
| 1 | AA | 1561 | C | C6-N1-C2 | 6.32 | 122.83 | 120.30 |
| 1 | AA | 2372 | A | O5'-P-OP2 | -6.32 | 100.01 | 105.70 |
| 1 | CA | 205 | G | O5'-P-OP2 | -6.32 | 100.01 | 105.70 |
| 1 | CA | 1626 | G | C2-N3-C4 | 6.32 | 115.06 | 111.90 |
| 1 | CA | 2740 | A | C8-N9-C4 | 6.32 | 108.33 | 105.80 |
| 1 | AA | 2301 | G | N1-C2-N3 | -6.32 | 120.11 | 123.90 |
| 1 | AA | 629 | U | O5'-P-OP2 | -6.31 | 100.02 | 105.70 |
| 1 | AA | 2791 | A | N1-C2-N3 | 6.31 | 132.46 | 129.30 |
| 1 | AA | 2835 | C | C5-C6-N1 | -6.31 | 117.84 | 121.00 |
| 1 | AA | 27 | G | O5'-P-OP2 | -6.31 | 100.02 | 105.70 |
| 1 | AA | 1021 | G | OP1-P-OP2 | 6.31 | 129.07 | 119.60 |
| 1 | CA | 2036 | C | C6-N1-C2 | 6.31 | 122.82 | 120.30 |
| 1 | AA | 1000 | C | O5'-P-OP2 | -6.31 | 100.02 | 105.70 |
| 1 | AA | 2346 | G | N3-C4-N9 | 6.31 | 129.78 | 126.00 |
| 1 | CA | 1565 | C | C6-N1-C2 | 6.31 | 122.82 | 120.30 |
| 1 | CA | 2286 | A | N7-C8-N9 | 6.31 | 116.95 | 113.80 |
| 1 | CA | 1789 | A | C5-C6-N6 | 6.31 | 128.75 | 123.70 |
| 34 | BA | 1442 | G | C6-C5-N7 | -6.30 | 126.62 | 130.40 |
| 34 | DA | 499 | A | C8-N9-C4 | 6.30 | 108.32 | 105.80 |
| 1 | AA | 470 | C | C2-N3-C4 | -6.30 | 116.75 | 119.90 |
| 1 | AA | 906 | G | O4'-C1'-N9 | -6.30 | 103.16 | 108.20 |
| 1 | AA | 540 | A | N1-C6-N6 | -6.30 | 114.82 | 118.60 |
| 1 | AA | 1359 | U | C2-N1-C1' | 6.30 | 125.26 | 117.70 |
| 1 | AA | 2621 | U | OP2-P-O3' | 6.30 | 119.06 | 105.20 |
| 1 | AA | 977 | G | C4-C5-N7 | -6.30 | 108.28 | 110.80 |
| 1 | AA | 1709 | C | N3-C4-C5 | 6.30 | 124.42 | 121.90 |
| 1 | AA | 2443 | U | N3-C4-C5 | 6.30 | 118.38 | 114.60 |
| 1 | AA | 2606 | C | N3-C2-O2 | -6.30 | 117.49 | 121.90 |
| 1 | AA | 2092 | G | C6-N1-C2 | -6.29 | 121.32 | 125.10 |
| 34 | BA | 1530 | G | N3-C4-C5 | 6.29 | 131.75 | 128.60 |
| 1 | AA | 1809 | U | N3-C2-O2 | 6.29 | 126.60 | 122.20 |
| 1 | AA | 2067 | C | C4-C5-C6 | 6.29 | 120.55 | 117.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2 | AB | 84 | C | N1-C2-O2 | 6.29 | 122.67 | 118.90 |
| 1 | AA | 2514 | G | O5'-P-OP1 | -6.29 | 100.04 | 105.70 |
| 1 | CA | 528 | A | C5-C6-N1 | -6.29 | 114.56 | 117.70 |
| 1 | AA | 993 | G | C5-C6-O6 | -6.29 | 124.83 | 128.60 |
| 1 | AA | 50 | G | N3-C4-N9 | 6.28 | 129.77 | 126.00 |
| 1 | AA | 1657 | C | N1-C2-N3 | 6.28 | 123.60 | 119.20 |
| 1 | AA | 2276 | C | C5-C6-N1 | -6.28 | 117.86 | 121.00 |
| 1 | AA | 2220 | A | O4'-C1'-N9 | 6.28 | 113.22 | 108.20 |
| 1 | AA | 2276 | C | C6-N1-C2 | 6.28 | 122.81 | 120.30 |
| 6 | AF | 74 | ARG | NE-CZ-NH1 | 6.28 | 123.44 | 120.30 |
| 34 | BA | 1417 | G | N3-C4-N9 | 6.28 | 129.77 | 126.00 |
| 1 | AA | 2291 | G | C5-C6-O6 | -6.28 | 124.83 | 128.60 |
| 1 | AA | 1281 | G | C6-C5-N7 | -6.28 | 126.64 | 130.40 |
| 1 | CA | 2287 | A | N3-C4-C5 | 6.28 | 131.19 | 126.80 |
| 1 | AA | 2049 | G | N9-C4-C5 | 6.27 | 107.91 | 105.40 |
| 1 | CA | 851 | U | C5-C6-N1 | -6.27 | 119.56 | 122.70 |
| 1 | CA | 1394 | U | O5'-P-OP2 | 6.27 | 118.23 | 110.70 |
| 1 | AA | 595 | A | N9-C4-C5 | 6.27 | 108.31 | 105.80 |
| 1 | CA | 562 | U | O5'-P-OP1 | -6.27 | 100.06 | 105.70 |
| 1 | AA | 1665 | G | N1-C6-O6 | -6.27 | 116.14 | 119.90 |
| 1 | CA | 2605 | U | N3-C4-O4 | -6.27 | 115.01 | 119.40 |
| 1 | CA | 768 | G | C5-C6-O6 | 6.27 | 132.36 | 128.60 |
| 1 | AA | 525 | G | C8-N9-C4 | 6.26 | 108.91 | 106.40 |
| 1 | AA | 747 | G | N9-C4-C5 | 6.26 | 107.91 | 105.40 |
| 1 | CA | 1313 | U | C2-N1-C1' | 6.26 | 125.22 | 117.70 |
| 1 | AA | 616 | G | N9-C4-C5 | 6.26 | 107.91 | 105.40 |
| 1 | AA | 1290 | G | C5-C6-O6 | 6.26 | 132.36 | 128.60 |
| 1 | AA | 1329 | G | N3-C4-N9 | 6.26 | 129.76 | 126.00 |
| 1 | AA | 85 | C | C2-N3-C4 | -6.26 | 116.77 | 119.90 |
| 1 | AA | 2341 | G | N3-C2-N2 | 6.25 | 124.28 | 119.90 |
| 1 | AA | 2451 | A | N1-C6-N6 | 6.25 | 122.35 | 118.60 |
| 1 | AA | 2791 | A | C2-N3-C4 | -6.25 | 107.47 | 110.60 |
| 1 | AA | 1290 | G | N1-C6-O6 | -6.25 | 116.15 | 119.90 |
| 34 | BA | 896 | C | C6-N1-C2 | 6.25 | 122.80 | 120.30 |
| 1 | CA | 16 | G | C8-N9-C4 | 6.25 | 108.90 | 106.40 |
| 1 | CA | 1899 | G | N3-C2-N2 | -6.25 | 115.52 | 119.90 |
| 1 | AA | 1069 | U | O5'-P-OP2 | -6.25 | 100.08 | 105.70 |
| 1 | AA | 1097 | G | C5-C6-O6 | -6.25 | 124.85 | 128.60 |
| 1 | AA | 1388 | A | C6-N1-C2 | -6.25 | 114.85 | 118.60 |
| 34 | BA | 297 | G | N9-C4-C5 | -6.25 | 102.90 | 105.40 |
| 1 | CA | 2387 | U | C5-C6-N1 | -6.25 | 119.58 | 122.70 |
| 1 | AA | 2383 | G | C5-C6-O6 | -6.25 | 124.85 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 820 | U | C2-N3-C4 | -6.24 | 123.25 | 127.00 |
| 1 | AA | 2052 | A | C5-C6-N6 | -6.24 | 118.70 | 123.70 |
| 1 | CA | 1425 | G | C4-C5-N7 | 6.24 | 113.30 | 110.80 |
| 1 | AA | 1612 | C | O5'-P-OP2 | -6.24 | 100.08 | 105.70 |
| 1 | AA | 2579 | G | N1-C6-O6 | -6.24 | 116.16 | 119.90 |
| 1 | CA | 665 | C | C6-N1-C2 | 6.24 | 122.80 | 120.30 |
| 1 | CA | 847 | U | C5-C4-O4 | 6.24 | 129.64 | 125.90 |
| 1 | AA | 1342 | G | N1-C2-N2 | -6.24 | 110.59 | 116.20 |
| 1 | AA | 1069 | U | N1-C2-N3 | 6.24 | 118.64 | 114.90 |
| 1 | AA | 1829 | U | C2-N3-C4 | -6.24 | 123.26 | 127.00 |
| 1 | AA | 2882 | G | N9-C4-C5 | 6.24 | 107.89 | 105.40 |
| 1 | CA | 728 | G | O5'-P-OP2 | -6.23 | 100.09 | 105.70 |
| 1 | CA | 2586 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 1 | AA | 422 | U | O4'-C1'-N1 | 6.23 | 113.19 | 108.20 |
| 1 | AA | 727 | G | O5'-P-OP1 | -6.23 | 100.09 | 105.70 |
| 2 | AB | 115 | G | OP1-P-OP2 | 6.23 | 128.95 | 119.60 |
| 1 | AA | 2387 | G | N7-C8-N9 | -6.23 | 109.99 | 113.10 |
| 1 | AA | 2798 | C | C6-N1-C2 | -6.23 | 117.81 | 120.30 |
| 1 | AA | 2553 | A | C4-C5-N7 | 6.22 | 113.81 | 110.70 |
| 1 | AA | 884 | C | C5-C6-N1 | -6.22 | 117.89 | 121.00 |
| 34 | BA | 1505 | G | N3-C4-C5 | 6.22 | 131.71 | 128.60 |
| 1 | CA | 834 | C | N1-C2-O2 | -6.22 | 115.17 | 118.90 |
| 1 | CA | 1351 | C | C6-N1-C2 | 6.22 | 122.79 | 120.30 |
| 1 | AA | 2384 | G | C5-C6-O6 | -6.21 | 124.87 | 128.60 |
| 1 | CA | 1774 | C | N3-C2-O2 | -6.21 | 117.55 | 121.90 |
| 1 | CA | 1781 | C | C5-C4-N4 | 6.21 | 124.55 | 120.20 |
| 34 | DA | 992 | U | P-O3'-C3' | 6.21 | 127.15 | 119.70 |
| 1 | AA | 2669 | A | O5'-P-OP2 | -6.21 | 100.11 | 105.70 |
| 1 | AA | 2162 | C | N3-C2-O2 | -6.20 | 117.56 | 121.90 |
| 1 | CA | 482 | A | N1-C2-N3 | 6.20 | 132.40 | 129.30 |
| 1 | AA | 1076 | G | N3-C2-N2 | 6.20 | 124.24 | 119.90 |
| 34 | BA | 442 | C | C6-N1-C2 | -6.20 | 117.82 | 120.30 |
| 1 | AA | 1721 | G | N3-C4-N9 | 6.20 | 129.72 | 126.00 |
| 1 | AA | 2576 | A | N9-C4-C5 | 6.20 | 108.28 | 105.80 |
| 1 | AA | 1312 | G | C6-N1-C2 | -6.19 | 121.38 | 125.10 |
| 1 | AA | 1253 | C | C2-N3-C4 | -6.19 | 116.80 | 119.90 |
| 4 | AD | 229 | VAL | CB-CA-C | -6.19 | 99.63 | 111.40 |
| 1 | CA | 1623 | G | C5-C6-N1 | -6.19 | 108.40 | 111.50 |
| 1 | CA | 2407 | G | N3-C4-C5 | -6.19 | 125.50 | 128.60 |
| 1 | AA | 2466 | G | C5-C6-O6 | 6.19 | 132.31 | 128.60 |
| 1 | CA | 1789 | A | N1-C6-N6 | -6.19 | 114.89 | 118.60 |
| 1 | CA | 2407 | G | N3-C4-N9 | 6.19 | 129.71 | 126.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 50 | G | C6-N1-C2 | -6.19 | 121.39 | 125.10 |
| 1 | AA | 830 | A | C4-C5-C6 | 6.19 | 120.09 | 117.00 |
| 1 | CA | 2415 | G | C5-C6-N1 | 6.19 | 114.59 | 111.50 |
| 1 | AA | 2898 | C | C2-N3-C4 | -6.18 | 116.81 | 119.90 |
| 34 | BA | 244 | U | N1-C2-O2 | 6.18 | 127.12 | 122.80 |
| 1 | AA | 1188 | A | N1-C6-N6 | 6.18 | 122.31 | 118.60 |
| 1 | AA | 1001 | G | N1-C2-N2 | 6.17 | 121.76 | 116.20 |
| 2 | AB | 86 | G | N9-C4-C5 | -6.17 | 102.93 | 105.40 |
| 34 | BA | 771 | G | N9-C4-C5 | 6.17 | 107.87 | 105.40 |
| 1 | CA | 2276 | G | C2-N3-C4 | 6.17 | 114.99 | 111.90 |
| 1 | AA | 2527 | C | C2-N3-C4 | -6.17 | 116.81 | 119.90 |
| 1 | AA | 1029 | A | N1-C6-N6 | -6.17 | 114.90 | 118.60 |
| 1 | AA | 2397 | C | N1-C2-O2 | -6.17 | 115.20 | 118.90 |
| 1 | AA | 2787 | C | C6-N1-C2 | -6.17 | 117.83 | 120.30 |
| 34 | DA | 901 | A | O5'-P-OP1 | -6.17 | 100.14 | 105.70 |
| 1 | AA | 2523 | U | C5-C6-N1 | -6.17 | 119.61 | 122.70 |
| 1 | CA | 1201 | C | N1-C2-O2 | -6.17 | 115.20 | 118.90 |
| 1 | CA | 2238 | G | O5'-P-OP1 | -6.17 | 100.15 | 105.70 |
| 34 | DA | 1529 | G | C4-N9-C1' | 6.17 | 134.52 | 126.50 |
| 1 | AA | 883 | G | C2-N3-C4 | 6.17 | 114.98 | 111.90 |
| 1 | AA | 1324 | A | C2-N3-C4 | -6.17 | 107.52 | 110.60 |
| 34 | DA | 754 | C | N1-C2-O2 | 6.17 | 122.60 | 118.90 |
| 1 | AA | 1821 | C | OP1-P-O3' | 6.16 | 118.76 | 105.20 |
| 1 | CA | 2588 | G | N3-C4-N9 | -6.16 | 122.30 | 126.00 |
| 1 | AA | 543 | G | O5'-P-OP1 | 6.16 | 118.09 | 110.70 |
| 1 | CA | 1837 | C | O5'-P-OP2 | 6.16 | 118.09 | 110.70 |
| 1 | AA | 593 | G | C5-C6-N1 | 6.16 | 114.58 | 111.50 |
| 1 | AA | 1026 | A | C4-C5-N7 | 6.16 | 113.78 | 110.70 |
| 1 | AA | 2101 | U | N1-C2-O2 | -6.16 | 118.49 | 122.80 |
| 1 | AA | 197 | C | N1-C2-O2 | -6.16 | 115.20 | 118.90 |
| 1 | AA | 352 | U | N1-C2-N3 | 6.16 | 118.60 | 114.90 |
| 1 | AA | 55 | A | N1-C2-N3 | 6.16 | 132.38 | 129.30 |
| 1 | AA | 2594 | G | N3-C2-N2 | 6.16 | 124.21 | 119.90 |
| 1 | AA | 851 | A | N3-C4-C5 | 6.16 | 131.11 | 126.80 |
| 1 | AA | 2583 | C | C5-C6-N1 | -6.16 | 117.92 | 121.00 |
| 1 | CA | 668 | G | O5'-P-OP1 | -6.16 | 100.16 | 105.70 |
| 1 | AA | 1312 | G | C5-C6-O6 | -6.15 | 124.91 | 128.60 |
| 1 | AA | 2090 | U | C5-C6-N1 | -6.15 | 119.62 | 122.70 |
| 1 | AA | 1688 | A | C8-N9-C4 | -6.15 | 103.34 | 105.80 |
| 34 | BA | 841 | U | C2-N1-C1' | 6.15 | 125.08 | 117.70 |
| 1 | AA | 1187 | U | C5-C4-O4 | -6.15 | 122.21 | 125.90 |
| 1 | AA | 2049 | G | C2-N3-C4 | 6.15 | 114.97 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2856 | G | O5'-P-OP1 | -6.15 | 100.17 | 105.70 |
| 1 | CA | 1963 | U | C2-N1-C1' | 6.15 | 125.08 | 117.70 |
| 1 | AA | 147 | U | N3-C4-C5 | 6.15 | 118.29 | 114.60 |
| 1 | AA | 962 | G | O5'-P-OP1 | -6.15 | 100.17 | 105.70 |
| 1 | CA | 1841 | U | OP1-P-OP2 | 6.14 | 128.81 | 119.60 |
| 1 | AA | 1053 | C | C2-N3-C4 | -6.14 | 116.83 | 119.90 |
| 1 | AA | 2426 | G | N1-C6-O6 | 6.14 | 123.58 | 119.90 |
| 1 | AA | 856 | G | N3-C2-N2 | 6.14 | 124.20 | 119.90 |
| 1 | AA | 1207 | C | C2-N3-C4 | -6.14 | 116.83 | 119.90 |
| 1 | AA | 2754 | A | N7-C8-N9 | -6.14 | 110.73 | 113.80 |
| 1 | CA | 2818 | G | N9-C4-C5 | -6.14 | 102.95 | 105.40 |
| 1 | AA | 40 | C | N1-C2-O2 | -6.13 | 115.22 | 118.90 |
| 1 | AA | 1741 | C | C5-C6-N1 | -6.13 | 117.93 | 121.00 |
| 1 | AA | 1655 | A | N1-C6-N6 | 6.13 | 122.28 | 118.60 |
| 1 | CA | 2280 | G | N1-C6-O6 | -6.13 | 116.22 | 119.90 |
| 34 | DA | 1405 | G | N3-C2-N2 | 6.13 | 124.19 | 119.90 |
| 1 | AA | 592 | U | N3-C2-O2 | 6.13 | 126.49 | 122.20 |
| 1 | AA | 1022 | C | OP2-P-O3' | 6.13 | 118.68 | 105.20 |
| 34 | BA | 1482 | G | N3-C4-N9 | 6.13 | 129.68 | 126.00 |
| 1 | AA | 185 | A | C6-C5-N7 | -6.13 | 128.01 | 132.30 |
| 1 | AA | 1246 | C | N3-C4-C5 | 6.13 | 124.35 | 121.90 |
| 1 | AA | 1966 | U | C5-C4-O4 | 6.13 | 129.58 | 125.90 |
| 1 | AA | 2073 | A | N9-C4-C5 | 6.13 | 108.25 | 105.80 |
| 1 | AA | 2531 | U | C2-N3-C4 | -6.13 | 123.32 | 127.00 |
| 34 | BA | 971 | G | O4'-C1'-N9 | 6.13 | 113.10 | 108.20 |
| 1 | AA | 1657 | C | N3-C2-O2 | -6.12 | 117.61 | 121.90 |
| 1 | AA | 2074 | G | C6-C5-N7 | 6.12 | 134.07 | 130.40 |
| 1 | AA | 1655 | A | C5-C6-N1 | 6.12 | 120.76 | 117.70 |
| 34 | BA | 1505 | G | C2-N3-C4 | -6.12 | 108.84 | 111.90 |
| 1 | CA | 1385 | G | N3-C4-C5 | 6.12 | 131.66 | 128.60 |
| 1 | CA | 2549 | G | C5-C6-O6 | -6.12 | 124.93 | 128.60 |
| 34 | BA | 1054 | C | O5'-P-OP2 | -6.12 | 100.19 | 105.70 |
| 1 | CA | 1850 | G | N1-C6-O6 | 6.12 | 123.57 | 119.90 |
| 34 | BA | 1530 | G | N3-C4-N9 | -6.12 | 122.33 | 126.00 |
| 2 | AB | 94 | C | C5-C4-N4 | 6.12 | 124.48 | 120.20 |
| 1 | CA | 265 | A | N1-C6-N6 | 6.12 | 122.27 | 118.60 |
| 1 | CA | 2029 | G | N1-C6-O6 | 6.12 | 123.57 | 119.90 |
| 1 | AA | 290 | G | C8-N9-C4 | 6.11 | 108.85 | 106.40 |
| 1 | CA | 1385 | G | C4-N9-C1' | -6.11 | 118.55 | 126.50 |
| 1 | CA | 420 | C | N1-C2-O2 | 6.11 | 122.57 | 118.90 |
| 1 | AA | 1344 | C | N3-C2-O2 | 6.11 | 126.18 | 121.90 |
| 1 | AA | 1921 | G | C5-C6-O6 | -6.11 | 124.93 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2701 | U | P-O3'-C3' | 6.11 | 127.03 | 119.70 |
| 2 | AB | 41 | U | C2-N3-C4 | -6.11 | 123.33 | 127.00 |
| 1 | CA | 1637 | A | N1-C6-N6 | -6.11 | 114.93 | 118.60 |
| 1 | AA | 2622 | C | N1-C2-O2 | 6.11 | 122.56 | 118.90 |
| 1 | AA | 1054 | C | N1-C2-O2 | -6.11 | 115.23 | 118.90 |
| 1 | AA | 1423 | G | N1-C2-N2 | -6.11 | 110.70 | 116.20 |
| 1 | CA | 774 | A | O5'-P-OP2 | -6.11 | 100.20 | 105.70 |
| 1 | CA | 1945 | G | C4-N9-C1' | 6.11 | 134.44 | 126.50 |
| 2 | CB | 22 | U | C5-C6-N1 | 6.11 | 125.75 | 122.70 |
| 1 | AA | 977 | G | O5'-P-OP2 | -6.11 | 100.20 | 105.70 |
| 1 | AA | 2611 | G | OP2-P-O3' | 6.11 | 118.63 | 105.20 |
| 1 | AA | 1179 | U | N1-C2-O2 | -6.10 | 118.53 | 122.80 |
| 1 | AA | 1571 | G | O5'-P-OP1 | -6.10 | 100.21 | 105.70 |
| 1 | AA | 2527 | C | N1-C2-O2 | -6.10 | 115.24 | 118.90 |
| 1 | AA | 2633 | A | C4-C5-C6 | -6.10 | 113.95 | 117.00 |
| 1 | CA | 2488 | A | C8-N9-C4 | 6.10 | 108.24 | 105.80 |
| 1 | AA | 748 | G | OP2-P-O3' | 6.10 | 118.62 | 105.20 |
| 34 | DA | 1183 | A | P-O3'-C3' | 6.10 | 127.02 | 119.70 |
| 1 | AA | 602 | G | C2-N3-C4 | 6.10 | 114.95 | 111.90 |
| 1 | AA | 916 | G | O5'-P-OP1 | -6.10 | 100.21 | 105.70 |
| 1 | AA | 1420 | G | OP1-P-OP2 | -6.10 | 110.45 | 119.60 |
| 1 | AA | 1782 | C | N3-C2-O2 | 6.10 | 126.17 | 121.90 |
| 2 | CB | 72 | G | C8-N9-C4 | 6.10 | 108.84 | 106.40 |
| 1 | AA | 2503 | U | C2-N3-C4 | -6.10 | 123.34 | 127.00 |
| 1 | CA | 1697 | G | C8-N9-C4 | 6.10 | 108.84 | 106.40 |
| 1 | AA | 2298 | A | N9-C1'-C2' | 6.09 | 121.92 | 114.00 |
| 1 | AA | 2459 | G | N1-C6-O6 | -6.09 | 116.24 | 119.90 |
| 1 | AA | 2732 | G | N1-C6-O6 | 6.09 | 123.56 | 119.90 |
| 1 | AA | 1665 | G | N1-C2-N2 | -6.09 | 110.72 | 116.20 |
| 1 | AA | 177 | G | N3-C2-N2 | 6.09 | 124.16 | 119.90 |
| 1 | AA | 202 | A | OP2-P-O3' | 6.09 | 118.60 | 105.20 |
| 1 | AA | 714 | U | C2-N3-C4 | -6.09 | 123.35 | 127.00 |
| 1 | AA | 723 | A | C6-N1-C2 | 6.09 | 122.25 | 118.60 |
| 1 | AA | 1448 | C | C5-C6-N1 | 6.09 | 124.04 | 121.00 |
| 13 | AP | 18 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 34 | DA | 1513 | A | OP1-P-OP2 | 6.09 | 128.74 | 119.60 |
| 1 | AA | 1393 | G | C5-C6-N1 | 6.09 | 114.54 | 111.50 |
| 1 | CA | 768 | G | C4-C5-N7 | -6.09 | 108.36 | 110.80 |
| 34 | DA | 754 | C | C6-N1-C2 | -6.09 | 117.86 | 120.30 |
| 1 | CA | 2287 | A | N1-C6-N6 | 6.09 | 122.25 | 118.60 |
| 1 | CA | 2444 | G | N1-C2-N3 | 6.09 | 127.55 | 123.90 |
| 1 | CA | 2576 | G | C8-N9-C4 | 6.09 | 108.83 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 34 | BA | 1515 | C | C5-C4-N4 | -6.08 | 115.94 | 120.20 |
| 1 | AA | 2263 | G | N1-C6-O6 | -6.08 | 116.25 | 119.90 |
| 1 | CA | 1412 | A | C8-N9-C4 | -6.08 | 103.37 | 105.80 |
| 1 | CA | 1602 | U | C6-N1-C2 | 6.08 | 124.65 | 121.00 |
| 1 | CA | 1110 | G | N3-C2-N2 | -6.08 | 115.64 | 119.90 |
| 1 | AA | 1033 | G | N3-C2-N2 | -6.08 | 115.65 | 119.90 |
| 1 | AA | 1254 | G | C6-N1-C2 | -6.08 | 121.45 | 125.10 |
| 1 | CA | 2337 | G | C5-C6-O6 | -6.08 | 124.95 | 128.60 |
| 1 | CA | 2490 | G | C5-C6-O6 | -6.08 | 124.95 | 128.60 |
| 1 | AA | 2632 | C | C6-N1-C2 | 6.07 | 122.73 | 120.30 |
| 1 | AA | 1044 | C | N1-C2-O2 | -6.07 | 115.26 | 118.90 |
| 34 | DA | 1431 | C | C6-N1-C2 | -6.07 | 117.87 | 120.30 |
| 1 | AA | 604 | C | N1-C2-O2 | -6.07 | 115.26 | 118.90 |
| 1 | CA | 773 | U | C5-C6-N1 | -6.07 | 119.66 | 122.70 |
| 1 | CA | 784 | A | O4'-C1'-N9 | 6.07 | 113.06 | 108.20 |
| 1 | CA | 962 | G | C5-C6-N1 | -6.07 | 108.47 | 111.50 |
| 1 | CA | 1692 | U | C2-N3-C4 | -6.07 | 123.36 | 127.00 |
| 1 | CA | 2822 | G | C4-C5-N7 | 6.07 | 113.23 | 110.80 |
| 1 | AA | 2559 | U | C5-C6-N1 | -6.07 | 119.67 | 122.70 |
| 34 | BA | 741 | G | C8-N9-C4 | -6.07 | 103.97 | 106.40 |
| 1 | CA | 185 | U | N1-C2-O2 | 6.07 | 127.05 | 122.80 |
| 1 | AA | 379 | G | N1-C6-O6 | 6.06 | 123.54 | 119.90 |
| 1 | AA | 2561 | G | C5-C6-O6 | -6.06 | 124.96 | 128.60 |
| 1 | CA | 2689 | U | N3-C2-O2 | -6.06 | 117.95 | 122.20 |
| 1 | AA | 46 | C | C6-N1-C2 | 6.06 | 122.72 | 120.30 |
| 1 | AA | 1983 | C | C6-N1-C2 | 6.06 | 122.72 | 120.30 |
| 1 | AA | 2882 | G | C4-C5-N7 | -6.06 | 108.38 | 110.80 |
| 1 | CA | 2092 | U | N3-C2-O2 | 6.06 | 126.44 | 122.20 |
| 1 | AA | 730 | C | N3-C4-N4 | -6.06 | 113.76 | 118.00 |
| 1 | CA | 827 | U | C6-N1-C2 | 6.06 | 124.64 | 121.00 |
| 1 | AA | 1617 | A | N1-C6-N6 | 6.06 | 122.23 | 118.60 |
| 1 | AA | 1704 | C | C2-N3-C4 | -6.06 | 116.87 | 119.90 |
| 1 | AA | 2005 | C | N1-C2-O2 | -6.06 | 115.27 | 118.90 |
| 1 | CA | 2057 | A | O5'-P-OP1 | 6.06 | 117.97 | 110.70 |
| 1 | CA | 1142(A) | A | C8-N9-C4 | -6.06 | 103.38 | 105.80 |
| 1 | AA | 1612 | C | C6-N1-C2 | 6.05 | 122.72 | 120.30 |
| 1 | AA | 2537 | G | C5-C6-N1 | 6.05 | 114.53 | 111.50 |
| 1 | CA | 794 | G | O5'-P-OP2 | -6.05 | 100.25 | 105.70 |
| 1 | CA | 2253 | G | C2-N3-C4 | -6.05 | 108.87 | 111.90 |
| 1 | AA | 1172 | A | C8-N9-C4 | -6.05 | 103.38 | 105.80 |
| 1 | CA | 1291 | C | N3-C4-C5 | 6.05 | 124.32 | 121.90 |
| 1 | AA | 2063 | U | N3-C4-O4 | 6.05 | 123.64 | 119.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 2115 | G | N3-C2-N2 | -6.05 | 115.66 | 119.90 |
| 34 | BA | 345 | C | C2-N3-C4 | 6.05 | 122.92 | 119.90 |
| 1 | AA | 831 | A | OP1-P-O3' | 6.05 | 118.51 | 105.20 |
| 1 | AA | 735 | U | C4-C5-C6 | 6.05 | 123.33 | 119.70 |
| 34 | BA | 297 | G | C5-C6-O6 | -6.05 | 124.97 | 128.60 |
| 1 | CA | 1966 | A | N7-C8-N9 | -6.05 | 110.78 | 113.80 |
| 1 | AA | 817 | G | C8-N9-C4 | 6.05 | 108.82 | 106.40 |
| 1 | AA | 1068 | G | N3-C2-N2 | -6.05 | 115.67 | 119.90 |
| 1 | AA | 1453 | C | N1-C2-O2 | -6.05 | 115.27 | 118.90 |
| 1 | AA | 1874 | C | C5-C6-N1 | -6.05 | 117.98 | 121.00 |
| 34 | BA | 1030(B) | C | N1-C2-O2 | 6.05 | 122.53 | 118.90 |
| 1 | CA | 2206 | G | C8-N9-C4 | 6.05 | 108.82 | 106.40 |
| 1 | AA | 621 | G | N9-C4-C5 | 6.04 | 107.82 | 105.40 |
| 1 | AA | 1037 | C | C4-C5-C6 | 6.04 | 120.42 | 117.40 |
| 34 | DA | 1158 | C | C2-N1-C1' | 6.04 | 125.44 | 118.80 |
| 1 | AA | 346 | A | C8-N9-C4 | 6.04 | 108.22 | 105.80 |
| 1 | AA | 2565 | G | C2-N3-C4 | 6.04 | 114.92 | 111.90 |
| 47 | DN | 44 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 1 | CA | 915 | C | N1-C2-O2 | 6.04 | 122.52 | 118.90 |
| 1 | AA | 2340 | A | C2-N3-C4 | -6.04 | 107.58 | 110.60 |
| 1 | AA | 2510 | C | C5-C4-N4 | 6.03 | 124.42 | 120.20 |
| 34 | BA | 1189 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 1 | CA | 1661 | G | N9-C4-C5 | -6.03 | 102.99 | 105.40 |
| 1 | AA | 1204 | C | C6-N1-C2 | 6.03 | 122.71 | 120.30 |
| 1 | AA | 1721 | G | C6-C5-N7 | -6.03 | 126.78 | 130.40 |
| 34 | BA | 529 | G | N1-C6-O6 | 6.03 | 123.52 | 119.90 |
| 34 | BA | 1482 | G | N3-C2-N2 | 6.03 | 124.12 | 119.90 |
| 1 | AA | 1314 | A | C5-C6-N1 | -6.03 | 114.69 | 117.70 |
| 34 | BA | 1067 | A | P-O3'-C3' | 6.02 | 126.93 | 119.70 |
| 34 | BA | 1519 | A | C8-N9-C4 | -6.02 | 103.39 | 105.80 |
| 1 | AA | 893 | C | N3-C4-C5 | 6.02 | 124.31 | 121.90 |
| 1 | AA | 991 | G | OP1-P-O3' | 6.02 | 118.45 | 105.20 |
| 2 | AB | 114 | C | C6-N1-C2 | 6.02 | 122.71 | 120.30 |
| 1 | AA | 279 | G | N7-C8-N9 | 6.02 | 116.11 | 113.10 |
| 1 | AA | 2843 | G | C8-N9-C4 | -6.02 | 103.99 | 106.40 |
| 1 | CA | 1842 | G | C5-C6-O6 | -6.02 | 124.99 | 128.60 |
| 1 | CA | 2001 | A | C5-C6-N1 | 6.02 | 120.71 | 117.70 |
| 1 | AA | 990 | A | N9-C4-C5 | -6.02 | 103.39 | 105.80 |
| 1 | AA | 2484 | G | N3-C4-C5 | -6.02 | 125.59 | 128.60 |
| 34 | DA | 23 | C | O5'-P-OP2 | 6.02 | 117.92 | 110.70 |
| 1 | AA | 2399 | U | C4-C5-C6 | 6.01 | 123.31 | 119.70 |
| 1 | CA | 1826 | G | C5-N7-C8 | 6.01 | 107.31 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 869 | U | C5-C6-N1 | 6.01 | 125.71 | 122.70 |
| 1 | AA | 15 | G | C5-C6-N1 | -6.01 | 108.49 | 111.50 |
| 1 | CA | 1427 | A | P-O3'-C3' | 6.01 | 126.91 | 119.70 |
| 1 | AA | 906 | G | C4-N9-C1' | -6.01 | 118.69 | 126.50 |
| 1 | AA | 2018 | C | N3-C4-C5 | 6.01 | 124.30 | 121.90 |
| 1 | AA | 806 | G | C5-C6-O6 | -6.01 | 125.00 | 128.60 |
| 1 | AA | 1694 | G | C6-C5-N7 | 6.01 | 134.00 | 130.40 |
| 1 | AA | 2299 | A | C6-C5-N7 | -6.01 | 128.09 | 132.30 |
| 1 | AA | 2759 | U | O5'-P-OP2 | -6.01 | 100.29 | 105.70 |
| 1 | CA | 1975 | G | C8-N9-C4 | 6.01 | 108.80 | 106.40 |
| 1 | CA | 2544 | G | C5-C6-O6 | -6.01 | 125.00 | 128.60 |
| 34 | DA | 355 | C | C6-N1-C2 | -6.01 | 117.90 | 120.30 |
| 1 | AA | 552 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 34 | DA | 754 | C | N3-C2-O2 | -6.00 | 117.70 | 121.90 |
| 1 | AA | 1924 | C | C4-C5-C6 | 6.00 | 120.40 | 117.40 |
| 2 | AB | 27 | C | O5'-P-OP2 | -6.00 | 100.30 | 105.70 |
| 1 | AA | 470 | C | OP1-P-OP2 | -6.00 | 110.60 | 119.60 |
| 34 | DA | 784 | C | N1-C2-O2 | -6.00 | 115.30 | 118.90 |
| 1 | AA | 1324 | A | N1-C2-N3 | 6.00 | 132.30 | 129.30 |
| 1 | AA | 2599 | A | O5'-P-OP1 | -6.00 | 100.30 | 105.70 |
| 1 | CA | 2032 | G | C8-N9-C4 | 6.00 | 108.80 | 106.40 |
| 1 | AA | 113 | C | C6-N1-C2 | 6.00 | 122.70 | 120.30 |
| 34 | BA | 442 | C | C5-C6-N1 | 6.00 | 124.00 | 121.00 |
| 1 | CA | 330 | A | N3-C4-C5 | 6.00 | 131.00 | 126.80 |
| 1 | AA | 1188 | A | C4-C5-N7 | 5.99 | 113.70 | 110.70 |
| 1 | AA | 1755 | C | N3-C4-C5 | 5.99 | 124.30 | 121.90 |
| 1 | AA | 223 | C | N3-C2-O2 | -5.99 | 117.71 | 121.90 |
| 1 | CA | 614 | U | N1-C2-N3 | 5.99 | 118.50 | 114.90 |
| 1 | AA | 540 | A | N9-C4-C5 | 5.99 | 108.20 | 105.80 |
| 1 | CA | 84 | A | O4'-C1'-N9 | 5.99 | 112.99 | 108.20 |
| 34 | BA | 1501 | C | C4-C5-C6 | 5.99 | 120.39 | 117.40 |
| 1 | CA | 1673 | U | N3-C4-C5 | 5.99 | 118.19 | 114.60 |
| 1 | AA | 2676 | G | N1-C6-O6 | 5.99 | 123.49 | 119.90 |
| 1 | AA | 2519 | C | C5-C4-N4 | 5.99 | 124.39 | 120.20 |
| 2 | AB | 7 | G | N1-C6-O6 | 5.99 | 123.49 | 119.90 |
| 1 | CA | 1332 | G | O5'-P-OP2 | -5.99 | 100.31 | 105.70 |
| 1 | AA | 1069 | U | C2-N3-C4 | -5.98 | 123.41 | 127.00 |
| 1 | AA | 1316 | C | C2-N3-C4 | -5.98 | 116.91 | 119.90 |
| 1 | CA | 2407 | G | C4-N9-C1' | 5.98 | 134.28 | 126.50 |
| 1 | AA | 1236 | G | C8-N9-C4 | 5.98 | 108.79 | 106.40 |
| 1 | AA | 1405 | A | N1-C2-N3 | -5.98 | 126.31 | 129.30 |
| 34 | BA | 836 | G | N1-C6-O6 | 5.98 | 123.49 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1832 | G | O5'-P-OP1 | -5.98 | 100.32 | 105.70 |
| 34 | BA | 760 | G | N1-C6-O6 | 5.98 | 123.49 | 119.90 |
| 1 | CA | 2503 | A | C5-C6-N6 | -5.98 | 118.92 | 123.70 |
| 1 | AA | 2453 | C | C2-N3-C4 | -5.98 | 116.91 | 119.90 |
| 1 | AA | 723 | A | C5-C6-N1 | -5.98 | 114.71 | 117.70 |
| 1 | AA | 2556 | G | N3-C2-N2 | -5.98 | 115.72 | 119.90 |
| 34 | BA | 290 | C | C6-N1-C2 | 5.98 | 122.69 | 120.30 |
| 1 | AA | 2613 | C | C4-C5-C6 | 5.98 | 120.39 | 117.40 |
| 55 | BV | 21 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 1 | AA | 635 | C | C6-N1-C2 | 5.97 | 122.69 | 120.30 |
| 1 | AA | 1233 | U | N3-C4-O4 | -5.97 | 115.22 | 119.40 |
| 1 | AA | 1296 | G | N1-C6-O6 | -5.97 | 116.32 | 119.90 |
| 34 | BA | 1036 | G | C4-N9-C1' | 5.97 | 134.26 | 126.50 |
| 1 | CA | 1064 | C | C2-N1-C1' | 5.97 | 125.37 | 118.80 |
| 1 | CA | 2373 | G | N3-C2-N2 | -5.97 | 115.72 | 119.90 |
| 34 | BA | 1442 | G | C4-C5-N7 | 5.97 | 113.19 | 110.80 |
| 1 | AA | 1805 | C | C2-N3-C4 | -5.97 | 116.92 | 119.90 |
| 1 | CA | 556 | G | N1-C6-O6 | 5.97 | 123.48 | 119.90 |
| 1 | AA | 785 | G | C4-C5-N7 | 5.97 | 113.19 | 110.80 |
| 1 | AA | 44 | G | N1-C6-O6 | -5.97 | 116.32 | 119.90 |
| 1 | AA | 846 | G | N3-C2-N2 | 5.97 | 124.08 | 119.90 |
| 1 | AA | 2576 | A | N1-C6-N6 | -5.97 | 115.02 | 118.60 |
| 1 | AA | 2895 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 1 | AA | 438 | G | N1-C2-N3 | 5.96 | 127.48 | 123.90 |
| 1 | AA | 1914 | C | N1-C2-O2 | -5.96 | 115.32 | 118.90 |
| 1 | AA | 2889 | C | O5'-P-OP2 | -5.96 | 100.33 | 105.70 |
| 1 | CA | 1021 | A | N7-C8-N9 | 5.96 | 116.78 | 113.80 |
| 1 | AA | 206 | G | N3-C2-N2 | -5.96 | 115.73 | 119.90 |
| 1 | AA | 481 | C | N3-C4-C5 | 5.96 | 124.28 | 121.90 |
| 1 | AA | 521 | G | C5-C6-O6 | 5.96 | 132.18 | 128.60 |
| 1 | CA | 945 | A | O4'-C1'-N9 | 5.96 | 112.97 | 108.20 |
| 1 | AA | 1539 | C | N1-C2-O2 | 5.96 | 122.47 | 118.90 |
| 1 | AA | 747 | G | C4-C5-N7 | -5.96 | 108.42 | 110.80 |
| 1 | AA | 194 | G | C6-C5-N7 | -5.95 | 126.83 | 130.40 |
| 1 | AA | 1845 | G | C4-C5-N7 | 5.95 | 113.18 | 110.80 |
| 1 | AA | 2327 | G | C8-N9-C4 | 5.95 | 108.78 | 106.40 |
| 1 | AA | 1244 | U | C2-N3-C4 | -5.95 | 123.43 | 127.00 |
| 1 | AA | 1369 | U | C6-N1-C2 | 5.95 | 124.57 | 121.00 |
| 1 | CA | 420 | C | N3-C2-O2 | -5.95 | 117.73 | 121.90 |
| 34 | BA | 1502 | A | C8-N9-C4 | -5.95 | 103.42 | 105.80 |
| 1 | CA | 1656 | C | C4-C5-C6 | -5.95 | 114.42 | 117.40 |
| 1 | AA | 995 | G | OP1-P-OP2 | -5.95 | 110.68 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1 | AA | 1067 | A | O5'-P-OP1 | -5.95 | 100.35 | 105.70 |
| 1 | CA | 176 | G | C8-N9-C4 | 5.95 | 108.78 | 106.40 |
| 1 | AA | 2557 | G | OP2-P-O3' | 5.95 | 118.28 | 105.20 |
| 1 | AA | 751 | G | O4'-C1'-N9 | 5.95 | 112.96 | 108.20 |
| 1 | AA | 958 | C | C5-C6-N1 | 5.95 | 123.97 | 121.00 |
| 1 | AA | 1252 | C | N3-C2-O2 | -5.95 | 117.74 | 121.90 |
| 34 | BA | 297 | G | C4-C5-N7 | 5.95 | 113.18 | 110.80 |
| 1 | CA | 2718 | G | N1-C6-O6 | 5.95 | 123.47 | 119.90 |
| 1 | CA | 2855 | C | C6-N1-C2 | -5.95 | 117.92 | 120.30 |
| 1 | AA | 1332 | A | C8-N9-C4 | -5.94 | 103.42 | 105.80 |
| 1 | CA | 265 | A | C6-C5-N7 | -5.94 | 128.14 | 132.30 |
| 34 | DA | 437 | U | O5'-P-OP1 | -5.94 | 100.35 | 105.70 |
| 1 | AA | 1866 | G | O5'-P-OP2 | -5.94 | 100.35 | 105.70 |
| 1 | AA | 354 | A | N7-C8-N9 | 5.94 | 116.77 | 113.80 |
| 1 | AA | 1696 | G | N1-C6-O6 | -5.94 | 116.34 | 119.90 |
| 1 | AA | 2355 | C | OP1-P-OP2 | 5.94 | 128.51 | 119.60 |
| 34 | BA | 764 | C | N3-C2-O2 | -5.94 | 117.74 | 121.90 |
| 34 | DA | 897 | C | C6-N1-C2 | 5.94 | 122.67 | 120.30 |
| 1 | AA | 615 | G | OP2-P-O3' | 5.94 | 118.26 | 105.20 |
| 1 | AA | 779 | C | N3-C2-O2 | 5.94 | 126.06 | 121.90 |
| 34 | BA | 771 | G | C8-N9-C4 | -5.93 | 104.03 | 106.40 |
| 1 | AA | 2595 | G | N3-C2-N2 | -5.93 | 115.75 | 119.90 |
| 1 | AA | 2700 | U | N3-C4-O4 | 5.93 | 123.55 | 119.40 |
| 1 | CA | 1407 | C | N1-C2-O2 | -5.93 | 115.34 | 118.90 |
| 1 | AA | 600 | G | O5'-P-OP2 | -5.93 | 100.37 | 105.70 |
| 1 | AA | 1659 | G | C8-N9-C4 | -5.93 | 104.03 | 106.40 |
| 1 | AA | 2162 | C | C5-C6-N1 | 5.93 | 123.96 | 121.00 |
| 34 | DA | 1527 | C | N3-C4-C5 | 5.93 | 124.27 | 121.90 |
| 1 | CA | 271(Y) | U | N3-C2-O2 | -5.92 | 118.05 | 122.20 |
| 1 | CA | 25 | U | N1-C2-O2 | -5.92 | 118.65 | 122.80 |
| 34 | DA | 1154 | G | C6-C5-N7 | -5.92 | 126.85 | 130.40 |
| 1 | AA | 1245 | C | O5'-P-OP2 | -5.92 | 100.37 | 105.70 |
| 1 | AA | 2641 | A | C5-C6-N6 | -5.92 | 118.96 | 123.70 |
| 1 | CA | 1372 | U | N3-C4-O4 | 5.92 | 123.55 | 119.40 |
| 1 | CA | 2324 | C | C6-N1-C2 | 5.92 | 122.67 | 120.30 |
| 1 | CA | 34 | C | N3-C2-O2 | -5.92 | 117.76 | 121.90 |
| 1 | AA | 350 | G | N9-C4-C5 | 5.92 | 107.77 | 105.40 |
| 1 | AA | 535 | C | N3-C2-O2 | -5.92 | 117.76 | 121.90 |
| 1 | CA | 2552 | U | N3-C4-C5 | 5.92 | 118.15 | 114.60 |
| 1 | AA | 103 | C | OP2-P-O3' | 5.92 | 118.22 | 105.20 |
| 1 | AA | 741 | U | C2-N3-C4 | -5.92 | 123.45 | 127.00 |
| 34 | DA | 579 | G | N1-C6-O6 | 5.92 | 123.45 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 127 | C | N1-C2-O2 | -5.91 | 115.35 | 118.90 |
| 1 | AA | 553 | A | C5-C6-N6 | -5.91 | 118.97 | 123.70 |
| 1 | AA | 2162 | C | C6-N1-C1' | -5.91 | 113.71 | 120.80 |
| 1 | AA | 553 | A | C5-C6-N1 | -5.91 | 114.75 | 117.70 |
| 1 | CA | 2080 | G | C5-N7-C8 | 5.91 | 107.25 | 104.30 |
| 1 | CA | 400 | G | N1-C6-O6 | 5.91 | 123.44 | 119.90 |
| 1 | CA | 2335 | A | O4'-C1'-N9 | 5.91 | 112.93 | 108.20 |
| 1 | CA | 2576 | G | O5'-P-OP2 | 5.91 | 117.79 | 110.70 |
| 1 | AA | 518 | G | C5-N7-C8 | 5.91 | 107.25 | 104.30 |
| 1 | AA | 846 | G | N3-C4-N9 | 5.91 | 129.54 | 126.00 |
| 1 | AA | 977 | G | O5'-P-OP1 | 5.91 | 117.79 | 110.70 |
| 1 | CA | 2487 | G | N9-C4-C5 | -5.91 | 103.04 | 105.40 |
| 1 | AA | 2258 | G | N7-C8-N9 | -5.90 | 110.15 | 113.10 |
| 1 | AA | 2616 | U | OP1-P-O3' | 5.90 | 118.19 | 105.20 |
| 24 | A0 | 12 | ASN | C-N-CA | -5.90 | 109.90 | 122.30 |
| 1 | AA | 1038 | C | C2-N3-C4 | -5.90 | 116.95 | 119.90 |
| 1 | AA | 2835 | C | C6-N1-C2 | 5.90 | 122.66 | 120.30 |
| 1 | AA | 279 | G | C6-C5-N7 | -5.90 | 126.86 | 130.40 |
| 1 | AA | 1924 | C | N3-C4-C5 | -5.90 | 119.54 | 121.90 |
| 1 | AA | 1961 | U | N3-C4-C5 | 5.90 | 118.14 | 114.60 |
| 1 | AA | 193 | A | C2-N3-C4 | 5.90 | 113.55 | 110.60 |
| 1 | AA | 996 | C | N3-C4-N4 | -5.90 | 113.87 | 118.00 |
| 1 | AA | 1175 | A | O5'-P-OP2 | -5.89 | 100.39 | 105.70 |
| 1 | AA | 1387 | U | N3-C2-O2 | 5.89 | 126.33 | 122.20 |
| 34 | BA | 1341 | U | N3-C2-O2 | -5.89 | 118.07 | 122.20 |
| 1 | CA | 1204 | A | N9-C4-C5 | -5.89 | 103.44 | 105.80 |
| 1 | CA | 1626 | G | C8-N9-C4 | -5.89 | 104.04 | 106.40 |
| 1 | CA | 2235 | G | N1-C6-O6 | 5.89 | 123.44 | 119.90 |
| 1 | AA | 2078 | G | N1-C6-O6 | -5.89 | 116.36 | 119.90 |
| 1 | AA | 126 | C | O5'-P-OP1 | -5.89 | 100.40 | 105.70 |
| 1 | AA | 1981 | G | OP2-P-O3' | 5.89 | 118.16 | 105.20 |
| 1 | AA | 338 | A | C5-N7-C8 | -5.89 | 100.95 | 103.90 |
| 1 | AA | 1184 | G | N9-C4-C5 | 5.89 | 107.76 | 105.40 |
| 1 | AA | 2033 | U | C5-C4-O4 | 5.89 | 129.43 | 125.90 |
| 1 | CA | 1850 | G | C5-C6-O6 | -5.89 | 125.07 | 128.60 |
| 1 | AA | 988 | U | O5'-P-OP2 | -5.89 | 100.40 | 105.70 |
| 1 | AA | 31 | C | O5'-P-OP1 | -5.89 | 100.40 | 105.70 |
| 1 | AA | 502 | G | C8-N9-C4 | 5.89 | 108.75 | 106.40 |
| 1 | AA | 1067 | A | C6-C5-N7 | -5.89 | 128.18 | 132.30 |
| 1 | AA | 2063 | U | N1-C2-O2 | -5.89 | 118.68 | 122.80 |
| 1 | AA | 2264 | G | C5-C6-O6 | 5.89 | 132.13 | 128.60 |
| 1 | CA | 12 | U | N1-C2-O2 | 5.89 | 126.92 | 122.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 34 | DA | 1158 | C | C6-N1-C2 | -5.89 | 117.94 | 120.30 |
| 1 | AA | 2189 | U | C2-N1-C1' | 5.88 | 124.76 | 117.70 |
| 1 | CA | 265 | A | C2-N3-C4 | -5.88 | 107.66 | 110.60 |
| 1 | CA | 2421 | G | C8-N9-C4 | 5.88 | 108.75 | 106.40 |
| 1 | CA | 2689 | U | C6-N1-C2 | -5.88 | 117.47 | 121.00 |
| 1 | AA | 1336 | C | OP2-P-O3' | 5.88 | 118.14 | 105.20 |
| 1 | AA | 1703 | C | N3-C4-C5 | 5.88 | 124.25 | 121.90 |
| 1 | AA | 2399 | U | C5-C6-N1 | -5.88 | 119.76 | 122.70 |
| 34 | DA | 219 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 34 | DA | 354 | G | C6-C5-N7 | -5.88 | 126.87 | 130.40 |
| 1 | AA | 708 | C | C5-C6-N1 | -5.88 | 118.06 | 121.00 |
| 29 | A5 | 16 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | CA | 1429 | G | C2-N3-C4 | 5.88 | 114.84 | 111.90 |
| 34 | BA | 659 | U | O5'-P-OP2 | -5.87 | 100.41 | 105.70 |
| 1 | AA | 2641 | A | C8-N9-C1' | -5.87 | 117.13 | 127.70 |
| 1 | AA | 2849 | G | N9-C4-C5 | -5.87 | 103.05 | 105.40 |
| 34 | DA | 1079 | G | O5'-P-OP1 | -5.87 | 100.42 | 105.70 |
| 1 | AA | 2553 | A | N1-C6-N6 | 5.87 | 122.12 | 118.60 |
| 34 | BA | 53 | A | C8-N9-C4 | -5.87 | 103.45 | 105.80 |
| 34 | DA | 1064 | G | P-O3'-C3' | 5.87 | 126.74 | 119.70 |
| 1 | AA | 887 | C | C2-N3-C4 | -5.87 | 116.97 | 119.90 |
| 1 | AA | 1188 | A | N7-C8-N9 | 5.87 | 116.73 | 113.80 |
| 1 | AA | 2381 | A | N1-C6-N6 | -5.87 | 115.08 | 118.60 |
| 34 | BA | 326 | G | C6-C5-N7 | -5.87 | 126.88 | 130.40 |
| 1 | AA | 639 | G | C4-C5-N7 | -5.87 | 108.45 | 110.80 |
| 1 | AA | 2521 | G | N9-C4-C5 | -5.87 | 103.05 | 105.40 |
| 1 | AA | 2529 | C | C4-C5-C6 | -5.87 | 114.47 | 117.40 |
| 1 | AA | 2571 | C | C4-C5-C6 | -5.87 | 114.47 | 117.40 |
| 1 | CA | 2617 | C | C6-N1-C2 | 5.87 | 122.65 | 120.30 |
| 1 | AA | 352 | U | OP1-P-O3' | 5.86 | 118.10 | 105.20 |
| 1 | AA | 1006 | C | C2-N1-C1' | -5.86 | 112.35 | 118.80 |
| 1 | CA | 1122 | G | C5-C6-O6 | -5.86 | 125.08 | 128.60 |
| 1 | AA | 1657 | C | C2-N3-C4 | -5.86 | 116.97 | 119.90 |
| 2 | AB | 114 | C | N3-C4-C5 | 5.86 | 124.24 | 121.90 |
| 34 | BA | 410 | G | C8-N9-C4 | -5.86 | 104.06 | 106.40 |
| 1 | CA | 2360 | A | N7-C8-N9 | -5.86 | 110.87 | 113.80 |
| 34 | BA | 1523 | G | OP1-P-OP2 | 5.86 | 128.39 | 119.60 |
| 1 | AA | 2039 | U | O5'-P-OP1 | -5.86 | 100.43 | 105.70 |
| 1 | AA | 2641 | A | C8-N9-C4 | -5.86 | 103.46 | 105.80 |
| 1 | CA | 2085 | C | N3-C4-C5 | 5.86 | 124.24 | 121.90 |
| 34 | BA | 1082 | G | C5-C6-O6 | -5.85 | 125.09 | 128.60 |
| 1 | AA | 22 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 592 | U | N3-C4-O4 | 5.85 | 123.50 | 119.40 |
| 1 | AA | 671 | A | C8-N9-C4 | -5.85 | 103.46 | 105.80 |
| 1 | AA | 710 | G | N3-C2-N2 | -5.85 | 115.80 | 119.90 |
| 1 | AA | 870 | G | N1-C6-O6 | -5.85 | 116.39 | 119.90 |
| 1 | AA | 1000 | C | N1-C2-O2 | -5.85 | 115.39 | 118.90 |
| 1 | AA | 1157 | A | C2-N3-C4 | -5.85 | 107.67 | 110.60 |
| 2 | CB | 91 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 1 | AA | 870 | G | N9-C4-C5 | 5.85 | 107.74 | 105.40 |
| 1 | AA | 833 | C | N3-C4-N4 | -5.85 | 113.91 | 118.00 |
| 1 | AA | 1845 | G | C5-C6-O6 | -5.85 | 125.09 | 128.60 |
| 1 | CA | 756 | C | N1-C2-O2 | -5.85 | 115.39 | 118.90 |
| 1 | CA | 2875 | C | C5-C6-N1 | -5.85 | 118.08 | 121.00 |
| 34 | DA | 1158 | C | N1-C2-O2 | 5.85 | 122.41 | 118.90 |
| 1 | AA | 1231 | G | C6-N1-C2 | -5.85 | 121.59 | 125.10 |
| 34 | BA | 758 | G | O5'-P-OP1 | 5.85 | 117.72 | 110.70 |
| 1 | AA | 1463 | C | OP1-P-OP2 | -5.85 | 110.83 | 119.60 |
| 1 | AA | 1870 | G | N1-C6-O6 | -5.85 | 116.39 | 119.90 |
| 1 | CA | 151 | C | C6-N1-C2 | 5.85 | 122.64 | 120.30 |
| 1 | CA | 1696 | G | O5'-P-OP2 | -5.85 | 100.44 | 105.70 |
| 1 | AA | 1423 | G | N3-C2-N2 | 5.84 | 123.99 | 119.90 |
| 1 | AA | 1593 | C | O5'-P-OP1 | -5.84 | 100.44 | 105.70 |
| 1 | AA | 2052 | A | C8-N9-C4 | 5.84 | 108.14 | 105.80 |
| 34 | BA | 1524 | C | N1-C2-N3 | 5.84 | 123.29 | 119.20 |
| 1 | CA | 1204 | A | N3-C4-C5 | 5.84 | 130.89 | 126.80 |
| 1 | CA | 2029 | G | C5-C6-O6 | -5.84 | 125.09 | 128.60 |
| 1 | AA | 645 | G | N9-C4-C5 | -5.84 | 103.06 | 105.40 |
| 1 | AA | 849 | A | N1-C6-N6 | -5.84 | 115.09 | 118.60 |
| 1 | CA | 2206 | G | C4-N9-C1' | -5.84 | 118.90 | 126.50 |
| 1 | AA | 491 | G | N7-C8-N9 | 5.84 | 116.02 | 113.10 |
| 1 | AA | 138 | G | OP1-P-OP2 | -5.84 | 110.84 | 119.60 |
| 1 | AA | 1961 | U | N1-C2-N3 | -5.84 | 111.40 | 114.90 |
| 1 | AA | 2043 | C | C5-C6-N1 | -5.84 | 118.08 | 121.00 |
| 1 | AA | 2605 | U | C2-N3-C4 | -5.84 | 123.50 | 127.00 |
| 1 | CA | 961 | C | N3-C4-C5 | 5.84 | 124.23 | 121.90 |
| 1 | CA | 596 | G | N1-C6-O6 | -5.84 | 116.40 | 119.90 |
| 1 | CA | 2023 | G | C5-C6-O6 | -5.83 | 125.10 | 128.60 |
| 1 | CA | 2546 | U | C5-C6-N1 | -5.83 | 119.78 | 122.70 |
| 1 | AA | 52 | A | N1-C2-N3 | 5.83 | 132.22 | 129.30 |
| 1 | AA | 1403 | U | N3-C2-O2 | -5.83 | 118.12 | 122.20 |
| 1 | AA | 2521 | G | C4-C5-N7 | 5.83 | 113.13 | 110.80 |
| 1 | AA | 2574 | U | N3-C2-O2 | -5.83 | 118.12 | 122.20 |
| 1 | AA | 1009 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2364 | A | C8-N9-C4 | 5.83 | 108.13 | 105.80 |
| 1 | AA | 331 | G | N3-C4-C5 | -5.83 | 125.69 | 128.60 |
| 1 | AA | 1401 | G | N1-C6-O6 | -5.83 | 116.41 | 119.90 |
| 1 | AA | 2542 | A | C2-N3-C4 | -5.83 | 107.69 | 110.60 |
| 1 | AA | 2802 | C | O4'-C1'-N1 | 5.83 | 112.86 | 108.20 |
| 1 | CA | 2867 | G | O4'-C1'-N9 | 5.83 | 112.86 | 108.20 |
| 1 | AA | 1728 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 1 | CA | 674 | G | N1-C6-O6 | 5.82 | 123.39 | 119.90 |
| 1 | AA | 808 | A | C2-N3-C4 | -5.82 | 107.69 | 110.60 |
| 1 | AA | 831 | A | C5-N7-C8 | 5.82 | 106.81 | 103.90 |
| 34 | DA | 687 | A | P-O3'-C3' | 5.82 | 126.69 | 119.70 |
| 1 | AA | 234 | G | C2-N3-C4 | -5.82 | 108.99 | 111.90 |
| 1 | AA | 817 | G | N3-C2-N2 | 5.82 | 123.97 | 119.90 |
| 1 | AA | 2501 | G | N3-C4-C5 | -5.82 | 125.69 | 128.60 |
| 1 | AA | 1185 | C | N1-C2-O2 | -5.82 | 115.41 | 118.90 |
| 1 | AA | 1637 | G | N1-C6-O6 | -5.82 | 116.41 | 119.90 |
| 34 | BA | 852 | G | O5'-P-OP2 | -5.82 | 100.46 | 105.70 |
| 1 | CA | 577 | G | N9-C4-C5 | -5.82 | 103.07 | 105.40 |
| 1 | CA | 2513 | G | C5-C6-O6 | -5.82 | 125.11 | 128.60 |
| 1 | CA | 1885 | A | C8-N9-C4 | 5.82 | 108.13 | 105.80 |
| 1 | CA | 2447 | G | O5'-P-OP2 | -5.82 | 100.47 | 105.70 |
| 1 | AA | 1513 | G | OP2-P-O3' | 5.81 | 117.99 | 105.20 |
| 34 | BA | 972 | C | C6-N1-C2 | -5.81 | 117.97 | 120.30 |
| 1 | CA | 1299 | G | C8-N9-C4 | -5.81 | 104.07 | 106.40 |
| 1 | AA | 892 | G | O4'-C1'-N9 | 5.81 | 112.85 | 108.20 |
| 1 | AA | 1020 | C | O5'-P-OP1 | -5.81 | 100.47 | 105.70 |
| 1 | CA | 1992 | G | N1-C6-O6 | -5.81 | 116.41 | 119.90 |
| 1 | AA | 1059 | C | C6-N1-C2 | 5.81 | 122.62 | 120.30 |
| 1 | AA | 1646 | C | C4-C5-C6 | 5.81 | 120.31 | 117.40 |
| 1 | AA | 2565 | G | C5-C6-N1 | 5.81 | 114.41 | 111.50 |
| 1 | AA | 2603 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 1 | CA | 2618 | G | C8-N9-C4 | 5.81 | 108.72 | 106.40 |
| 1 | AA | 2265 | G | N7-C8-N9 | -5.81 | 110.20 | 113.10 |
| 1 | AA | 2303 | U | C5-C6-N1 | -5.81 | 119.80 | 122.70 |
| 1 | CA | 2724 | C | N3-C4-C5 | 5.81 | 124.22 | 121.90 |
| 1 | AA | 85 | C | C5-C6-N1 | -5.81 | 118.10 | 121.00 |
| 1 | CA | 2070 | G | N1-C2-N3 | 5.80 | 127.38 | 123.90 |
| 1 | AA | 1302 | G | N9-C4-C5 | -5.80 | 103.08 | 105.40 |
| 1 | AA | 2022 | G | OP1-P-OP2 | 5.80 | 128.30 | 119.60 |
| 1 | AA | 107 | G | N1-C6-O6 | -5.80 | 116.42 | 119.90 |
| 13 | AP | 18 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | CA | 2273 | A | O5'-P-OP2 | -5.80 | 100.48 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 976 | G | C6-N1-C2 | -5.80 | 121.62 | 125.10 |
| 1 | AA | 1018 | A | OP1-P-OP2 | -5.80 | 110.90 | 119.60 |
| 1 | AA | 2093 | A | C2-N3-C4 | -5.80 | 107.70 | 110.60 |
| 1 | AA | 2824 | C | N1-C2-O2 | -5.80 | 115.42 | 118.90 |
| 1 | CA | 1235 | G | N1-C6-O6 | 5.80 | 123.38 | 119.90 |
| 1 | AA | 123 | G | C5-C6-O6 | -5.80 | 125.12 | 128.60 |
| 1 | AA | 853 | C | C4-C5-C6 | -5.80 | 114.50 | 117.40 |
| 1 | AA | 2565 | G | N3-C4-N9 | 5.80 | 129.48 | 126.00 |
| 34 | BA | 600 | C | O5'-P-OP2 | -5.80 | 100.48 | 105.70 |
| 1 | AA | 560 | C | C5-C6-N1 | -5.79 | 118.10 | 121.00 |
| 34 | DA | 884 | U | N1-C2-O2 | -5.79 | 118.75 | 122.80 |
| 1 | AA | 1029 | A | O5'-P-OP2 | -5.79 | 100.49 | 105.70 |
| 1 | AA | 1410 | G | C5-C6-O6 | -5.79 | 125.12 | 128.60 |
| 1 | AA | 1920 | U | N3-C2-O2 | -5.79 | 118.15 | 122.20 |
| 1 | AA | 1965 | U | C2-N3-C4 | -5.79 | 123.53 | 127.00 |
| 1 | CA | 1279 | G | C2-N3-C4 | -5.79 | 109.00 | 111.90 |
| 1 | CA | 1698 | A | C8-N9-C4 | -5.79 | 103.48 | 105.80 |
| 1 | AA | 426 | G | C8-N9-C4 | 5.79 | 108.72 | 106.40 |
| 1 | AA | 2561 | G | N1-C6-O6 | 5.79 | 123.37 | 119.90 |
| 1 | AA | 2002 | G | C8-N9-C4 | -5.79 | 104.08 | 106.40 |
| 1 | AA | 894 | U | C6-N1-C1' | 5.79 | 129.30 | 121.20 |
| 1 | AA | 918 | U | C5-C4-O4 | -5.78 | 122.43 | 125.90 |
| 1 | AA | 1030 | A | N1-C6-N6 | -5.78 | 115.13 | 118.60 |
| 1 | AA | 1069 | U | C5-C6-N1 | -5.78 | 119.81 | 122.70 |
| 1 | AA | 2243 | C | C4-C5-C6 | 5.78 | 120.29 | 117.40 |
| 1 | AA | 2738 | A | C2-N3-C4 | -5.78 | 107.71 | 110.60 |
| 1 | CA | 2372 | G | C8-N9-C4 | -5.78 | 104.09 | 106.40 |
| 1 | AA | 2871 | G | C5-C6-O6 | -5.78 | 125.13 | 128.60 |
| 34 | BA | 335 | C | N1-C2-O2 | 5.78 | 122.37 | 118.90 |
| 1 | CA | 1855 | G | C8-N9-C4 | 5.78 | 108.71 | 106.40 |
| 1 | AA | 235 | C | N3-C4-C5 | 5.78 | 124.21 | 121.90 |
| 1 | AA | 716 | G | OP1-P-OP2 | -5.78 | 110.93 | 119.60 |
| 1 | AA | 2553 | A | C5-N7-C8 | -5.78 | 101.01 | 103.90 |
| 1 | CA | 2490 | G | N9-C4-C5 | -5.78 | 103.09 | 105.40 |
| 1 | CA | 2847 | U | C5-C4-O4 | -5.78 | 122.43 | 125.90 |
| 1 | AA | 960 | C | C5-C6-N1 | -5.78 | 118.11 | 121.00 |
| 1 | AA | 2378 | A | N1-C6-N6 | 5.78 | 122.06 | 118.60 |
| 1 | CA | 686 | G | O4'-C1'-N9 | 5.78 | 112.82 | 108.20 |
| 34 | BA | 266 | G | C6-C5-N7 | -5.77 | 126.94 | 130.40 |
| 1 | AA | 542 | C | N3-C4-N4 | 5.77 | 122.04 | 118.00 |
| 1 | CA | 1496 | A | C8-N9-C4 | -5.77 | 103.49 | 105.80 |
| 1 | AA | 2082 | A | C2-N3-C4 | -5.77 | 107.72 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20 | AW | 17 | VAL | CB-CA-C | -5.77 | 100.44 | 111.40 |
| 1 | AA | 491 | G | C8-N9-C4 | -5.77 | 104.09 | 106.40 |
| 1 | AA | 1691 | C | N1-C2-O2 | 5.77 | 122.36 | 118.90 |
| 1 | AA | 2264 | G | C4-C5-N7 | -5.77 | 108.49 | 110.80 |
| 34 | BA | 321 | A | O5'-P-OP2 | -5.77 | 100.51 | 105.70 |
| 1 | CA | 670 | A | O4'-C1'-N9 | -5.77 | 103.58 | 108.20 |
| 34 | DA | 910 | C | C6-N1-C2 | 5.77 | 122.61 | 120.30 |
| 1 | AA | 1623 | U | N3-C2-O2 | -5.77 | 118.16 | 122.20 |
| 1 | AA | 2481 | A | OP2-P-O3' | 5.77 | 117.89 | 105.20 |
| 1 | AA | 2607 | G | N1-C6-O6 | -5.77 | 116.44 | 119.90 |
| 1 | AA | 1312 | G | C2-N3-C4 | 5.77 | 114.78 | 111.90 |
| 1 | AA | 1814 | A | N9-C4-C5 | 5.77 | 108.11 | 105.80 |
| 1 | AA | 852 | G | N1-C6-O6 | -5.76 | 116.44 | 119.90 |
| 1 | AA | 980 | C | C6-N1-C2 | 5.76 | 122.61 | 120.30 |
| 1 | AA | 1240 | G | N1-C2-N2 | 5.76 | 121.39 | 116.20 |
| 1 | CA | 704 | G | O4'-C1'-N9 | 5.76 | 112.81 | 108.20 |
| 1 | CA | 799 | G | C5-C6-O6 | -5.76 | 125.14 | 128.60 |
| 1 | CA | 2361 | A | C2-N3-C4 | -5.76 | 107.72 | 110.60 |
| 1 | CA | 1977 | A | C5-C6-N6 | 5.76 | 128.31 | 123.70 |
| 1 | AA | 361 | C | C6-N1-C2 | 5.76 | 122.60 | 120.30 |
| 1 | AA | 801 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 1 | AA | 2029 | C | C6-N1-C2 | -5.76 | 118.00 | 120.30 |
| 1 | AA | 2066 | C | N1-C2-N3 | 5.76 | 123.23 | 119.20 |
| 34 | BA | 266 | G | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 2 | AB | 1 | U | N1-C2-O2 | 5.76 | 126.83 | 122.80 |
| 1 | CA | 1021 | A | C8-N9-C4 | -5.76 | 103.50 | 105.80 |
| 1 | CA | 2742 | C | C6-N1-C2 | 5.76 | 122.60 | 120.30 |
| 1 | AA | 556 | C | C2-N3-C4 | -5.76 | 117.02 | 119.90 |
| 1 | AA | 1431 | G | O4'-C1'-N9 | 5.76 | 112.80 | 108.20 |
| 1 | AA | 2346 | G | C6-C5-N7 | -5.76 | 126.95 | 130.40 |
| 1 | AA | 2387 | G | C8-N9-C4 | 5.76 | 108.70 | 106.40 |
| 34 | BA | 615 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 1 | AA | 2585 | C | C5-C6-N1 | -5.75 | 118.12 | 121.00 |
| 34 | BA | 769 | G | O5'-P-OP1 | 5.75 | 117.60 | 110.70 |
| 34 | BA | 1442 | G | C2-N3-C4 | -5.75 | 109.02 | 111.90 |
| 1 | CA | 2028 | U | N3-C2-O2 | -5.75 | 118.17 | 122.20 |
| 34 | DA | 1054 | C | O4'-C1'-N1 | 5.75 | 112.80 | 108.20 |
| 1 | AA | 1751 | G | N1-C6-O6 | -5.75 | 116.45 | 119.90 |
| 1 | AA | 2609 | G | C4-C5-N7 | 5.75 | 113.10 | 110.80 |
| 1 | CA | 528 | A | N1-C2-N3 | 5.75 | 132.17 | 129.30 |
| 1 | CA | 2824 | C | C5-C4-N4 | -5.75 | 116.18 | 120.20 |
| 57 | DX | 20 | U | C2-N1-C1' | 5.75 | 124.60 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 960 | C | C6-N1-C2 | 5.75 | 122.60 | 120.30 |
| 1 | CA | 829 | A | N1-C6-N6 | 5.75 | 122.05 | 118.60 |
| 1 | CA | 1672 | C | C6-N1-C2 | -5.75 | 118.00 | 120.30 |
| 1 | AA | 1983 | C | C5-C6-N1 | -5.75 | 118.13 | 121.00 |
| 1 | CA | 1781 | C | C6-N1-C1' | 5.74 | 127.69 | 120.80 |
| 1 | AA | 894 | U | C2-N1-C1' | -5.74 | 110.81 | 117.70 |
| 1 | AA | 2460 | A | C8-N9-C4 | -5.74 | 103.50 | 105.80 |
| 1 | CA | 2003 | G | O5'-P-OP1 | -5.74 | 100.53 | 105.70 |
| 1 | AA | 2528 | G | C4-C5-N7 | -5.74 | 108.50 | 110.80 |
| 1 | AA | 784 | C | C6-N1-C2 | 5.74 | 122.59 | 120.30 |
| 1 | AA | 1313 | U | N3-C4-O4 | -5.74 | 115.38 | 119.40 |
| 1 | AA | 2219 | U | C4-C5-C6 | 5.74 | 123.14 | 119.70 |
| 1 | AA | 2655 | G | N9-C4-C5 | -5.74 | 103.11 | 105.40 |
| 34 | BA | 1397 | C | C5-C4-N4 | 5.74 | 124.22 | 120.20 |
| 1 | AA | 560 | C | N1-C2-N3 | 5.74 | 123.22 | 119.20 |
| 1 | AA | 457 | G | C5-C6-O6 | -5.74 | 125.16 | 128.60 |
| 1 | AA | 1370 | G | N1-C2-N3 | 5.74 | 127.34 | 123.90 |
| 1 | AA | 2264 | G | N3-C4-N9 | -5.74 | 122.56 | 126.00 |
| 1 | AA | 2345 | A | P-O3'-C3' | 5.74 | 126.58 | 119.70 |
| 1 | AA | 2643 | G | OP1-P-OP2 | 5.73 | 128.20 | 119.60 |
| 1 | AA | 2849 | G | N7-C8-N9 | -5.73 | 110.23 | 113.10 |
| 2 | AB | 63 | G | O5'-P-OP2 | -5.73 | 100.54 | 105.70 |
| 1 | AA | 59 | G | C5-C6-O6 | -5.73 | 125.16 | 128.60 |
| 1 | AA | 430 | U | N3-C2-O2 | -5.73 | 118.19 | 122.20 |
| 1 | AA | 725 | C | N1-C2-O2 | -5.73 | 115.46 | 118.90 |
| 1 | AA | 2696 | U | C5-C6-N1 | -5.73 | 119.83 | 122.70 |
| 34 | BA | 890 | G | N3-C2-N2 | 5.73 | 123.91 | 119.90 |
| 1 | CA | 383 | U | O4'-C1'-N1 | 5.73 | 112.79 | 108.20 |
| 1 | AA | 240 | A | N1-C2-N3 | -5.73 | 126.43 | 129.30 |
| 1 | AA | 827 | G | N3-C2-N2 | -5.73 | 115.89 | 119.90 |
| 1 | AA | 2472 | U | O5'-P-OP1 | -5.73 | 100.54 | 105.70 |
| 1 | CA | 563 | G | C4-C5-N7 | 5.73 | 113.09 | 110.80 |
| 1 | CA | 1797 | C | N3-C4-C5 | 5.73 | 124.19 | 121.90 |
| 1 | CA | 2377 | A | C2-N3-C4 | -5.73 | 107.73 | 110.60 |
| 1 | CA | 2647 | U | C5-C6-N1 | -5.73 | 119.83 | 122.70 |
| 1 | AA | 131 | C | N1-C2-O2 | 5.73 | 122.34 | 118.90 |
| 1 | AA | 395 | C | N1-C2-O2 | -5.73 | 115.46 | 118.90 |
| 1 | CA | 2407 | G | C8-N9-C1' | -5.73 | 119.55 | 127.00 |
| 34 | DA | 266 | G | C5-N7-C8 | -5.73 | 101.44 | 104.30 |
| 1 | AA | 1849 | U | N3-C4-C5 | 5.73 | 118.04 | 114.60 |
| 1 | AA | 715 | G | C4-C5-N7 | 5.73 | 113.09 | 110.80 |
| 1 | AA | 1208 | G | C5-N7-C8 | 5.73 | 107.16 | 104.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1042 | A | N1-C6-N6 | -5.72 | 115.17 | 118.60 |
| 1 | CA | 2050 | C | N3-C4-C5 | 5.72 | 124.19 | 121.90 |
| 1 | AA | 125 | A | C8-N9-C4 | 5.72 | 108.09 | 105.80 |
| 1 | AA | 621 | G | C8-N9-C4 | -5.72 | 104.11 | 106.40 |
| 1 | AA | 1097 | G | C4-C5-N7 | 5.72 | 113.09 | 110.80 |
| 1 | AA | 1721 | G | N9-C4-C5 | -5.72 | 103.11 | 105.40 |
| 1 | CA | 2242 | G | C8-N9-C4 | 5.72 | 108.69 | 106.40 |
| 1 | CA | 147 | U | C5-C6-N1 | -5.72 | 119.84 | 122.70 |
| 1 | AA | 1321 | A | C5-N7-C8 | 5.72 | 106.76 | 103.90 |
| 1 | AA | 2776 | G | C8-N9-C4 | 5.72 | 108.69 | 106.40 |
| 4 | AD | 111 | LEU | CA-CB-CG | 5.72 | 128.45 | 115.30 |
| 1 | AA | 2461 | U | N3-C4-O4 | 5.72 | 123.40 | 119.40 |
| 1 | AA | 1296 | G | N7-C8-N9 | -5.72 | 110.24 | 113.10 |
| 1 | AA | 1415 | G | C5-C6-O6 | -5.72 | 125.17 | 128.60 |
| 1 | AA | 1484 | U | N3-C4-O4 | 5.71 | 123.40 | 119.40 |
| 1 | AA | 583 | C | C5-C6-N1 | -5.71 | 118.14 | 121.00 |
| 1 | AA | 891 | C | N3-C4-C5 | 5.71 | 124.18 | 121.90 |
| 1 | AA | 2581 | G | C5-C6-N1 | 5.71 | 114.35 | 111.50 |
| 1 | AA | 2604 | G | OP2-P-O3' | 5.71 | 117.76 | 105.20 |
| 1 | CA | 2523 | G | N3-C4-N9 | 5.71 | 129.43 | 126.00 |
| 1 | CA | 2772 | C | C6-N1-C2 | -5.71 | 118.02 | 120.30 |
| 34 | BA | 554 | C | N1-C2-O2 | -5.71 | 115.48 | 118.90 |
| 1 | CA | 1355 | G | N3-C4-C5 | -5.71 | 125.75 | 128.60 |
| 1 | AA | 2745 | G | N3-C2-N2 | -5.70 | 115.91 | 119.90 |
| 34 | DA | 266 | G | P-O3'-C3' | 5.70 | 126.55 | 119.70 |
| 1 | AA | 782 | A | C5-C6-N1 | -5.70 | 114.85 | 117.70 |
| 1 | AA | 1179 | U | C2-N3-C4 | -5.70 | 123.58 | 127.00 |
| 1 | CA | 1977 | A | C4-C5-N7 | -5.70 | 107.85 | 110.70 |
| 1 | CA | 2541 | A | N1-C2-N3 | 5.70 | 132.15 | 129.30 |
| 1 | AA | 123 | G | C2-N3-C4 | 5.70 | 114.75 | 111.90 |
| 1 | CA | 474 | G | N3-C4-C5 | -5.70 | 125.75 | 128.60 |
| 1 | CA | 1212 | G | N3-C4-C5 | -5.70 | 125.75 | 128.60 |
| 1 | AA | 107 | G | C5-C6-N1 | 5.70 | 114.35 | 111.50 |
| 1 | AA | 200 | A | N1-C2-N3 | 5.70 | 132.15 | 129.30 |
| 1 | CA | 410 | G | N1-C6-O6 | -5.70 | 116.48 | 119.90 |
| 2 | CB | 10 | C | C6-N1-C2 | -5.70 | 118.02 | 120.30 |
| 1 | AA | 1487 | G | N1-C2-N2 | 5.70 | 121.33 | 116.20 |
| 1 | AA | 184 | A | P-O3'-C3' | 5.70 | 126.53 | 119.70 |
| 1 | AA | 471 | C | C6-N1-C2 | -5.70 | 118.02 | 120.30 |
| 1 | AA | 491 | G | C4-C5-N7 | 5.70 | 113.08 | 110.80 |
| 1 | AA | 2783 | G | C8-N9-C4 | 5.70 | 108.68 | 106.40 |
| 1 | CA | 2019 | A | C5-N7-C8 | 5.70 | 106.75 | 103.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1204 | A | C5-C6-N1 | -5.69 | 114.85 | 117.70 |
| 1 | CA | 1313 | U | O4'-C1'-N1 | 5.69 | 112.76 | 108.20 |
| 2 | CB | 115 | G | C8-N9-C4 | 5.69 | 108.68 | 106.40 |
| 1 | AA | 419 | C | O5'-P-OP1 | -5.69 | 100.58 | 105.70 |
| 1 | AA | 1438 | A | C5-C6-N1 | 5.69 | 120.55 | 117.70 |
| 1 | AA | 139 | A | N1-C2-N3 | 5.69 | 132.15 | 129.30 |
| 1 | AA | 1817 | A | C8-N9-C4 | 5.69 | 108.08 | 105.80 |
| 1 | AA | 2448 | G | OP1-P-O3' | 5.69 | 117.72 | 105.20 |
| 1 | CA | 2848 | G | O4'-C1'-N9 | 5.69 | 112.75 | 108.20 |
| 1 | AA | 2052 | A | C4-C5-N7 | 5.69 | 113.54 | 110.70 |
| 1 | CA | 1788 | C | N3-C4-C5 | -5.69 | 119.62 | 121.90 |
| 1 | CA | 2718 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 1 | AA | 541 | C | N3-C4-C5 | 5.69 | 124.17 | 121.90 |
| 1 | AA | 847 | A | N1-C2-N3 | 5.69 | 132.14 | 129.30 |
| 1 | AA | 2096 | U | N1-C2-O2 | -5.69 | 118.82 | 122.80 |
| 1 | AA | 2117 | C | O5'-P-OP2 | -5.69 | 100.58 | 105.70 |
| 1 | AA | 2544 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 1 | CA | 1613 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 1 | CA | 2077 | A | N1-C6-N6 | 5.69 | 122.01 | 118.60 |
| 34 | DA | 1500 | A | N1-C6-N6 | 5.69 | 122.01 | 118.60 |
| 1 | AA | 2052 | A | N9-C4-C5 | -5.69 | 103.53 | 105.80 |
| 1 | AA | 1427 | G | C5-C6-O6 | -5.68 | 125.19 | 128.60 |
| 1 | AA | 2552 | C | N3-C4-C5 | 5.68 | 124.17 | 121.90 |
| 34 | BA | 1464 | G | N1-C6-O6 | 5.68 | 123.31 | 119.90 |
| 1 | CA | 2425 | A | C5-C6-N1 | 5.68 | 120.54 | 117.70 |
| 34 | DA | 886 | G | N9-C4-C5 | -5.68 | 103.13 | 105.40 |
| 1 | AA | 518 | G | N7-C8-N9 | -5.68 | 110.26 | 113.10 |
| 1 | AA | 715 | G | OP2-P-O3' | 5.68 | 117.70 | 105.20 |
| 1 | AA | 2364 | A | O5'-P-OP1 | -5.68 | 100.59 | 105.70 |
| 1 | AA | 2511 | C | N1-C2-O2 | -5.68 | 115.49 | 118.90 |
| 1 | CA | 981 | A | C8-N9-C4 | 5.68 | 108.07 | 105.80 |
| 1 | CA | 1842 | G | N9-C4-C5 | -5.68 | 103.13 | 105.40 |
| 1 | AA | 833 | C | N3-C4-C5 | 5.68 | 124.17 | 121.90 |
| 1 | AA | 2372 | A | O5'-P-OP1 | 5.68 | 117.51 | 110.70 |
| 1 | AA | 2561 | G | C5-N7-C8 | -5.68 | 101.46 | 104.30 |
| 1 | AA | 2659 | U | C6-N1-C2 | 5.68 | 124.41 | 121.00 |
| 1 | AA | 2707 | C | C6-N1-C2 | 5.68 | 122.57 | 120.30 |
| 1 | AA | 2837 | C | N1-C2-O2 | -5.68 | 115.49 | 118.90 |
| 1 | CA | 529 | A | C5-N7-C8 | -5.68 | 101.06 | 103.90 |
| 1 | CA | 1204 | A | C6-C5-N7 | -5.68 | 128.33 | 132.30 |
| 1 | AA | 2773 | C | O5'-P-OP1 | -5.67 | 100.59 | 105.70 |
| 1 | CA | 560 | C | C5-C6-N1 | -5.67 | 118.16 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1292 | U | N1-C2-O2 | -5.67 | 118.83 | 122.80 |
| 1 | CA | 2517 | C | N3-C4-C5 | 5.67 | 124.17 | 121.90 |
| 1 | CA | 2373 | G | N1-C6-O6 | 5.67 | 123.30 | 119.90 |
| 1 | AA | 200 | A | C4-C5-C6 | 5.67 | 119.84 | 117.00 |
| 1 | AA | 2528 | G | C6-C5-N7 | 5.67 | 133.80 | 130.40 |
| 1 | AA | 2625 | U | C5-C4-O4 | 5.67 | 129.30 | 125.90 |
| 1 | AA | 2887 | G | N1-C6-O6 | -5.67 | 116.50 | 119.90 |
| 1 | CA | 188 | G | N3-C2-N2 | 5.67 | 123.87 | 119.90 |
| 34 | DA | 532 | A | OP1-P-O3' | 5.67 | 117.68 | 105.20 |
| 1 | AA | 830 | A | C8-N9-C4 | -5.67 | 103.53 | 105.80 |
| 1 | AA | 1438 | A | N9-C4-C5 | -5.67 | 103.53 | 105.80 |
| 34 | BA | 44 | G | N3-C2-N2 | -5.67 | 115.93 | 119.90 |
| 1 | CA | 668 | G | C2-N3-C4 | -5.67 | 109.07 | 111.90 |
| 1 | CA | 2593 | U | N3-C4-C5 | 5.67 | 118.00 | 114.60 |
| 1 | AA | 1695 | C | C2-N1-C1' | -5.67 | 112.57 | 118.80 |
| 1 | AA | 2370 | G | C2-N3-C4 | -5.67 | 109.07 | 111.90 |
| 1 | AA | 2397 | C | C2-N3-C4 | -5.67 | 117.07 | 119.90 |
| 1 | AA | 2802 | C | C5-C6-N1 | -5.67 | 118.17 | 121.00 |
| 34 | BA | 1505 | G | C5-C6-N1 | -5.67 | 108.67 | 111.50 |
| 1 | AA | 526 | A | N1-C2-N3 | 5.66 | 132.13 | 129.30 |
| 1 | AA | 954 | C | C2-N3-C4 | -5.66 | 117.07 | 119.90 |
| 1 | AA | 2696 | U | C2-N3-C4 | -5.66 | 123.60 | 127.00 |
| 1 | CA | 918 | A | O5'-P-OP1 | -5.66 | 100.60 | 105.70 |
| 1 | AA | 713 | G | OP2-P-O3' | 5.66 | 117.66 | 105.20 |
| 1 | AA | 20 | C | N3-C4-N4 | -5.66 | 114.04 | 118.00 |
| 34 | BA | 1442 | G | N1-C6-O6 | 5.66 | 123.30 | 119.90 |
| 1 | CA | 426 | C | N3-C2-O2 | -5.66 | 117.94 | 121.90 |
| 1 | CA | 1385 | G | O4'-C1'-N9 | 5.66 | 112.73 | 108.20 |
| 1 | AA | 957 | A | N1-C6-N6 | -5.66 | 115.20 | 118.60 |
| 1 | AA | 2498 | G | N3-C4-N9 | 5.66 | 129.40 | 126.00 |
| 1 | AA | 1037 | C | N3-C4-C5 | 5.65 | 124.16 | 121.90 |
| 1 | AA | 1849 | U | C2-N3-C4 | -5.65 | 123.61 | 127.00 |
| 34 | BA | 110 | C | N1-C2-O2 | 5.65 | 122.29 | 118.90 |
| 1 | AA | 2089 | G | N9-C4-C5 | 5.65 | 107.66 | 105.40 |
| 1 | AA | 2823 | A | N1-C6-N6 | -5.65 | 115.21 | 118.60 |
| 34 | BA | 1442 | G | C8-N9-C4 | -5.65 | 104.14 | 106.40 |
| 34 | BA | 1502 | A | C6-C5-N7 | -5.65 | 128.34 | 132.30 |
| 1 | CA | 1499 | C | N3-C4-C5 | 5.65 | 124.16 | 121.90 |
| 1 | AA | 1070 | G | C6-C5-N7 | -5.65 | 127.01 | 130.40 |
| 1 | AA | 1810 | U | C5-C4-O4 | -5.65 | 122.51 | 125.90 |
| 1 | CA | 1901 | A | O5'-P-OP1 | -5.65 | 100.62 | 105.70 |
| 1 | AA | 1488 | G | C8-N9-C4 | -5.65 | 104.14 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2797 | C | N3-C2-O2 | -5.65 | 117.95 | 121.90 |
| 34 | BA | 277 | C | C2-N3-C4 | -5.64 | 117.08 | 119.90 |
| 34 | BA | 567 | G | O5'-P-OP1 | -5.64 | 100.62 | 105.70 |
| 1 | CA | 1681 | G | C5-N7-C8 | -5.64 | 101.48 | 104.30 |
| 1 | AA | 870 | G | C5-C6-O6 | 5.64 | 131.99 | 128.60 |
| 1 | AA | 1805 | C | N3-C2-O2 | -5.64 | 117.95 | 121.90 |
| 1 | AA | 2520 | G | N3-C4-C5 | -5.64 | 125.78 | 128.60 |
| 1 | AA | 2602 | A | OP1-P-OP2 | -5.64 | 111.14 | 119.60 |
| 1 | AA | 2292 | G | OP2-P-O3' | 5.64 | 117.61 | 105.20 |
| 1 | AA | 1712 | A | C8-N9-C4 | -5.64 | 103.54 | 105.80 |
| 1 | AA | 2538 | G | C5-C6-O6 | 5.64 | 131.98 | 128.60 |
| 1 | AA | 2632 | C | C2-N1-C1' | -5.64 | 112.60 | 118.80 |
| 1 | AA | 371 | A | N1-C2-N3 | 5.64 | 132.12 | 129.30 |
| 1 | AA | 1015 | C | C5-C6-N1 | 5.64 | 123.82 | 121.00 |
| 1 | AA | 1252 | C | C4-C5-C6 | 5.64 | 120.22 | 117.40 |
| 1 | AA | 2693 | C | C6-N1-C2 | -5.64 | 118.05 | 120.30 |
| 1 | CA | 2605 | U | N3-C4-C5 | 5.64 | 117.98 | 114.60 |
| 1 | AA | 2346 | G | C8-N9-C1' | -5.63 | 119.67 | 127.00 |
| 34 | DA | 1405 | G | N3-C4-N9 | 5.63 | 129.38 | 126.00 |
| 1 | CA | 778 | G | C4-C5-N7 | 5.63 | 113.05 | 110.80 |
| 1 | CA | 2085 | C | C5-C4-N4 | -5.63 | 116.26 | 120.20 |
| 1 | AA | 491 | G | C5-N7-C8 | -5.63 | 101.48 | 104.30 |
| 1 | AA | 663 | G | N1-C6-O6 | -5.63 | 116.52 | 119.90 |
| 34 | BA | 123 | C | C6-N1-C2 | 5.63 | 122.55 | 120.30 |
| 1 | CA | 2318 | G | O4'-C1'-N9 | 5.63 | 112.71 | 108.20 |
| 1 | CA | 2387 | U | C2-N1-C1' | -5.63 | 110.94 | 117.70 |
| 1 | AA | 1813 | C | O5'-P-OP2 | 5.63 | 117.45 | 110.70 |
| 34 | BA | 115 | G | P-O3'-C3' | 5.63 | 126.45 | 119.70 |
| 1 | CA | 1616 | A | C2-N3-C4 | -5.63 | 107.78 | 110.60 |
| 1 | AA | 2650 | G | N3-C4-N9 | 5.63 | 129.38 | 126.00 |
| 1 | CA | 2503 | A | N1-C6-N6 | 5.63 | 121.98 | 118.60 |
| 34 | DA | 795 | C | C2-N3-C4 | -5.63 | 117.09 | 119.90 |
| 1 | AA | 783 | C | C6-N1-C2 | 5.62 | 122.55 | 120.30 |
| 1 | AA | 2898 | C | N3-C4-N4 | -5.62 | 114.06 | 118.00 |
| 34 | DA | 894 | G | C5-C6-O6 | -5.62 | 125.22 | 128.60 |
| 1 | AA | 1023 | G | C8-N9-C4 | -5.62 | 104.15 | 106.40 |
| 1 | AA | 1742 | G | C4-C5-N7 | 5.62 | 113.05 | 110.80 |
| 1 | AA | 2544 | G | N1-C6-O6 | 5.62 | 123.27 | 119.90 |
| 1 | AA | 877 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 1 | AA | 2503 | U | N3-C4-C5 | 5.62 | 117.97 | 114.60 |
| 1 | CA | 1501 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 1 | AA | 2504 | U | N3-C2-O2 | -5.62 | 118.27 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1029 | A | O5'-P-OP1 | 5.62 | 117.44 | 110.70 |
| 1 | AA | 1243 | U | C5-C6-N1 | -5.62 | 119.89 | 122.70 |
| 1 | AA | 2520 | G | N1-C6-O6 | -5.62 | 116.53 | 119.90 |
| 1 | AA | 2607 | G | N3-C4-N9 | -5.62 | 122.63 | 126.00 |
| 1 | CA | 34 | C | C5-C6-N1 | 5.62 | 123.81 | 121.00 |
| 34 | BA | 1526 | G | C5-C6-N1 | 5.61 | 114.31 | 111.50 |
| 1 | CA | 2456 | C | C6-N1-C2 | 5.61 | 122.55 | 120.30 |
| 1 | AA | 1463 | C | N3-C4-N4 | 5.61 | 121.93 | 118.00 |
| 1 | AA | 777 | C | N1-C2-N3 | 5.61 | 123.13 | 119.20 |
| 1 | AA | 707 | G | N1-C6-O6 | 5.61 | 123.26 | 119.90 |
| 1 | AA | 874 | U | C5-C6-N1 | -5.61 | 119.90 | 122.70 |
| 1 | AA | 1020 | C | N3-C4-C5 | 5.61 | 124.14 | 121.90 |
| 1 | AA | 2074 | G | N9-C4-C5 | 5.61 | 107.64 | 105.40 |
| 1 | AA | 2898 | C | C5-C6-N1 | -5.61 | 118.20 | 121.00 |
| 34 | DA | 97 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 1 | AA | 252 | C | C6-N1-C2 | 5.61 | 122.54 | 120.30 |
| 1 | CA | 845 | G | O4'-C1'-N9 | 5.61 | 112.69 | 108.20 |
| 34 | DA | 320 | C | C6-N1-C2 | 5.61 | 122.54 | 120.30 |
| 1 | CA | 1552 | G | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 1 | AA | 2450 | U | C2-N3-C4 | -5.60 | 123.64 | 127.00 |
| 1 | AA | 1412 | A | N9-C4-C5 | -5.60 | 103.56 | 105.80 |
| 1 | AA | 1712 | A | N9-C4-C5 | 5.60 | 108.04 | 105.80 |
| 1 | AA | 2331 | G | N9-C1'-C2' | 5.60 | 121.28 | 114.00 |
| 34 | BA | 1113 | C | C5-C6-N1 | 5.60 | 123.80 | 121.00 |
| 1 | AA | 438 | G | C8-N9-C4 | -5.60 | 104.16 | 106.40 |
| 1 | AA | 2400 | A | OP1-P-OP2 | -5.60 | 111.20 | 119.60 |
| 34 | BA | 254 | G | O5'-P-OP1 | -5.60 | 100.66 | 105.70 |
| 1 | CA | 1945 | G | C8-N9-C1' | -5.60 | 119.72 | 127.00 |
| 1 | CA | 2674 | G | C8-N9-C4 | 5.60 | 108.64 | 106.40 |
| 1 | AA | 2064 | A | O5'-P-OP1 | 5.60 | 117.42 | 110.70 |
| 2 | AB | 72 | G | C2-N3-C4 | -5.60 | 109.10 | 111.90 |
| 1 | CA | 532 | A | O4'-C1'-N9 | 5.60 | 112.68 | 108.20 |
| 1 | CA | 945 | A | N7-C8-N9 | 5.60 | 116.60 | 113.80 |
| 34 | DA | 1502 | A | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 1 | AA | 352 | U | N3-C2-O2 | -5.60 | 118.28 | 122.20 |
| 1 | AA | 370 | A | N9-C4-C5 | -5.60 | 103.56 | 105.80 |
| 1 | AA | 353 | G | C5-C6-O6 | -5.59 | 125.24 | 128.60 |
| 1 | AA | 2529 | C | O4'-C1'-N1 | 5.59 | 112.68 | 108.20 |
| 1 | CA | 1139 | G | O5'-P-OP2 | -5.59 | 100.67 | 105.70 |
| 1 | CA | 1695 | G | O5'-P-OP2 | -5.59 | 100.67 | 105.70 |
| 1 | CA | 2618 | G | N1-C6-O6 | -5.59 | 116.54 | 119.90 |
| 1 | CA | 2031 | A | C4-C5-C6 | 5.59 | 119.80 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 34 | DA | 65 | U | P-O3'-C3' | 5.59 | 126.41 | 119.70 |
| 2 | CB | 10 | C | N3-C2-O2 | -5.59 | 117.99 | 121.90 |
| 1 | AA | 141 | C | OP2-P-O3' | 5.59 | 117.49 | 105.20 |
| 1 | AA | 2331 | G | N3-C2-N2 | -5.59 | 115.99 | 119.90 |
| 1 | AA | 2674 | A | C8-N9-C4 | -5.59 | 103.56 | 105.80 |
| 34 | BA | 1509 | C | N1-C2-O2 | -5.59 | 115.55 | 118.90 |
| 1 | AA | 736 | A | N7-C8-N9 | -5.59 | 111.01 | 113.80 |
| 1 | AA | 2502 | G | N3-C2-N2 | 5.59 | 123.81 | 119.90 |
| 34 | BA | 1464 | G | C5-C6-O6 | -5.59 | 125.25 | 128.60 |
| 1 | CA | 1977 | A | N1-C6-N6 | -5.59 | 115.25 | 118.60 |
| 34 | DA | 290 | C | N3-C4-C5 | 5.58 | 124.13 | 121.90 |
| 1 | AA | 12 | U | O4'-C1'-N1 | -5.58 | 103.73 | 108.20 |
| 1 | CA | 2645 | G | N1-C6-O6 | 5.58 | 123.25 | 119.90 |
| 1 | CA | 265 | A | C4-C5-N7 | 5.58 | 113.49 | 110.70 |
| 1 | CA | 2523 | G | C4-C5-C6 | 5.58 | 122.15 | 118.80 |
| 34 | DA | 1499 | A | C8-N9-C4 | 5.58 | 108.03 | 105.80 |
| 1 | AA | 1232 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | AA | 2529 | C | C2-N3-C4 | 5.58 | 122.69 | 119.90 |
| 1 | AA | 2599 | A | OP1-P-O3' | 5.58 | 117.47 | 105.20 |
| 1 | CA | 1899 | G | C4-C5-N7 | 5.58 | 113.03 | 110.80 |
| 1 | CA | 2876 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | AA | 724 | A | C4-C5-N7 | -5.58 | 107.91 | 110.70 |
| 1 | AA | 808 | A | N1-C6-N6 | 5.58 | 121.95 | 118.60 |
| 1 | AA | 2022 | G | C2-N3-C4 | 5.58 | 114.69 | 111.90 |
| 1 | CA | 2253 | G | C8-N9-C4 | 5.58 | 108.63 | 106.40 |
| 1 | AA | 847 | A | N9-C4-C5 | 5.57 | 108.03 | 105.80 |
| 1 | AA | 2770 | A | N1-C2-N3 | -5.57 | 126.51 | 129.30 |
| 20 | AW | 18 | ARG | NE-CZ-NH1 | 5.57 | 123.09 | 120.30 |
| 1 | AA | 859 | C | C6-N1-C2 | 5.57 | 122.53 | 120.30 |
| 1 | AA | 2657 | G | N9-C4-C5 | -5.57 | 103.17 | 105.40 |
| 1 | CA | 1629 | U | C5-C6-N1 | 5.57 | 125.49 | 122.70 |
| 1 | AA | 943 | C | C2-N1-C1' | 5.57 | 124.92 | 118.80 |
| 1 | CA | 963 | U | C6-N1-C2 | 5.57 | 124.34 | 121.00 |
| 1 | AA | 507 | G | O5'-P-OP2 | -5.57 | 100.69 | 105.70 |
| 1 | AA | 639 | G | N1-C6-O6 | -5.57 | 116.56 | 119.90 |
| 1 | AA | 2431 | U | C6-N1-C2 | 5.57 | 124.34 | 121.00 |
| 34 | BA | 770 | C | OP1-P-OP2 | -5.57 | 111.25 | 119.60 |
| 34 | BA | 1344 | C | O5'-P-OP2 | -5.57 | 100.69 | 105.70 |
| 1 | AA | 137 | G | N3-C4-N9 | 5.56 | 129.34 | 126.00 |
| 1 | AA | 721 | G | N3-C2-N2 | 5.56 | 123.79 | 119.90 |
| 1 | AA | 742 | G | C4-C5-N7 | -5.56 | 108.58 | 110.80 |
| 1 | AA | 1002 | A | O5'-P-OP2 | -5.56 | 100.69 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | AA | 1183 | G | O5'-P-OP1 | -5.56 | 100.69 | 105.70 |
| 1 | AA | 1187 | U | N3-C4-O4 | 5.56 | 123.29 | 119.40 |
| 1 | AA | 1273 | G | C5-N7-C8 | 5.56 | 107.08 | 104.30 |
| 1 | CA | 798 | G | C5-C6-O6 | 5.56 | 131.94 | 128.60 |
| 1 | CA | 2431 | U | C5-C6-N1 | -5.56 | 119.92 | 122.70 |
| 1 | AA | 706 | C | C6-N1-C2 | 5.56 | 122.52 | 120.30 |
| 1 | CA | 2576 | G | N7-C8-N9 | -5.56 | 110.32 | 113.10 |
| 1 | AA | 1312 | G | N3-C4-N9 | 5.56 | 129.34 | 126.00 |
| 1 | AA | 1432 | C | N1-C2-O2 | -5.56 | 115.56 | 118.90 |
| 1 | AA | 2708 | U | C5-C6-N1 | -5.56 | 119.92 | 122.70 |
| 1 | CA | 12 | U | N3-C2-O2 | -5.56 | 118.31 | 122.20 |
| 1 | CA | 2571 | C | C2-N3-C4 | -5.56 | 117.12 | 119.90 |
| 1 | AA | 1029 | A | C4-C5-N7 | -5.56 | 107.92 | 110.70 |
| 1 | AA | 1274 | G | C5-C6-O6 | 5.56 | 131.94 | 128.60 |
| 1 | AA | 2727 | G | O5'-P-OP1 | 5.56 | 117.37 | 110.70 |
| 1 | CA | 1653 | G | N1-C2-N3 | 5.56 | 127.23 | 123.90 |
| 1 | AA | 801 | C | C5-C6-N1 | -5.56 | 118.22 | 121.00 |
| 1 | AA | 2570 | C | N3-C4-C5 | 5.56 | 124.12 | 121.90 |
| 1 | CA | 743 | G | N1-C2-N2 | -5.56 | 111.20 | 116.20 |
| 1 | CA | 2822 | G | C6-C5-N7 | -5.56 | 127.07 | 130.40 |
| 1 | CA | 2824 | C | N1-C2-O2 | -5.56 | 115.57 | 118.90 |
| 1 | AA | 2831 | A | N1-C2-N3 | 5.55 | 132.08 | 129.30 |
| 1 | CA | 1634 | A | C6-N1-C2 | -5.55 | 115.27 | 118.60 |
| 1 | AA | 174 | U | N1-C2-N3 | 5.55 | 118.23 | 114.90 |
| 1 | AA | 663 | G | C5-C6-O6 | 5.55 | 131.93 | 128.60 |
| 1 | AA | 1474 | C | N1-C2-O2 | -5.55 | 115.57 | 118.90 |
| 1 | AA | 1751 | G | C5-C6-O6 | 5.55 | 131.93 | 128.60 |
| 34 | BA | 243 | A | OP1-P-OP2 | 5.55 | 127.93 | 119.60 |
| 34 | BA | 884 | U | N3-C2-O2 | 5.55 | 126.09 | 122.20 |
| 1 | CA | 673 | C | O5'-P-OP2 | -5.55 | 100.70 | 105.70 |
| 1 | AA | 2346 | G | OP2-P-O3' | 5.55 | 117.41 | 105.20 |
| 1 | AA | 2620 | G | C6-N1-C2 | -5.55 | 121.77 | 125.10 |
| 1 | AA | 2663 | C | C6-N1-C2 | 5.55 | 122.52 | 120.30 |
| 34 | BA | 792 | A | O4'-C1'-N9 | 5.55 | 112.64 | 108.20 |
| 1 | CA | 665 | C | N3-C4-C5 | 5.55 | 124.12 | 121.90 |
| 1 | CA | 1997 | G | C5'-C4'-O4' | 5.55 | 115.76 | 109.10 |
| 1 | AA | 2583 | C | C6-N1-C2 | 5.55 | 122.52 | 120.30 |
| 1 | CA | 1288 | U | N3-C2-O2 | -5.55 | 118.32 | 122.20 |
| 1 | CA | 2082 | A | C8-N9-C4 | -5.55 | 103.58 | 105.80 |
| 1 | AA | 320 | C | C6-N1-C2 | 5.54 | 122.52 | 120.30 |
| 1 | AA | 31 | C | C2-N1-C1' | -5.54 | 112.70 | 118.80 |
| 1 | AA | 1240 | G | C5-C6-O6 | -5.54 | 125.27 | 128.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 2422 | G | O5'-P-OP1 | -5.54 | 100.71 | 105.70 |
| 1 | CA | 827 | U | C2-N3-C4 | -5.54 | 123.67 | 127.00 |
| 1 | AA | 1683 | C | C4-C5-C6 | 5.54 | 120.17 | 117.40 |
| 1 | CA | 2273 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 1 | AA | 709 | G | OP1-P-OP2 | -5.54 | 111.29 | 119.60 |
| 1 | AA | 2876 | U | C4-C5-C6 | 5.54 | 123.02 | 119.70 |
| 1 | CA | 1768 | U | C5-C4-O4 | 5.54 | 129.22 | 125.90 |
| 1 | CA | 2570 | G | C4-C5-N7 | -5.54 | 108.58 | 110.80 |
| 1 | AA | 644 | G | C5-C6-N1 | 5.54 | 114.27 | 111.50 |
| 1 | AA | 1438 | A | C8-N9-C4 | 5.54 | 108.02 | 105.80 |
| 1 | AA | 18 | C | C4-C5-C6 | 5.54 | 120.17 | 117.40 |
| 1 | CA | 973 | A | N1-C6-N6 | -5.54 | 115.28 | 118.60 |
| 1 | AA | 209 | G | C8-N9-C4 | 5.53 | 108.61 | 106.40 |
| 1 | AA | 1014 | U | N3-C4-O4 | -5.53 | 115.53 | 119.40 |
| 1 | AA | 2802 | C | N1-C2-O2 | -5.53 | 115.58 | 118.90 |
| 1 | AA | 2051 | G | N3-C2-N2 | -5.53 | 116.03 | 119.90 |
| 1 | AA | 471 | C | OP1-P-OP2 | -5.53 | 111.31 | 119.60 |
| 1 | AA | 784 | C | N3-C2-O2 | 5.53 | 125.77 | 121.90 |
| 1 | AA | 800 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 1 | AA | 605 | G | C2-N3-C4 | -5.53 | 109.14 | 111.90 |
| 1 | AA | 799 | A | N1-C6-N6 | 5.53 | 121.92 | 118.60 |
| 1 | AA | 2641 | A | C4-C5-N7 | 5.53 | 113.46 | 110.70 |
| 1 | AA | 2712 | C | C6-N1-C2 | 5.53 | 122.51 | 120.30 |
| 1 | CA | 2550 | G | N1-C2-N3 | 5.53 | 127.22 | 123.90 |
| 1 | CA | 2855 | C | C5-C6-N1 | 5.53 | 123.76 | 121.00 |
| 1 | AA | 1290 | G | N3-C2-N2 | 5.53 | 123.77 | 119.90 |
| 1 | AA | 1385 | G | C8-N9-C4 | 5.53 | 108.61 | 106.40 |
| 1 | AA | 1925 | G | O5'-P-OP1 | -5.53 | 100.73 | 105.70 |
| 1 | AA | 2775 | G | N1-C6-O6 | -5.53 | 116.58 | 119.90 |
| 1 | CA | 1047 | G | N3-C4-N9 | 5.53 | 129.31 | 126.00 |
| 1 | CA | 2287 | A | C5-C6-N1 | -5.53 | 114.94 | 117.70 |
| 1 | CA | 2608 | G | O5'-P-OP2 | -5.53 | 100.73 | 105.70 |
| 4 | CD | 229 | VAL | CB-CA-C | -5.53 | 100.90 | 111.40 |
| 1 | AA | 1964 | C | C4-C5-C6 | -5.52 | 114.64 | 117.40 |
| 1 | AA | 23 | G | N9-C4-C5 | 5.52 | 107.61 | 105.40 |
| 1 | AA | 2273 | C | N1-C2-N3 | 5.52 | 123.07 | 119.20 |
| 1 | AA | 2745 | G | N1-C2-N3 | 5.52 | 127.21 | 123.90 |
| 34 | BA | 353 | A | OP2-P-O3' | 5.52 | 117.35 | 105.20 |
| 1 | CA | 315 | G | O5'-P-OP2 | -5.52 | 100.73 | 105.70 |
| 1 | CA | 1698 | A | C4-C5-C6 | 5.52 | 119.76 | 117.00 |
| 1 | CA | 2618 | G | C5-N7-C8 | 5.52 | 107.06 | 104.30 |
| 1 | AA | 279 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 593 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 34 | BA | 1530 | G | C4-N9-C1' | -5.52 | 119.32 | 126.50 |
| 1 | CA | 2050 | C | C2-N3-C4 | -5.52 | 117.14 | 119.90 |
| 1 | CA | 2598 | A | C2-N3-C4 | -5.52 | 107.84 | 110.60 |
| 34 | DA | 1484 | C | C5-C4-N4 | -5.52 | 116.34 | 120.20 |
| 1 | AA | 31 | C | C6-N1-C1' | 5.52 | 127.42 | 120.80 |
| 1 | AA | 2096 | U | N3-C4-C5 | -5.52 | 111.29 | 114.60 |
| 1 | CA | 33 | U | N3-C2-O2 | -5.52 | 118.34 | 122.20 |
| 1 | CA | 2067 | G | C8-N9-C4 | -5.52 | 104.19 | 106.40 |
| 34 | DA | 1522 | U | OP2-P-O3' | 5.52 | 117.34 | 105.20 |
| 1 | AA | 2050 | U | N3-C4-O4 | -5.52 | 115.54 | 119.40 |
| 1 | AA | 2641 | A | C2-N3-C4 | -5.52 | 107.84 | 110.60 |
| 1 | AA | 2359 | C | N3-C2-O2 | -5.51 | 118.04 | 121.90 |
| 34 | BA | 893 | C | N3-C4-N4 | 5.51 | 121.86 | 118.00 |
| 1 | CA | 2604 | U | N1-C2-O2 | 5.51 | 126.66 | 122.80 |
| 1 | AA | 16 | G | N1-C6-O6 | -5.51 | 116.59 | 119.90 |
| 34 | BA | 1407 | C | N3-C2-O2 | 5.51 | 125.76 | 121.90 |
| 1 | CA | 599 | G | N3-C4-N9 | 5.51 | 129.31 | 126.00 |
| 1 | AA | 2221 | A | C8-N9-C4 | -5.51 | 103.59 | 105.80 |
| 1 | CA | 1021 | A | C4-C5-N7 | 5.51 | 113.46 | 110.70 |
| 1 | AA | 488 | C | N1-C2-O2 | -5.51 | 115.59 | 118.90 |
| 1 | AA | 530 | A | N7-C8-N9 | 5.51 | 116.56 | 113.80 |
| 1 | AA | 981 | C | N1-C2-O2 | -5.51 | 115.59 | 118.90 |
| 1 | AA | 1834 | A | OP2-P-O3' | 5.51 | 117.32 | 105.20 |
| 1 | AA | 2676 | G | N3-C4-N9 | 5.51 | 129.31 | 126.00 |
| 34 | DA | 576 | G | N9-C4-C5 | -5.51 | 103.20 | 105.40 |
| 34 | DA | 705 | U | O5'-P-OP2 | -5.51 | 100.74 | 105.70 |
| 1 | AA | 26 | G | N3-C4-C5 | -5.51 | 125.85 | 128.60 |
| 1 | AA | 236 | G | N1-C6-O6 | 5.51 | 123.20 | 119.90 |
| 1 | AA | 449 | A | OP1-P-OP2 | -5.51 | 111.34 | 119.60 |
| 1 | AA | 1314 | A | C2-N3-C4 | -5.51 | 107.85 | 110.60 |
| 1 | AA | 1719 | C | N3-C2-O2 | 5.51 | 125.75 | 121.90 |
| 1 | AA | 2584 | A | OP1-P-O3' | 5.51 | 117.32 | 105.20 |
| 34 | BA | 322 | C | C6-N1-C2 | 5.51 | 122.50 | 120.30 |
| 1 | CA | 2557 | G | N1-C2-N2 | -5.50 | 111.25 | 116.20 |
| 1 | AA | 2398 | C | C5-C4-N4 | 5.50 | 124.05 | 120.20 |
| 34 | DA | 489 | C | C6-N1-C2 | -5.50 | 118.10 | 120.30 |
| 1 | AA | 2556 | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 34 | BA | 321 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 1 | CA | 2559 | C | C6-N1-C2 | 5.50 | 122.50 | 120.30 |
| 1 | CA | 2560 | C | C5-C4-N4 | -5.50 | 116.35 | 120.20 |
| 1 | AA | 398 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | AA | 1371 | G | C2-N3-C4 | 5.50 | 114.65 | 111.90 |
| 1 | AA | 2456 | G | C5-C6-O6 | -5.50 | 125.30 | 128.60 |
| 1 | AA | 22 | C | N3-C2-O2 | -5.50 | 118.05 | 121.90 |
| 1 | AA | 549 | U | C2-N3-C4 | -5.50 | 123.70 | 127.00 |
| 1 | AA | 781 | A | N1-C6-N6 | 5.50 | 121.90 | 118.60 |
| 1 | AA | 1359 | U | N3-C2-O2 | -5.50 | 118.35 | 122.20 |
| 1 | AA | 1674 | G | O5'-P-OP1 | -5.50 | 100.75 | 105.70 |
| 1 | CA | 2454 | G | C5-C6-O6 | 5.50 | 131.90 | 128.60 |
| 1 | AA | 714 | U | N1-C2-O2 | -5.50 | 118.95 | 122.80 |
| 1 | AA | 721 | G | C6-N1-C2 | 5.50 | 128.40 | 125.10 |
| 1 | AA | 2113 | U | N1-C2-N3 | 5.50 | 118.20 | 114.90 |
| 1 | AA | 2233 | G | C5-C6-O6 | 5.50 | 131.90 | 128.60 |
| 1 | AA | 2312 | G | N9-C4-C5 | 5.50 | 107.60 | 105.40 |
| 1 | AA | 2566 | U | O5'-P-OP1 | -5.50 | 100.75 | 105.70 |
| 1 | AA | 17 | G | C6-N1-C2 | -5.49 | 121.80 | 125.10 |
| 1 | AA | 118 | U | OP1-P-OP2 | -5.49 | 111.36 | 119.60 |
| 1 | AA | 1427 | G | C4-C5-N7 | 5.49 | 113.00 | 110.80 |
| 1 | AA | 2373 | A | N1-C6-N6 | 5.49 | 121.90 | 118.60 |
| 2 | AB | 101 | G | O5'-P-OP2 | 5.49 | 117.29 | 110.70 |
| 1 | CA | 704 | G | N3-C4-N9 | 5.49 | 129.30 | 126.00 |
| 1 | AA | 585 | U | C4-C5-C6 | -5.49 | 116.41 | 119.70 |
| 34 | BA | 244 | U | N3-C2-O2 | -5.49 | 118.36 | 122.20 |
| 1 | CA | 692 | C | N3-C4-N4 | -5.49 | 114.16 | 118.00 |
| 1 | AA | 1296 | G | N3-C2-N2 | 5.49 | 123.74 | 119.90 |
| 1 | AA | 2529 | C | O5'-P-OP1 | 5.49 | 117.29 | 110.70 |
| 2 | AB | 83 | G | N1-C6-O6 | -5.49 | 116.61 | 119.90 |
| 1 | CA | 945 | A | N3-C4-N9 | -5.49 | 123.01 | 127.40 |
| 1 | AA | 83 | A | O4'-C1'-N9 | 5.49 | 112.59 | 108.20 |
| 1 | AA | 455 | A | C5'-C4'-C3' | -5.49 | 107.22 | 116.00 |
| 1 | AA | 1157 | A | C5-N7-C8 | -5.49 | 101.16 | 103.90 |
| 1 | AA | 1597 | C | C5-C4-N4 | -5.49 | 116.36 | 120.20 |
| 1 | AA | 2446 | A | N1-C6-N6 | -5.49 | 115.31 | 118.60 |
| 1 | AA | 2798 | C | C4-C5-C6 | 5.48 | 120.14 | 117.40 |
| 34 | BA | 1520 | G | N1-C6-O6 | 5.48 | 123.19 | 119.90 |
| 1 | AA | 410 | U | O4'-C1'-N1 | 5.48 | 112.58 | 108.20 |
| 1 | CA | 2539 | C | C5-C6-N1 | -5.48 | 118.26 | 121.00 |
| 34 | DA | 1416 | G | C8-N9-C4 | 5.48 | 108.59 | 106.40 |
| 1 | AA | 551 | A | C5-C6-N6 | 5.48 | 128.08 | 123.70 |
| 1 | AA | 2252 | C | O5'-P-OP2 | -5.48 | 100.77 | 105.70 |
| 34 | BA | 1414 | U | C6-N1-C2 | 5.48 | 124.29 | 121.00 |
| 1 | CA | 1965 | C | N1-C2-O2 | -5.48 | 115.61 | 118.90 |
| 1 | AA | 614 | C | N3-C4-C5 | 5.47 | 124.09 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | AA | 1028 | C | C5-C6-N1 | 5.47 | 123.74 | 121.00 |
| 1 | AA | 2757 | G | C8-N9-C4 | 5.47 | 108.59 | 106.40 |
| 34 | BA | 953 | G | O5'-P-OP2 | -5.47 | 100.77 | 105.70 |
| 1 | CA | 746 | A | O4'-C1'-N9 | 5.47 | 112.58 | 108.20 |
| 1 | AA | 2775 | G | O5'-P-OP2 | -5.47 | 100.78 | 105.70 |
| 1 | AA | 2271 | G | N1-C2-N2 | -5.47 | 111.28 | 116.20 |
| 34 | BA | 771 | G | N3-C2-N2 | -5.47 | 116.07 | 119.90 |
| 1 | CA | 933 | A | C4-C5-N7 | 5.47 | 113.44 | 110.70 |
| 1 | CA | 2287 | A | C5-N7-C8 | -5.47 | 101.17 | 103.90 |
| 1 | CA | 2221 | G | C5-C6-O6 | 5.47 | 131.88 | 128.60 |
| 1 | AA | 1180 | C | N1-C2-O2 | -5.47 | 115.62 | 118.90 |
| 1 | AA | 1984 | C | C4-C5-C6 | -5.47 | 114.67 | 117.40 |
| 1 | CA | 1142(A) | A | N7-C8-N9 | 5.47 | 116.53 | 113.80 |
| 1 | AA | 2451 | A | C8-N9-C4 | -5.46 | 103.61 | 105.80 |
| 34 | BA | 1074 | G | N1-C6-O6 | 5.46 | 123.18 | 119.90 |
| 1 | CA | 1125 | G | C8-N9-C4 | 5.46 | 108.59 | 106.40 |
| 1 | CA | 1661 | G | N7-C8-N9 | -5.46 | 110.37 | 113.10 |
| 1 | CA | 806 | C | C4-C5-C6 | -5.46 | 114.67 | 117.40 |
| 1 | CA | 2424 | C | N1-C2-O2 | -5.46 | 115.62 | 118.90 |
| 1 | AA | 784 | C | N1-C2-O2 | -5.46 | 115.62 | 118.90 |
| 1 | AA | 1617 | A | C5-C6-N6 | -5.46 | 119.33 | 123.70 |
| 1 | AA | 2024 | G | C8-N9-C4 | 5.46 | 108.58 | 106.40 |
| 1 | AA | 2375 | C | N3-C2-O2 | -5.46 | 118.08 | 121.90 |
| 34 | BA | 785 | G | N1-C6-O6 | 5.46 | 123.18 | 119.90 |
| 1 | CA | 34 | C | C6-N1-C2 | -5.46 | 118.11 | 120.30 |
| 1 | CA | 2254 | C | OP2-P-O3' | 5.46 | 117.21 | 105.20 |
| 34 | DA | 1442 | G | P-O3'-C3' | 5.46 | 126.25 | 119.70 |
| 1 | AA | 888 | A | N1-C6-N6 | 5.46 | 121.88 | 118.60 |
| 1 | AA | 2250 | G | OP2-P-O3' | 5.46 | 117.21 | 105.20 |
| 34 | BA | 886 | G | N3-C2-N2 | -5.46 | 116.08 | 119.90 |
| 1 | CA | 1022 | G | N3-C4-N9 | -5.46 | 122.72 | 126.00 |
| 1 | CA | 57 | C | N1-C2-O2 | -5.46 | 115.63 | 118.90 |
| 1 | AA | 412 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 1 | AA | 1264 | G | C6-C5-N7 | -5.46 | 127.13 | 130.40 |
| 1 | CA | 1812 | A | O5'-P-OP1 | -5.46 | 100.79 | 105.70 |
| 1 | AA | 841 | G | C8-N9-C4 | 5.45 | 108.58 | 106.40 |
| 1 | AA | 872 | C | C2-N3-C4 | -5.45 | 117.17 | 119.90 |
| 1 | CA | 1022 | G | N9-C4-C5 | 5.45 | 107.58 | 105.40 |
| 1 | CA | 2610 | C | O5'-P-OP1 | -5.45 | 100.79 | 105.70 |
| 1 | AA | 2751 | A | N7-C8-N9 | -5.45 | 111.07 | 113.80 |
| 2 | AB | 79 | C | N3-C4-C5 | -5.45 | 119.72 | 121.90 |
| 1 | AA | 2636 | G | N3-C2-N2 | -5.45 | 116.08 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2 | AB | 99 | G | C4-C5-N7 | 5.45 | 112.98 | 110.80 |
| 1 | CA | 1807 | G | N9-C4-C5 | -5.45 | 103.22 | 105.40 |
| 34 | DA | 1405 | G | N1-C2-N2 | -5.45 | 111.29 | 116.20 |
| 1 | AA | 818 | G | N1-C6-O6 | -5.45 | 116.63 | 119.90 |
| 1 | AA | 2776 | G | N1-C6-O6 | 5.45 | 123.17 | 119.90 |
| 1 | CA | 2766 | G | C4-C5-N7 | 5.45 | 112.98 | 110.80 |
| 1 | CA | 1259 | G | N1-C2-N2 | -5.45 | 111.30 | 116.20 |
| 1 | AA | 843 | C | C4-C5-C6 | 5.45 | 120.12 | 117.40 |
| 1 | CA | 2540 | C | N3-C4-C5 | 5.45 | 124.08 | 121.90 |
| 34 | DA | 510 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 34 | DA | 1502 | A | N7-C8-N9 | 5.45 | 116.52 | 113.80 |
| 1 | CA | 1282 | U | C5-C4-O4 | 5.44 | 129.17 | 125.90 |
| 1 | CA | 2690 | C | N1-C2-O2 | -5.44 | 115.63 | 118.90 |
| 1 | AA | 555 | G | OP2-P-O3' | 5.44 | 117.17 | 105.20 |
| 1 | AA | 1253 | C | C4-C5-C6 | 5.44 | 120.12 | 117.40 |
| 1 | AA | 2259 | A | N1-C2-N3 | 5.44 | 132.02 | 129.30 |
| 1 | CA | 1425 | G | N3-C4-N9 | 5.44 | 129.26 | 126.00 |
| 34 | DA | 897 | C | C5-C6-N1 | -5.44 | 118.28 | 121.00 |
| 1 | AA | 725 | C | N3-C2-O2 | 5.44 | 125.71 | 121.90 |
| 1 | AA | 2251 | G | OP1-P-OP2 | -5.44 | 111.44 | 119.60 |
| 1 | AA | 2890 | C | N3-C2-O2 | -5.44 | 118.09 | 121.90 |
| 34 | BA | 881 | G | O5'-P-OP1 | 5.44 | 117.23 | 110.70 |
| 1 | AA | 542 | C | OP2-P-O3' | 5.44 | 117.17 | 105.20 |
| 1 | AA | 2077 | C | C2-N1-C1' | -5.44 | 112.82 | 118.80 |
| 1 | CA | 2579 | C | C6-N1-C2 | -5.44 | 118.12 | 120.30 |
| 1 | AA | 2622 | C | O5'-P-OP2 | -5.44 | 100.81 | 105.70 |
| 1 | CA | 1692 | U | N3-C2-O2 | 5.44 | 126.01 | 122.20 |
| 1 | CA | 2023 | G | C6-C5-N7 | -5.44 | 127.14 | 130.40 |
| 1 | AA | 1360 | C | C2-N3-C4 | -5.43 | 117.18 | 119.90 |
| 1 | CA | 945 | A | C5-C6-N6 | -5.43 | 119.35 | 123.70 |
| 1 | CA | 1407 | C | N3-C2-O2 | 5.43 | 125.70 | 121.90 |
| 1 | CA | 2424 | C | C5-C6-N1 | -5.43 | 118.28 | 121.00 |
| 1 | AA | 1014 | U | OP2-P-O3' | 5.43 | 117.15 | 105.20 |
| 1 | AA | 1426 | G | N7-C8-N9 | -5.43 | 110.38 | 113.10 |
| 1 | AA | 1835 | C | OP1-P-OP2 | -5.43 | 111.45 | 119.60 |
| 1 | AA | 2443 | U | C5-C6-N1 | -5.43 | 119.98 | 122.70 |
| 1 | AA | 2538 | G | C2-N3-C4 | -5.43 | 109.18 | 111.90 |
| 1 | CA | 583 | G | N3-C2-N2 | -5.43 | 116.10 | 119.90 |
| 1 | CA | 2832 | U | C6-N1-C2 | 5.43 | 124.26 | 121.00 |
| 1 | AA | 2475 | C | C5-C6-N1 | -5.43 | 118.28 | 121.00 |
| 1 | CA | 1208 | C | OP2-P-O3' | 5.43 | 117.15 | 105.20 |
| 1 | CA | 2690 | C | C2-N1-C1' | -5.43 | 112.83 | 118.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2233 | G | C4-C5-N7 | -5.43 | 108.63 | 110.80 |
| 1 | AA | 2497 | G | C8-N9-C4 | 5.43 | 108.57 | 106.40 |
| 1 | CA | 786 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 1 | AA | 839 | G | O5'-P-OP1 | -5.43 | 100.82 | 105.70 |
| 1 | AA | 1796 | C | N3-C4-C5 | 5.43 | 124.07 | 121.90 |
| 34 | BA | 1193 | G | O5'-P-OP1 | -5.43 | 100.82 | 105.70 |
| 1 | CA | 599 | G | N3-C4-C5 | -5.43 | 125.89 | 128.60 |
| 1 | AA | 1735 | U | N3-C4-O4 | -5.42 | 115.60 | 119.40 |
| 1 | AA | 2367 | C | O5'-P-OP1 | -5.42 | 100.82 | 105.70 |
| 1 | AA | 2370 | G | N1-C2-N2 | -5.42 | 111.32 | 116.20 |
| 34 | DA | 1158 | C | N3-C2-O2 | -5.42 | 118.10 | 121.90 |
| 1 | AA | 1955 | G | C4-N9-C1' | 5.42 | 133.55 | 126.50 |
| 1 | AA | 2619 | G | C6-N1-C2 | -5.42 | 121.85 | 125.10 |
| 1 | CA | 2772 | C | N3-C4-C5 | -5.42 | 119.73 | 121.90 |
| 1 | AA | 2113 | U | C4-C5-C6 | 5.42 | 122.95 | 119.70 |
| 1 | AA | 2434 | A | O4'-C1'-N9 | 5.42 | 112.54 | 108.20 |
| 1 | CA | 2740 | A | N7-C8-N9 | -5.42 | 111.09 | 113.80 |
| 1 | CA | 2755 | C | C5-C6-N1 | 5.42 | 123.71 | 121.00 |
| 1 | CA | 2832 | U | C5-C6-N1 | -5.42 | 119.99 | 122.70 |
| 1 | AA | 2095 | C | OP2-P-O3' | 5.42 | 117.12 | 105.20 |
| 1 | AA | 2502 | G | N3-C4-N9 | 5.42 | 129.25 | 126.00 |
| 1 | AA | 2715 | C | C4-C5-C6 | 5.42 | 120.11 | 117.40 |
| 1 | CA | 2601 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 1 | CA | 2710 | C | C6-N1-C2 | 5.42 | 122.47 | 120.30 |
| 1 | AA | 182 | U | C4-C5-C6 | 5.42 | 122.95 | 119.70 |
| 1 | AA | 887 | C | C5-C6-N1 | -5.42 | 118.29 | 121.00 |
| 1 | AA | 1048 | G | O5'-P-OP2 | -5.42 | 100.83 | 105.70 |
| 1 | AA | 2229 | A | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 34 | BA | 1515 | C | N3-C4-C5 | 5.42 | 124.07 | 121.90 |
| 39 | DF | 87 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | AA | 552 | C | C6-N1-C2 | -5.42 | 118.13 | 120.30 |
| 1 | CA | 1801 | G | O4'-C1'-N9 | 5.42 | 112.53 | 108.20 |
| 1 | AA | 145 | G | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 1 | AA | 1006 | C | C6-N1-C1' | 5.41 | 127.30 | 120.80 |
| 1 | AA | 1234 | A | C5-C6-N6 | -5.41 | 119.37 | 123.70 |
| 1 | AA | 1264 | G | N9-C4-C5 | -5.41 | 103.23 | 105.40 |
| 34 | BA | 1496 | C | C6-N1-C2 | 5.41 | 122.47 | 120.30 |
| 1 | AA | 417 | A | N1-C6-N6 | 5.41 | 121.85 | 118.60 |
| 1 | CA | 945 | A | C6-N1-C2 | 5.41 | 121.85 | 118.60 |
| 1 | AA | 1807 | G | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 1 | CA | 673 | C | N1-C2-O2 | -5.41 | 115.65 | 118.90 |
| 1 | AA | 992 | G | N1-C2-N2 | -5.41 | 111.33 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1374 | G | C5-C6-O6 | -5.41 | 125.36 | 128.60 |
| 1 | AA | 1440 | U | N1-C2-O2 | 5.41 | 126.59 | 122.80 |
| 1 | AA | 2708 | U | C2-N3-C4 | -5.41 | 123.75 | 127.00 |
| 1 | AA | 1385 | G | C5-C6-N1 | 5.41 | 114.20 | 111.50 |
| 1 | CA | 1489 | U | C5-C4-O4 | 5.41 | 129.14 | 125.90 |
| 1 | CA | 1696 | G | N1-C6-O6 | -5.41 | 116.66 | 119.90 |
| 34 | DA | 266 | G | C2-N3-C4 | -5.41 | 109.20 | 111.90 |
| 1 | AA | 1265 | A | N1-C6-N6 | 5.41 | 121.84 | 118.60 |
| 1 | AA | 1378 | G | C6-C5-N7 | -5.41 | 127.16 | 130.40 |
| 1 | AA | 2029 | C | C4-C5-C6 | 5.41 | 120.10 | 117.40 |
| 1 | AA | 2072 | C | C4-C5-C6 | 5.41 | 120.10 | 117.40 |
| 1 | AA | 2427 | G | N1-C6-O6 | 5.41 | 123.14 | 119.90 |
| 1 | CA | 2511 | U | N3-C4-O4 | -5.41 | 115.62 | 119.40 |
| 34 | DA | 1484 | C | N3-C2-O2 | 5.41 | 125.68 | 121.90 |
| 1 | AA | 554 | A | C5-N7-C8 | -5.40 | 101.20 | 103.90 |
| 1 | AA | 887 | C | C4-C5-C6 | 5.40 | 120.10 | 117.40 |
| 1 | AA | 1204 | C | C2-N3-C4 | -5.40 | 117.20 | 119.90 |
| 1 | AA | 2497 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 1 | AA | 2565 | G | N3-C4-C5 | -5.40 | 125.90 | 128.60 |
| 1 | AA | 2637 | G | C6-C5-N7 | 5.40 | 133.64 | 130.40 |
| 34 | DA | 1484 | C | N3-C4-C5 | 5.40 | 124.06 | 121.90 |
| 1 | AA | 1030 | A | N7-C8-N9 | -5.40 | 111.10 | 113.80 |
| 1 | AA | 2479 | C | OP2-P-O3' | 5.40 | 117.08 | 105.20 |
| 1 | AA | 2882 | G | C6-C5-N7 | 5.40 | 133.64 | 130.40 |
| 1 | CA | 2285 | C | O5'-P-OP2 | -5.40 | 100.84 | 105.70 |
| 1 | AA | 2788 | A | C5-C6-N6 | 5.40 | 128.02 | 123.70 |
| 34 | BA | 1403 | C | N3-C4-N4 | -5.40 | 114.22 | 118.00 |
| 1 | AA | 1026 | A | C5-N7-C8 | -5.40 | 101.20 | 103.90 |
| 1 | AA | 1067 | A | N1-C6-N6 | 5.40 | 121.84 | 118.60 |
| 1 | AA | 2083 | G | C5-C6-N1 | 5.40 | 114.20 | 111.50 |
| 1 | CA | 786 | C | O5'-P-OP1 | -5.40 | 100.84 | 105.70 |
| 1 | CA | 1653 | G | N1-C6-O6 | -5.40 | 116.66 | 119.90 |
| 1 | CA | 1899 | G | C5-N7-C8 | -5.40 | 101.60 | 104.30 |
| 1 | AA | 1050 | C | N3-C2-O2 | 5.39 | 125.68 | 121.90 |
| 1 | AA | 2118 | U | OP2-P-O3' | 5.39 | 117.07 | 105.20 |
| 1 | AA | 800 | C | C5-C6-N1 | -5.39 | 118.30 | 121.00 |
| 1 | AA | 1598 | C | C4-C5-C6 | 5.39 | 120.10 | 117.40 |
| 1 | AA | 1457 | C | N3-C2-O2 | -5.39 | 118.13 | 121.90 |
| 1 | CA | 2221 | G | C8-N9-C4 | -5.39 | 104.24 | 106.40 |
| 1 | AA | 596 | G | C8-N9-C4 | -5.39 | 104.25 | 106.40 |
| 1 | CA | 577 | G | C5-C6-O6 | -5.39 | 125.37 | 128.60 |
| 1 | AA | 231 | G | OP1-P-OP2 | -5.39 | 111.52 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 1 | AA | 558 | G | C4-C5-C6 | -5.39 | 115.57 | 118.80 |
| 1 | AA | 585 | U | N3-C2-O2 | -5.39 | 118.43 | 122.20 |
| 1 | AA | 894 | U | C4-C5-C6 | 5.39 | 122.93 | 119.70 |
| 1 | AA | 2285 | A | C8-N9-C4 | 5.39 | 107.95 | 105.80 |
| 1 | AA | 2477 | C | C6-N1-C2 | 5.39 | 122.45 | 120.30 |
| 1 | AA | 2487 | C | C6-N1-C2 | -5.39 | 118.14 | 120.30 |
| 34 | DA | 913 | A | P-O3'-C3' | 5.39 | 126.16 | 119.70 |
| 1 | AA | 1613 | A | N1-C2-N3 | -5.38 | 126.61 | 129.30 |
| 1 | AA | 1846 | A | N1-C2-N3 | 5.38 | 131.99 | 129.30 |
| 1 | AA | 2494 | G | N1-C6-O6 | 5.38 | 123.13 | 119.90 |
| 34 | BA | 43 | C | C6-N1-C2 | 5.38 | 122.45 | 120.30 |
| 34 | BA | 317 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 1 | CA | 2536 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 1 | AA | 2344 | U | C5-C6-N1 | -5.38 | 120.01 | 122.70 |
| 1 | AA | 2461 | U | C5-C4-O4 | -5.38 | 122.67 | 125.90 |
| 1 | AA | 2620 | G | C5-C6-O6 | -5.38 | 125.37 | 128.60 |
| 2 | AB | 62 | C | N1-C2-O2 | -5.38 | 115.67 | 118.90 |
| 1 | CA | 2519 | U | N1-C2-O2 | -5.38 | 119.03 | 122.80 |
| 1 | AA | 601 | A | C5-C6-N6 | 5.38 | 128.00 | 123.70 |
| 1 | AA | 2287 | C | C5'-C4'-O4' | -5.38 | 102.64 | 109.10 |
| 34 | BA | 1520 | G | C4-C5-N7 | 5.38 | 112.95 | 110.80 |
| 1 | CA | 1626 | G | C4-C5-N7 | -5.38 | 108.65 | 110.80 |
| 1 | CA | 2452 | C | OP2-P-O3' | 5.38 | 117.04 | 105.20 |
| 1 | CA | 2439 | A | C5'-C4'-O4' | -5.38 | 102.64 | 109.10 |
| 1 | AA | 808 | A | C4-C5-C6 | 5.38 | 119.69 | 117.00 |
| 1 | AA | 1306 | G | OP2-P-O3' | 5.38 | 117.03 | 105.20 |
| 1 | AA | 2093 | A | O5'-P-OP2 | -5.38 | 100.86 | 105.70 |
| 1 | AA | 2475 | C | N3-C4-N4 | -5.38 | 114.23 | 118.00 |
| 34 | BA | 801 | U | C5-C6-N1 | -5.38 | 120.01 | 122.70 |
| 1 | CA | 847 | U | N1-C2-N3 | 5.38 | 118.13 | 114.90 |
| 1 | CA | 1992 | G | P-O3'-C3' | 5.38 | 126.15 | 119.70 |
| 1 | CA | 2360 | A | C8-N9-C4 | 5.38 | 107.95 | 105.80 |
| 1 | AA | 1232 | G | N1-C2-N3 | -5.38 | 120.67 | 123.90 |
| 16 | AS | 25 | ARG | NE-CZ-NH1 | -5.38 | 117.61 | 120.30 |
| 1 | CA | 271(M) | G | OP1-P-O3' | 5.38 | 117.03 | 105.20 |
| 1 | CA | 1794 | U | N1-C2-N3 | 5.38 | 118.12 | 114.90 |
| 1 | CA | 2708 | G | N9-C4-C5 | -5.38 | 103.25 | 105.40 |
| 1 | AA | 1804 | A | O5'-P-OP1 | 5.38 | 117.15 | 110.70 |
| 1 | AA | 777 | C | C2-N3-C4 | -5.37 | 117.21 | 119.90 |
| 1 | AA | 1020 | C | OP1-P-O3' | 5.37 | 117.02 | 105.20 |
| 1 | CA | 515 | A | C2-N3-C4 | 5.37 | 113.29 | 110.60 |
| 34 | DA | 354 | G | C4-N9-C1' | 5.37 | 133.49 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1169 | C | N3-C4-C5 | 5.37 | 124.05 | 121.90 |
| 1 | AA | 2502 | G | C4-C5-N7 | 5.37 | 112.95 | 110.80 |
| 2 | AB | 84 | C | C2-N1-C1' | 5.37 | 124.71 | 118.80 |
| 1 | CA | 2032 | G | N1-C6-O6 | -5.37 | 116.68 | 119.90 |
| 34 | DA | 1529 | G | C8-N9-C1' | -5.37 | 120.02 | 127.00 |
| 1 | AA | 730 | C | N3-C2-O2 | -5.37 | 118.14 | 121.90 |
| 1 | AA | 1921 | G | N3-C4-N9 | 5.37 | 129.22 | 126.00 |
| 1 | AA | 2021 | C | N1-C2-O2 | -5.37 | 115.68 | 118.90 |
| 34 | BA | 1401 | G | C5-C6-N1 | -5.37 | 108.81 | 111.50 |
| 1 | AA | 1329 | G | N9-C4-C5 | -5.37 | 103.25 | 105.40 |
| 1 | AA | 2264 | G | C5-C6-N1 | -5.37 | 108.82 | 111.50 |
| 1 | AA | 2427 | G | N3-C2-N2 | -5.37 | 116.14 | 119.90 |
| 1 | AA | 2427 | G | C5-C6-N1 | 5.37 | 114.18 | 111.50 |
| 1 | AA | 2639 | G | N3-C2-N2 | 5.37 | 123.66 | 119.90 |
| 1 | AA | 2713 | C | C4-C5-C6 | 5.37 | 120.08 | 117.40 |
| 1 | CA | 321 | G | O4'-C1'-N9 | 5.37 | 112.50 | 108.20 |
| 1 | CA | 1989 | G | O5'-P-OP1 | -5.37 | 100.87 | 105.70 |
| 1 | AA | 2797 | C | N1-C2-O2 | 5.37 | 122.12 | 118.90 |
| 1 | AA | 2883 | A | C5-N7-C8 | -5.37 | 101.22 | 103.90 |
| 1 | CA | 1425 | G | C5-C6-O6 | -5.37 | 125.38 | 128.60 |
| 1 | AA | 899 | G | C5-C6-O6 | 5.37 | 131.82 | 128.60 |
| 1 | AA | 2588 | G | N1-C2-N2 | 5.37 | 121.03 | 116.20 |
| 1 | CA | 1266 | G | C5-C6-O6 | -5.37 | 125.38 | 128.60 |
| 1 | AA | 780 | G | C5-N7-C8 | 5.36 | 106.98 | 104.30 |
| 1 | AA | 2001 | C | C6-N1-C2 | -5.36 | 118.16 | 120.30 |
| 1 | CA | 782 | A | C5-C6-N6 | -5.36 | 119.41 | 123.70 |
| 34 | DA | 329 | A | N1-C6-N6 | 5.36 | 121.82 | 118.60 |
| 34 | DA | 915 | A | O5'-P-OP2 | -5.36 | 100.87 | 105.70 |
| 1 | AA | 1985 | U | OP1-P-O3' | 5.36 | 117.00 | 105.20 |
| 1 | AA | 2050 | U | N1-C2-O2 | 5.36 | 126.55 | 122.80 |
| 2 | AB | 102 | A | N1-C6-N6 | 5.36 | 121.82 | 118.60 |
| 1 | AA | 1329 | G | C8-N9-C4 | 5.36 | 108.54 | 106.40 |
| 1 | AA | 1802 | C | C2-N3-C4 | -5.36 | 117.22 | 119.90 |
| 1 | AA | 2513 | C | C6-N1-C2 | 5.36 | 122.44 | 120.30 |
| 34 | BA | 527 | G | C8-N9-C4 | -5.36 | 104.25 | 106.40 |
| 34 | BA | 889 | A | O5'-P-OP2 | -5.36 | 100.88 | 105.70 |
| 1 | AA | 2245 | U | N1-C2-N3 | 5.36 | 118.12 | 114.90 |
| 1 | AA | 2433 | G | N1-C6-O6 | 5.36 | 123.11 | 119.90 |
| 1 | CA | 2893 | G | N3-C4-C5 | -5.36 | 125.92 | 128.60 |
| 1 | AA | 912 | C | N3-C4-C5 | -5.36 | 119.76 | 121.90 |
| 1 | AA | 2399 | U | N1-C2-O2 | -5.36 | 119.05 | 122.80 |
| 1 | CA | 2581 | G | O5'-P-OP2 | -5.36 | 100.88 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1055 | A | C2-N3-C4 | 5.36 | 113.28 | 110.60 |
| 1 | AA | 2043 | C | N3-C4-C5 | 5.36 | 124.04 | 121.90 |
| 1 | AA | 2069 | U | C5-C4-O4 | -5.36 | 122.69 | 125.90 |
| 1 | AA | 2513 | C | C5-C6-N1 | -5.36 | 118.32 | 121.00 |
| 1 | AA | 2802 | C | C6-N1-C1' | 5.36 | 127.23 | 120.80 |
| 1 | AA | 2825 | C | N1-C2-O2 | 5.36 | 122.11 | 118.90 |
| 34 | BA | 404 | U | N3-C2-O2 | -5.36 | 118.45 | 122.20 |
| 34 | BA | 852 | G | C8-N9-C4 | 5.36 | 108.54 | 106.40 |
| 1 | AA | 800 | C | N3-C4-C5 | 5.35 | 124.04 | 121.90 |
| 1 | AA | 880 | U | O5'-P-OP1 | -5.35 | 100.88 | 105.70 |
| 1 | AA | 2427 | G | N1-C2-N2 | 5.35 | 121.02 | 116.20 |
| 1 | AA | 468 | G | C5-C6-O6 | -5.35 | 125.39 | 128.60 |
| 1 | AA | 869 | U | C6-N1-C2 | -5.35 | 117.79 | 121.00 |
| 1 | AA | 1324 | A | N9-C4-C5 | 5.35 | 107.94 | 105.80 |
| 34 | BA | 317 | G | C6-C5-N7 | -5.35 | 127.19 | 130.40 |
| 1 | CA | 31 | C | C2-N3-C4 | -5.35 | 117.22 | 119.90 |
| 1 | CA | 176 | G | N9-C4-C5 | -5.35 | 103.26 | 105.40 |
| 1 | CA | 2897 | U | C2-N1-C1' | 5.35 | 124.12 | 117.70 |
| 1 | AA | 181 | C | N1-C2-O2 | -5.35 | 115.69 | 118.90 |
| 1 | AA | 788 | G | O5'-P-OP1 | -5.35 | 100.89 | 105.70 |
| 1 | AA | 845 | G | N7-C8-N9 | -5.35 | 110.43 | 113.10 |
| 2 | AB | 7 | G | C5-N7-C8 | -5.35 | 101.63 | 104.30 |
| 34 | BA | 1406 | U | C5-C6-N1 | -5.35 | 120.03 | 122.70 |
| 1 | CA | 2835 | A | OP1-P-O3' | 5.35 | 116.97 | 105.20 |
| 1 | AA | 2498 | G | N3-C4-C5 | -5.35 | 125.93 | 128.60 |
| 2 | AB | 109 | C | O4'-C1'-N1 | 5.35 | 112.48 | 108.20 |
| 1 | CA | 2448 | A | N1-C6-N6 | 5.35 | 121.81 | 118.60 |
| 1 | CA | 2645 | G | C6-C5-N7 | -5.35 | 127.19 | 130.40 |
| 1 | AA | 203 | G | OP2-P-O3' | 5.34 | 116.96 | 105.20 |
| 34 | BA | 1407 | C | C6-N1-C2 | 5.34 | 122.44 | 120.30 |
| 34 | DA | 830 | G | N1-C6-O6 | 5.34 | 123.11 | 119.90 |
| 1 | AA | 77 | A | C2-N3-C4 | -5.34 | 107.93 | 110.60 |
| 1 | AA | 2277 | U | N1-C2-O2 | -5.34 | 119.06 | 122.80 |
| 1 | CA | 1416 | G | O4'-C1'-N9 | 5.34 | 112.47 | 108.20 |
| 1 | AA | 1487 | G | N3-C2-N2 | -5.34 | 116.16 | 119.90 |
| 1 | AA | 2043 | C | C2-N3-C4 | -5.34 | 117.23 | 119.90 |
| 1 | AA | 2393 | C | C5-C6-N1 | -5.34 | 118.33 | 121.00 |
| 1 | AA | 2657 | G | N1-C6-O6 | 5.34 | 123.11 | 119.90 |
| 1 | CA | 185 | U | N3-C4-O4 | -5.34 | 115.66 | 119.40 |
| 1 | CA | 418 | G | C8-N9-C4 | 5.34 | 108.54 | 106.40 |
| 1 | CA | 1842 | G | C8-N9-C4 | 5.34 | 108.54 | 106.40 |
| 34 | DA | 866 | C | N3-C2-O2 | -5.34 | 118.16 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 737 | G | N7-C8-N9 | -5.34 | 110.43 | 113.10 |
| 1 | AA | 1725 | G | C6-C5-N7 | -5.34 | 127.20 | 130.40 |
| 1 | AA | 2271 | G | N3-C2-N2 | 5.34 | 123.64 | 119.90 |
| 34 | BA | 299 | G | N1-C6-O6 | 5.34 | 123.10 | 119.90 |
| 1 | AA | 502 | G | N7-C8-N9 | -5.34 | 110.43 | 113.10 |
| 1 | AA | 1457 | C | N1-C2-O2 | 5.34 | 122.10 | 118.90 |
| 1 | AA | 1842 | G | C4-C5-N7 | -5.34 | 108.67 | 110.80 |
| 1 | CA | 2877 | G | N1-C6-O6 | 5.34 | 123.10 | 119.90 |
| 34 | DA | 367 | U | N3-C4-O4 | 5.34 | 123.14 | 119.40 |
| 34 | BA | 1484 | C | C6-N1-C2 | 5.33 | 122.43 | 120.30 |
| 1 | AA | 413 | G | N3-C4-C5 | -5.33 | 125.93 | 128.60 |
| 1 | AA | 2586 | G | C5-C6-N1 | 5.33 | 114.17 | 111.50 |
| 1 | AA | 1434 | G | C5-N7-C8 | 5.33 | 106.97 | 104.30 |
| 1 | AA | 2542 | A | C5-C6-N1 | -5.33 | 115.03 | 117.70 |
| 34 | BA | 438 | G | C8-N9-C4 | -5.33 | 104.27 | 106.40 |
| 1 | CA | 2867 | G | N3-C4-C5 | 5.33 | 131.27 | 128.60 |
| 1 | AA | 40 | C | C2-N3-C4 | -5.33 | 117.23 | 119.90 |
| 1 | AA | 2756 | C | O5'-P-OP1 | -5.33 | 100.90 | 105.70 |
| 38 | BE | 53 | LEU | CA-CB-CG | 5.33 | 127.56 | 115.30 |
| 1 | CA | 435 | C | N1-C2-O2 | 5.33 | 122.10 | 118.90 |
| 1 | CA | 659 | C | C5-C6-N1 | -5.33 | 118.33 | 121.00 |
| 1 | AA | 55 | A | O5'-P-OP1 | -5.33 | 100.90 | 105.70 |
| 1 | AA | 990 | A | C6-N1-C2 | -5.33 | 115.40 | 118.60 |
| 1 | AA | 2039 | U | C4-C5-C6 | 5.33 | 122.90 | 119.70 |
| 1 | AA | 2533 | C | C5-C6-N1 | -5.33 | 118.34 | 121.00 |
| 1 | CA | 1809 | A | C5-C6-N6 | -5.33 | 119.44 | 123.70 |
| 1 | CA | 2448 | A | O5'-P-OP1 | -5.33 | 100.91 | 105.70 |
| 57 | DX | 17 | C | C2-N1-C1' | 5.33 | 124.66 | 118.80 |
| 1 | AA | 205 | A | C8-N9-C4 | 5.33 | 107.93 | 105.80 |
| 1 | AA | 1011 | G | C5-C6-N1 | -5.33 | 108.84 | 111.50 |
| 1 | AA | 2617 | U | O5'-P-OP2 | -5.33 | 100.91 | 105.70 |
| 1 | CA | 2292 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 1 | CA | 2595 | G | O5'-P-OP2 | 5.33 | 117.09 | 110.70 |
| 1 | AA | 471 | C | N1-C2-N3 | 5.32 | 122.93 | 119.20 |
| 1 | AA | 1728 | G | C5-C6-O6 | -5.32 | 125.41 | 128.60 |
| 34 | BA | 529 | G | C5-C6-O6 | -5.32 | 125.41 | 128.60 |
| 35 | BB | 9 | GLU | N-CA-C | 5.32 | 125.37 | 111.00 |
| 1 | CA | 1937 | A | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |
| 1 | CA | 769 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 1 | CA | 1406 | U | N3-C4-O4 | -5.32 | 115.67 | 119.40 |
| 1 | AA | 888 | A | C2-N3-C4 | -5.32 | 107.94 | 110.60 |
| 1 | AA | 1218 | G | O4'-C1'-N9 | 5.32 | 112.46 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1593 | C | N3-C4-C5 | -5.32 | 119.77 | 121.90 |
| 1 | AA | 2312 | G | N7-C8-N9 | 5.32 | 115.76 | 113.10 |
| 1 | AA | 2477 | C | N3-C4-N4 | -5.32 | 114.28 | 118.00 |
| 2 | AB | 73 | A | OP1-P-OP2 | 5.32 | 127.58 | 119.60 |
| 1 | CA | 2043 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 1 | CA | 2402 | C | N1-C2-O2 | -5.32 | 115.71 | 118.90 |
| 1 | AA | 550 | U | O5'-P-OP2 | -5.32 | 100.91 | 105.70 |
| 1 | AA | 1518 | A | N7-C8-N9 | 5.32 | 116.46 | 113.80 |
| 1 | AA | 2735 | G | C2-N3-C4 | 5.32 | 114.56 | 111.90 |
| 34 | BA | 1417 | G | C8-N9-C4 | 5.32 | 108.53 | 106.40 |
| 1 | AA | 1745 | A | N9-C1'-C2' | 5.32 | 120.91 | 114.00 |
| 1 | AA | 2454 | C | C4-C5-C6 | 5.32 | 120.06 | 117.40 |
| 2 | AB | 15 | A | N9-C4-C5 | -5.32 | 103.67 | 105.80 |
| 1 | CA | 1400 | G | C8-N9-C4 | -5.32 | 104.27 | 106.40 |
| 1 | AA | 315 | C | C6-N1-C2 | 5.32 | 122.43 | 120.30 |
| 1 | AA | 1299 | A | N7-C8-N9 | -5.32 | 111.14 | 113.80 |
| 1 | CA | 2513 | G | N1-C6-O6 | 5.32 | 123.09 | 119.90 |
| 1 | CA | 2080 | G | N7-C8-N9 | -5.31 | 110.44 | 113.10 |
| 1 | AA | 98 | U | N3-C4-O4 | -5.31 | 115.68 | 119.40 |
| 1 | AA | 555 | G | C8-N9-C1' | 5.31 | 133.91 | 127.00 |
| 1 | AA | 2015 | U | O5'-P-OP1 | -5.31 | 100.92 | 105.70 |
| 34 | BA | 811 | C | C6-N1-C2 | 5.31 | 122.42 | 120.30 |
| 1 | CA | 1675 | C | C6-N1-C2 | -5.31 | 118.17 | 120.30 |
| 34 | DA | 17 | U | N1-C2-O2 | 5.31 | 126.52 | 122.80 |
| 34 | DA | 1154 | G | C4-C5-N7 | 5.31 | 112.92 | 110.80 |
| 1 | AA | 644 | G | N1-C2-N2 | -5.31 | 111.42 | 116.20 |
| 1 | AA | 1384 | G | N1-C2-N3 | 5.31 | 127.09 | 123.90 |
| 1 | AA | 184 | A | C5-N7-C8 | -5.31 | 101.25 | 103.90 |
| 1 | AA | 395 | C | N1-C2-N3 | 5.31 | 122.92 | 119.20 |
| 1 | CA | 1047 | G | N3-C4-C5 | -5.31 | 125.95 | 128.60 |
| 1 | CA | 2496 | C | N3-C4-N4 | -5.31 | 114.28 | 118.00 |
| 1 | AA | 584 | G | C5-C6-N1 | 5.31 | 114.15 | 111.50 |
| 1 | AA | 893 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 1 | AA | 1273 | G | N7-C8-N9 | -5.31 | 110.45 | 113.10 |
| 1 | AA | 2024 | G | N9-C4-C5 | -5.31 | 103.28 | 105.40 |
| 1 | CA | 185 | U | N3-C2-O2 | -5.31 | 118.48 | 122.20 |
| 1 | CA | 408 | G | O5'-P-OP2 | -5.31 | 100.92 | 105.70 |
| 1 | AA | 1248 | G | C5-C6-N1 | 5.31 | 114.15 | 111.50 |
| 34 | BA | 830 | G | OP1-P-OP2 | -5.31 | 111.64 | 119.60 |
| 1 | AA | 334 | A | C8-N9-C4 | 5.30 | 107.92 | 105.80 |
| 1 | AA | 511 | C | O5'-P-OP1 | -5.30 | 100.93 | 105.70 |
| 1 | AA | 1344 | C | N1-C2-O2 | -5.30 | 115.72 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1474 | C | C5-C6-N1 | -5.30 | 118.35 | 121.00 |
| 1 | AA | 2583 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 34 | BA | 1406 | U | O5'-P-OP2 | -5.30 | 100.92 | 105.70 |
| 1 | CA | 2337 | G | C6-C5-N7 | -5.30 | 127.22 | 130.40 |
| 1 | AA | 354 | A | C4-C5-C6 | -5.30 | 114.35 | 117.00 |
| 34 | BA | 733 | A | OP1-P-OP2 | 5.30 | 127.56 | 119.60 |
| 1 | AA | 358 | C | N1-C2-O2 | -5.30 | 115.72 | 118.90 |
| 1 | AA | 1370 | G | OP1-P-O3' | 5.30 | 116.86 | 105.20 |
| 1 | AA | 2598 | C | N3-C4-C5 | 5.30 | 124.02 | 121.90 |
| 34 | BA | 1286 | A | C8-N9-C4 | -5.30 | 103.68 | 105.80 |
| 1 | CA | 852 | G | C5-C6-O6 | 5.30 | 131.78 | 128.60 |
| 1 | CA | 2067 | G | N3-C4-C5 | -5.30 | 125.95 | 128.60 |
| 1 | AA | 505 | A | O4'-C1'-N9 | 5.30 | 112.44 | 108.20 |
| 1 | CA | 1238 | G | O5'-P-OP2 | -5.30 | 100.93 | 105.70 |
| 1 | CA | 1697 | G | N9-C4-C5 | -5.30 | 103.28 | 105.40 |
| 1 | AA | 2587 | C | C6-N1-C1' | -5.30 | 114.44 | 120.80 |
| 1 | AA | 236 | G | C5-C6-O6 | -5.30 | 125.42 | 128.60 |
| 1 | AA | 1385 | G | N3-C4-N9 | 5.30 | 129.18 | 126.00 |
| 1 | AA | 1872 | U | OP1-P-O3' | 5.30 | 116.85 | 105.20 |
| 1 | AA | 793 | A | O5'-P-OP2 | 5.29 | 117.05 | 110.70 |
| 1 | AA | 817 | G | N9-C4-C5 | -5.29 | 103.28 | 105.40 |
| 1 | CA | 2200 | C | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 1 | AA | 238 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 1 | AA | 472 | G | N1-C2-N3 | -5.29 | 120.72 | 123.90 |
| 1 | AA | 1169 | C | C2-N3-C4 | -5.29 | 117.25 | 119.90 |
| 1 | AA | 1757 | C | N1-C2-O2 | -5.29 | 115.73 | 118.90 |
| 1 | AA | 2831 | A | N1-C6-N6 | 5.29 | 121.78 | 118.60 |
| 1 | CA | 659 | C | C6-N1-C2 | 5.29 | 122.42 | 120.30 |
| 1 | AA | 1281 | G | N1-C2-N3 | 5.29 | 127.07 | 123.90 |
| 1 | AA | 74 | G | N1-C6-O6 | 5.29 | 123.07 | 119.90 |
| 1 | AA | 227 | C | C5-C4-N4 | -5.29 | 116.50 | 120.20 |
| 1 | AA | 1714 | G | N1-C6-O6 | -5.29 | 116.73 | 119.90 |
| 1 | AA | 1844 | G | N9-C4-C5 | -5.29 | 103.28 | 105.40 |
| 1 | AA | 2729 | U | N1-C2-O2 | -5.29 | 119.10 | 122.80 |
| 1 | AA | 2849 | G | N1-C2-N2 | -5.29 | 111.44 | 116.20 |
| 1 | CA | 840 | C | N1-C2-O2 | -5.29 | 115.73 | 118.90 |
| 1 | CA | 1697 | G | C5-C6-O6 | -5.29 | 125.43 | 128.60 |
| 1 | AA | 1617 | A | C4-C5-N7 | 5.29 | 113.34 | 110.70 |
| 1 | CA | 1850 | G | C6-C5-N7 | -5.29 | 127.23 | 130.40 |
| 1 | AA | 1154 | U | OP1-P-O3' | 5.29 | 116.83 | 105.20 |
| 1 | AA | 1236 | G | O5'-P-OP1 | -5.29 | 100.94 | 105.70 |
| 1 | CA | 513 | A | C2-N3-C4 | -5.29 | 107.96 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 671 | C | C5-C6-N1 | 5.29 | 123.64 | 121.00 |
| 1 | CA | 840 | C | N3-C4-N4 | 5.29 | 121.70 | 118.00 |
| 1 | CA | 945 | A | C5-C6-N1 | -5.29 | 115.06 | 117.70 |
| 1 | CA | 1647 | G | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 1 | CA | 1809 | A | N1-C6-N6 | 5.29 | 121.77 | 118.60 |
| 1 | AA | 976 | G | N3-C2-N2 | -5.28 | 116.20 | 119.90 |
| 1 | AA | 1643 | A | N7-C8-N9 | -5.28 | 111.16 | 113.80 |
| 1 | AA | 1952 | G | C5-N7-C8 | 5.28 | 106.94 | 104.30 |
| 1 | AA | 2608 | U | C6-N1-C2 | 5.28 | 124.17 | 121.00 |
| 34 | BA | 860 | A | C8-N9-C4 | -5.28 | 103.69 | 105.80 |
| 1 | AA | 1243 | U | N1-C2-O2 | -5.28 | 119.10 | 122.80 |
| 1 | AA | 2060 | G | N1-C6-O6 | -5.28 | 116.73 | 119.90 |
| 1 | CA | 692 | C | C5-C4-N4 | 5.28 | 123.90 | 120.20 |
| 34 | DA | 204 | U | C2-N1-C1' | 5.28 | 124.04 | 117.70 |
| 1 | AA | 418 | G | C6-C5-N7 | -5.28 | 127.23 | 130.40 |
| 1 | CA | 942 | G | C8-N9-C4 | 5.28 | 108.51 | 106.40 |
| 1 | AA | 564 | G | C2-N3-C4 | 5.28 | 114.54 | 111.90 |
| 1 | AA | 2045 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 34 | BA | 332 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 1 | CA | 816 | C | OP1-P-O3' | 5.28 | 116.81 | 105.20 |
| 1 | AA | 2598 | C | C5-C4-N4 | -5.28 | 116.51 | 120.20 |
| 1 | AA | 2871 | G | N1-C6-O6 | 5.28 | 123.07 | 119.90 |
| 1 | CA | 2521 | C | N1-C2-O2 | -5.28 | 115.73 | 118.90 |
| 1 | AA | 206 | G | N1-C6-O6 | 5.28 | 123.06 | 119.90 |
| 1 | AA | 1019 | G | N3-C2-N2 | -5.28 | 116.21 | 119.90 |
| 1 | AA | 1080 | G | OP1-P-OP2 | 5.28 | 127.51 | 119.60 |
| 1 | AA | 1710 | C | C4-C5-C6 | 5.28 | 120.04 | 117.40 |
| 1 | AA | 853 | C | N3-C4-N4 | -5.27 | 114.31 | 118.00 |
| 34 | BA | 991 | U | P-O3'-C3' | 5.27 | 126.03 | 119.70 |
| 1 | CA | 2359 | C | C5-C4-N4 | 5.27 | 123.89 | 120.20 |
| 1 | AA | 126 | C | OP1-P-OP2 | 5.27 | 127.51 | 119.60 |
| 1 | AA | 1535 | U | O5'-P-OP1 | -5.27 | 100.95 | 105.70 |
| 1 | CA | 2592 | G | C8-N9-C4 | -5.27 | 104.29 | 106.40 |
| 1 | AA | 418 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 1 | CA | 1832 | C | N3-C2-O2 | 5.27 | 125.59 | 121.90 |
| 1 | AA | 559 | U | C6-N1-C2 | 5.27 | 124.16 | 121.00 |
| 1 | AA | 2019 | G | N1-C2-N2 | -5.27 | 111.46 | 116.20 |
| 1 | AA | 2085 | C | O5'-P-OP1 | -5.27 | 100.96 | 105.70 |
| 1 | AA | 2459 | G | N3-C2-N2 | 5.27 | 123.59 | 119.90 |
| 34 | BA | 533 | A | O5'-P-OP1 | -5.27 | 100.96 | 105.70 |
| 1 | AA | 2335 | G | C6-C5-N7 | -5.27 | 127.24 | 130.40 |
| 1 | AA | 2707 | C | N1-C2-O2 | 5.27 | 122.06 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 34 | BA | 1458 | G | C8-N9-C4 | 5.27 | 108.51 | 106.40 |
| 34 | DA | 60 | A | P-O3'-C3' | 5.27 | 126.02 | 119.70 |
| 1 | AA | 969 | C | N1-C2-O2 | -5.27 | 115.74 | 118.90 |
| 34 | BA | 518 | C | N3-C2-O2 | -5.27 | 118.21 | 121.90 |
| 1 | CA | 2413 | G | N1-C6-O6 | 5.27 | 123.06 | 119.90 |
| 1 | AA | 841 | G | OP1-P-OP2 | -5.26 | 111.70 | 119.60 |
| 1 | AA | 969 | C | N3-C2-O2 | 5.26 | 125.58 | 121.90 |
| 1 | AA | 1024 | G | C5-C6-O6 | 5.26 | 131.76 | 128.60 |
| 1 | AA | 1925 | G | N7-C8-N9 | 5.26 | 115.73 | 113.10 |
| 34 | BA | 1508 | G | C4-C5-N7 | -5.26 | 108.69 | 110.80 |
| 1 | CA | 2239 | G | C8-N9-C4 | 5.26 | 108.50 | 106.40 |
| 34 | DA | 1465 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 1 | AA | 591 | U | N3-C4-O4 | -5.26 | 115.72 | 119.40 |
| 1 | AA | 723 | A | N7-C8-N9 | -5.26 | 111.17 | 113.80 |
| 1 | AA | 2081 | A | O4'-C1'-N9 | 5.26 | 112.41 | 108.20 |
| 1 | AA | 2773 | C | N3-C4-C5 | 5.26 | 124.00 | 121.90 |
| 1 | AA | 2303 | U | C5-C4-O4 | 5.26 | 129.06 | 125.90 |
| 34 | BA | 1340 | A | C8-N9-C4 | 5.26 | 107.90 | 105.80 |
| 34 | DA | 619 | U | N3-C2-O2 | -5.26 | 118.52 | 122.20 |
| 1 | AA | 1404 | G | C5-C6-O6 | 5.26 | 131.76 | 128.60 |
| 1 | AA | 1674 | G | OP1-P-O3' | 5.26 | 116.77 | 105.20 |
| 1 | AA | 1688 | A | C5-N7-C8 | -5.26 | 101.27 | 103.90 |
| 1 | AA | 2788 | A | C6-C5-N7 | 5.26 | 135.98 | 132.30 |
| 1 | AA | 2902 | G | C4-C5-N7 | 5.26 | 112.90 | 110.80 |
| 34 | BA | 389 | A | N1-C6-N6 | 5.26 | 121.76 | 118.60 |
| 1 | CA | 1505 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 34 | DA | 533 | A | C8-N9-C4 | -5.26 | 103.70 | 105.80 |
| 1 | AA | 735 | U | N1-C2-N3 | 5.26 | 118.06 | 114.90 |
| 1 | AA | 1231 | G | OP1-P-O3' | 5.26 | 116.76 | 105.20 |
| 1 | AA | 1744 | G | N1-C6-O6 | 5.26 | 123.05 | 119.90 |
| 1 | CA | 1217 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 1 | CA | 1421 | G | N1-C6-O6 | 5.26 | 123.05 | 119.90 |
| 1 | CA | 1531 | C | C2-N1-C1' | 5.26 | 124.58 | 118.80 |
| 1 | CA | 1774 | C | C6-N1-C2 | -5.26 | 118.20 | 120.30 |
| 1 | AA | 2734 | A | N7-C8-N9 | -5.25 | 111.17 | 113.80 |
| 1 | CA | 2406 | U | O4'-C1'-N1 | -5.25 | 104.00 | 108.20 |
| 1 | CA | 2516 | G | C2-N3-C4 | -5.25 | 109.27 | 111.90 |
| 1 | AA | 193 | A | C5-C6-N1 | 5.25 | 120.33 | 117.70 |
| 34 | BA | 1279 | A | N7-C8-N9 | 5.25 | 116.43 | 113.80 |
| 1 | CA | 1813 | G | C8-N9-C4 | 5.25 | 108.50 | 106.40 |
| 1 | CA | 2195 | C | OP1-P-O3' | 5.25 | 116.76 | 105.20 |
| 1 | AA | 2539 | C | C6-N1-C2 | 5.25 | 122.40 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | CA | 664 | C | N3-C4-C5 | 5.25 | 124.00 | 121.90 |
| 1 | CA | 744 | G | N1-C6-O6 | 5.25 | 123.05 | 119.90 |
| 1 | CA | 1877 | A | N1-C6-N6 | 5.25 | 121.75 | 118.60 |
| 1 | CA | 2003 | G | C5-C6-O6 | 5.25 | 131.75 | 128.60 |
| 1 | CA | 2399 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 34 | DA | 831 | U | C6-N1-C2 | -5.25 | 117.85 | 121.00 |
| 1 | AA | 615 | G | O5'-P-OP2 | -5.25 | 100.98 | 105.70 |
| 1 | AA | 1312 | G | N3-C4-C5 | -5.25 | 125.98 | 128.60 |
| 1 | AA | 1921 | G | C4-C5-N7 | 5.25 | 112.90 | 110.80 |
| 34 | BA | 841 | U | C6-N1-C2 | -5.25 | 117.85 | 121.00 |
| 34 | DA | 38 | G | C8-N9-C4 | 5.25 | 108.50 | 106.40 |
| 1 | AA | 596 | G | N3-C4-C5 | -5.25 | 125.98 | 128.60 |
| 1 | AA | 848 | G | C2-N3-C4 | -5.25 | 109.28 | 111.90 |
| 34 | BA | 1437 | C | N3-C2-O2 | -5.25 | 118.23 | 121.90 |
| 1 | CA | 987 | G | O5'-P-OP2 | 5.25 | 117.00 | 110.70 |
| 1 | AA | 193 | A | N1-C6-N6 | -5.24 | 115.45 | 118.60 |
| 1 | AA | 1026 | A | C5-C6-N6 | -5.24 | 119.51 | 123.70 |
| 1 | AA | 1098 | C | C6-N1-C2 | -5.24 | 118.20 | 120.30 |
| 1 | AA | 358 | C | C4-C5-C6 | 5.24 | 120.02 | 117.40 |
| 1 | AA | 961 | C | N3-C4-C5 | -5.24 | 119.80 | 121.90 |
| 1 | AA | 1954 | A | O5'-P-OP1 | -5.24 | 100.98 | 105.70 |
| 34 | BA | 155 | C | N1-C2-O2 | 5.24 | 122.05 | 118.90 |
| 1 | AA | 1728 | G | N7-C8-N9 | 5.24 | 115.72 | 113.10 |
| 1 | AA | 1753 | U | N1-C2-O2 | 5.24 | 126.47 | 122.80 |
| 34 | BA | 572 | A | C8-N9-C4 | 5.24 | 107.90 | 105.80 |
| 1 | CA | 1348 | G | N1-C6-O6 | 5.24 | 123.04 | 119.90 |
| 1 | CA | 1355 | G | N1-C6-O6 | -5.24 | 116.76 | 119.90 |
| 34 | DA | 813 | U | OP1-P-OP2 | -5.24 | 111.74 | 119.60 |
| 1 | AA | 1785 | C | C4-C5-C6 | 5.24 | 120.02 | 117.40 |
| 1 | CA | 2521 | C | C6-N1-C2 | 5.24 | 122.39 | 120.30 |
| 1 | AA | 2346 | G | C4-N9-C1' | 5.24 | 133.31 | 126.50 |
| 1 | AA | 2398 | C | C2-N1-C1' | -5.24 | 113.04 | 118.80 |
| 34 | BA | 1524 | C | C6-N1-C2 | -5.24 | 118.21 | 120.30 |
| 1 | AA | 32 | C | O5'-P-OP2 | -5.23 | 100.99 | 105.70 |
| 1 | AA | 2403 | G | O5'-P-OP2 | -5.23 | 100.99 | 105.70 |
| 1 | CA | 614 | U | N1-C2-O2 | 5.23 | 126.46 | 122.80 |
| 1 | CA | 2593 | U | N3-C4-O4 | -5.23 | 115.74 | 119.40 |
| 1 | CA | 2828 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 1 | AA | 1839 | U | N3-C2-O2 | 5.23 | 125.86 | 122.20 |
| 1 | AA | 2370 | G | N3-C2-N2 | 5.23 | 123.56 | 119.90 |
| 1 | AA | 2839 | C | C6-N1-C2 | 5.23 | 122.39 | 120.30 |
| 1 | AA | 1678 | A | C5-C6-N1 | -5.23 | 115.08 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | AA | 1688 | A | N7-C8-N9 | 5.23 | 116.42 | 113.80 |
| 1 | AA | 1171 | G | C5-C6-O6 | -5.23 | 125.46 | 128.60 |
| 34 | BA | 596 | C | C6-N1-C2 | 5.23 | 122.39 | 120.30 |
| 1 | AA | 581 | G | N3-C2-N2 | 5.23 | 123.56 | 119.90 |
| 1 | AA | 740 | C | N3-C4-N4 | -5.23 | 114.34 | 118.00 |
| 1 | AA | 1807 | G | C8-N9-C4 | 5.23 | 108.49 | 106.40 |
| 1 | AA | 2303 | U | C4-C5-C6 | 5.23 | 122.84 | 119.70 |
| 1 | AA | 2480 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | AA | 2590 | G | N3-C2-N2 | 5.23 | 123.56 | 119.90 |
| 1 | AA | 2799 | U | N3-C4-C5 | 5.23 | 117.74 | 114.60 |
| 1 | AA | 2858 | G | N1-C6-O6 | -5.23 | 116.76 | 119.90 |
| 1 | AA | 321 | C | C4-C5-C6 | 5.23 | 120.01 | 117.40 |
| 1 | AA | 1184 | G | C8-N9-C4 | -5.23 | 104.31 | 106.40 |
| 1 | AA | 2863 | C | C5-C6-N1 | -5.23 | 118.39 | 121.00 |
| 34 | BA | 869 | G | N1-C6-O6 | 5.23 | 123.04 | 119.90 |
| 1 | AA | 500 | G | N1-C2-N3 | 5.22 | 127.03 | 123.90 |
| 1 | AA | 1440 | U | OP1-P-OP2 | -5.22 | 111.76 | 119.60 |
| 1 | AA | 2441 | G | OP1-P-OP2 | -5.22 | 111.76 | 119.60 |
| 18 | CU | 74 | LEU | CA-CB-CG | 5.22 | 127.32 | 115.30 |
| 34 | BA | 795 | C | N1-C2-O2 | -5.22 | 115.77 | 118.90 |
| 1 | CA | 2066 | C | O5'-P-OP1 | -5.22 | 101.00 | 105.70 |
| 1 | AA | 199 | C | C2-N1-C1' | -5.22 | 113.06 | 118.80 |
| 1 | AA | 1849 | U | N1-C2-O2 | -5.22 | 119.14 | 122.80 |
| 1 | AA | 2637 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 1 | AA | 512 | C | OP1-P-O3' | 5.22 | 116.68 | 105.20 |
| 1 | AA | 615 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 1 | AA | 2572 | C | C4-C5-C6 | 5.22 | 120.01 | 117.40 |
| 1 | AA | 2879 | G | C5-C6-N1 | -5.22 | 108.89 | 111.50 |
| 34 | BA | 787 | A | OP2-P-O3' | 5.22 | 116.68 | 105.20 |
| 1 | CA | 154(A) | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 1 | AA | 250 | G | C5-C6-O6 | -5.22 | 125.47 | 128.60 |
| 1 | AA | 1835 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 2 | AB | 90 | A | N7-C8-N9 | -5.22 | 111.19 | 113.80 |
| 34 | DA | 175 | C | C6-N1-C2 | -5.22 | 118.21 | 120.30 |
| 1 | AA | 974 | G | C6-C5-N7 | -5.22 | 127.27 | 130.40 |
| 1 | AA | 1659 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 1 | AA | 2576 | A | C5-C6-N6 | 5.22 | 127.87 | 123.70 |
| 1 | AA | 2783 | G | C5-C6-O6 | -5.22 | 125.47 | 128.60 |
| 1 | CA | 241 | A | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 1 | AA | 410 | U | C4-C5-C6 | 5.21 | 122.83 | 119.70 |
| 1 | CA | 1284 | A | N9-C4-C5 | -5.21 | 103.71 | 105.80 |
| 34 | DA | 577 | G | OP2-P-O3' | 5.21 | 116.67 | 105.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | AA | 1301 | U | C4-C5-C6 | -5.21 | 116.57 | 119.70 |
| 1 | CA | 2570 | G | C5-C6-O6 | 5.21 | 131.73 | 128.60 |
| 1 | AA | 558 | G | C5-C6-N1 | 5.21 | 114.11 | 111.50 |
| 1 | AA | 2014 | G | C2'-C3'-O3' | 5.21 | 122.04 | 113.70 |
| 1 | AA | 2033 | U | C6-N1-C2 | -5.21 | 117.87 | 121.00 |
| 1 | AA | 2504 | U | OP2-P-O3' | 5.21 | 116.67 | 105.20 |
| 1 | CA | 2085 | C | C2-N3-C4 | -5.21 | 117.29 | 119.90 |
| 2 | CB | 30 | C | C2-N1-C1' | 5.21 | 124.53 | 118.80 |
| 1 | AA | 2858 | G | N3-C2-N2 | 5.21 | 123.55 | 119.90 |
| 1 | CA | 2822 | G | N9-C4-C5 | -5.21 | 103.32 | 105.40 |
| 1 | AA | 990 | A | C8-N9-C1' | -5.21 | 118.32 | 127.70 |
| 1 | AA | 1704 | C | OP2-P-O3' | 5.21 | 116.66 | 105.20 |
| 1 | AA | 2006 | G | OP2-P-O3' | 5.21 | 116.66 | 105.20 |
| 1 | AA | 2320 | G | C5-N7-C8 | -5.21 | 101.70 | 104.30 |
| 1 | AA | 2676 | G | C5-C6-O6 | -5.21 | 125.47 | 128.60 |
| 1 | CA | 1350 | C | N1-C2-O2 | -5.21 | 115.78 | 118.90 |
| 1 | CA | 1355 | G | C2-N3-C4 | 5.21 | 114.50 | 111.90 |
| 1 | AA | 1024 | G | C8-N9-C4 | 5.21 | 108.48 | 106.40 |
| 1 | AA | 1200 | G | OP1-P-OP2 | -5.21 | 111.79 | 119.60 |
| 1 | AA | 2101 | U | C4-C5-C6 | 5.21 | 122.82 | 119.70 |
| 1 | CA | 411 | G | O4'-C1'-N9 | -5.21 | 104.03 | 108.20 |
| 1 | AA | 22 | C | C5-C4-N4 | 5.21 | 123.84 | 120.20 |
| 34 | BA | 552 | U | C5-C6-N1 | -5.21 | 120.10 | 122.70 |
| 2 | CB | 56 | G | N3-C4-C5 | -5.21 | 126.00 | 128.60 |
| 1 | AA | 65 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 1 | AA | 995 | G | N7-C8-N9 | 5.20 | 115.70 | 113.10 |
| 1 | AA | 2633 | A | O5'-P-OP1 | -5.20 | 101.02 | 105.70 |
| 1 | CA | 426 | C | N1-C2-O2 | 5.20 | 122.02 | 118.90 |
| 1 | CA | 1964 | G | O4'-C1'-N9 | -5.20 | 104.04 | 108.20 |
| 34 | BA | 822 | C | C6-N1-C2 | 5.20 | 122.38 | 120.30 |
| 1 | CA | 948 | G | N9-C4-C5 | 5.20 | 107.48 | 105.40 |
| 1 | CA | 961 | C | OP1-P-OP2 | 5.20 | 127.40 | 119.60 |
| 1 | AA | 472 | G | C5-C6-O6 | -5.20 | 125.48 | 128.60 |
| 1 | AA | 1646 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 1 | AA | 1967 | G | N1-C2-N3 | 5.20 | 127.02 | 123.90 |
| 1 | AA | 2389 | A | N1-C6-N6 | 5.20 | 121.72 | 118.60 |
| 1 | AA | 2632 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 1 | AA | 2826 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 1 | CA | 1374 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 1 | CA | 1885 | A | N7-C8-N9 | -5.20 | 111.20 | 113.80 |
| 34 | BA | 768 | A | N1-C2-N3 | 5.20 | 131.90 | 129.30 |
| 34 | BA | 1511 | G | C8-N9-C4 | 5.20 | 108.48 | 106.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 474 | G | C6-N1-C2 | -5.20 | 121.98 | 125.10 |
| 1 | AA | 187 | C | N3-C4-C5 | 5.20 | 123.98 | 121.90 |
| 1 | AA | 1697 | G | OP1-P-OP2 | -5.20 | 111.81 | 119.60 |
| 1 | AA | 2303 | U | N1-C2-N3 | 5.20 | 118.02 | 114.90 |
| 1 | CA | 2599 | G | C6-C5-N7 | 5.20 | 133.52 | 130.40 |
| 1 | AA | 31 | C | N3-C4-N4 | -5.20 | 114.36 | 118.00 |
| 1 | AA | 479 | C | C5-C6-N1 | -5.20 | 118.40 | 121.00 |
| 34 | BA | 1471 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 1 | CA | 2431 | U | N3-C4-C5 | 5.20 | 117.72 | 114.60 |
| 34 | DA | 1481 | U | C5-C4-O4 | 5.20 | 129.02 | 125.90 |
| 1 | AA | 2561 | G | C6-C5-N7 | -5.19 | 127.28 | 130.40 |
| 1 | AA | 2294 | G | N9-C4-C5 | -5.19 | 103.32 | 105.40 |
| 1 | AA | 2619 | G | N1-C2-N3 | 5.19 | 127.02 | 123.90 |
| 1 | AA | 2877 | G | O4'-C1'-N9 | 5.19 | 112.36 | 108.20 |
| 1 | CA | 1611 | C | N1-C2-O2 | 5.19 | 122.02 | 118.90 |
| 1 | CA | 1721 | G | C5-C6-O6 | -5.19 | 125.48 | 128.60 |
| 1 | CA | 2356 | C | C6-N1-C2 | 5.19 | 122.38 | 120.30 |
| 1 | AA | 898 | U | C5-C6-N1 | -5.19 | 120.10 | 122.70 |
| 34 | BA | 791 | G | O5'-P-OP2 | 5.19 | 116.93 | 110.70 |
| 1 | CA | 795 | C | C4-C5-C6 | 5.19 | 120.00 | 117.40 |
| 2 | CB | 15 | A | C8-N9-C4 | 5.19 | 107.88 | 105.80 |
| 1 | AA | 1332 | A | O5'-P-OP2 | -5.19 | 101.03 | 105.70 |
| 1 | AA | 2221 | A | O5'-P-OP2 | 5.19 | 116.93 | 110.70 |
| 1 | CA | 1778 | U | C5-C6-N1 | -5.19 | 120.11 | 122.70 |
| 1 | AA | 884 | C | C4-C5-C6 | 5.19 | 119.99 | 117.40 |
| 1 | AA | 999 | G | N1-C2-N2 | -5.19 | 111.53 | 116.20 |
| 1 | AA | 1097 | G | N1-C6-O6 | 5.19 | 123.01 | 119.90 |
| 1 | AA | 1254 | G | C5-C6-O6 | -5.19 | 125.49 | 128.60 |
| 1 | AA | 1343 | C | N3-C4-N4 | -5.19 | 114.37 | 118.00 |
| 1 | AA | 2374 | G | N7-C8-N9 | -5.19 | 110.51 | 113.10 |
| 1 | CA | 826 | U | N3-C4-O4 | -5.19 | 115.77 | 119.40 |
| 1 | CA | 1155 | A | OP1-P-O3' | 5.19 | 116.61 | 105.20 |
| 1 | CA | 1372 | U | C5-C4-O4 | -5.19 | 122.79 | 125.90 |
| 1 | AA | 479 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 1 | AA | 551 | A | C4-C5-N7 | -5.18 | 108.11 | 110.70 |
| 1 | AA | 2017 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 1 | AA | 2281 | A | N1-C6-N6 | 5.18 | 121.71 | 118.60 |
| 1 | AA | 2726 | A | C8-N9-C4 | 5.18 | 107.87 | 105.80 |
| 1 | AA | 2761 | A | N7-C8-N9 | -5.18 | 111.21 | 113.80 |
| 34 | BA | 1482 | G | C8-N9-C1' | -5.18 | 120.26 | 127.00 |
| 1 | AA | 438 | G | N3-C2-N2 | -5.18 | 116.27 | 119.90 |
| 1 | AA | 2260 | C | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 1210 | A | OP2-P-O3' | 5.18 | 116.60 | 105.20 |
| 1 | CA | 1976 | U | C2-N3-C4 | -5.18 | 123.89 | 127.00 |
| 1 | AA | 74 | G | N3-C4-C5 | 5.18 | 131.19 | 128.60 |
| 1 | AA | 1078 | A | C8-N9-C4 | 5.18 | 107.87 | 105.80 |
| 1 | AA | 1472 | G | C5-C6-N1 | 5.18 | 114.09 | 111.50 |
| 1 | AA | 1983 | C | C4-C5-C6 | 5.18 | 119.99 | 117.40 |
| 1 | CA | 2508 | G | N1-C6-O6 | -5.18 | 116.79 | 119.90 |
| 1 | AA | 1242 | G | C8-N9-C4 | 5.18 | 108.47 | 106.40 |
| 1 | AA | 2056 | U | N1-C2-N3 | 5.18 | 118.01 | 114.90 |
| 1 | CA | 556 | G | C5-C6-O6 | -5.18 | 125.49 | 128.60 |
| 1 | CA | 1251 | C | OP1-P-OP2 | 5.18 | 127.37 | 119.60 |
| 1 | CA | 2046 | G | C8-N9-C4 | 5.18 | 108.47 | 106.40 |
| 1 | CA | 2647 | U | C6-N1-C2 | 5.18 | 124.11 | 121.00 |
| 1 | AA | 1811 | A | OP1-P-O3' | 5.18 | 116.59 | 105.20 |
| 1 | CA | 1374 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 34 | DA | 691 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 1 | AA | 1247 | C | C5-C4-N4 | -5.18 | 116.58 | 120.20 |
| 34 | BA | 266 | G | C8-N9-C4 | -5.18 | 104.33 | 106.40 |
| 1 | CA | 17 | G | OP1-P-OP2 | -5.18 | 111.83 | 119.60 |
| 1 | CA | 501 | A | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 1 | CA | 934 | G | C6-C5-N7 | -5.18 | 127.29 | 130.40 |
| 1 | CA | 2526 | G | N1-C6-O6 | 5.18 | 123.01 | 119.90 |
| 34 | DA | 557 | G | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 1 | AA | 1299 | A | C5-C6-N6 | -5.17 | 119.56 | 123.70 |
| 34 | BA | 760 | G | C5-C6-O6 | -5.17 | 125.50 | 128.60 |
| 1 | CA | 823 | G | C5-C6-N1 | 5.17 | 114.09 | 111.50 |
| 14 | AQ | 2 | LEU | CA-CB-CG | 5.17 | 127.20 | 115.30 |
| 34 | BA | 1227 | A | C2-N3-C4 | -5.17 | 108.01 | 110.60 |
| 1 | CA | 791 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |
| 1 | AA | 74 | G | C4-C5-N7 | 5.17 | 112.87 | 110.80 |
| 1 | AA | 816 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 1 | AA | 1024 | G | N1-C6-O6 | -5.17 | 116.80 | 119.90 |
| 1 | AA | 1361 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 1 | AA | 1612 | C | N1-C2-O2 | -5.17 | 115.80 | 118.90 |
| 1 | AA | 2051 | G | N9-C4-C5 | 5.17 | 107.47 | 105.40 |
| 1 | AA | 2400 | A | O4'-C1'-N9 | 5.17 | 112.34 | 108.20 |
| 18 | AU | 20 | LEU | CB-CG-CD1 | -5.17 | 102.21 | 111.00 |
| 19 | AV | 35 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 1 | CA | 1989 | G | C4-C5-N7 | 5.17 | 112.87 | 110.80 |
| 1 | AA | 884 | C | OP1-P-OP2 | -5.17 | 111.84 | 119.60 |
| 1 | AA | 454 | U | OP1-P-O3' | 5.17 | 116.57 | 105.20 |
| 1 | AA | 859 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1387 | U | N1-C2-O2 | -5.17 | 119.18 | 122.80 |
| 2 | AB | 15 | A | C8-N9-C4 | 5.17 | 107.87 | 105.80 |
| 1 | CA | 987 | G | C4-N9-C1' | -5.17 | 119.78 | 126.50 |
| 1 | AA | 1155 | C | C6-N1-C2 | -5.17 | 118.23 | 120.30 |
| 1 | AA | 1401 | G | C5-C6-O6 | 5.17 | 131.70 | 128.60 |
| 1 | AA | 2075 | G | O5'-P-OP2 | -5.17 | 101.05 | 105.70 |
| 1 | AA | 2550 | C | C6-N1-C2 | 5.17 | 122.37 | 120.30 |
| 1 | CA | 185 | U | C5-C6-N1 | -5.17 | 120.12 | 122.70 |
| 1 | AA | 455 | A | C5-C6-N1 | -5.17 | 115.12 | 117.70 |
| 1 | AA | 1281 | G | N1-C6-O6 | 5.16 | 123.00 | 119.90 |
| 1 | AA | 1623 | U | OP2-P-O3' | 5.16 | 116.56 | 105.20 |
| 2 | AB | 62 | C | OP1-P-OP2 | 5.16 | 127.35 | 119.60 |
| 1 | CA | 666 | G | N1-C2-N2 | -5.16 | 111.55 | 116.20 |
| 1 | CA | 2863 | C | N3-C4-C5 | 5.16 | 123.97 | 121.90 |
| 1 | AA | 777 | C | N3-C2-O2 | -5.16 | 118.29 | 121.90 |
| 34 | DA | 866 | C | N1-C2-O2 | 5.16 | 122.00 | 118.90 |
| 1 | AA | 200 | A | C2-N3-C4 | -5.16 | 108.02 | 110.60 |
| 1 | AA | 971 | C | C2-N3-C4 | -5.16 | 117.32 | 119.90 |
| 1 | AA | 2114 | U | N1-C2-O2 | 5.16 | 126.41 | 122.80 |
| 1 | AA | 2117 | C | OP2-P-O3' | 5.16 | 116.55 | 105.20 |
| 1 | CA | 2063 | C | OP2-P-O3' | 5.16 | 116.55 | 105.20 |
| 34 | DA | 1527 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 1 | AA | 310 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 1 | AA | 2016 | C | N3-C4-C5 | -5.16 | 119.84 | 121.90 |
| 1 | AA | 2035 | A | N9-C4-C5 | -5.16 | 103.74 | 105.80 |
| 1 | CA | 1647 | G | C6-C5-N7 | 5.16 | 133.50 | 130.40 |
| 1 | CA | 2032 | G | N7-C8-N9 | -5.16 | 110.52 | 113.10 |
| 2 | CB | 80 | U | C5-C4-O4 | 5.16 | 129.00 | 125.90 |
| 2 | AB | 55 | U | N1-C2-O2 | -5.16 | 119.19 | 122.80 |
| 1 | CA | 2292 | C | C6-N1-C2 | 5.16 | 122.36 | 120.30 |
| 1 | CA | 2720 | U | N3-C2-O2 | -5.16 | 118.59 | 122.20 |
| 34 | BA | 1477 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 1 | CA | 827 | U | N3-C4-C5 | 5.16 | 117.69 | 114.60 |
| 1 | CA | 2766 | G | C4-N9-C1' | 5.16 | 133.20 | 126.50 |
| 1 | AA | 1405 | A | C6-N1-C2 | 5.15 | 121.69 | 118.60 |
| 34 | BA | 872 | A | O4'-C1'-N9 | 5.15 | 112.32 | 108.20 |
| 1 | CA | 2642 | G | OP2-P-O3' | 5.15 | 116.54 | 105.20 |
| 1 | AA | 45 | C | O4'-C1'-N1 | 5.15 | 112.32 | 108.20 |
| 1 | AA | 818 | G | C4-C5-N7 | -5.15 | 108.74 | 110.80 |
| 1 | AA | 1757 | C | N3-C2-O2 | 5.15 | 125.51 | 121.90 |
| 2 | AB | 48 | A | N1-C6-N6 | 5.15 | 121.69 | 118.60 |
| 1 | CA | 715 | G | O5'-P-OP2 | -5.15 | 101.06 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | CA | 997 | G | O5'-P-OP1 | -5.15 | 101.06 | 105.70 |
| 1 | CA | 1019 | U | C5-C4-O4 | 5.15 | 128.99 | 125.90 |
| 1 | AA | 239 | G | C8-N9-C4 | -5.15 | 104.34 | 106.40 |
| 1 | AA | 1434 | G | N3-C4-C5 | -5.15 | 126.03 | 128.60 |
| 1 | AA | 1515 | C | N1-C2-O2 | -5.15 | 115.81 | 118.90 |
| 34 | BA | 786 | G | N1-C6-O6 | -5.15 | 116.81 | 119.90 |
| 1 | CA | 225 | A | O5'-P-OP2 | -5.15 | 101.06 | 105.70 |
| 4 | CD | 52 | ARG | NE-CZ-NH1 | -5.15 | 117.72 | 120.30 |
| 34 | DA | 1487 | G | C8-N9-C4 | -5.15 | 104.34 | 106.40 |
| 1 | AA | 1232 | G | C6-C5-N7 | 5.15 | 133.49 | 130.40 |
| 34 | BA | 753 | A | OP1-P-O3' | 5.15 | 116.53 | 105.20 |
| 1 | AA | 816 | G | N3-C2-N2 | 5.15 | 123.50 | 119.90 |
| 1 | AA | 2115 | G | C5-C6-O6 | -5.15 | 125.51 | 128.60 |
| 1 | AA | 2274 | U | N1-C2-N3 | 5.15 | 117.99 | 114.90 |
| 34 | DA | 1079 | G | C8-N9-C4 | -5.15 | 104.34 | 106.40 |
| 34 | BA | 1482 | G | N9-C4-C5 | -5.15 | 103.34 | 105.40 |
| 1 | CA | 410 | G | C5-C6-O6 | 5.15 | 131.69 | 128.60 |
| 1 | CA | 2655 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 1 | AA | 724 | A | N9-C4-C5 | 5.14 | 107.86 | 105.80 |
| 1 | AA | 621 | G | N3-C4-C5 | -5.14 | 126.03 | 128.60 |
| 1 | AA | 1917 | C | OP2-P-O3' | 5.14 | 116.51 | 105.20 |
| 1 | AA | 2364 | A | N9-C4-C5 | -5.14 | 103.74 | 105.80 |
| 1 | CA | 127 | A | O5'-P-OP2 | -5.14 | 101.07 | 105.70 |
| 2 | AB | 12 | C | O5'-P-OP1 | -5.14 | 101.07 | 105.70 |
| 1 | AA | 2511 | C | N3-C2-O2 | 5.14 | 125.50 | 121.90 |
| 1 | AA | 2547 | G | C8-N9-C4 | -5.14 | 104.34 | 106.40 |
| 1 | AA | 2801 | C | N3-C4-C5 | 5.14 | 123.96 | 121.90 |
| 1 | AA | 2897 | U | N3-C4-C5 | 5.14 | 117.68 | 114.60 |
| 1 | CA | 2608 | G | C5-C6-O6 | 5.14 | 131.68 | 128.60 |
| 34 | DA | 1154 | G | O4'-C1'-N9 | 5.14 | 112.31 | 108.20 |
| 1 | AA | 1963 | C | N3-C2-O2 | 5.14 | 125.50 | 121.90 |
| 1 | AA | 2231 | G | N1-C6-O6 | 5.14 | 122.98 | 119.90 |
| 1 | AA | 2243 | C | C5-C6-N1 | -5.14 | 118.43 | 121.00 |
| 1 | CA | 2286 | A | C8-N9-C4 | -5.14 | 103.75 | 105.80 |
| 1 | AA | 2510 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 34 | BA | 821 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |
| 1 | CA | 850 | C | O5'-P-OP1 | -5.14 | 101.08 | 105.70 |
| 1 | CA | 2454 | G | N1-C6-O6 | -5.14 | 116.82 | 119.90 |
| 34 | DA | 1119 | C | C6-N1-C2 | -5.14 | 118.25 | 120.30 |
| 34 | DA | 1201 | A | P-O3'-C3' | 5.14 | 125.86 | 119.70 |
| 1 | AA | 1236 | G | N7-C8-N9 | -5.13 | 110.53 | 113.10 |
| 1 | AA | 1344 | C | C6-N1-C2 | 5.13 | 122.35 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 2048 | C | OP2-P-O3' | 5.13 | 116.50 | 105.20 |
| 34 | DA | 1004 | A | O4'-C1'-N9 | 5.13 | 112.31 | 108.20 |
| 59 | BZ | 378 | VAL | CB-CA-C | -5.13 | 101.65 | 111.40 |
| 1 | CA | 668 | G | OP2-P-O3' | 5.13 | 116.49 | 105.20 |
| 34 | DA | 865 | A | C2-N3-C4 | -5.13 | 108.03 | 110.60 |
| 1 | AA | 131 | C | O5'-P-OP2 | -5.13 | 101.08 | 105.70 |
| 1 | AA | 2011 | G | N3-C2-N2 | 5.13 | 123.49 | 119.90 |
| 1 | AA | 2456 | G | O5'-P-OP1 | -5.13 | 101.08 | 105.70 |
| 34 | BA | 800 | G | O5'-P-OP2 | -5.13 | 101.08 | 105.70 |
| 1 | CA | 934 | G | N1-C6-O6 | 5.13 | 122.98 | 119.90 |
| 1 | CA | 1331 | A | N1-C2-N3 | 5.13 | 131.87 | 129.30 |
| 1 | AA | 137 | G | N3-C4-C5 | -5.13 | 126.04 | 128.60 |
| 34 | BA | 974 | A | N1-C6-N6 | 5.13 | 121.68 | 118.60 |
| 1 | AA | 1154 | U | C5-C4-O4 | 5.12 | 128.97 | 125.90 |
| 34 | BA | 1036 | G | C8-N9-C1' | -5.12 | 120.34 | 127.00 |
| 1 | CA | 1684 | C | N1-C2-O2 | -5.12 | 115.83 | 118.90 |
| 1 | AA | 199 | C | C6-N1-C2 | 5.12 | 122.35 | 120.30 |
| 1 | AA | 1742 | G | C5-C6-O6 | -5.12 | 125.53 | 128.60 |
| 34 | DA | 354 | G | C8-N9-C1' | -5.12 | 120.34 | 127.00 |
| 1 | AA | 24 | G | O5'-P-OP1 | -5.12 | 101.09 | 105.70 |
| 1 | AA | 1843 | A | C4-C5-N7 | -5.12 | 108.14 | 110.70 |
| 1 | AA | 2217 | C | OP1-P-O3' | 5.12 | 116.47 | 105.20 |
| 1 | AA | 2560 | G | O5'-P-OP1 | -5.12 | 101.09 | 105.70 |
| 1 | CA | 540 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 1 | CA | 668 | G | N3-C4-C5 | 5.12 | 131.16 | 128.60 |
| 1 | CA | 708 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 1 | CA | 2616 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 1 | AA | 826 | U | C5-C4-O4 | -5.12 | 122.83 | 125.90 |
| 1 | AA | 1772 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 2 | AB | 118 | G | C8-N9-C4 | 5.12 | 108.45 | 106.40 |
| 34 | DA | 1501 | C | C4-C5-C6 | 5.12 | 119.96 | 117.40 |
| 1 | AA | 354 | A | C8-N9-C1' | 5.12 | 136.91 | 127.70 |
| 1 | AA | 1033 | G | N9-C4-C5 | 5.12 | 107.45 | 105.40 |
| 1 | AA | 2056 | U | C4-C5-C6 | 5.12 | 122.77 | 119.70 |
| 34 | BA | 354 | G | O5'-P-OP2 | -5.12 | 101.09 | 105.70 |
| 1 | CA | 2525 | G | O5'-P-OP2 | -5.12 | 101.09 | 105.70 |
| 1 | CA | 28 | A | N1-C6-N6 | -5.12 | 115.53 | 118.60 |
| 1 | CA | 1647 | G | O5'-P-OP1 | -5.12 | 101.09 | 105.70 |
| 1 | AA | 1303 | C | C4-C5-C6 | 5.12 | 119.96 | 117.40 |
| 1 | AA | 1380 | G | N9-C4-C5 | 5.12 | 107.45 | 105.40 |
| 1 | AA | 2257 | U | C6-N1-C2 | 5.12 | 124.07 | 121.00 |
| 1 | AA | 2535 | G | C6-C5-N7 | -5.12 | 127.33 | 130.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 2896 | G | N3-C2-N2 | -5.12 | 116.32 | 119.90 |
| 34 | BA | 518 | C | N1-C2-O2 | 5.12 | 121.97 | 118.90 |
| 1 | CA | 387 | U | OP1-P-O3' | 5.12 | 116.45 | 105.20 |
| 1 | CA | 1579 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 1 | AA | 54 | G | N1-C6-O6 | -5.11 | 116.83 | 119.90 |
| 1 | AA | 192 | C | N3-C4-C5 | 5.11 | 123.95 | 121.90 |
| 1 | AA | 434 | G | N3-C4-C5 | -5.11 | 126.04 | 128.60 |
| 1 | AA | 2847 | G | C4-C5-C6 | 5.11 | 121.87 | 118.80 |
| 2 | CB | 85 | G | N9-C4-C5 | -5.11 | 103.36 | 105.40 |
| 1 | CA | 298 | G | N9-C4-C5 | -5.11 | 103.36 | 105.40 |
| 57 | DX | 74 | C | OP2-P-O3' | -5.11 | 93.95 | 105.20 |
| 1 | AA | 738 | C | C2-N3-C4 | -5.11 | 117.34 | 119.90 |
| 1 | AA | 837 | C | N3-C4-C5 | 5.11 | 123.94 | 121.90 |
| 1 | AA | 2251 | G | N7-C8-N9 | -5.11 | 110.55 | 113.10 |
| 1 | CA | 866 | A | OP1-P-O3' | 5.11 | 116.44 | 105.20 |
| 1 | CA | 2598 | A | N1-C6-N6 | 5.11 | 121.67 | 118.60 |
| 1 | AA | 2467 | G | N1-C2-N2 | -5.11 | 111.60 | 116.20 |
| 34 | BA | 1483 | A | O5'-P-OP1 | -5.11 | 101.10 | 105.70 |
| 1 | CA | 385 | C | N1-C2-O2 | 5.11 | 121.97 | 118.90 |
| 1 | AA | 474 | U | C5-C4-O4 | 5.11 | 128.97 | 125.90 |
| 1 | CA | 827 | U | C5-C6-N1 | -5.11 | 120.15 | 122.70 |
| 1 | CA | 1681 | G | C4-C5-N7 | 5.11 | 112.84 | 110.80 |
| 1 | AA | 581 | G | O5'-P-OP2 | -5.11 | 101.11 | 105.70 |
| 1 | AA | 1655 | A | N1-C2-N3 | -5.11 | 126.75 | 129.30 |
| 1 | AA | 1829 | U | C5-C6-N1 | -5.11 | 120.15 | 122.70 |
| 1 | AA | 1062 | G | C8-N9-C4 | -5.10 | 104.36 | 106.40 |
| 1 | CA | 571 | A | OP1-P-OP2 | -5.10 | 111.94 | 119.60 |
| 1 | CA | 1799 | G | C4-C5-N7 | -5.10 | 108.76 | 110.80 |
| 1 | CA | 2242 | G | N7-C8-N9 | -5.10 | 110.55 | 113.10 |
| 1 | AA | 471 | C | N1-C2-O2 | -5.10 | 115.84 | 118.90 |
| 1 | AA | 1961 | U | O5'-P-OP1 | -5.10 | 101.11 | 105.70 |
| 2 | AB | 108 | U | C6-N1-C2 | 5.10 | 124.06 | 121.00 |
| 34 | BA | 7 | G | N3-C4-C5 | 5.10 | 131.15 | 128.60 |
| 1 | CA | 2258 | C | N3-C4-C5 | 5.10 | 123.94 | 121.90 |
| 1 | CA | 2708 | G | N3-C4-C5 | 5.10 | 131.15 | 128.60 |
| 1 | AA | 479 | C | C5-C4-N4 | 5.10 | 123.77 | 120.20 |
| 1 | AA | 2530 | A | N1-C6-N6 | 5.10 | 121.66 | 118.60 |
| 1 | AA | 584 | G | C2-N3-C4 | 5.10 | 114.45 | 111.90 |
| 1 | CA | 453 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 1 | CA | 2242 | G | C5-N7-C8 | 5.10 | 106.85 | 104.30 |
| 1 | CA | 2435 | A | N7-C8-N9 | 5.10 | 116.35 | 113.80 |
| 1 | CA | 2732 | G | N1-C6-O6 | -5.10 | 116.84 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 704 | U | C6-N1-C2 | 5.10 | 124.06 | 121.00 |
| 1 | AA | 1025 | G | C5-C6-N1 | 5.10 | 114.05 | 111.50 |
| 1 | AA | 1385 | G | C5-C6-O6 | -5.10 | 125.54 | 128.60 |
| 1 | AA | 1551 | C | C6-N1-C2 | -5.10 | 118.26 | 120.30 |
| 1 | AA | 1647 | G | N7-C8-N9 | -5.10 | 110.55 | 113.10 |
| 1 | AA | 2340 | A | N7-C8-N9 | -5.10 | 111.25 | 113.80 |
| 1 | AA | 2743 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 1 | CA | 516 | C | C6-N1-C2 | 5.10 | 122.34 | 120.30 |
| 1 | CA | 1779 | U | C5-C4-O4 | -5.10 | 122.84 | 125.90 |
| 1 | AA | 2256 | U | N3-C4-O4 | -5.10 | 115.83 | 119.40 |
| 1 | AA | 876 | A | C4-C5-N7 | 5.09 | 113.25 | 110.70 |
| 34 | BA | 890 | G | N1-C6-O6 | -5.09 | 116.84 | 119.90 |
| 1 | CA | 1788 | C | C4-C5-C6 | 5.09 | 119.95 | 117.40 |
| 1 | AA | 866 | A | OP2-P-O3' | 5.09 | 116.41 | 105.20 |
| 6 | AF | 38 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | CA | 482 | A | C4-C5-C6 | 5.09 | 119.55 | 117.00 |
| 1 | CA | 1681 | G | C2-N3-C4 | -5.09 | 109.35 | 111.90 |
| 1 | AA | 632 | A | C8-N9-C4 | 5.09 | 107.84 | 105.80 |
| 1 | AA | 814 | U | C2-N3-C4 | -5.09 | 123.94 | 127.00 |
| 1 | AA | 1068 | G | N3-C4-N9 | -5.09 | 122.94 | 126.00 |
| 1 | AA | 1412 | A | N7-C8-N9 | -5.09 | 111.25 | 113.80 |
| 1 | AA | 1815 | A | C5-C6-N1 | -5.09 | 115.15 | 117.70 |
| 1 | AA | 2238 | C | C2-N3-C4 | -5.09 | 117.35 | 119.90 |
| 34 | BA | 345 | C | N3-C4-C5 | -5.09 | 119.86 | 121.90 |
| 34 | BA | 524 | G | C5-C6-O6 | -5.09 | 125.55 | 128.60 |
| 34 | BA | 807 | A | N1-C6-N6 | -5.09 | 115.55 | 118.60 |
| 34 | DA | 1373 | G | N3-C4-C5 | -5.09 | 126.05 | 128.60 |
| 34 | DA | 1482 | G | C8-N9-C1' | -5.09 | 120.38 | 127.00 |
| 1 | AA | 645 | G | N3-C2-N2 | 5.09 | 123.46 | 119.90 |
| 1 | AA | 762 | G | C6-C5-N7 | -5.09 | 127.35 | 130.40 |
| 1 | AA | 2553 | A | C5-C6-N6 | -5.09 | 119.63 | 123.70 |
| 1 | AA | 358 | C | C5-C6-N1 | -5.09 | 118.46 | 121.00 |
| 1 | CA | 2057 | A | O5'-P-OP2 | -5.09 | 101.12 | 105.70 |
| 1 | AA | 742 | G | C5-C6-O6 | 5.09 | 131.65 | 128.60 |
| 1 | AA | 1449 | C | O5'-P-OP1 | -5.09 | 101.12 | 105.70 |
| 1 | AA | 2467 | G | N1-C6-O6 | -5.09 | 116.85 | 119.90 |
| 1 | AA | 2686 | G | C8-N9-C4 | -5.09 | 104.36 | 106.40 |
| 1 | CA | 40 | C | C5-C6-N1 | -5.09 | 118.46 | 121.00 |
| 1 | AA | 913 | A | C2-N3-C4 | -5.08 | 108.06 | 110.60 |
| 1 | CA | 798 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 1 | AA | 414 | U | N3-C2-O2 | 5.08 | 125.76 | 122.20 |
| 1 | AA | 2335 | G | C4-C5-N7 | 5.08 | 112.83 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|-------|-------------|----------|
| 1 | AA | 2515 | A | C6-C5-N7 | -5.08 | 128.74 | 132.30 |
| 1 | AA | 2723 | A | N9-C4-C5 | -5.08 | 103.77 | 105.80 |
| 1 | CA | 2331 | G | C2-N3-C4 | -5.08 | 109.36 | 111.90 |
| 1 | AA | 781 | A | C5-C6-N6 | -5.08 | 119.63 | 123.70 |
| 1 | AA | 2484 | G | C6-N1-C2 | -5.08 | 122.05 | 125.10 |
| 1 | AA | 2773 | C | N1-C2-O2 | -5.08 | 115.85 | 118.90 |
| 20 | AW | 18 | ARG | NE-CZ-NH2 | -5.08 | 117.76 | 120.30 |
| 34 | BA | 580 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 1 | CA | 1181 | C | C6-N1-C2 | 5.08 | 122.33 | 120.30 |
| 1 | AA | 1617 | A | N9-C4-C5 | -5.08 | 103.77 | 105.80 |
| 1 | AA | 1544 | C | OP1-P-O3' | 5.08 | 116.37 | 105.20 |
| 1 | AA | 25 | U | C2-N3-C4 | -5.08 | 123.95 | 127.00 |
| 1 | AA | 1365 | G | OP2-P-O3' | 5.08 | 116.37 | 105.20 |
| 1 | AA | 1441 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 1 | AA | 1809 | U | N1-C2-N3 | -5.08 | 111.85 | 114.90 |
| 1 | AA | 2701 | U | C6-N1-C2 | -5.08 | 117.95 | 121.00 |
| 1 | CA | 1687 | G | N3-C2-N2 | 5.08 | 123.45 | 119.90 |
| 1 | AA | 32 | C | C5-C6-N1 | -5.08 | 118.46 | 121.00 |
| 1 | AA | 240 | A | C6-C5-N7 | 5.08 | 135.85 | 132.30 |
| 1 | AA | 1026 | A | C8-N9-C4 | 5.08 | 107.83 | 105.80 |
| 1 | AA | 2759 | U | C5-C6-N1 | -5.08 | 120.16 | 122.70 |
| 2 | AB | 103 | G | N1-C6-O6 | 5.08 | 122.95 | 119.90 |
| 34 | DA | 7 | G | C8-N9-C1' | 5.08 | 133.60 | 127.00 |
| 34 | DA | 907 | A | OP2-P-O3' | 5.08 | 116.37 | 105.20 |
| 1 | AA | 2019 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 1 | AA | 2233 | G | N1-C6-O6 | -5.07 | 116.86 | 119.90 |
| 1 | AA | 2441 | G | N1-C2-N3 | 5.07 | 126.94 | 123.90 |
| 1 | AA | 2801 | C | C2-N3-C4 | -5.07 | 117.36 | 119.90 |
| 34 | BA | 423 | G | N3-C4-N9 | 5.07 | 129.04 | 126.00 |
| 34 | DA | 532 | A | P-O3'-C3' | 5.07 | 125.79 | 119.70 |
| 1 | AA | 630 | U | N3-C2-O2 | 5.07 | 125.75 | 122.20 |
| 1 | AA | 2059 | G | N7-C8-N9 | -5.07 | 110.56 | 113.10 |
| 1 | AA | 225 | C | N3-C4-C5 | 5.07 | 123.93 | 121.90 |
| 1 | AA | 2638 | C | C2-N3-C4 | -5.07 | 117.36 | 119.90 |
| 1 | CA | 1644 | C | N3-C4-C5 | -5.07 | 119.87 | 121.90 |
| 1 | AA | 1275 | G | N1-C6-O6 | 5.07 | 122.94 | 119.90 |
| 1 | AA | 2272 | C | C4-C5-C6 | 5.07 | 119.93 | 117.40 |
| 34 | BA | 1030(B) | C | N3-C2-O2 | -5.07 | 118.35 | 121.90 |
| 1 | AA | 199 | C | C5-C4-N4 | 5.07 | 123.75 | 120.20 |
| 1 | AA | 536 | U | N1-C2-O2 | -5.07 | 119.25 | 122.80 |
| 2 | AB | 64 | C | C5-C6-N1 | -5.07 | 118.47 | 121.00 |
| 5 | AE | 47 | VAL | CB-CA-C | -5.07 | 101.77 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 1054 | C | C6-N1-C2 | 5.07 | 122.33 | 120.30 |
| 1 | AA | 2276 | C | C2-N3-C4 | -5.07 | 117.37 | 119.90 |
| 1 | AA | 2576 | A | C8-N9-C4 | -5.07 | 103.77 | 105.80 |
| 34 | BA | 605 | U | C5-C4-O4 | 5.07 | 128.94 | 125.90 |
| 34 | BA | 1458 | G | C5-C6-O6 | -5.07 | 125.56 | 128.60 |
| 34 | DA | 904 | C | C5-C4-N4 | -5.07 | 116.65 | 120.20 |
| 1 | AA | 1376 | C | C5-C6-N1 | -5.06 | 118.47 | 121.00 |
| 1 | CA | 1687 | G | OP2-P-O3' | 5.06 | 116.34 | 105.20 |
| 1 | CA | 2712 | U | N3-C4-C5 | 5.06 | 117.64 | 114.60 |
| 34 | BA | 578 | C | C2-N3-C4 | -5.06 | 117.37 | 119.90 |
| 1 | AA | 1240 | G | C5-C6-N1 | 5.06 | 114.03 | 111.50 |
| 1 | AA | 1720 | U | O4'-C1'-N1 | 5.06 | 112.25 | 108.20 |
| 1 | AA | 2344 | U | N3-C4-O4 | -5.06 | 115.86 | 119.40 |
| 34 | BA | 598 | U | N3-C4-O4 | 5.06 | 122.94 | 119.40 |
| 1 | AA | 17 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 1 | AA | 1585 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 1 | AA | 2611 | G | N1-C6-O6 | -5.06 | 116.86 | 119.90 |
| 34 | BA | 546 | G | N9-C4-C5 | 5.06 | 107.42 | 105.40 |
| 1 | CA | 116 | C | O5'-P-OP2 | -5.06 | 101.15 | 105.70 |
| 34 | DA | 758 | G | C5-C6-O6 | 5.06 | 131.63 | 128.60 |
| 1 | AA | 174 | U | OP2-P-O3' | 5.06 | 116.33 | 105.20 |
| 1 | AA | 733 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | AA | 2403 | G | O4'-C1'-N9 | 5.06 | 112.25 | 108.20 |
| 1 | AA | 2437 | A | N1-C6-N6 | 5.06 | 121.63 | 118.60 |
| 29 | A5 | 20 | ARG | NE-CZ-NH1 | -5.06 | 117.77 | 120.30 |
| 1 | CA | 1680 | U | N1-C2-O2 | -5.06 | 119.26 | 122.80 |
| 1 | CA | 2167 | U | C2-N1-C1' | 5.06 | 123.77 | 117.70 |
| 1 | AA | 1258 | A | C6-N1-C2 | -5.06 | 115.57 | 118.60 |
| 1 | AA | 2775 | G | C5-C6-O6 | 5.06 | 131.63 | 128.60 |
| 1 | CA | 1129 | A | OP1-P-OP2 | 5.06 | 127.18 | 119.60 |
| 1 | AA | 1545 | C | C5-C6-N1 | -5.05 | 118.47 | 121.00 |
| 1 | CA | 660 | G | C5-C6-O6 | 5.05 | 131.63 | 128.60 |
| 1 | CA | 1256 | G | N1-C6-O6 | 5.05 | 122.93 | 119.90 |
| 1 | CA | 2439 | A | N1-C6-N6 | 5.05 | 121.63 | 118.60 |
| 1 | CA | 2523 | G | C4-N9-C1' | 5.05 | 133.07 | 126.50 |
| 1 | CA | 2625 | G | C8-N9-C4 | 5.05 | 108.42 | 106.40 |
| 34 | DA | 1502 | A | C5-C6-N6 | -5.05 | 119.66 | 123.70 |
| 1 | AA | 730 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 1 | AA | 2016 | C | C4-C5-C6 | 5.05 | 119.93 | 117.40 |
| 1 | AA | 2701 | U | N3-C2-O2 | -5.05 | 118.66 | 122.20 |
| 1 | CA | 2277 | G | N9-C4-C5 | 5.05 | 107.42 | 105.40 |
| 1 | AA | 2375 | C | C5-C4-N4 | 5.05 | 123.74 | 120.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 50 | BQ | 9 | VAL | CB-CA-C | -5.05 | 101.80 | 111.40 |
| 34 | DA | 1517 | G | O5'-P-OP2 | -5.05 | 101.15 | 105.70 |
| 1 | AA | 2682 | A | N1-C6-N6 | -5.05 | 115.57 | 118.60 |
| 1 | CA | 1531 | C | C5-C6-N1 | 5.05 | 123.53 | 121.00 |
| 1 | CA | 1784 | A | C8-N9-C4 | 5.05 | 107.82 | 105.80 |
| 1 | AA | 655 | G | O5'-P-OP2 | -5.05 | 101.16 | 105.70 |
| 1 | AA | 893 | C | C2-N1-C1' | -5.05 | 113.25 | 118.80 |
| 1 | AA | 2828 | G | OP1-P-OP2 | 5.05 | 127.17 | 119.60 |
| 34 | BA | 770 | C | N3-C2-O2 | -5.05 | 118.37 | 121.90 |
| 1 | CA | 794 | G | N1-C2-N2 | -5.05 | 111.66 | 116.20 |
| 1 | AA | 632 | A | N7-C8-N9 | -5.05 | 111.28 | 113.80 |
| 1 | AA | 875 | U | N1-C2-O2 | -5.05 | 119.27 | 122.80 |
| 1 | AA | 2074 | G | C4-C5-N7 | -5.05 | 108.78 | 110.80 |
| 34 | BA | 337 | C | N1-C2-O2 | 5.05 | 121.93 | 118.90 |
| 1 | CA | 2496 | C | C5-C4-N4 | 5.05 | 123.73 | 120.20 |
| 1 | AA | 592 | U | N1-C2-N3 | 5.04 | 117.93 | 114.90 |
| 34 | BA | 852 | G | N7-C8-N9 | -5.04 | 110.58 | 113.10 |
| 1 | AA | 739 | C | OP1-P-OP2 | -5.04 | 112.03 | 119.60 |
| 1 | AA | 1653 | C | N3-C4-C5 | -5.04 | 119.88 | 121.90 |
| 1 | AA | 2578 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 1 | AA | 2883 | A | C8-N9-C4 | -5.04 | 103.78 | 105.80 |
| 34 | BA | 769 | G | OP2-P-O3' | 5.04 | 116.30 | 105.20 |
| 1 | AA | 201 | G | N7-C8-N9 | -5.04 | 110.58 | 113.10 |
| 1 | AA | 1848 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 1 | CA | 125 | G | O4'-C1'-N9 | -5.04 | 104.17 | 108.20 |
| 1 | CA | 528 | A | C4-C5-N7 | 5.04 | 113.22 | 110.70 |
| 1 | CA | 2286 | A | C4-C5-N7 | 5.04 | 113.22 | 110.70 |
| 34 | DA | 784 | C | N3-C2-O2 | 5.04 | 125.43 | 121.90 |
| 1 | AA | 1418 | U | C2-N1-C1' | 5.04 | 123.75 | 117.70 |
| 1 | AA | 2243 | C | C2-N3-C4 | -5.04 | 117.38 | 119.90 |
| 1 | CA | 2415 | G | C5-C6-O6 | -5.04 | 125.58 | 128.60 |
| 1 | AA | 953 | U | OP2-P-O3' | 5.04 | 116.28 | 105.20 |
| 1 | AA | 1256 | U | OP1-P-OP2 | -5.04 | 112.04 | 119.60 |
| 1 | AA | 1824 | C | N3-C4-C5 | 5.04 | 123.92 | 121.90 |
| 1 | CA | 141 | A | O4'-C1'-N9 | 5.04 | 112.23 | 108.20 |
| 1 | CA | 2413 | G | N3-C2-N2 | -5.04 | 116.37 | 119.90 |
| 34 | DA | 319 | G | N1-C6-O6 | -5.04 | 116.88 | 119.90 |
| 34 | DA | 646 | U | N3-C2-O2 | -5.04 | 118.67 | 122.20 |
| 34 | DA | 1063 | C | C5-C6-N1 | 5.04 | 123.52 | 121.00 |
| 1 | CA | 856 | C | C3'-C2'-C1' | -5.04 | 97.47 | 101.50 |
| 1 | AA | 17 | G | C5-C6-N1 | 5.04 | 114.02 | 111.50 |
| 1 | AA | 199 | C | C2-N3-C4 | -5.04 | 117.38 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | AA | 777 | C | C5-C6-N1 | -5.04 | 118.48 | 121.00 |
| 1 | AA | 1398 | U | OP1-P-OP2 | -5.04 | 112.05 | 119.60 |
| 1 | AA | 555 | G | C4-C5-C6 | -5.03 | 115.78 | 118.80 |
| 1 | AA | 2057 | G | O4'-C1'-N9 | 5.03 | 112.23 | 108.20 |
| 34 | BA | 1430 | C | N3-C4-N4 | -5.03 | 114.48 | 118.00 |
| 1 | CA | 1797 | C | C2-N3-C4 | -5.03 | 117.38 | 119.90 |
| 1 | AA | 448 | U | N3-C4-O4 | -5.03 | 115.88 | 119.40 |
| 1 | AA | 2416 | C | C2-N1-C1' | -5.03 | 113.27 | 118.80 |
| 2 | AB | 80 | U | C6-N1-C2 | 5.03 | 124.02 | 121.00 |
| 1 | CA | 663 | G | C4-C5-N7 | -5.03 | 108.79 | 110.80 |
| 1 | CA | 1425 | G | C8-N9-C1' | -5.03 | 120.46 | 127.00 |
| 1 | CA | 2043 | C | N3-C2-O2 | -5.03 | 118.38 | 121.90 |
| 1 | AA | 596 | G | C2-N3-C4 | 5.03 | 114.42 | 111.90 |
| 1 | AA | 610 | C | C5-C6-N1 | 5.03 | 123.52 | 121.00 |
| 1 | AA | 1589 | A | C8-N9-C4 | -5.03 | 103.79 | 105.80 |
| 1 | AA | 2026 | G | N1-C6-O6 | 5.03 | 122.92 | 119.90 |
| 1 | CA | 47 | C | C5-C6-N1 | -5.03 | 118.48 | 121.00 |
| 1 | CA | 753 | C | O5'-P-OP2 | 5.03 | 116.74 | 110.70 |
| 1 | CA | 1901 | A | C5-C6-N1 | 5.03 | 120.22 | 117.70 |
| 1 | CA | 2570 | G | O5'-P-OP1 | -5.03 | 101.17 | 105.70 |
| 1 | AA | 2229 | A | N1-C6-N6 | 5.03 | 121.62 | 118.60 |
| 1 | AA | 723 | A | N1-C6-N6 | 5.03 | 121.62 | 118.60 |
| 1 | AA | 1924 | C | OP2-P-O3' | 5.03 | 116.26 | 105.20 |
| 1 | AA | 2384 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 1 | AA | 2902 | G | C5-N7-C8 | -5.03 | 101.79 | 104.30 |
| 1 | CA | 1397 | U | O4'-C1'-N1 | 5.03 | 112.22 | 108.20 |
| 1 | CA | 2040 | C | C5-C6-N1 | -5.03 | 118.49 | 121.00 |
| 1 | CA | 2489 | G | OP2-P-O3' | 5.03 | 116.26 | 105.20 |
| 1 | CA | 2538 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 1 | AA | 126 | C | N1-C2-O2 | -5.03 | 115.89 | 118.90 |
| 1 | AA | 874 | U | O5'-P-OP2 | -5.03 | 101.18 | 105.70 |
| 1 | AA | 1256 | U | C5-C6-N1 | -5.03 | 120.19 | 122.70 |
| 1 | AA | 1713 | G | O4'-C1'-N9 | 5.03 | 112.22 | 108.20 |
| 34 | BA | 1445 | C | C6-N1-C2 | -5.03 | 118.29 | 120.30 |
| 34 | DA | 322 | C | C6-N1-C2 | 5.03 | 122.31 | 120.30 |
| 1 | AA | 1665 | G | N3-C4-N9 | 5.02 | 129.01 | 126.00 |
| 1 | CA | 460 | A | C4-C5-C6 | 5.02 | 119.51 | 117.00 |
| 34 | DA | 31 | G | N3-C4-C5 | 5.02 | 131.11 | 128.60 |
| 1 | AA | 279 | G | C4-C5-C6 | 5.02 | 121.81 | 118.80 |
| 1 | AA | 549 | U | OP2-P-O3' | 5.02 | 116.25 | 105.20 |
| 1 | AA | 777 | C | C4-C5-C6 | 5.02 | 119.91 | 117.40 |
| 1 | AA | 1645 | C | C5-C6-N1 | -5.02 | 118.49 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | AA | 1814 | A | C8-N9-C4 | -5.02 | 103.79 | 105.80 |
| 1 | AA | 1925 | G | O5'-P-OP2 | -5.02 | 101.18 | 105.70 |
| 1 | AA | 2277 | U | N3-C2-O2 | 5.02 | 125.72 | 122.20 |
| 1 | CA | 671 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | CA | 1284 | A | C5-C6-N6 | -5.02 | 119.68 | 123.70 |
| 1 | AA | 831 | A | N7-C8-N9 | -5.02 | 111.29 | 113.80 |
| 34 | BA | 1457 | G | C4-C5-N7 | -5.02 | 108.79 | 110.80 |
| 1 | CA | 2003 | G | N1-C6-O6 | -5.02 | 116.89 | 119.90 |
| 18 | CU | 28 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 1 | AA | 183 | G | OP2-P-O3' | 5.02 | 116.24 | 105.20 |
| 1 | AA | 462 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 1 | AA | 1181 | G | C5-C6-N1 | 5.02 | 114.01 | 111.50 |
| 1 | AA | 1930 | C | C4-C5-C6 | 5.02 | 119.91 | 117.40 |
| 23 | AZ | 86 | VAL | CB-CA-C | -5.02 | 101.86 | 111.40 |
| 1 | CA | 2291 | U | C5-C4-O4 | 5.02 | 128.91 | 125.90 |
| 1 | CA | 2589 | A | C2-N3-C4 | -5.02 | 108.09 | 110.60 |
| 1 | AA | 495 | G | C8-N9-C4 | 5.02 | 108.41 | 106.40 |
| 1 | AA | 854 | U | N1-C2-N3 | 5.02 | 117.91 | 114.90 |
| 1 | AA | 1178 | A | OP1-P-OP2 | 5.02 | 127.13 | 119.60 |
| 1 | AA | 1941 | A | N9-C4-C5 | -5.02 | 103.79 | 105.80 |
| 2 | AB | 43 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 34 | BA | 821 | G | C2-N3-C4 | 5.02 | 114.41 | 111.90 |
| 1 | CA | 573 | G | C2-N3-C4 | 5.02 | 114.41 | 111.90 |
| 1 | CA | 1387 | C | C6-N1-C2 | -5.02 | 118.29 | 120.30 |
| 1 | CA | 1470 | G | N3-C4-C5 | 5.02 | 131.11 | 128.60 |
| 57 | DX | 20 | U | N1-C2-O2 | 5.02 | 126.31 | 122.80 |
| 1 | CA | 246 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 1 | CA | 1180 | C | C6-N1-C2 | 5.02 | 122.31 | 120.30 |
| 1 | CA | 1786 | A | OP1-P-O3' | 5.02 | 116.23 | 105.20 |
| 1 | AA | 470 | C | C6-N1-C2 | 5.01 | 122.31 | 120.30 |
| 1 | AA | 661 | G | N3-C2-N2 | -5.01 | 116.39 | 119.90 |
| 1 | AA | 1479 | U | C6-N1-C2 | 5.01 | 124.01 | 121.00 |
| 1 | AA | 1567 | G | C8-N9-C4 | -5.01 | 104.39 | 106.40 |
| 1 | AA | 2567 | U | OP1-P-OP2 | -5.01 | 112.08 | 119.60 |
| 34 | BA | 599 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 1 | CA | 778 | G | C5-C6-O6 | -5.01 | 125.59 | 128.60 |
| 1 | CA | 2438 | U | O5'-P-OP2 | -5.01 | 101.19 | 105.70 |
| 1 | AA | 31 | C | N1-C2-O2 | -5.01 | 115.89 | 118.90 |
| 1 | AA | 1495 | G | C8-N9-C4 | 5.01 | 108.41 | 106.40 |
| 1 | AA | 2044 | U | C4-C5-C6 | 5.01 | 122.71 | 119.70 |
| 1 | AA | 820 | U | C5-C6-N1 | -5.01 | 120.19 | 122.70 |
| 1 | AA | 854 | U | N3-C2-O2 | -5.01 | 118.69 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1 | AA | 1369 | U | N1-C2-N3 | -5.01 | 111.89 | 114.90 |
| 1 | AA | 2723 | A | N1-C6-N6 | 5.01 | 121.61 | 118.60 |
| 1 | AA | 2724 | U | N1-C2-O2 | 5.01 | 126.31 | 122.80 |
| 1 | CA | 133 | C | N3-C4-C5 | 5.01 | 123.91 | 121.90 |
| 1 | CA | 992 | C | N3-C4-C5 | 5.01 | 123.91 | 121.90 |
| 1 | CA | 1268 | A | OP1-P-O3' | 5.01 | 116.22 | 105.20 |
| 1 | AA | 1812 | C | C6-N1-C1' | -5.01 | 114.79 | 120.80 |
| 1 | AA | 1962 | U | N1-C2-N3 | 5.01 | 117.91 | 114.90 |
| 1 | CA | 709 | U | O5'-P-OP1 | 5.01 | 116.71 | 110.70 |
| 1 | CA | 2614 | A | N1-C6-N6 | -5.01 | 115.59 | 118.60 |
| 1 | AA | 176 | G | C4-C5-N7 | 5.01 | 112.80 | 110.80 |
| 1 | AA | 1612 | C | C5-C4-N4 | -5.01 | 116.69 | 120.20 |
| 1 | AA | 2877 | G | N3-C4-N9 | -5.01 | 123.00 | 126.00 |
| 1 | CA | 379 | G | OP2-P-O3' | 5.01 | 116.22 | 105.20 |
| 1 | AA | 738 | C | C5-C6-N1 | -5.01 | 118.50 | 121.00 |
| 1 | AA | 1485 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |
| 1 | AA | 2696 | U | C4-C5-C6 | 5.01 | 122.70 | 119.70 |
| 2 | AB | 114 | C | C5-C6-N1 | -5.01 | 118.50 | 121.00 |
| 34 | BA | 862 | C | OP2-P-O3' | 5.01 | 116.22 | 105.20 |
| 1 | CA | 2547 | U | N3-C4-O4 | 5.01 | 122.91 | 119.40 |
| 1 | AA | 704 | U | N3-C4-O4 | -5.00 | 115.90 | 119.40 |
| 1 | AA | 1020 | C | N3-C4-N4 | -5.00 | 114.50 | 118.00 |
| 1 | AA | 2627 | U | N3-C2-O2 | -5.00 | 118.70 | 122.20 |
| 1 | AA | 2798 | C | N3-C4-C5 | -5.00 | 119.90 | 121.90 |
| 1 | CA | 2876 | G | N9-C4-C5 | -5.00 | 103.40 | 105.40 |
| 1 | AA | 331 | G | N1-C6-O6 | -5.00 | 116.90 | 119.90 |
| 1 | AA | 1359 | U | O4'-C1'-N1 | 5.00 | 112.20 | 108.20 |
| 1 | AA | 1437 | U | N1-C2-O2 | 5.00 | 126.30 | 122.80 |
| 1 | AA | 2451 | A | C5'-C4'-O4' | -5.00 | 103.09 | 109.10 |
| 1 | AA | 2625 | U | N3-C4-O4 | -5.00 | 115.90 | 119.40 |
| 2 | AB | 106 | G | C4-C5-N7 | 5.00 | 112.80 | 110.80 |
| 1 | CA | 1899 | G | N1-C2-N2 | 5.00 | 120.70 | 116.20 |
| 34 | DA | 804 | U | C5-C4-O4 | 5.00 | 128.90 | 125.90 |
| 1 | AA | 1214 | G | N1-C2-N2 | -5.00 | 111.70 | 116.20 |
| 1 | AA | 2530 | A | C4-C5-C6 | 5.00 | 119.50 | 117.00 |
| 1 | CA | 2517 | C | C5-C4-N4 | -5.00 | 116.70 | 120.20 |
| 1 | CA | 2600 | A | N1-C2-N3 | 5.00 | 131.80 | 129.30 |
| 2 | CB | 105 | A | C8-N9-C4 | 5.00 | 107.80 | 105.80 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 28 | A4 | 59 | PHE | Peptide |
| 1 | AA | 537 | G | Sidechain |
| 35 | BB | 8 | LYS | Peptide |
| 53 | BT | 9 | ASN | Peptide |
| 53 | DT | 9 | ASN | Peptide |
| 59 | DZ | 159 | ALA | 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 | 61861 | 0 | 31186 | 660 | 2 |
| 1 | CA | 61771 | 0 | 31146 | 786 | 0 |
| 2 | AB | 2573 | 0 | 1306 | 15 | 0 |
| 2 | CB | 2573 | 0 | 1306 | 26 | 0 |
| 3 | AC | 1063 | 0 | 1091 | 140 | 5 |
| 3 | CC | 1063 | 0 | 1089 | 150 | 10 |
| 4 | AD | 2136 | 0 | 2218 | 55 | 0 |
| 4 | CD | 2142 | 0 | 2229 | 67 | 0 |
| 5 | AE | 1559 | 0 | 1618 | 48 | 0 |
| 5 | CE | 1559 | 0 | 1618 | 42 | 0 |
| 6 | AF | 1584 | 0 | 1625 | 39 | 0 |
| 6 | CF | 1580 | 0 | 1619 | 50 | 0 |
| 7 | AG | 1425 | 0 | 1443 | 47 | 0 |
| 7 | CG | 1424 | 0 | 1434 | 42 | 0 |
| 8 | AH | 1330 | 0 | 1407 | 24 | 0 |
| 8 | CH | 1330 | 0 | 1407 | 42 | 0 |
| 9 | AK | 641 | 0 | 309 | 11 | 0 |
| 9 | CK | 641 | 0 | 309 | 13 | 0 |
| 10 | AL | 498 | 0 | 521 | 17 | 0 |
| 10 | CL | 498 | 0 | 521 | 21 | 0 |
| 11 | AN | 1117 | 0 | 1184 | 26 | 0 |
| 11 | CN | 1117 | 0 | 1184 | 21 | 0 |
| 12 | AO | 933 | 0 | 996 | 29 | 0 |
| 12 | CO | 933 | 0 | 996 | 22 | 0 |
| 13 | AP | 1139 | 0 | 1223 | 34 | 0 |
| 13 | CP | 1135 | 0 | 1212 | 47 | 0 |
| 14 | AQ | 1122 | 0 | 1179 | 36 | 0 |
| 14 | CQ | 1122 | 0 | 1179 | 36 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15 | AR | 968 | 0 | 1033 | 19 | 0 |
| 15 | CR | 968 | 0 | 1033 | 27 | 0 |
| 16 | AS | 877 | 0 | 938 | 20 | 0 |
| 16 | CS | 870 | 0 | 923 | 35 | 0 |
| 17 | AT | 1091 | 0 | 1151 | 31 | 0 |
| 17 | CT | 1083 | 0 | 1136 | 28 | 0 |
| 18 | AU | 959 | 0 | 1019 | 25 | 0 |
| 18 | CU | 959 | 0 | 1019 | 30 | 0 |
| 19 | AV | 771 | 0 | 830 | 13 | 0 |
| 19 | CV | 771 | 0 | 830 | 19 | 0 |
| 20 | AW | 886 | 0 | 940 | 15 | 0 |
| 20 | CW | 886 | 0 | 940 | 18 | 0 |
| 21 | AX | 750 | 0 | 814 | 20 | 0 |
| 21 | CX | 750 | 0 | 814 | 19 | 0 |
| 22 | AY | 806 | 0 | 881 | 29 | 0 |
| 22 | CY | 806 | 0 | 882 | 37 | 0 |
| 23 | AZ | 1349 | 0 | 1355 | 38 | 0 |
| 23 | CZ | 1360 | 0 | 1363 | 41 | 0 |
| 24 | A0 | 653 | 0 | 674 | 20 | 0 |
| 24 | C0 | 653 | 0 | 674 | 20 | 0 |
| 25 | A1 | 755 | 0 | 826 | 20 | 0 |
| 25 | C1 | 755 | 0 | 826 | 20 | 0 |
| 26 | A2 | 588 | 0 | 643 | 9 | 0 |
| 26 | C2 | 588 | 0 | 643 | 14 | 0 |
| 27 | A3 | 469 | 0 | 518 | 6 | 0 |
| 27 | C3 | 464 | 0 | 514 | 8 | 0 |
| 28 | A4 | 558 | 0 | 545 | 22 | 0 |
| 28 | C4 | 532 | 0 | 506 | 20 | 0 |
| 29 | A5 | 455 | 0 | 465 | 7 | 0 |
| 29 | C5 | 455 | 0 | 465 | 11 | 0 |
| 30 | A6 | 453 | 0 | 473 | 13 | 0 |
| 30 | C6 | 449 | 0 | 469 | 13 | 0 |
| 31 | A7 | 418 | 0 | 467 | 11 | 0 |
| 31 | C7 | 418 | 0 | 467 | 9 | 0 |
| 32 | A8 | 517 | 0 | 582 | 23 | 0 |
| 32 | C8 | 517 | 0 | 582 | 19 | 0 |
| 33 | A9 | 307 | 0 | 335 | 8 | 0 |
| 33 | C9 | 307 | 0 | 335 | 11 | 0 |
| 34 | BA | 32185 | 0 | 16245 | 438 | 0 |
| 34 | DA | 32312 | 0 | 16308 | 510 | 1 |
| 35 | BB | 1846 | 0 | 1867 | 80 | 0 |
| 35 | DB | 1825 | 0 | 1828 | 101 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 36 | BC | 1552 | 0 | 1546 | 52 | 0 |
| 36 | DC | 1544 | 0 | 1524 | 65 | 0 |
| 37 | BD | 1659 | 0 | 1676 | 58 | 0 |
| 37 | DD | 1678 | 0 | 1718 | 53 | 0 |
| 38 | BE | 1129 | 0 | 1185 | 42 | 0 |
| 38 | DE | 1133 | 0 | 1191 | 41 | 0 |
| 39 | BF | 812 | 0 | 804 | 18 | 0 |
| 39 | DF | 820 | 0 | 814 | 23 | 0 |
| 40 | BG | 1231 | 0 | 1238 | 21 | 0 |
| 40 | DG | 1235 | 0 | 1249 | 31 | 0 |
| 41 | BH | 1088 | 0 | 1126 | 39 | 0 |
| 41 | DH | 1088 | 0 | 1126 | 37 | 0 |
| 42 | BI | 986 | 0 | 995 | 39 | 0 |
| 42 | DI | 978 | 0 | 966 | 42 | 0 |
| 43 | BJ | 709 | 0 | 650 | 34 | 0 |
| 43 | DJ | 714 | 0 | 672 | 33 | 0 |
| 44 | BK | 833 | 0 | 836 | 23 | 0 |
| 44 | DK | 833 | 0 | 836 | 16 | 0 |
| 45 | BL | 930 | 0 | 980 | 10 | 0 |
| 45 | DL | 930 | 0 | 980 | 30 | 0 |
| 46 | BM | 966 | 0 | 1024 | 33 | 0 |
| 46 | DM | 950 | 0 | 988 | 39 | 0 |
| 47 | BN | 492 | 0 | 529 | 22 | 0 |
| 47 | DN | 492 | 0 | 531 | 33 | 0 |
| 48 | BO | 728 | 0 | 760 | 17 | 0 |
| 48 | DO | 728 | 0 | 760 | 14 | 0 |
| 49 | BP | 681 | 0 | 697 | 27 | 0 |
| 49 | DP | 677 | 0 | 686 | 20 | 0 |
| 50 | BQ | 823 | 0 | 891 | 24 | 0 |
| 50 | DQ | 823 | 0 | 891 | 23 | 0 |
| 51 | BR | 555 | 0 | 618 | 16 | 0 |
| 51 | DR | 555 | 0 | 618 | 20 | 0 |
| 52 | BS | 661 | 0 | 675 | 39 | 0 |
| 52 | DS | 646 | 0 | 644 | 25 | 0 |
| 53 | BT | 728 | 0 | 798 | 29 | 0 |
| 53 | DT | 731 | 0 | 807 | 22 | 0 |
| 54 | BU | 199 | 0 | 208 | 7 | 0 |
| 54 | DU | 199 | 0 | 208 | 5 | 0 |
| 55 | BV | 277 | 0 | 140 | 3 | 0 |
| 55 | DV | 252 | 0 | 130 | 3 | 0 |
| 56 | BW | 1599 | 0 | 830 | 26 | 0 |
| 56 | DW | 1552 | 0 | 794 | 21 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | BX | 1635 | 0 | 838 | 15 | 0 |
| 57 | DX | 1635 | 0 | 839 | 25 | 0 |
| 58 | BY | 1581 | 0 | 805 | 21 | 0 |
| 58 | DY | 1561 | 0 | 796 | 18 | 0 |
| 59 | BZ | 5663 | 0 | 5746 | 246 | 10 |
| 59 | DZ | 5682 | 0 | 5766 | 192 | 6 |
| 60 | A0 | 5 | 0 | 0 | 0 | 0 |
| 60 | A1 | 2 | 0 | 0 | 0 | 0 |
| 60 | A2 | 1 | 0 | 0 | 0 | 0 |
| 60 | A4 | 1 | 0 | 0 | 0 | 0 |
| 60 | A5 | 1 | 0 | 0 | 0 | 0 |
| 60 | A6 | 1 | 0 | 0 | 0 | 0 |
| 60 | A7 | 1 | 0 | 0 | 0 | 0 |
| 60 | A8 | 2 | 0 | 0 | 0 | 0 |
| 60 | A9 | 1 | 0 | 0 | 0 | 0 |
| 60 | AA | 834 | 0 | 0 | 0 | 0 |
| 60 | AB | 23 | 0 | 0 | 0 | 0 |
| 60 | AD | 10 | 0 | 0 | 0 | 0 |
| 60 | AE | 5 | 0 | 0 | 0 | 0 |
| 60 | AF | 5 | 0 | 0 | 0 | 0 |
| 60 | AG | 2 | 0 | 0 | 0 | 0 |
| 60 | AH | 1 | 0 | 0 | 0 | 0 |
| 60 | AN | 3 | 0 | 0 | 0 | 0 |
| 60 | AO | 1 | 0 | 0 | 0 | 0 |
| 60 | AP | 2 | 0 | 0 | 0 | 0 |
| 60 | AQ | 3 | 0 | 0 | 0 | 0 |
| 60 | AR | 1 | 0 | 0 | 0 | 0 |
| 60 | AU | 4 | 0 | 0 | 0 | 0 |
| 60 | AV | 1 | 0 | 0 | 0 | 0 |
| 60 | AW | 4 | 0 | 0 | 0 | 0 |
| 60 | AX | 2 | 0 | 0 | 0 | 0 |
| 60 | AY | 1 | 0 | 0 | 0 | 0 |
| 60 | AZ | 1 | 0 | 0 | 0 | 0 |
| 60 | BA | 213 | 0 | 0 | 0 | 0 |
| 60 | BB | 1 | 0 | 0 | 0 | 0 |
| 60 | BD | 1 | 0 | 0 | 0 | 0 |
| 60 | BE | 1 | 0 | 0 | 0 | 0 |
| 60 | BF | 1 | 0 | 0 | 0 | 0 |
| 60 | BK | 1 | 0 | 0 | 0 | 0 |
| 60 | BL | 2 | 0 | 0 | 0 | 0 |
| 60 | BM | 1 | 0 | 0 | 0 | 0 |
| 60 | BN | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 60 | BT | 1 | 0 | 0 | 0 | 0 |
| 60 | BV | 1 | 0 | 0 | 0 | 0 |
| 60 | BW | 2 | 0 | 0 | 0 | 0 |
| 60 | BX | 15 | 0 | 0 | 0 | 0 |
| 60 | BY | 2 | 0 | 0 | 0 | 0 |
| 60 | BZ | 1 | 0 | 0 | 0 | 0 |
| 60 | C0 | 2 | 0 | 0 | 0 | 0 |
| 60 | C3 | 1 | 0 | 0 | 0 | 0 |
| 60 | C5 | 1 | 0 | 0 | 0 | 0 |
| 60 | C7 | 1 | 0 | 0 | 0 | 0 |
| 60 | C8 | 1 | 0 | 0 | 0 | 0 |
| 60 | CA | 664 | 0 | 0 | 0 | 0 |
| 60 | CB | 13 | 0 | 0 | 0 | 0 |
| 60 | CD | 4 | 0 | 0 | 0 | 0 |
| 60 | CE | 6 | 0 | 0 | 0 | 0 |
| 60 | CF | 6 | 0 | 0 | 0 | 0 |
| 60 | CG | 1 | 0 | 0 | 0 | 0 |
| 60 | CN | 1 | 0 | 0 | 0 | 0 |
| 60 | CO | 2 | 0 | 0 | 0 | 0 |
| 60 | CP | 1 | 0 | 0 | 0 | 0 |
| 60 | CQ | 4 | 0 | 0 | 0 | 0 |
| 60 | CR | 2 | 0 | 0 | 0 | 0 |
| 60 | CU | 1 | 0 | 0 | 0 | 0 |
| 60 | CV | 2 | 0 | 0 | 0 | 0 |
| 60 | CY | 1 | 0 | 0 | 0 | 0 |
| 60 | DA | 168 | 0 | 0 | 0 | 0 |
| 60 | DD | 1 | 0 | 0 | 0 | 0 |
| 60 | DE | 2 | 0 | 0 | 0 | 0 |
| 60 | DF | 1 | 0 | 0 | 0 | 0 |
| 60 | DJ | 1 | 0 | 0 | 0 | 0 |
| 60 | DK | 2 | 0 | 0 | 0 | 0 |
| 60 | DT | 1 | 0 | 0 | 0 | 0 |
| 60 | DW | 1 | 0 | 0 | 0 | 0 |
| 60 | DX | 1 | 0 | 0 | 0 | 0 |
| 60 | DZ | 1 | 0 | 0 | 0 | 0 |
| 61 | AA | 1 | 0 | 0 | 0 | 0 |
| 62 | A4 | 1 | 0 | 0 | 0 | 0 |
| 62 | A5 | 1 | 0 | 0 | 0 | 0 |
| 62 | A6 | 1 | 0 | 0 | 0 | 0 |
| 62 | A9 | 1 | 0 | 0 | 0 | 0 |
| 62 | AY | 1 | 0 | 0 | 0 | 0 |
| 62 | BN | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 62 | C4 | 1 | 0 | 0 | 0 | 0 |
| 62 | C5 | 1 | 0 | 0 | 0 | 0 |
| 62 | C6 | 1 | 0 | 0 | 0 | 0 |
| 62 | C9 | 1 | 0 | 0 | 0 | 0 |
| 62 | CY | 1 | 0 | 0 | 0 | 0 |
| 62 | DN | 1 | 0 | 0 | 0 | 0 |
| 63 | BD | 8 | 0 | 0 | 1 | 0 |
| 63 | DD | 8 | 0 | 0 | 1 | 0 |
| 64 | BZ | 28 | 0 | 12 | 6 | 0 |
| 64 | DZ | 28 | 0 | 12 | 7 | 0 |
| 65 | A0 | 6 | 0 | 0 | 0 | 0 |
| 65 | A1 | 1 | 0 | 0 | 0 | 0 |
| 65 | A3 | 1 | 0 | 0 | 0 | 0 |
| 65 | A5 | 3 | 0 | 0 | 0 | 0 |
| 65 | A6 | 2 | 0 | 0 | 0 | 0 |
| 65 | A7 | 4 | 0 | 0 | 1 | 0 |
| 65 | A8 | 10 | 0 | 0 | 1 | 0 |
| 65 | AA | 1408 | 0 | 0 | 48 | 0 |
| 65 | AB | 36 | 0 | 0 | 1 | 0 |
| 65 | AD | 15 | 0 | 0 | 1 | 0 |
| 65 | AE | 19 | 0 | 0 | 1 | 0 |
| 65 | AF | 7 | 0 | 0 | 0 | 0 |
| 65 | AG | 3 | 0 | 0 | 0 | 0 |
| 65 | AH | 1 | 0 | 0 | 0 | 0 |
| 65 | AN | 2 | 0 | 0 | 0 | 0 |
| 65 | AO | 1 | 0 | 0 | 0 | 0 |
| 65 | AP | 15 | 0 | 0 | 2 | 0 |
| 65 | AQ | 4 | 0 | 0 | 2 | 0 |
| 65 | AR | 2 | 0 | 0 | 2 | 0 |
| 65 | AS | 1 | 0 | 0 | 0 | 0 |
| 65 | AT | 2 | 0 | 0 | 0 | 0 |
| 65 | AU | 5 | 0 | 0 | 0 | 0 |
| 65 | AV | 2 | 0 | 0 | 0 | 0 |
| 65 | AW | 2 | 0 | 0 | 0 | 0 |
| 65 | AX | 3 | 0 | 0 | 0 | 0 |
| 65 | AZ | 1 | 0 | 0 | 0 | 0 |
| 65 | BA | 212 | 0 | 0 | 13 | 0 |
| 65 | BD | 2 | 0 | 0 | 0 | 0 |
| 65 | BE | 2 | 0 | 0 | 0 | 0 |
| 65 | BL | 1 | 0 | 0 | 0 | 0 |
| 65 | BM | 1 | 0 | 0 | 0 | 0 |
| 65 | BV | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 65 | BW | 3 | 0 | 0 | 0 | 0 |
| 65 | BX | 8 | 0 | 0 | 0 | 0 |
| 65 | BY | 1 | 0 | 0 | 0 | 0 |
| 65 | BZ | 2 | 0 | 0 | 0 | 0 |
| 65 | C0 | 6 | 0 | 0 | 1 | 0 |
| 65 | C1 | 2 | 0 | 0 | 0 | 0 |
| 65 | C3 | 2 | 0 | 0 | 0 | 0 |
| 65 | C6 | 1 | 0 | 0 | 1 | 0 |
| 65 | C7 | 1 | 0 | 0 | 0 | 0 |
| 65 | C8 | 3 | 0 | 0 | 0 | 0 |
| 65 | CA | 985 | 0 | 0 | 52 | 0 |
| 65 | CB | 9 | 0 | 0 | 1 | 0 |
| 65 | CD | 14 | 0 | 0 | 0 | 0 |
| 65 | CE | 13 | 0 | 0 | 1 | 0 |
| 65 | CF | 7 | 0 | 0 | 0 | 0 |
| 65 | CN | 2 | 0 | 0 | 0 | 0 |
| 65 | CP | 10 | 0 | 0 | 1 | 0 |
| 65 | CQ | 1 | 0 | 0 | 0 | 0 |
| 65 | CR | 1 | 0 | 0 | 0 | 0 |
| 65 | CT | 3 | 0 | 0 | 0 | 0 |
| 65 | CU | 2 | 0 | 0 | 0 | 0 |
| 65 | CV | 1 | 0 | 0 | 0 | 0 |
| 65 | CY | 1 | 0 | 0 | 0 | 0 |
| 65 | DA | 155 | 0 | 0 | 6 | 0 |
| 65 | DE | 4 | 0 | 0 | 0 | 0 |
| 65 | DJ | 1 | 0 | 0 | 0 | 0 |
| 65 | DK | 2 | 0 | 0 | 0 | 0 |
| 65 | DL | 1 | 0 | 0 | 0 | 0 |
| 65 | DW | 2 | 0 | 0 | 0 | 0 |
| 65 | DX | 1 | 0 | 0 | 0 | 0 |
| All | All | 313372 | 0 | 210866 | 5329 | 17 |

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 11.

All (5329) 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:CA:1860:G:H5' | 3:CC:206:LYS:CD | 1.27 | 1.64 |
| 1:CA:1860:G:H5'' | 3:CC:206:LYS:CG | 1.28 | 1.64 |
| 1:AA:1891:G:C5' | 3:AC:206:LYS:HD2 | 1.35 | 1.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1860:G:C5' | 3:CC:206:LYS:HD2 | 1.25 | 1.53 |
| 1:CA:1860:G:C5' | 3:CC:206:LYS:CG | 1.84 | 1.50 |
| 1:CA:1860:G:C5' | 3:CC:206:LYS:CD | 1.76 | 1.45 |
| 1:CA:1053:C:H42 | 1:CA:1107:G:N2 | 1.04 | 1.41 |
| 1:CA:1053:C:N4 | 1:CA:1107:G:H22 | 1.16 | 1.38 |
| 1:CA:1860:G:C4' | 3:CC:206:LYS:HD2 | 1.53 | 1.35 |
| 1:CA:1860:G:H4' | 3:CC:206:LYS:CD | 1.59 | 1.32 |
| 1:AA:1891:G:C4' | 3:AC:206:LYS:HD2 | 1.58 | 1.31 |
| 1:AA:1891:G:C5' | 3:AC:206:LYS:CD | 2.09 | 1.31 |
| 1:CA:1860:G:C4' | 3:CC:206:LYS:CD | 2.06 | 1.29 |
| 1:AA:1891:G:H4' | 3:AC:206:LYS:CD | 1.60 | 1.29 |
| 1:AA:1891:G:H5'' | 3:AC:206:LYS:CG | 1.68 | 1.22 |
| 1:AA:1891:G:H5' | 3:AC:206:LYS:HD2 | 1.20 | 1.09 |
| 1:CA:1798:U:H5' | 4:CD:259:THR:HG22 | 1.34 | 1.09 |
| 1:AA:1891:G:H5'' | 3:AC:206:LYS:HG2 | 1.36 | 1.06 |
| 1:AA:1891:G:O3' | 3:AC:206:LYS:HG3 | 1.54 | 1.05 |
| 1:AA:2198:A:HO2' | 3:AC:45:HIS:CD2 | 1.74 | 1.04 |
| 1:CA:1860:G:C4' | 3:CC:206:LYS:HG3 | 1.87 | 1.02 |
| 1:CA:2132:U:N3 | 3:CC:6:LYS:HE3 | 1.74 | 1.02 |
| 1:CA:1860:G:C4' | 3:CC:206:LYS:CG | 2.32 | 1.02 |
| 1:AA:1249:A:H2 | 1:AA:1287:A:H62 | 1.06 | 1.02 |
| 1:CA:1860:G:H5' | 3:CC:206:LYS:CE | 1.90 | 1.01 |
| 1:CA:1053:C:N4 | 1:CA:1107:G:N2 | 1.87 | 1.00 |
| 1:AA:9:U:H3 | 1:AA:2641:A:H2 | 1.08 | 0.99 |
| 21:AX:31:HIS:HD2 | 21:AX:33:LYS:H | 1.07 | 0.99 |
| 59:BZ:99:ARG:HB3 | 59:BZ:99:ARG:HH11 | 1.26 | 0.99 |
| 1:AA:1829:U:H5' | 4:AD:259:THR:HG22 | 1.43 | 0.98 |
| 1:CA:1860:G:H4' | 3:CC:206:LYS:HD3 | 1.42 | 0.98 |
| 1:CA:1860:G:H5'' | 3:CC:206:LYS:HG3 | 1.38 | 0.98 |
| 1:AA:2198:A:O2' | 3:AC:45:HIS:CD2 | 2.17 | 0.98 |
| 1:AA:1891:G:H5'' | 3:AC:206:LYS:CD | 1.86 | 0.96 |
| 1:AA:1405:A:H61 | 1:AA:1418:U:H3 | 1.10 | 0.96 |
| 59:BZ:13:ARG:HH12 | 59:BZ:247:ARG:HH22 | 1.11 | 0.96 |
| 21:CX:35:THR:HG22 | 21:CX:38:GLU:H | 1.30 | 0.95 |
| 1:AA:535:C:OP1 | 65:AA:4769:HOH:O | 1.83 | 0.95 |
| 1:CA:1204:A:H2 | 1:CA:1241:A:H62 | 1.14 | 0.95 |
| 1:AA:1891:G:C4' | 3:AC:206:LYS:CD | 2.26 | 0.95 |
| 59:DZ:119:GLU:OE1 | 59:DZ:156:ARG:NH1 | 2.00 | 0.94 |
| 34:BA:160:A:N6 | 34:BA:345:C:OP2 | 2.01 | 0.94 |
| 35:BB:16:HIS:HB2 | 35:BB:204:ASN:HB3 | 1.49 | 0.94 |
| 13:AP:39:LYS:NZ | 65:AP:307:HOH:O | 2.00 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1736:A:H62 | 1:AA:1745:A:H2 | 1.13 | 0.94 |
| 1:AA:1891:G:C5' | 3:AC:206:LYS:CG | 2.42 | 0.93 |
| 1:CA:1689:A:H62 | 1:CA:1698:A:H2 | 1.04 | 0.93 |
| 1:AA:1090:G:O2' | 1:AA:1157:A:N6 | 2.01 | 0.93 |
| 34:DA:1086:U:H3 | 34:DA:1099:G:H22 | 1.16 | 0.92 |
| 1:CA:397:G:N7 | 65:CA:4556:HOH:O | 2.03 | 0.92 |
| 1:CA:1860:G:H5'' | 3:CC:206:LYS:HG2 | 0.94 | 0.92 |
| 34:BA:1158:C:H5 | 34:BA:1181:G:H1 | 1.19 | 0.90 |
| 1:CA:1021:A:H62 | 1:CA:1141:U:H3 | 1.15 | 0.90 |
| 1:AA:1065:U:HO2' | 1:AA:1067:A:H2 | 1.18 | 0.90 |
| 1:AA:2511:C:OP1 | 65:AA:5078:HOH:O | 1.87 | 0.89 |
| 22:CY:102:CYS:SG | 22:CY:103:GLY:N | 2.42 | 0.89 |
| 20:AW:12:ILE:HD13 | 20:AW:17:VAL:HG22 | 1.55 | 0.89 |
| 59:BZ:78:ARG:HG3 | 59:BZ:78:ARG:HH11 | 1.38 | 0.89 |
| 23:AZ:29:TYR:HB3 | 23:AZ:34:ASN:HD22 | 1.37 | 0.89 |
| 34:BA:975:A:H4' | 34:BA:976:G:H5'' | 1.56 | 0.88 |
| 3:CC:31:LYS:NZ | 3:CC:181:PHE:O | 2.06 | 0.88 |
| 34:BA:964:A:OP1 | 65:BA:2060:HOH:O | 1.88 | 0.88 |
| 17:CT:55:ASN:H | 17:CT:59:THR:HG22 | 1.36 | 0.87 |
| 34:BA:937:A:OP2 | 65:BA:2015:HOH:O | 1.92 | 0.87 |
| 3:AC:31:LYS:NZ | 3:AC:181:PHE:O | 2.06 | 0.87 |
| 6:CF:185:ASP:HA | 6:CF:188:ARG:HD3 | 1.57 | 0.87 |
| 35:DB:185:ILE:HG22 | 35:DB:199:TYR:HB2 | 1.55 | 0.86 |
| 3:AC:52:PRO:HG2 | 3:AC:53:ARG:HD3 | 1.57 | 0.86 |
| 34:DA:975:A:H4' | 34:DA:976:G:H5'' | 1.58 | 0.86 |
| 1:CA:2714:G:OP2 | 65:CA:3993:HOH:O | 1.91 | 0.86 |
| 34:DA:376:G:H5'' | 49:DP:5:ARG:HD3 | 1.58 | 0.86 |
| 3:CC:52:PRO:HG2 | 3:CC:53:ARG:HD3 | 1.57 | 0.86 |
| 24:C0:10:THR:HG22 | 24:C0:12:ASN:H | 1.40 | 0.85 |
| 1:AA:1716:A:OP2 | 65:AA:5038:HOH:O | 1.94 | 0.85 |
| 1:AA:2201:C:O4' | 3:AC:169:THR:HG22 | 1.76 | 0.85 |
| 22:AY:54:LYS:HA | 22:AY:56:PRO:HD3 | 1.58 | 0.85 |
| 44:BK:79:SER:HA | 44:BK:104:GLN:HB2 | 1.59 | 0.85 |
| 13:CP:100:LEU:HD12 | 13:CP:112:LEU:HD11 | 1.57 | 0.84 |
| 18:AU:108:GLU:OE2 | 18:AU:112:ARG:NH1 | 2.10 | 0.84 |
| 59:BZ:169:GLY:HA3 | 59:BZ:174:PHE:HA | 1.59 | 0.84 |
| 43:BJ:35:SER:HB3 | 43:BJ:73:ASP:HB2 | 1.58 | 0.84 |
| 34:BA:1502:A:H2 | 34:BA:1505:G:H1 | 1.24 | 0.84 |
| 1:AA:1891:G:H4' | 3:AC:206:LYS:HD3 | 1.56 | 0.84 |
| 1:AA:1356:G:OP2 | 31:A7:9:ARG:NH1 | 2.10 | 0.84 |
| 34:DA:1166:G:N2 | 34:DA:1170:A:OP2 | 2.09 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 59:BZ:405:PRO:HD2 | 59:BZ:406:GLU:HG2 | 1.60 | 0.83 |
| 34:BA:538:G:H5'' | 45:BL:114:LYS:HB2 | 1.60 | 0.83 |
| 34:BA:664:G:H22 | 34:BA:741:G:H1 | 1.24 | 0.83 |
| 1:CA:1603:A:OP1 | 65:CA:4478:HOH:O | 1.95 | 0.83 |
| 12:AO:2:ILE:HD12 | 12:AO:6:THR:HG21 | 1.59 | 0.83 |
| 1:CA:2178:C:O2' | 3:CC:169:THR:HB | 1.76 | 0.83 |
| 34:DA:656:C:O2' | 48:DO:28:GLN:NE2 | 2.12 | 0.83 |
| 14:AQ:111:GLU:OE1 | 14:AQ:133:ARG:NH2 | 2.13 | 0.82 |
| 1:AA:2297:C:OP2 | 30:A6:6:ARG:NH1 | 2.12 | 0.82 |
| 1:AA:1094:A:OP2 | 1:AA:1155:C:N4 | 2.12 | 0.82 |
| 34:DA:922:G:H4' | 38:DE:20:GLN:HA | 1.59 | 0.82 |
| 13:CP:39:LYS:HB2 | 13:CP:45:LEU:HG | 1.61 | 0.82 |
| 1:CA:1860:G:H4' | 3:CC:206:LYS:CG | 2.03 | 0.82 |
| 1:CA:2206:G:H3' | 1:CA:2207:G:C8 | 2.15 | 0.82 |
| 3:AC:54:ARG:NH2 | 3:AC:56:ASP:HB3 | 1.95 | 0.82 |
| 8:CH:98:LEU:HD22 | 8:CH:125:VAL:HG23 | 1.61 | 0.82 |
| 1:AA:1100:A:H62 | 1:AA:1151:U:H3 | 1.29 | 0.81 |
| 1:AA:2128:G:H1 | 1:AA:2205:C:H42 | 1.27 | 0.81 |
| 43:DJ:49:VAL:HG23 | 47:DN:41:ARG:HB2 | 1.61 | 0.81 |
| 5:AE:179:GLU:HB3 | 5:AE:181:LEU:HD22 | 1.60 | 0.81 |
| 34:BA:1129:C:H5'' | 42:BI:16:ARG:HH12 | 1.46 | 0.81 |
| 34:DA:653:A:OP1 | 41:DH:56:LYS:NZ | 2.13 | 0.81 |
| 38:DE:122:GLU:O | 38:DE:126:ARG:NH1 | 2.14 | 0.81 |
| 59:BZ:97:SER:O | 59:BZ:99:ARG:N | 2.12 | 0.81 |
| 45:DL:24:VAL:HG11 | 45:DL:27:LEU:HD22 | 1.62 | 0.81 |
| 35:BB:69:LEU:HB3 | 35:BB:162:ILE:HG22 | 1.60 | 0.81 |
| 3:CC:54:ARG:NH2 | 3:CC:56:ASP:HB3 | 1.95 | 0.81 |
| 53:DT:10:LEU:HB3 | 53:DT:12:ALA:H | 1.45 | 0.81 |
| 1:AA:927:G:N2 | 1:AA:944:C:N3 | 2.29 | 0.80 |
| 24:A0:11:ARG:O | 24:A0:14:ARG:NH2 | 2.14 | 0.80 |
| 1:CA:1019:U:H3 | 1:CA:1142(A):A:H62 | 1.27 | 0.80 |
| 58:DY:19:G:N2 | 58:DY:56:C:N3 | 2.29 | 0.80 |
| 35:BB:111:ARG:HG2 | 35:BB:111:ARG:HH11 | 1.46 | 0.80 |
| 1:AA:2299:A:H62 | 1:AA:2356:U:H3 | 1.27 | 0.80 |
| 59:BZ:357:ARG:NH1 | 59:BZ:373:ASP:OD1 | 2.15 | 0.79 |
| 40:BG:111:ARG:NH1 | 40:BG:113:GLU:OE2 | 2.15 | 0.79 |
| 34:DA:664:G:H22 | 34:DA:741:G:H1 | 1.25 | 0.79 |
| 7:CG:80:PHE:O | 7:CG:82:LEU:N | 2.15 | 0.79 |
| 1:AA:1219:A:H1' | 1:AA:1220:U:H5'' | 1.62 | 0.79 |
| 34:BA:376:G:H5'' | 49:BP:5:ARG:HG2 | 1.64 | 0.79 |
| 36:BC:37:GLN:NE2 | 47:BN:52:GLN:OE1 | 2.16 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:2132:U:C4 | 3:CC:6:LYS:HE3 | 2.18 | 0.79 |
| 38:DE:74:GLY:HA3 | 38:DE:116:THR:HG22 | 1.64 | 0.79 |
| 34:BA:656:C:O2' | 48:BO:28:GLN:NE2 | 2.15 | 0.79 |
| 41:DH:51:VAL:HG11 | 41:DH:60:ARG:HH11 | 1.46 | 0.79 |
| 1:CA:529:A:N6 | 1:CA:2041:U:O2 | 2.15 | 0.79 |
| 24:C0:11:ARG:O | 24:C0:14:ARG:NH2 | 2.16 | 0.79 |
| 59:BZ:380:LEU:HD21 | 59:BZ:389:LEU:HD21 | 1.64 | 0.79 |
| 17:AT:55:ASN:H | 17:AT:59:THR:HG22 | 1.45 | 0.79 |
| 1:CA:1860:G:C3' | 3:CC:206:LYS:HG3 | 2.12 | 0.79 |
| 1:AA:1891:G:C4' | 3:AC:206:LYS:CG | 2.61 | 0.79 |
| 1:CA:2287:A:H62 | 1:CA:2344:U:H3 | 1.30 | 0.79 |
| 34:DA:115:G:OP1 | 65:DA:1871:HOH:O | 2.01 | 0.79 |
| 59:BZ:363:ARG:HH11 | 59:BZ:363:ARG:HG2 | 1.46 | 0.79 |
| 34:DA:1320:C:N3 | 52:DS:36:ARG:NH2 | 2.31 | 0.78 |
| 1:CA:1860:G:C5' | 3:CC:206:LYS:HG2 | 1.77 | 0.78 |
| 59:BZ:480:GLN:O | 59:BZ:482:ALA:N | 2.17 | 0.78 |
| 28:C4:36:CYS:SG | 28:C4:37:SER:N | 2.55 | 0.78 |
| 22:AY:92:ASN:H | 22:AY:92:ASN:HD22 | 1.29 | 0.78 |
| 58:DY:7:A:H61 | 58:DY:66:U:H3 | 1.30 | 0.78 |
| 4:AD:69:ARG:NH2 | 4:AD:128:GLY:O | 2.16 | 0.78 |
| 35:BB:115:LEU:HD13 | 35:BB:145:LEU:HB3 | 1.65 | 0.78 |
| 1:CA:2296:U:OP2 | 16:CS:9:ARG:NH2 | 2.17 | 0.78 |
| 1:CA:880:G:H22 | 1:CA:898:C:H1' | 1.46 | 0.78 |
| 59:BZ:169:GLY:O | 59:BZ:173:THR:OG1 | 2.02 | 0.78 |
| 1:CA:1817:G:OP1 | 4:CD:88:ARG:NH2 | 2.16 | 0.78 |
| 1:CA:631:A:OP1 | 13:CP:65:ARG:NH1 | 2.16 | 0.78 |
| 36:BC:58:GLU:HB3 | 43:BJ:92:THR:HG21 | 1.65 | 0.78 |
| 24:C0:5:LYS:NZ | 57:DX:2:G:OP1 | 2.17 | 0.78 |
| 42:BI:17:VAL:HG21 | 42:BI:81:ILE:HG22 | 1.65 | 0.77 |
| 4:CD:148:GLU:HB2 | 4:CD:151:LYS:HD2 | 1.66 | 0.77 |
| 1:CA:528:A:O2' | 1:CA:529:A:H5'' | 1.83 | 0.77 |
| 14:AQ:21:THR:HG21 | 14:AQ:101:ARG:HD3 | 1.64 | 0.77 |
| 1:AA:1100:A:N6 | 1:AA:1151:U:H3 | 1.81 | 0.77 |
| 35:BB:150:SER:O | 35:BB:153:ARG:NH1 | 2.17 | 0.77 |
| 36:DC:70:VAL:HG22 | 36:DC:72:LYS:H | 1.49 | 0.77 |
| 34:DA:344:A:H5'' | 34:DA:345:C:H5 | 1.48 | 0.77 |
| 21:AX:31:HIS:CD2 | 21:AX:33:LYS:H | 1.98 | 0.77 |
| 22:AY:92:ASN:HB2 | 22:AY:94:LYS:H | 1.48 | 0.77 |
| 3:AC:20:VAL:O | 3:AC:21:TYR:HB2 | 1.83 | 0.77 |
| 34:DA:48:C:OP2 | 65:DA:1871:HOH:O | 2.03 | 0.77 |
| 39:DF:87:ARG:HH11 | 39:DF:87:ARG:HG3 | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:AZ:117:LEU:HD11 | 23:AZ:144:LEU:HD22 | 1.66 | 0.77 |
| 59:BZ:329:ARG:HH11 | 59:BZ:331:TYR:HE1 | 1.33 | 0.77 |
| 19:AV:98:GLU:OE2 | 19:AV:100:ARG:NH1 | 2.17 | 0.77 |
| 56:BW:5:G:H2' | 56:BW:6:G:H8 | 1.50 | 0.77 |
| 3:AC:27:ALA:O | 3:AC:30:VAL:HG22 | 1.85 | 0.77 |
| 36:DC:179:ARG:NH1 | 36:DC:206:GLU:OE1 | 2.17 | 0.77 |
| 15:AR:33:ARG:NH1 | 15:AR:115:GLU:OE2 | 2.16 | 0.77 |
| 53:BT:10:LEU:HB3 | 53:BT:12:ALA:H | 1.50 | 0.76 |
| 1:AA:1007:G:OP1 | 65:AA:4764:HOH:O | 2.03 | 0.76 |
| 3:CC:20:VAL:O | 3:CC:21:TYR:HB2 | 1.83 | 0.76 |
| 1:CA:1155:A:H5'' | 18:CU:55:ARG:HH11 | 1.50 | 0.76 |
| 3:AC:24:ASP:O | 3:AC:28:ARG:HG3 | 1.85 | 0.76 |
| 1:AA:992:G:OP2 | 65:AA:4762:HOH:O | 2.03 | 0.76 |
| 59:BZ:78:ARG:HH11 | 59:BZ:78:ARG:CG | 1.96 | 0.76 |
| 1:CA:1031:G:H21 | 33:C9:36:GLN:HE22 | 1.31 | 0.76 |
| 15:AR:67:LEU:HD13 | 15:AR:76:VAL:HG21 | 1.67 | 0.76 |
| 3:CC:24:ASP:O | 3:CC:28:ARG:HG3 | 1.85 | 0.76 |
| 1:AA:1829:U:OP2 | 4:AD:274:ARG:NH2 | 2.19 | 0.76 |
| 34:DA:1224:G:O2' | 34:DA:1322:C:OP1 | 2.04 | 0.76 |
| 59:BZ:148:LEU:O | 59:BZ:152:THR:OG1 | 2.04 | 0.76 |
| 59:DZ:247:ARG:NH1 | 59:DZ:251:ILE:HD11 | 2.00 | 0.76 |
| 1:AA:1740:U:O2' | 4:AD:14:ARG:NH2 | 2.18 | 0.76 |
| 1:CA:1310:G:OP2 | 31:C7:9:ARG:NH1 | 2.19 | 0.76 |
| 34:DA:1103:C:OP1 | 35:DB:96:ARG:NH2 | 2.18 | 0.76 |
| 1:AA:1016:C:OP2 | 65:AA:5195:HOH:O | 2.03 | 0.76 |
| 1:CA:1039:G:O6 | 1:CA:1116:C:N4 | 2.19 | 0.76 |
| 1:CA:827:U:OP1 | 65:CA:4250:HOH:O | 2.02 | 0.76 |
| 1:AA:2658:C:OP2 | 1:AA:2745:G:O2' | 2.02 | 0.76 |
| 56:BW:50:U:H3 | 56:BW:64:A:H61 | 1.33 | 0.76 |
| 3:CC:27:ALA:O | 3:CC:30:VAL:HG22 | 1.85 | 0.76 |
| 59:DZ:165:GLN:HE21 | 59:DZ:260:LEU:H | 1.33 | 0.76 |
| 1:CA:271(R):G:H5'' | 25:C1:97:LEU:HD21 | 1.66 | 0.76 |
| 56:DW:76:F3N:H8 | 56:DW:76:F3N:H5' | 1.66 | 0.76 |
| 1:CA:878:A:N6 | 1:CA:899:A:O2' | 2.18 | 0.76 |
| 1:AA:1891:G:C3' | 3:AC:206:LYS:HG3 | 2.16 | 0.76 |
| 1:CA:731:C:OP2 | 65:CA:4229:HOH:O | 2.02 | 0.75 |
| 6:AF:195:ASP:HB3 | 6:AF:198:ALA:H | 1.50 | 0.75 |
| 1:AA:894:U:OP2 | 65:AA:4336:HOH:O | 2.02 | 0.75 |
| 56:BW:19:G:H1 | 56:BW:56:C:H42 | 1.33 | 0.75 |
| 1:CA:301:G:OP2 | 22:CY:84:ARG:NH2 | 2.18 | 0.75 |
| 59:BZ:373:ASP:OD2 | 59:BZ:374:LEU:N | 2.18 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:614(B):G:H2' | 6:CF:44:ARG:HH11 | 1.51 | 0.75 |
| 4:CD:96:HIS:HD2 | 4:CD:102:LYS:HG2 | 1.52 | 0.75 |
| 59:DZ:129:LYS:HD3 | 59:DZ:521:SER:HB2 | 1.67 | 0.75 |
| 1:AA:2227:G:H5' | 1:AA:2228:G:N7 | 2.02 | 0.75 |
| 1:AA:139:A:H8 | 1:AA:1454:C:HO2' | 1.34 | 0.75 |
| 1:AA:927:G:H2' | 1:AA:928:G:H8 | 1.52 | 0.75 |
| 34:DA:838:G:H1 | 34:DA:848:C:H42 | 1.34 | 0.75 |
| 34:DA:677:U:H3 | 34:DA:713:G:H22 | 1.35 | 0.75 |
| 4:CD:125:ILE:HB | 39:DF:81:ILE:HD11 | 1.68 | 0.75 |
| 15:AR:3:HIS:NE2 | 65:AR:5101:HOH:O | 2.20 | 0.75 |
| 20:CW:34:ASN:OD1 | 20:CW:37:ARG:NH2 | 2.18 | 0.75 |
| 1:CA:1024:G:OP2 | 65:CA:4575:HOH:O | 2.03 | 0.75 |
| 1:CA:2138:C:H42 | 1:CA:2153:G:H1 | 1.35 | 0.75 |
| 34:DA:1255:G:OP1 | 43:DJ:45:ARG:NH2 | 2.19 | 0.74 |
| 34:BA:504:C:OP1 | 65:BA:2083:HOH:O | 2.04 | 0.74 |
| 1:CA:370:G:N7 | 65:CA:3748:HOH:O | 2.20 | 0.74 |
| 15:CR:55:ALA:HB2 | 15:CR:79:LEU:HD13 | 1.69 | 0.74 |
| 59:DZ:116:PRO:O | 59:DZ:118:SER:N | 2.21 | 0.74 |
| 1:AA:1151:U:H2' | 1:AA:1152:G:C8 | 2.22 | 0.74 |
| 1:AA:2122:G:H1 | 1:AA:2211:U:H3 | 1.33 | 0.74 |
| 37:BD:49:ARG:H | 37:BD:49:ARG:HE | 1.35 | 0.74 |
| 1:CA:2099:U:H3 | 1:CA:2190:G:H1 | 1.35 | 0.74 |
| 34:DA:619:U:N3 | 37:DD:134:ASP:OD1 | 2.21 | 0.74 |
| 59:DZ:-66:MET:N | 59:DZ:-46:VAL:O | 2.19 | 0.74 |
| 59:DZ:203:GLU:OE2 | 59:DZ:203:GLU:N | 2.20 | 0.74 |
| 3:CC:48:LEU:HB3 | 3:CC:50:ILE:HD12 | 1.70 | 0.74 |
| 46:DM:58:GLU:O | 46:DM:62:ASN:ND2 | 2.20 | 0.74 |
| 34:DA:992:U:H3 | 34:DA:1044:A:H62 | 1.36 | 0.74 |
| 1:AA:427:G:N7 | 65:AA:4917:HOH:O | 2.19 | 0.74 |
| 34:DA:953:G:H5' | 34:DA:965:A:H61 | 1.51 | 0.74 |
| 1:CA:1860:G:O3' | 3:CC:206:LYS:HG3 | 1.88 | 0.74 |
| 44:DK:92:GLU:OE2 | 51:DR:87:ARG:NH1 | 2.21 | 0.74 |
| 34:BA:165:C:H2' | 34:BA:166:G:C8 | 2.23 | 0.74 |
| 1:AA:1405:A:N6 | 1:AA:1418:U:H3 | 1.84 | 0.73 |
| 43:DJ:29:ARG:HB2 | 43:DJ:84:GLN:HE22 | 1.53 | 0.73 |
| 59:DZ:21:ILE:HD11 | 59:DZ:117:GLN:HE22 | 1.51 | 0.73 |
| 1:CA:2646:C:OP2 | 1:CA:2732:G:O2' | 2.06 | 0.73 |
| 13:CP:38:GLN:O | 13:CP:40:SER:N | 2.22 | 0.73 |
| 34:BA:560:U:OP2 | 65:BA:1956:HOH:O | 2.07 | 0.73 |
| 1:CA:1842:G:O2' | 4:CD:253:GLN:NE2 | 2.21 | 0.73 |
| 1:AA:2825:C:H5' | 29:A5:29:THR:HG21 | 1.68 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:CA:517:C:OP1 | 29:C5:16:ARG:NH2 | 2.22 | 0.73 |
| 35:BB:16:HIS:O | 35:BB:18:GLY:N | 2.21 | 0.73 |
| 59:DZ:363:ARG:HG2 | 59:DZ:363:ARG:HH11 | 1.53 | 0.73 |
| 59:BZ:13:ARG:HH12 | 59:BZ:247:ARG:NH2 | 1.84 | 0.73 |
| 34:BA:1305:G:N2 | 34:BA:1331:G:H1' | 2.02 | 0.73 |
| 1:CA:2176:A:O2' | 3:CC:45:HIS:CD2 | 2.41 | 0.73 |
| 1:AA:1873:G:O2' | 4:AD:253:GLN:NE2 | 2.22 | 0.73 |
| 20:AW:4:LYS:HE2 | 20:AW:6:ILE:HD11 | 1.70 | 0.73 |
| 34:DA:1075:C:OP1 | 35:DB:179:LYS:NZ | 2.22 | 0.73 |
| 5:AE:127:ASP:OD2 | 65:AE:406:HOH:O | 2.07 | 0.73 |
| 1:CA:2177:C:O2 | 3:CC:173:HIS:CE1 | 2.42 | 0.73 |
| 23:CZ:45:ASP:OD2 | 23:CZ:49:ARG:NH1 | 2.22 | 0.73 |
| 37:BD:178:VAL:O | 37:BD:180:GLY:N | 2.21 | 0.73 |
| 41:DH:29:SER:HB3 | 41:DH:32:LYS:HG3 | 1.70 | 0.73 |
| 1:AA:1055:A:OP2 | 11:AN:37:LYS:NZ | 2.22 | 0.73 |
| 35:BB:7:VAL:HG11 | 35:BB:221:LEU:HD23 | 1.70 | 0.73 |
| 34:DA:1030(A):G:N2 | 34:DA:1030(D):A:OP2 | 2.20 | 0.73 |
| 34:DA:137:C:H42 | 34:DA:226:G:H1 | 1.37 | 0.73 |
| 12:AO:97:ARG:NH1 | 34:BA:339:C:OP2 | 2.20 | 0.73 |
| 1:AA:2324:U:H5' | 7:AG:88:ILE:HD11 | 1.71 | 0.73 |
| 15:CR:33:ARG:NH2 | 29:C5:57:VAL:O | 2.22 | 0.73 |
| 1:AA:2859:U:O4 | 17:AT:23:ARG:NH2 | 2.21 | 0.73 |
| 7:CG:38:VAL:HG22 | 7:CG:93:THR:HG23 | 1.71 | 0.73 |
| 34:BA:166:G:H2' | 34:BA:167:G:H8 | 1.53 | 0.72 |
| 28:C4:61:ARG:HG3 | 52:DS:42:PRO:HG3 | 1.71 | 0.72 |
| 38:DE:100:VAL:O | 38:DE:107:ARG:NH2 | 2.22 | 0.72 |
| 34:BA:558:G:OP1 | 65:BA:1960:HOH:O | 2.07 | 0.72 |
| 1:AA:929:G:N2 | 1:AA:941:U:O2 | 2.22 | 0.72 |
| 34:BA:505:G:N7 | 65:BA:2082:HOH:O | 2.22 | 0.72 |
| 6:AF:185:ASP:HA | 6:AF:188:ARG:HD3 | 1.71 | 0.72 |
| 49:BP:53:VAL:HG13 | 49:BP:79:VAL:HG22 | 1.70 | 0.72 |
| 56:DW:11:C:H42 | 56:DW:24:G:H1 | 1.36 | 0.72 |
| 34:BA:1030(C):G:N7 | 34:BA:1031:G:N2 | 2.37 | 0.72 |
| 1:AA:1001:G:OP2 | 14:AQ:14:ARG:NH2 | 2.22 | 0.72 |
| 1:AA:1065:U:H3 | 1:AA:1188:A:H62 | 1.35 | 0.72 |
| 42:DI:16:ARG:HB2 | 42:DI:64:THR:HG23 | 1.70 | 0.72 |
| 1:CA:2357:U:OP1 | 24:C0:20:ARG:NH1 | 2.22 | 0.72 |
| 36:BC:40:ARG:NH2 | 36:BC:55:VAL:O | 2.22 | 0.72 |
| 35:DB:178:ARG:HH22 | 41:DH:68:ARG:HH22 | 1.35 | 0.72 |
| 1:CA:991:C:OP2 | 65:CA:4148:HOH:O | 2.08 | 0.72 |
| 1:AA:831:A:OP2 | 65:AA:4557:HOH:O | 2.08 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:323:G:HO2' | 1:CA:1205:U:H3 | 0.75 | 0.72 |
| 1:CA:2046:G:H5' | 29:C5:19:ARG:HA | 1.70 | 0.72 |
| 59:BZ:102:ASP:OD2 | 59:BZ:329:ARG:NH2 | 2.22 | 0.72 |
| 34:BA:167:G:H2' | 34:BA:168:G:H8 | 1.55 | 0.72 |
| 42:BI:128:ARG:NH2 | 57:BX:33:U:OP2 | 2.21 | 0.72 |
| 1:AA:1657:C:OP1 | 65:AA:5025:HOH:O | 2.07 | 0.72 |
| 38:DE:88:LYS:HB3 | 38:DE:123:LEU:HB2 | 1.71 | 0.72 |
| 34:BA:1054:C:OP2 | 65:BA:1976:HOH:O | 2.07 | 0.72 |
| 35:DB:69:LEU:HB3 | 35:DB:162:ILE:HG22 | 1.70 | 0.72 |
| 34:DA:1065:U:OP2 | 34:DA:1190:G:N2 | 2.22 | 0.72 |
| 50:DQ:66:SER:O | 50:DQ:70:ARG:NH1 | 2.23 | 0.72 |
| 1:AA:467:U:O2 | 6:AF:46:ARG:NH2 | 2.23 | 0.72 |
| 20:AW:2:GLU:OE2 | 20:AW:72:LYS:HE2 | 1.90 | 0.72 |
| 59:BZ:13:ARG:NH1 | 59:BZ:247:ARG:HH22 | 1.86 | 0.72 |
| 59:BZ:363:ARG:NH1 | 59:BZ:363:ARG:HG2 | 2.01 | 0.72 |
| 12:CO:63:VAL:HG12 | 12:CO:106:LEU:HD11 | 1.72 | 0.72 |
| 1:CA:2445:G:OP1 | 6:CF:74:ARG:NH2 | 2.23 | 0.72 |
| 34:DA:1239:A:H4' | 34:DA:1240:U:H5' | 1.70 | 0.72 |
| 42:BI:40:LEU:O | 42:BI:42:ARG:N | 2.23 | 0.71 |
| 1:AA:1189:A:OP1 | 11:AN:25:ARG:NH2 | 2.23 | 0.71 |
| 1:AA:1151:U:H2' | 1:AA:1152:G:H8 | 1.51 | 0.71 |
| 1:CA:1622:G:OP2 | 65:CA:3921:HOH:O | 2.08 | 0.71 |
| 3:AC:48:LEU:HB3 | 3:AC:50:ILE:HD12 | 1.70 | 0.71 |
| 17:AT:60:THR:HG22 | 17:AT:77:PRO:HA | 1.70 | 0.71 |
| 48:DO:5:LYS:HD3 | 48:DO:5:LYS:H | 1.55 | 0.71 |
| 6:CF:53:THR:HG22 | 6:CF:56:GLU:HG3 | 1.71 | 0.71 |
| 1:AA:2337:G:OP2 | 65:AA:5135:HOH:O | 2.06 | 0.71 |
| 59:DZ:466:LEU:HG | 59:DZ:472:VAL:HG21 | 1.71 | 0.71 |
| 59:DZ:82:ILE:HD12 | 59:DZ:101:LEU:HB3 | 1.72 | 0.71 |
| 1:CA:1754:C:OP1 | 17:CT:96:ARG:NH1 | 2.22 | 0.71 |
| 37:DD:187:ARG:NH2 | 37:DD:193:ASP:OD2 | 2.23 | 0.71 |
| 1:CA:641:C:O2' | 1:CA:2350:C:OP1 | 2.04 | 0.71 |
| 14:AQ:14:ARG:HG2 | 14:AQ:41:TRP:HH2 | 1.55 | 0.71 |
| 45:DL:32:PHE:HB3 | 45:DL:84:LEU:HD11 | 1.72 | 0.71 |
| 1:AA:1891:G:C4' | 3:AC:206:LYS:HG3 | 2.20 | 0.71 |
| 1:CA:775:G:N3 | 65:CA:4199:HOH:O | 2.23 | 0.71 |
| 1:AA:2291:G:N7 | 24:A0:14:ARG:NH1 | 2.37 | 0.71 |
| 34:BA:1226:C:O2' | 46:BM:111:LYS:NZ | 2.23 | 0.71 |
| 1:CA:2124:G:H4' | 3:CC:175:PRO:HG3 | 1.72 | 0.71 |
| 1:CA:740:U:OP2 | 65:CA:4169:HOH:O | 2.07 | 0.71 |
| 34:DA:1238:A:OP2 | 65:DA:1861:HOH:O | 2.07 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:107:VAL:HG11 | 8:CH:162:ILE:HD11 | 1.70 | 0.71 |
| 59:BZ:396:ARG:HG3 | 59:BZ:396:ARG:HH21 | 1.56 | 0.71 |
| 1:CA:971:C:OP2 | 65:CA:4574:HOH:O | 2.07 | 0.71 |
| 34:BA:255:G:H1' | 50:BQ:16:GLN:HE21 | 1.54 | 0.71 |
| 3:AC:51:ASP:HB3 | 3:AC:57:GLN:OE1 | 1.91 | 0.71 |
| 3:CC:51:ASP:HB3 | 3:CC:57:GLN:OE1 | 1.91 | 0.71 |
| 41:BH:10:LEU:HD22 | 41:BH:83:ILE:HD11 | 1.72 | 0.71 |
| 59:DZ:225:GLU:HA | 59:DZ:228:MET:HB3 | 1.72 | 0.71 |
| 59:DZ:466:LEU:HA | 59:DZ:470:PHE:HD2 | 1.56 | 0.71 |
| 48:DO:39:LEU:HD13 | 48:DO:56:LEU:HB2 | 1.73 | 0.71 |
| 1:CA:2823:A:OP1 | 5:CE:159:HIS:NE2 | 2.21 | 0.71 |
| 19:AV:40:LEU:HB2 | 19:AV:46:VAL:HG13 | 1.72 | 0.71 |
| 3:AC:55:SER:O | 3:AC:57:GLN:N | 2.22 | 0.70 |
| 59:BZ:87:HIS:O | 59:BZ:89:ASP:N | 2.24 | 0.70 |
| 59:DZ:169:GLY:H | 59:DZ:170:ARG:HH12 | 1.39 | 0.70 |
| 1:AA:1391:C:OP2 | 65:AA:3960:HOH:O | 2.08 | 0.70 |
| 1:CA:2022:U:OP1 | 65:CA:4131:HOH:O | 2.07 | 0.70 |
| 47:DN:21:TYR:OH | 47:DN:23:ARG:NH2 | 2.24 | 0.70 |
| 34:BA:427:U:OP1 | 37:BD:13:ARG:NH2 | 2.23 | 0.70 |
| 59:BZ:114:VAL:CG1 | 59:BZ:156:ARG:HH12 | 2.05 | 0.70 |
| 52:BS:32:LYS:HA | 52:BS:50:ALA:HB3 | 1.72 | 0.70 |
| 36:BC:150:LYS:HG3 | 36:BC:169:ALA:HB2 | 1.73 | 0.70 |
| 38:BE:43:LEU:HD21 | 38:BE:132:ALA:HB1 | 1.73 | 0.70 |
| 38:BE:100:VAL:O | 38:BE:107:ARG:NH2 | 2.24 | 0.70 |
| 1:AA:1891:G:H4' | 3:AC:206:LYS:CG | 2.21 | 0.70 |
| 3:CC:55:SER:O | 3:CC:57:GLN:N | 2.22 | 0.70 |
| 34:BA:953:G:H5' | 34:BA:965:A:H61 | 1.56 | 0.70 |
| 7:CG:101:ILE:HG22 | 7:CG:105:LYS:HE2 | 1.73 | 0.70 |
| 31:A7:24:THR:HG22 | 31:A7:27:GLY:H | 1.56 | 0.70 |
| 1:CA:1860:G:H5' | 3:CC:206:LYS:HD2 | 0.85 | 0.70 |
| 1:CA:1026:U:OP1 | 65:CA:4575:HOH:O | 2.09 | 0.70 |
| 1:AA:325:G:OP2 | 22:AY:84:ARG:NH2 | 2.24 | 0.70 |
| 38:DE:75:THR:OG1 | 38:DE:117:ASP:O | 2.07 | 0.70 |
| 36:BC:181:ASN:HD22 | 36:BC:204:LEU:HB2 | 1.57 | 0.70 |
| 10:CL:99:ILE:HG23 | 10:CL:103:GLN:HB2 | 1.74 | 0.70 |
| 17:CT:54:ARG:HA | 17:CT:59:THR:HB | 1.72 | 0.70 |
| 59:BZ:329:ARG:NH1 | 59:BZ:331:TYR:HE1 | 1.89 | 0.70 |
| 15:CR:67:LEU:HD13 | 15:CR:76:VAL:HG21 | 1.73 | 0.70 |
| 59:BZ:546:ILE:HG23 | 59:BZ:590:ILE:HG13 | 1.73 | 0.70 |
| 1:CA:1108:U:C5 | 1:CA:1109:C:C5 | 2.79 | 0.70 |
| 1:AA:2442:A:OP1 | 65:AA:4780:HOH:O | 2.08 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BK:19:ALA:HB3 | 44:BK:82:VAL:HG22 | 1.73 | 0.70 |
| 41:DH:119:LEU:HD13 | 41:DH:123:GLU:HG2 | 1.74 | 0.70 |
| 1:AA:2299:A:H2 | 1:AA:2358:A:H62 | 1.40 | 0.70 |
| 59:BZ:165:GLN:HE21 | 59:BZ:259:PHE:HB3 | 1.56 | 0.70 |
| 1:AA:2459:G:OP2 | 65:AA:4485:HOH:O | 2.08 | 0.70 |
| 42:BI:23:ASN:HD22 | 42:BI:25:LYS:HG2 | 1.57 | 0.70 |
| 38:DE:80:ILE:HD13 | 41:DH:104:ARG:HH21 | 1.56 | 0.69 |
| 46:DM:37:THR:O | 46:DM:55:ARG:NH1 | 2.24 | 0.69 |
| 3:CC:25:GLU:HA | 3:CC:28:ARG:HD2 | 1.74 | 0.69 |
| 39:BF:28:ARG:O | 39:BF:32:ASN:ND2 | 2.24 | 0.69 |
| 37:BD:15:GLU:HG3 | 37:BD:63:LYS:HD3 | 1.74 | 0.69 |
| 7:CG:64:THR:HB | 7:CG:94:LEU:HD21 | 1.74 | 0.69 |
| 3:AC:57:GLN:O | 3:AC:57:GLN:HG3 | 1.93 | 0.69 |
| 1:CA:1528:A:OP2 | 65:CA:3946:HOH:O | 2.09 | 0.69 |
| 34:DA:254:G:OP1 | 50:DQ:66:SER:OG | 2.10 | 0.69 |
| 7:CG:64:THR:HG21 | 7:CG:92:VAL:HG11 | 1.74 | 0.69 |
| 1:CA:1762:A:N1 | 65:CA:4246:HOH:O | 2.25 | 0.69 |
| 10:CL:106:GLU:HA | 10:CL:109:LYS:HD3 | 1.74 | 0.69 |
| 32:C8:10:ALA:HB3 | 32:C8:62:LEU:HD21 | 1.73 | 0.69 |
| 34:BA:1086:U:H3 | 34:BA:1099:G:H22 | 1.38 | 0.69 |
| 3:AC:183:PRO:HG2 | 3:AC:184:GLU:OE2 | 1.92 | 0.69 |
| 1:AA:2801:C:OP1 | 5:AE:61:ARG:NH2 | 2.25 | 0.69 |
| 1:CA:1419:A:OP2 | 65:CA:4417:HOH:O | 2.09 | 0.69 |
| 35:DB:120:ALA:O | 35:DB:122:PHE:N | 2.25 | 0.69 |
| 1:AA:1221:G:H1' | 1:AA:1222:A:H5' | 1.75 | 0.69 |
| 17:CT:65:LYS:HE2 | 17:CT:67:SER:HB2 | 1.75 | 0.69 |
| 3:CC:15:VAL:O | 3:CC:16:ASP:HB3 | 1.92 | 0.69 |
| 43:DJ:30:SER:O | 43:DJ:81:THR:OG1 | 2.10 | 0.69 |
| 29:A5:16:ARG:HG3 | 29:A5:17:ASP:N | 2.08 | 0.69 |
| 42:BI:3:GLN:OE1 | 42:BI:20:ARG:NH2 | 2.21 | 0.69 |
| 59:BZ:227:ILE:HG23 | 59:BZ:237:PRO:HG2 | 1.74 | 0.69 |
| 34:BA:1191:A:H5'' | 36:BC:4:LYS:HZ2 | 1.58 | 0.69 |
| 1:AA:1324:A:OP1 | 15:AR:36:THR:HG23 | 1.91 | 0.69 |
| 3:AC:15:VAL:O | 3:AC:16:ASP:HB3 | 1.92 | 0.69 |
| 1:AA:483:A:H5'' | 65:AA:5243:HOH:O | 1.93 | 0.69 |
| 9:AK:73:GLY:O | 9:AK:75:GLN:N | 2.24 | 0.69 |
| 34:BA:356:A:N3 | 34:BA:368:U:O2' | 2.24 | 0.69 |
| 1:CA:526:A:OP1 | 65:CA:4143:HOH:O | 2.10 | 0.69 |
| 1:AA:671:A:H2' | 1:AA:672:G:O4' | 1.93 | 0.69 |
| 3:CC:46:ALA:HB3 | 3:CC:172:ILE:CG2 | 2.23 | 0.69 |
| 3:CC:46:ALA:HB3 | 3:CC:172:ILE:HG22 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DA:353:A:H5' | 34:DA:353:A:H8 | 1.57 | 0.69 |
| 22:AY:102:CYS:SG | 22:AY:103:GLY:N | 2.66 | 0.69 |
| 59:DZ:26:THR:OG1 | 64:DZ:702:GDP:O1B | 2.10 | 0.68 |
| 34:DA:1060:C:C5 | 36:DC:2:GLY:HA3 | 2.28 | 0.68 |
| 3:AC:46:ALA:HB3 | 3:AC:172:ILE:HG22 | 1.75 | 0.68 |
| 1:AA:553:A:C8 | 1:AA:553:A:H3' | 2.28 | 0.68 |
| 3:CC:183:PRO:HG2 | 3:CC:184:GLU:OE2 | 1.93 | 0.68 |
| 4:CD:276:LYS:H | 4:CD:276:LYS:HD3 | 1.58 | 0.68 |
| 1:CA:1061:U:H4' | 1:CA:1070:A:H1' | 1.75 | 0.68 |
| 1:AA:2146:G:H1 | 1:AA:2196:C:H42 | 1.41 | 0.68 |
| 44:DK:99:GLN:HG2 | 44:DK:105:VAL:HG21 | 1.74 | 0.68 |
| 46:BM:17:VAL:O | 46:BM:20:THR:OG1 | 2.09 | 0.68 |
| 1:AA:2200:C:O2' | 3:AC:169:THR:HB | 1.93 | 0.68 |
| 17:AT:54:ARG:HA | 17:AT:59:THR:HB | 1.76 | 0.68 |
| 3:AC:25:GLU:HA | 3:AC:28:ARG:HD2 | 1.75 | 0.68 |
| 59:BZ:87:HIS:HB3 | 59:BZ:90:PHE:HB3 | 1.75 | 0.68 |
| 37:DD:150:GLU:HA | 37:DD:153:ARG:HE | 1.59 | 0.68 |
| 1:AA:932:C:H3' | 1:AA:933:C:H5'' | 1.75 | 0.68 |
| 34:BA:1255:G:O2' | 34:BA:1258:G:O2' | 2.10 | 0.68 |
| 3:CC:30:VAL:HG23 | 3:CC:31:LYS:H | 1.58 | 0.68 |
| 34:DA:1060:C:H5 | 36:DC:2:GLY:HA3 | 1.58 | 0.68 |
| 56:DW:27:G:H1 | 56:DW:43:C:H42 | 1.40 | 0.68 |
| 34:DA:117:G:OP2 | 65:DA:1839:HOH:O | 2.11 | 0.68 |
| 46:DM:14:ARG:HG3 | 46:DM:44:ARG:HH11 | 1.58 | 0.68 |
| 34:DA:983:A:N1 | 34:DA:1222:G:N2 | 2.41 | 0.68 |
| 2:CB:76:G:N7 | 65:CB:3103:HOH:O | 2.25 | 0.68 |
| 28:C4:44:THR:O | 28:C4:46:GLN:N | 2.26 | 0.68 |
| 34:DA:976:G:H5' | 34:DA:1358:U:O2' | 1.94 | 0.68 |
| 1:AA:2007:G:OP2 | 65:AA:4909:HOH:O | 2.11 | 0.68 |
| 34:DA:1255:G:P | 43:DJ:45:ARG:HH22 | 2.16 | 0.68 |
| 22:AY:102:CYS:SG | 22:AY:104:GLY:N | 2.63 | 0.68 |
| 41:BH:114:THR:OG1 | 41:BH:117:GLY:O | 2.11 | 0.68 |
| 16:CS:5:THR:N | 16:CS:8:GLU:OE1 | 2.26 | 0.68 |
| 1:AA:1431:G:O2' | 1:AA:1442:U:O2 | 2.10 | 0.68 |
| 34:DA:1004:A:H62 | 34:DA:1037:C:H2' | 1.59 | 0.68 |
| 5:CE:97:LYS:N | 5:CE:100:GLU:OE1 | 2.24 | 0.68 |
| 3:AC:30:VAL:HG23 | 3:AC:31:LYS:H | 1.58 | 0.68 |
| 1:CA:1604:C:OP2 | 65:CA:4479:HOH:O | 2.11 | 0.68 |
| 1:CA:299:A:H5'' | 22:CY:86:ARG:HH21 | 1.59 | 0.68 |
| 58:BY:60:U:H5'' | 58:BY:61:C:H5 | 1.56 | 0.68 |
| 1:AA:2586:G:OP1 | 65:AA:4113:HOH:O | 2.11 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:307:G:H21 | 1:CA:330:A:H62 | 1.42 | 0.68 |
| 35:BB:60:ASP:OD1 | 35:BB:64:ARG:NH2 | 2.26 | 0.68 |
| 5:CE:12:THR:HG21 | 17:CT:11:GLU:OE2 | 1.92 | 0.68 |
| 3:CC:30:VAL:HG23 | 3:CC:31:LYS:N | 2.09 | 0.68 |
| 56:BW:5:G:H2' | 56:BW:6:G:C8 | 2.30 | 0.68 |
| 3:AC:30:VAL:HG23 | 3:AC:31:LYS:N | 2.09 | 0.67 |
| 59:BZ:114:VAL:HG23 | 59:BZ:152:THR:HB | 1.75 | 0.67 |
| 47:DN:23:ARG:HH11 | 47:DN:30:ALA:HB2 | 1.58 | 0.67 |
| 1:AA:1114:G:N2 | 1:AA:1141:A:O3' | 2.27 | 0.67 |
| 42:DI:99:LEU:HB3 | 42:DI:101:PHE:CE1 | 2.29 | 0.67 |
| 3:AC:46:ALA:HB3 | 3:AC:172:ILE:CG2 | 2.23 | 0.67 |
| 1:CA:813:U:H2' | 1:CA:814:C:C6 | 2.30 | 0.67 |
| 12:CO:64:ARG:HG2 | 12:CO:79:PHE:CG | 2.29 | 0.67 |
| 26:A2:9:GLN:HE22 | 26:A2:56:GLN:HB3 | 1.58 | 0.67 |
| 4:AD:206:LEU:HD22 | 4:AD:211:ARG:HG2 | 1.75 | 0.67 |
| 1:CA:2611:U:C4 | 29:C5:3:LYS:HG2 | 2.30 | 0.67 |
| 23:CZ:150:LEU:H | 23:CZ:172:ALA:HB3 | 1.59 | 0.67 |
| 1:CA:882:G:H2' | 1:CA:883:G:H8 | 1.59 | 0.67 |
| 1:AA:2457:G:OP1 | 6:AF:74:ARG:NH2 | 2.27 | 0.67 |
| 37:BD:178:VAL:HG12 | 37:BD:179:GLU:H | 1.58 | 0.67 |
| 34:DA:1502:A:H2 | 34:DA:1505:G:H1 | 1.38 | 0.67 |
| 42:BI:43:ALA:O | 42:BI:45:ALA:N | 2.28 | 0.67 |
| 46:DM:25:ILE:HG23 | 46:DM:29:ARG:HB3 | 1.75 | 0.67 |
| 3:CC:176:VAL:HG11 | 3:CC:190:ILE:HD13 | 1.76 | 0.67 |
| 1:AA:2227:G:H3' | 1:AA:2228:G:C8 | 2.30 | 0.67 |
| 6:CF:101:LEU:O | 6:CF:106:ARG:NH1 | 2.26 | 0.67 |
| 48:DO:41:GLU:HA | 48:DO:44:LYS:HD2 | 1.75 | 0.67 |
| 38:DE:102:ALA:HB1 | 38:DE:106:PRO:HG2 | 1.75 | 0.67 |
| 1:AA:399:G:OP2 | 25:A1:69:LYS:NZ | 2.24 | 0.67 |
| 8:CH:9:ILE:HB | 8:CH:50:VAL:HB | 1.74 | 0.67 |
| 1:AA:626:A:H4' | 1:AA:627:G:H5' | 1.76 | 0.67 |
| 34:DA:1305:G:N2 | 34:DA:1331:G:H1' | 2.09 | 0.67 |
| 38:BE:110:LEU:HD13 | 38:BE:118:ILE:HD13 | 1.77 | 0.67 |
| 9:AK:26:LEU:HA | 9:AK:84:GLU:HA | 1.74 | 0.67 |
| 1:CA:1547:C:H2' | 1:CA:1548:C:H6 | 1.60 | 0.67 |
| 51:DR:56:THR:HB | 51:DR:58:LEU:HD23 | 1.77 | 0.67 |
| 34:BA:353:A:H5' | 34:BA:353:A:H8 | 1.60 | 0.67 |
| 1:CA:2070:G:OP2 | 65:CA:4420:HOH:O | 2.12 | 0.67 |
| 37:BD:111:ALA:HB2 | 37:BD:120:LEU:HD12 | 1.75 | 0.67 |
| 34:DA:1316:G:OP1 | 47:DN:17:LYS:NZ | 2.25 | 0.67 |
| 1:CA:1430:C:H2' | 1:CA:1431:U:C6 | 2.30 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:BC:50:ALA:HB1 | 36:BC:70:VAL:HG21 | 1.74 | 0.67 |
| 36:DC:52:LEU:HD23 | 36:DC:55:VAL:HG23 | 1.75 | 0.67 |
| 1:CA:1057:A:O2' | 1:CA:1058:G:OP1 | 2.09 | 0.67 |
| 34:DA:920:U:H2' | 34:DA:921:U:C6 | 2.29 | 0.67 |
| 3:CC:57:GLN:O | 3:CC:57:GLN:HG3 | 1.93 | 0.67 |
| 28:C4:16:CYS:SG | 28:C4:17:GLY:N | 2.67 | 0.67 |
| 1:AA:2772:G:N7 | 65:AA:4053:HOH:O | 2.27 | 0.67 |
| 43:DJ:17:ASP:OD1 | 43:DJ:70:ARG:NH1 | 2.26 | 0.67 |
| 1:CA:2114:A:N1 | 1:CA:2171:A:N6 | 2.40 | 0.67 |
| 44:BK:18:ARG:NH1 | 44:BK:20:TYR:OH | 2.27 | 0.67 |
| 1:CA:2104:G:H1 | 1:CA:2185:C:H42 | 1.42 | 0.67 |
| 2:AB:7:G:OP2 | 65:AB:3127:HOH:O | 2.11 | 0.67 |
| 1:AA:2396:G:OP2 | 24:A0:55:ARG:NH1 | 2.26 | 0.67 |
| 1:CA:1022:G:N7 | 11:CN:66:LYS:HE2 | 2.10 | 0.67 |
| 42:BI:128:ARG:NH1 | 57:BX:35:A:OP2 | 2.27 | 0.67 |
| 59:DZ:494:GLU:HG2 | 59:DZ:511:LYS:HG2 | 1.75 | 0.67 |
| 34:DA:560:U:O2' | 34:DA:561:U:OP2 | 2.13 | 0.67 |
| 3:CC:42:VAL:HG13 | 3:CC:43:GLU:N | 2.10 | 0.67 |
| 1:CA:2286:A:H4' | 1:CA:2287:A:O4' | 1.95 | 0.67 |
| 59:BZ:20:HIS:ND1 | 59:BZ:115:GLU:HB3 | 2.09 | 0.67 |
| 1:CA:2177:C:O2 | 3:CC:173:HIS:HE1 | 1.78 | 0.67 |
| 44:BK:34:ASP:HB3 | 44:BK:40:ILE:HD11 | 1.75 | 0.67 |
| 37:BD:187:ARG:NH1 | 37:BD:190:ASP:OD1 | 2.28 | 0.67 |
| 45:BL:53:ARG:HG3 | 45:BL:93:LEU:HD21 | 1.76 | 0.67 |
| 3:AC:42:VAL:HG13 | 3:AC:43:GLU:N | 2.10 | 0.66 |
| 1:AA:925:A:H61 | 1:AA:945:A:H1' | 1.59 | 0.66 |
| 9:AK:70:GLU:O | 9:AK:72:ASP:N | 2.28 | 0.66 |
| 1:CA:1970:A:OP1 | 65:CA:3914:HOH:O | 2.12 | 0.66 |
| 3:AC:31:LYS:NZ | 3:AC:180:SER:O | 2.28 | 0.66 |
| 40:BG:111:ARG:NH2 | 40:BG:126:ASP:OD2 | 2.28 | 0.66 |
| 59:DZ:329:ARG:HD3 | 59:DZ:331:TYR:CZ | 2.31 | 0.66 |
| 1:AA:1154:U:HO2' | 1:AA:1155:C:H6 | 1.43 | 0.66 |
| 34:BA:1303:C:OP1 | 65:BA:2008:HOH:O | 2.14 | 0.66 |
| 37:BD:107:ARG:HH22 | 37:BD:194:LEU:HD11 | 1.59 | 0.66 |
| 1:AA:237:G:OP1 | 65:AA:4920:HOH:O | 2.13 | 0.66 |
| 9:CK:73:GLY:O | 9:CK:75:GLN:N | 2.21 | 0.66 |
| 1:AA:1249:A:H2 | 1:AA:1287:A:N6 | 1.88 | 0.66 |
| 1:CA:2590:A:OP2 | 4:CD:238:GLY:HA2 | 1.94 | 0.66 |
| 4:CD:8:PRO:HB3 | 4:CD:14:ARG:HB2 | 1.76 | 0.66 |
| 57:DX:73:A:H5'' | 57:DX:74:C:H5' | 1.76 | 0.66 |
| 10:AL:106:GLU:HA | 10:AL:109:LYS:HD3 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DB:52:GLU:O | 35:DB:56:ARG:HG2 | 1.96 | 0.66 |
| 56:BW:51:U:H2' | 56:BW:52:G:H8 | 1.60 | 0.66 |
| 34:BA:1069:C:OP2 | 65:BA:1906:HOH:O | 2.13 | 0.66 |
| 1:CA:2136:C:O2' | 1:CA:2137:C:O5' | 2.13 | 0.66 |
| 59:DZ:181:LEU:HD12 | 59:DZ:216:LEU:HD21 | 1.78 | 0.66 |
| 3:CC:63:VAL:O | 3:CC:161:ARG:HA | 1.96 | 0.66 |
| 34:BA:1221:G:OP1 | 34:BA:1320:C:N4 | 2.23 | 0.66 |
| 43:DJ:38:ILE:HD11 | 43:DJ:71:LEU:HD23 | 1.78 | 0.66 |
| 22:AY:15:VAL:HG21 | 22:AY:42:VAL:HG11 | 1.78 | 0.66 |
| 42:DI:28:VAL:HG22 | 42:DI:63:ILE:HB | 1.76 | 0.66 |
| 34:DA:1054:C:C4 | 56:DW:34:G:H1' | 2.29 | 0.66 |
| 1:AA:1711:A:OP1 | 65:AA:5092:HOH:O | 2.13 | 0.66 |
| 37:BD:22:LYS:HB2 | 63:BD:501:SF4:S4 | 2.36 | 0.66 |
| 36:DC:59:ARG:HG3 | 36:DC:64:VAL:HG13 | 1.77 | 0.66 |
| 34:BA:166:G:H2' | 34:BA:167:G:C8 | 2.30 | 0.66 |
| 1:CA:1341:U:OP2 | 1:CA:1394:U:O2' | 2.11 | 0.66 |
| 3:AC:176:VAL:HG11 | 3:AC:190:ILE:HD13 | 1.76 | 0.66 |
| 1:CA:833:U:O2 | 13:CP:55:ARG:NH2 | 2.29 | 0.66 |
| 34:BA:1348:U:H4' | 42:BI:120:ARG:HD2 | 1.77 | 0.66 |
| 35:DB:201:ILE:HG21 | 35:DB:214:ILE:HG21 | 1.78 | 0.66 |
| 1:CA:855:G:O2' | 24:C0:27:GLU:OE2 | 2.14 | 0.66 |
| 3:CC:65:LEU:HB3 | 3:CC:189:ASN:ND2 | 2.11 | 0.66 |
| 34:DA:1239:A:H62 | 34:DA:1299:A:H62 | 1.41 | 0.66 |
| 34:BA:193:C:H2' | 34:BA:194:C:H6 | 1.61 | 0.66 |
| 59:DZ:264:LEU:HB2 | 64:DZ:702:GDP:C6 | 2.31 | 0.65 |
| 3:AC:65:LEU:HB3 | 3:AC:189:ASN:ND2 | 2.11 | 0.65 |
| 1:AA:1079:U:OP1 | 33:A9:9:ARG:NH2 | 2.29 | 0.65 |
| 20:AW:18:ARG:NH1 | 20:AW:76:VAL:O | 2.29 | 0.65 |
| 17:CT:56:GLY:O | 17:CT:59:THR:HG23 | 1.96 | 0.65 |
| 1:CA:1671:U:HO2' | 1:CA:1673:U:H5 | 1.44 | 0.65 |
| 1:CA:1332:G:OP1 | 65:CA:4126:HOH:O | 2.14 | 0.65 |
| 18:CU:76:TYR:OH | 18:CU:92:ARG:NH1 | 2.28 | 0.65 |
| 1:CA:1604:C:OP2 | 65:CA:4478:HOH:O | 2.15 | 0.65 |
| 1:CA:300:A:P | 22:CY:86:ARG:HH22 | 2.19 | 0.65 |
| 34:DA:222:U:H2' | 34:DA:223:U:C6 | 2.30 | 0.65 |
| 3:AC:41:THR:O | 3:AC:42:VAL:HB | 1.94 | 0.65 |
| 1:CA:1315:C:OP2 | 65:CA:4126:HOH:O | 2.15 | 0.65 |
| 34:DA:266:G:H5'' | 34:DA:268:C:H41 | 1.62 | 0.65 |
| 3:AC:63:VAL:O | 3:AC:161:ARG:HA | 1.95 | 0.65 |
| 7:AG:179:PRO:HB2 | 28:A4:42:PHE:HE1 | 1.61 | 0.65 |
| 28:C4:40:HIS:HB3 | 28:C4:43:TYR:HB2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:CC:206:LYS:NZ | 3:CC:206:LYS:HB3 | 2.12 | 0.65 |
| 7:AG:137:GLU:HG2 | 7:AG:152:LEU:HD13 | 1.78 | 0.65 |
| 42:DI:43:ALA:HA | 42:DI:74:ILE:HD13 | 1.77 | 0.65 |
| 17:AT:16:ARG:NH2 | 17:AT:83:ILE:O | 2.29 | 0.65 |
| 35:DB:162:ILE:HD11 | 35:DB:184:VAL:HG22 | 1.78 | 0.65 |
| 34:BA:1304:G:OP2 | 65:BA:2008:HOH:O | 2.15 | 0.65 |
| 3:CC:41:THR:O | 3:CC:42:VAL:HB | 1.94 | 0.65 |
| 59:BZ:191:ASP:O | 59:BZ:266:ASN:ND2 | 2.22 | 0.65 |
| 35:BB:195:ASP:O | 41:BH:68:ARG:NH2 | 2.30 | 0.65 |
| 35:DB:91:PRO:HG3 | 35:DB:155:LEU:HD23 | 1.79 | 0.65 |
| 34:BA:200:G:H1 | 34:BA:217:C:H42 | 1.43 | 0.65 |
| 1:CA:2327:A:H2' | 1:CA:2328:A:C8 | 2.31 | 0.65 |
| 13:AP:50:ARG:HD3 | 32:A8:7:HIS:CD2 | 2.32 | 0.65 |
| 34:BA:642:A:N3 | 41:BH:113:SER:OG | 2.30 | 0.65 |
| 1:CA:1495:A:H2' | 1:CA:1496:A:C8 | 2.32 | 0.65 |
| 35:DB:100:GLY:O | 35:DB:104:ASN:N | 2.25 | 0.65 |
| 42:BI:42:ARG:NH1 | 42:BI:71:SER:OG | 2.29 | 0.65 |
| 37:DD:127:THR:HB | 37:DD:132:ARG:HA | 1.79 | 0.65 |
| 34:DA:1000:U:H3 | 34:DA:1041:A:H61 | 1.44 | 0.65 |
| 59:BZ:160:ARG:HD2 | 59:BZ:160:ARG:H | 1.61 | 0.65 |
| 20:AW:14:PRO:HG2 | 20:AW:78:GLU:HG2 | 1.77 | 0.65 |
| 1:AA:2138:G:N2 | 1:AA:2184:G:OP1 | 2.26 | 0.65 |
| 1:AA:1087:C:H42 | 1:AA:1160:G:H1 | 1.45 | 0.65 |
| 34:DA:403:C:OP1 | 37:DD:137:SER:OG | 2.14 | 0.65 |
| 19:CV:21:ARG:HG2 | 19:CV:91:TYR:CD2 | 2.31 | 0.65 |
| 1:AA:2199:C:O2 | 3:AC:173:HIS:CE1 | 2.50 | 0.65 |
| 47:DN:22:THR:HB | 47:DN:33:VAL:HB | 1.79 | 0.65 |
| 1:CA:816:C:OP2 | 65:CA:4596:HOH:O | 2.13 | 0.65 |
| 59:DZ:610:VAL:HG13 | 59:DZ:659:LEU:HD11 | 1.78 | 0.65 |
| 1:AA:2776:G:OP2 | 65:AA:4635:HOH:O | 2.13 | 0.65 |
| 34:BA:1369:C:H2' | 34:BA:1370:G:C8 | 2.31 | 0.65 |
| 23:AZ:53:ILE:HG22 | 23:AZ:71:VAL:HG12 | 1.79 | 0.65 |
| 1:AA:1891:G:H5' | 3:AC:206:LYS:CD | 2.00 | 0.64 |
| 20:CW:65:LEU:HD12 | 20:CW:68:ARG:HE | 1.62 | 0.64 |
| 3:AC:206:LYS:NZ | 3:AC:206:LYS:HB3 | 2.12 | 0.64 |
| 56:DW:3:C:O2 | 56:DW:70:G:N2 | 2.17 | 0.64 |
| 37:DD:61:LYS:NZ | 37:DD:207:TYR:OH | 2.31 | 0.64 |
| 1:AA:1093:G:HO2' | 1:AA:1156:G:H1 | 1.44 | 0.64 |
| 34:DA:1129:C:H2' | 34:DA:1139:G:N7 | 2.11 | 0.64 |
| 1:AA:1219:A:H4' | 1:AA:1220:U:OP1 | 1.97 | 0.64 |
| 41:BH:73:ASP:OD2 | 41:BH:75:ARG:NH1 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:41:GLN:NE2 | 7:AG:154:GLY:O | 2.30 | 0.64 |
| 41:DH:86:ILE:HG21 | 41:DH:133:LEU:HD13 | 1.78 | 0.64 |
| 1:CA:848:G:H2' | 1:CA:849:A:C8 | 2.33 | 0.64 |
| 30:A6:44:ARG:HB3 | 30:A6:44:ARG:NH1 | 2.12 | 0.64 |
| 30:C6:13:CYS:SG | 30:C6:47:THR:HG21 | 2.37 | 0.64 |
| 57:BX:61:C:H2' | 57:BX:62:C:H6 | 1.62 | 0.64 |
| 3:AC:69:LEU:O | 3:AC:178:LYS:HG3 | 1.98 | 0.64 |
| 23:CZ:117:LEU:HD12 | 23:CZ:174:VAL:HG22 | 1.80 | 0.64 |
| 34:BA:1318:A:H1' | 52:BS:37:ARG:HH21 | 1.61 | 0.64 |
| 1:CA:1082:U:H4' | 10:CL:117:THR:HB | 1.78 | 0.64 |
| 1:AA:2460:A:OP1 | 65:AA:5078:HOH:O | 2.14 | 0.64 |
| 1:AA:2601:A:OP1 | 65:AA:4557:HOH:O | 2.14 | 0.64 |
| 42:DI:8:GLY:N | 42:DI:15:ALA:O | 2.27 | 0.64 |
| 3:AC:68:GLY:N | 3:AC:189:ASN:HD21 | 1.96 | 0.64 |
| 1:CA:1800:C:OP2 | 4:CD:183:ARG:NH2 | 2.29 | 0.64 |
| 34:DA:396:G:OP1 | 59:DZ:349:LYS:NZ | 2.31 | 0.64 |
| 36:BC:52:LEU:HD23 | 36:BC:53:ALA:H | 1.63 | 0.64 |
| 10:CL:81:ALA:HB1 | 10:CL:99:ILE:HD11 | 1.79 | 0.64 |
| 1:CA:1250:G:N7 | 13:CP:18:ARG:NH2 | 2.45 | 0.64 |
| 12:CO:35:VAL:HG23 | 12:CO:65:THR:HG23 | 1.78 | 0.64 |
| 34:DA:189(F):U:O2 | 50:DQ:63:ARG:NH2 | 2.30 | 0.64 |
| 1:AA:630:U:OP1 | 6:AF:102:PRO:HA | 1.98 | 0.64 |
| 37:DD:18:LYS:NZ | 37:DD:31:CYS:SG | 2.71 | 0.64 |
| 1:AA:9:U:N3 | 1:AA:2641:A:H2 | 1.89 | 0.64 |
| 1:CA:528:A:C2 | 1:CA:2043:C:H4' | 2.33 | 0.64 |
| 22:AY:92:ASN:HB2 | 22:AY:94:LYS:N | 2.12 | 0.64 |
| 59:DZ:170:ARG:N | 59:DZ:170:ARG:HH11 | 1.96 | 0.64 |
| 36:BC:114:PRO:O | 36:BC:118:GLN:NE2 | 2.31 | 0.64 |
| 23:AZ:157:LEU:HD21 | 23:AZ:163:LEU:HD13 | 1.79 | 0.64 |
| 1:AA:239:G:OP2 | 32:A8:13:ARG:NH2 | 2.31 | 0.64 |
| 35:DB:204:ASN:OD1 | 35:DB:205:ASP:N | 2.31 | 0.64 |
| 19:CV:62:LEU:HD23 | 19:CV:93:GLU:HG2 | 1.80 | 0.64 |
| 34:BA:1158:C:H5 | 34:BA:1181:G:N1 | 1.95 | 0.64 |
| 7:AG:41:GLN:HB3 | 7:AG:43:LEU:HD22 | 1.79 | 0.64 |
| 1:CA:2424:C:O2 | 1:CA:2429:G:O2' | 2.14 | 0.64 |
| 34:BA:1182:G:H4' | 34:BA:1183:A:H5' | 1.80 | 0.64 |
| 45:BL:7:ILE:HA | 45:BL:10:LEU:HD12 | 1.80 | 0.64 |
| 28:C4:24:THR:OG1 | 28:C4:25:TYR:N | 2.27 | 0.64 |
| 46:BM:59:TYR:O | 46:BM:63:THR:OG1 | 2.15 | 0.64 |
| 3:CC:69:LEU:O | 3:CC:178:LYS:HG3 | 1.97 | 0.64 |
| 35:BB:54:THR:HG21 | 35:BB:201:ILE:HD11 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:BY:8:4SU:H4' | 58:BY:48:C:H4' | 1.80 | 0.64 |
| 1:CA:2243:U:H2' | 1:CA:2244:U:C6 | 2.33 | 0.63 |
| 15:CR:21:TYR:OH | 15:CR:43:GLU:HG2 | 1.98 | 0.63 |
| 1:AA:791:G:OP1 | 65:AA:4626:HOH:O | 2.15 | 0.63 |
| 4:AD:122:ASP:OD1 | 4:AD:122:ASP:N | 2.24 | 0.63 |
| 7:AG:48:GLU:HA | 7:AG:51:ARG:HE | 1.62 | 0.63 |
| 59:BZ:82:ILE:HD12 | 59:BZ:101:LEU:HD23 | 1.80 | 0.63 |
| 3:CC:31:LYS:NZ | 3:CC:180:SER:O | 2.28 | 0.63 |
| 3:AC:29:LEU:O | 3:AC:32:GLU:N | 2.32 | 0.63 |
| 34:DA:986:A:O2' | 52:DS:55:LYS:O | 2.16 | 0.63 |
| 59:DZ:363:ARG:CG | 59:DZ:363:ARG:HH11 | 2.09 | 0.63 |
| 13:AP:125:VAL:HG21 | 13:AP:138:LEU:HD21 | 1.80 | 0.63 |
| 11:CN:123:TYR:OH | 11:CN:130:HIS:NE2 | 2.31 | 0.63 |
| 50:DQ:81:ARG:HB3 | 50:DQ:84:LEU:HD12 | 1.80 | 0.63 |
| 8:AH:90:LYS:HD3 | 8:AH:159:GLU:HG2 | 1.79 | 0.63 |
| 34:BA:600:C:H2' | 34:BA:601:C:C6 | 2.33 | 0.63 |
| 59:DZ:117:GLN:O | 59:DZ:121:VAL:N | 2.30 | 0.63 |
| 3:AC:44:VAL:CG2 | 3:AC:176:VAL:HG21 | 2.28 | 0.63 |
| 35:DB:213:LEU:HD22 | 35:DB:214:ILE:HD13 | 1.80 | 0.63 |
| 59:DZ:-53:ASP:H | 59:DZ:-50:GLN:NE2 | 1.97 | 0.63 |
| 12:CO:25:LEU:HD12 | 12:CO:38:VAL:HG12 | 1.80 | 0.63 |
| 30:A6:13:CYS:SG | 30:A6:47:THR:HG21 | 2.39 | 0.63 |
| 3:CC:7:ARG:O | 3:CC:11:LEU:HD23 | 1.99 | 0.63 |
| 44:DK:98:LEU:O | 44:DK:101:SER:OG | 2.06 | 0.63 |
| 3:AC:7:ARG:O | 3:AC:11:LEU:HD23 | 1.99 | 0.63 |
| 52:BS:63:THR:OG1 | 52:BS:65:ASN:ND2 | 2.32 | 0.63 |
| 14:AQ:10:ARG:HG2 | 14:AQ:11:LYS:HG3 | 1.80 | 0.63 |
| 59:BZ:73:PHE:CE2 | 59:BZ:78:ARG:NH1 | 2.67 | 0.63 |
| 49:DP:5:ARG:HB3 | 49:DP:67:THR:HG23 | 1.80 | 0.63 |
| 58:DY:12:U:H3 | 58:DY:23:A:H61 | 1.45 | 0.63 |
| 11:AN:46:VAL:HG23 | 11:AN:48:MET:HG2 | 1.80 | 0.63 |
| 42:DI:99:LEU:HB3 | 42:DI:101:PHE:HE1 | 1.62 | 0.63 |
| 34:DA:1130:A:O2' | 42:DI:3:GLN:OE1 | 2.17 | 0.63 |
| 34:BA:421:U:OP2 | 34:BA:422:C:N4 | 2.30 | 0.63 |
| 59:BZ:184:LYS:HD2 | 59:BZ:198:GLU:OE2 | 1.98 | 0.63 |
| 1:CA:1860:G:C5' | 3:CC:206:LYS:HG3 | 1.88 | 0.63 |
| 34:DA:986:A:H1' | 52:DS:55:LYS:HA | 1.81 | 0.63 |
| 34:DA:1118:C:OP1 | 42:DI:104:ARG:NH1 | 2.32 | 0.63 |
| 3:CC:68:GLY:N | 3:CC:189:ASN:HD21 | 1.96 | 0.63 |
| 20:CW:18:ARG:NH1 | 20:CW:76:VAL:O | 2.31 | 0.63 |
| 49:DP:52:ASP:O | 49:DP:54:GLU:N | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1143:A:OP1 | 11:CN:25:ARG:NH2 | 2.31 | 0.63 |
| 1:AA:1218:G:O2' | 1:AA:1219:A:O4' | 2.16 | 0.63 |
| 17:CT:39:ARG:NH2 | 34:DA:345:C:OP2 | 2.32 | 0.63 |
| 3:AC:6:LYS:HG3 | 3:AC:7:ARG:N | 2.14 | 0.63 |
| 4:AD:71:ASP:OD2 | 4:AD:103:ARG:NH2 | 2.32 | 0.63 |
| 1:CA:96:G:H4' | 26:C2:48:HIS:CD2 | 2.33 | 0.63 |
| 3:CC:6:LYS:HG3 | 3:CC:7:ARG:N | 2.14 | 0.63 |
| 1:AA:990:A:OP2 | 65:AA:4345:HOH:O | 2.16 | 0.63 |
| 59:BZ:78:ARG:HG3 | 59:BZ:78:ARG:NH1 | 2.07 | 0.63 |
| 53:BT:9:ASN:HB3 | 53:BT:10:LEU:HD12 | 1.80 | 0.63 |
| 3:CC:44:VAL:CG2 | 3:CC:176:VAL:HG21 | 2.28 | 0.63 |
| 37:DD:103:ASN:OD1 | 37:DD:114:ARG:NE | 2.28 | 0.63 |
| 59:BZ:127:LYS:HG3 | 59:BZ:520:GLY:HA3 | 1.81 | 0.63 |
| 34:BA:992:U:O2 | 34:BA:1043:C:N4 | 2.32 | 0.63 |
| 43:DJ:5:ARG:N | 43:DJ:73:ASP:OD1 | 2.32 | 0.63 |
| 34:BA:1525:G:OP1 | 44:BK:120:ARG:NH2 | 2.32 | 0.63 |
| 39:DF:23:LYS:HG2 | 39:DF:61:LEU:HD21 | 1.81 | 0.63 |
| 3:CC:29:LEU:O | 3:CC:32:GLU:N | 2.31 | 0.62 |
| 1:CA:2176:A:H2' | 1:CA:2177:C:C6 | 2.34 | 0.62 |
| 1:AA:2045:G:H5' | 1:AA:2629:C:H4' | 1.79 | 0.62 |
| 59:BZ:238:THR:HG23 | 59:BZ:241:GLU:HB2 | 1.80 | 0.62 |
| 34:BA:972:C:O2' | 43:BJ:55:LYS:O | 2.16 | 0.62 |
| 15:CR:56:LYS:NZ | 15:CR:90:ARG:O | 2.32 | 0.62 |
| 42:DI:128:ARG:NH2 | 57:DX:33:U:OP2 | 2.32 | 0.62 |
| 1:AA:2152:U:H4' | 1:AA:2155:G:H4' | 1.81 | 0.62 |
| 57:DX:9:G:O2' | 57:DX:10:G:N7 | 2.24 | 0.62 |
| 38:BE:68:GLU:HG2 | 38:BE:70:PRO:HD3 | 1.81 | 0.62 |
| 6:CF:185:ASP:OD1 | 6:CF:188:ARG:NH1 | 2.31 | 0.62 |
| 50:BQ:45:HIS:HB3 | 50:BQ:72:ARG:HB3 | 1.82 | 0.62 |
| 1:AA:1199:C:OP1 | 18:AU:92:ARG:NH1 | 2.32 | 0.62 |
| 35:BB:17:PHE:HB2 | 35:BB:44:LEU:HD21 | 1.81 | 0.62 |
| 3:AC:68:GLY:H | 3:AC:189:ASN:HD21 | 1.47 | 0.62 |
| 1:AA:1480:A:H61 | 1:AA:1605:A:H62 | 1.47 | 0.62 |
| 1:CA:2785:C:OP1 | 5:CE:41:LYS:NZ | 2.32 | 0.62 |
| 35:BB:155:LEU:HD21 | 35:BB:159:PRO:HD3 | 1.82 | 0.62 |
| 1:CA:2206:G:H3' | 1:CA:2207:G:N7 | 2.15 | 0.62 |
| 1:CA:731:C:OP1 | 65:CA:4291:HOH:O | 2.16 | 0.62 |
| 36:BC:19:GLU:HB3 | 36:BC:40:ARG:HH22 | 1.65 | 0.62 |
| 21:AX:57:LEU:HD21 | 21:AX:78:LYS:HE2 | 1.80 | 0.62 |
| 1:CA:2839:G:H5' | 15:CR:46:GLY:HA2 | 1.81 | 0.62 |
| 1:AA:1501:U:OP1 | 15:AR:77:ARG:NH1 | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:CF:155:LEU:HD23 | 6:CF:186:ILE:HG13 | 1.81 | 0.62 |
| 34:BA:598:U:H4' | 41:BH:94:TYR:CD2 | 2.34 | 0.62 |
| 1:CA:1798:U:OP2 | 4:CD:274:ARG:NH2 | 2.32 | 0.62 |
| 36:DC:58:GLU:HB3 | 43:DJ:92:THR:HG21 | 1.82 | 0.62 |
| 34:DA:1228:C:OP1 | 46:DM:115:LYS:N | 2.30 | 0.62 |
| 1:AA:611:U:H2' | 1:AA:612:C:C6 | 2.35 | 0.62 |
| 36:DC:65:ALA:HA | 36:DC:100:ALA:HB3 | 1.81 | 0.62 |
| 34:DA:1133:G:H2' | 34:DA:1134:G:H8 | 1.63 | 0.62 |
| 34:DA:406:G:H5' | 37:DD:5:ILE:HD11 | 1.82 | 0.62 |
| 34:BA:153:C:H42 | 34:BA:168:G:H1 | 1.48 | 0.62 |
| 1:CA:2788:C:O2' | 1:CA:2809:A:N3 | 2.30 | 0.62 |
| 48:BO:17:ARG:HG3 | 48:BO:17:ARG:HH11 | 1.64 | 0.62 |
| 34:DA:958:A:N6 | 52:DS:77:THR:O | 2.32 | 0.62 |
| 1:AA:927:G:H2' | 1:AA:928:G:C8 | 2.34 | 0.62 |
| 56:BW:63:G:H2' | 56:BW:64:A:O4' | 2.00 | 0.62 |
| 35:DB:16:HIS:CG | 35:DB:17:PHE:H | 2.17 | 0.62 |
| 26:C2:1:MET:N | 26:C2:52:ASP:OD1 | 2.23 | 0.62 |
| 34:DA:1318:A:H1' | 52:DS:37:ARG:HD3 | 1.80 | 0.62 |
| 3:CC:53:ARG:HD3 | 3:CC:53:ARG:H | 1.65 | 0.62 |
| 1:AA:1154:U:O2' | 1:AA:1155:C:H6 | 1.82 | 0.62 |
| 34:DA:1073:U:H2' | 34:DA:1074:G:H8 | 1.65 | 0.62 |
| 1:AA:798:A:H5' | 20:AW:90:ARG:HA | 1.82 | 0.62 |
| 30:C6:6:ARG:NH1 | 30:C6:26:ASN:HB2 | 2.14 | 0.62 |
| 1:AA:957:A:H2' | 14:AQ:9:TYR:OH | 2.00 | 0.62 |
| 13:AP:59:LEU:HD11 | 32:A8:10:ALA:HB2 | 1.81 | 0.62 |
| 34:BA:255:G:H1' | 50:BQ:16:GLN:NE2 | 2.15 | 0.62 |
| 6:CF:101:LEU:HD12 | 6:CF:102:PRO:HD2 | 1.82 | 0.62 |
| 34:DA:523:A:H61 | 45:DL:92:ASP:HB2 | 1.64 | 0.62 |
| 42:BI:99:LEU:HB3 | 42:BI:101:PHE:HE1 | 1.64 | 0.62 |
| 3:CC:11:LEU:HD12 | 3:CC:33:LEU:HA | 1.82 | 0.62 |
| 3:AC:53:ARG:H | 3:AC:53:ARG:HD3 | 1.65 | 0.62 |
| 1:AA:2209:G:O2' | 1:AA:2210:C:OP1 | 2.18 | 0.62 |
| 1:AA:202:A:H2' | 1:AA:203:G:O4' | 2.00 | 0.62 |
| 1:CA:993:G:OP1 | 18:CU:50:ARG:NH2 | 2.32 | 0.62 |
| 34:BA:1062:U:H2' | 34:BA:1063:C:C6 | 2.35 | 0.62 |
| 1:AA:1405:A:N1 | 1:AA:1418:U:O4 | 2.33 | 0.61 |
| 59:BZ:319:ASP:OD1 | 59:BZ:363:ARG:NH2 | 2.33 | 0.61 |
| 34:DA:991:U:H4' | 34:DA:992:U:OP1 | 1.99 | 0.61 |
| 1:CA:2805:G:H2' | 1:CA:2807:G:C8 | 2.35 | 0.61 |
| 1:CA:2328:A:H2' | 1:CA:2329:G:C8 | 2.35 | 0.61 |
| 34:BA:877:C:H5" | 41:BH:88:LYS:HD3 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:AF:28:ILE:O | 6:AF:30:PRO:HD3 | 1.99 | 0.61 |
| 34:DA:460:G:O6 | 34:DA:470:C:H5'' | 2.00 | 0.61 |
| 19:AV:49:THR:O | 19:AV:49:THR:HG22 | 2.00 | 0.61 |
| 1:AA:1529:G:O6 | 1:AA:1553:A:N6 | 2.33 | 0.61 |
| 19:CV:98:GLU:OE1 | 19:CV:100:ARG:NH1 | 2.33 | 0.61 |
| 35:DB:13:ALA:N | 35:DB:14:GLY:HA3 | 2.15 | 0.61 |
| 1:CA:2355:C:H1' | 24:C0:39:ARG:HH21 | 1.63 | 0.61 |
| 19:AV:76:LYS:HB2 | 19:AV:81:TYR:HB3 | 1.82 | 0.61 |
| 1:CA:1109:C:H2' | 1:CA:1110:G:C8 | 2.35 | 0.61 |
| 59:BZ:328:ILE:O | 59:BZ:374:LEU:HB2 | 2.00 | 0.61 |
| 34:DA:1010:G:N2 | 34:DA:1020:U:O2 | 2.34 | 0.61 |
| 7:AG:110:ALA:HB1 | 7:AG:140:ILE:HG23 | 1.82 | 0.61 |
| 34:BA:1123:A:H61 | 34:BA:1149:C:H42 | 1.49 | 0.61 |
| 34:DA:1002:G:C4 | 34:DA:1003:G:H8 | 2.18 | 0.61 |
| 49:BP:75:ARG:O | 49:BP:78:GLY:N | 2.27 | 0.61 |
| 14:AQ:12:GLN:HG2 | 14:AQ:73:PRO:HD2 | 1.83 | 0.61 |
| 14:CQ:85:LYS:HG2 | 24:C0:7:LEU:HB3 | 1.82 | 0.61 |
| 1:CA:2238:G:N7 | 65:CA:4455:HOH:O | 2.31 | 0.61 |
| 34:DA:1302:U:OP2 | 46:DM:21:TYR:OH | 2.10 | 0.61 |
| 34:BA:266:G:H5'' | 34:BA:268:C:H41 | 1.65 | 0.61 |
| 5:CE:59:VAL:HG21 | 5:CE:74:PRO:HB3 | 1.82 | 0.61 |
| 1:CA:1876:A:H2' | 1:CA:1877:A:C8 | 2.35 | 0.61 |
| 1:AA:1834:A:H4' | 4:AD:259:THR:HG23 | 1.83 | 0.61 |
| 59:DZ:659:LEU:HD12 | 59:DZ:669:PHE:HD1 | 1.66 | 0.61 |
| 4:AD:71:ASP:HB3 | 4:AD:103:ARG:HH22 | 1.66 | 0.61 |
| 1:CA:1081:U:OP1 | 10:CL:125:ARG:NH1 | 2.33 | 0.61 |
| 4:CD:142:VAL:HG13 | 4:CD:191:ALA:HB1 | 1.81 | 0.61 |
| 28:A4:10:VAL:HG21 | 28:A4:29:PRO:HG3 | 1.81 | 0.61 |
| 14:CQ:138:ASP:OD2 | 23:CZ:81:ARG:NH1 | 2.34 | 0.61 |
| 1:CA:1019:U:HO2' | 1:CA:1021:A:H2 | 1.48 | 0.61 |
| 34:DA:1022:G:H2' | 34:DA:1023:G:H8 | 1.64 | 0.61 |
| 42:DI:8:GLY:HA2 | 42:DI:79:LEU:HD23 | 1.83 | 0.61 |
| 34:DA:1062:U:H2' | 34:DA:1063:C:C6 | 2.35 | 0.61 |
| 58:DY:51:U:H3 | 58:DY:63:G:H1 | 1.46 | 0.61 |
| 7:AG:161:THR:HG22 | 7:AG:163:ALA:H | 1.65 | 0.61 |
| 28:A4:44:THR:O | 28:A4:46:GLN:N | 2.34 | 0.61 |
| 36:BC:134:ILE:HG23 | 36:BC:151:VAL:HB | 1.83 | 0.61 |
| 1:CA:300:A:OP2 | 22:CY:86:ARG:NH2 | 2.34 | 0.61 |
| 30:A6:44:ARG:HH11 | 30:A6:44:ARG:HB3 | 1.66 | 0.61 |
| 1:AA:1604:C:OP2 | 1:AA:1605:A:O2' | 2.19 | 0.61 |
| 23:AZ:72:ARG:NH2 | 23:AZ:97:GLU:O | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:959:A:HO2' | 34:DA:984:C:HO2' | 1.43 | 0.61 |
| 59:BZ:509:HIS:HB3 | 59:BZ:571:SER:H | 1.66 | 0.61 |
| 1:AA:625:G:O2' | 1:AA:702:A:N6 | 2.34 | 0.61 |
| 1:AA:354:A:H2 | 1:AA:1255:A:HO2' | 1.49 | 0.61 |
| 34:DA:1312:G:H5' | 52:DS:5:LEU:HD11 | 1.81 | 0.61 |
| 1:AA:542:C:OP1 | 29:A5:16:ARG:NH2 | 2.30 | 0.61 |
| 42:DI:3:GLN:HG2 | 42:DI:20:ARG:HE | 1.64 | 0.61 |
| 36:DC:125:GLU:HG3 | 36:DC:190:ARG:O | 2.01 | 0.61 |
| 5:AE:117:MET:SD | 5:AE:136:ARG:HB3 | 2.41 | 0.61 |
| 34:BA:1255:G:OP1 | 43:BJ:45:ARG:NH2 | 2.33 | 0.61 |
| 7:AG:41:GLN:HE22 | 7:AG:153:ARG:HB3 | 1.66 | 0.61 |
| 56:BW:9:A:N3 | 56:BW:45:U:H2' | 2.16 | 0.61 |
| 43:BJ:40:LEU:HB2 | 43:BJ:69:ASN:HB2 | 1.83 | 0.61 |
| 1:AA:2348:A:H61 | 24:A0:43:THR:CG2 | 2.14 | 0.61 |
| 35:BB:100:GLY:O | 35:BB:104:ASN:N | 2.27 | 0.61 |
| 42:DI:51:ARG:HG2 | 42:DI:56:LEU:HD21 | 1.83 | 0.61 |
| 1:CA:2169:A:H2' | 1:CA:2170:A:C8 | 2.36 | 0.61 |
| 1:CA:1816:G:O6 | 4:CD:35:LYS:NZ | 2.23 | 0.61 |
| 1:AA:2348:A:H61 | 24:A0:43:THR:HG21 | 1.65 | 0.60 |
| 58:DY:33:U:H2' | 58:DY:35:A:OP2 | 2.01 | 0.60 |
| 13:CP:138:LEU:HD23 | 13:CP:145:PRO:HG3 | 1.82 | 0.60 |
| 59:DZ:491:VAL:HG21 | 59:DZ:597:GLY:HA3 | 1.83 | 0.60 |
| 35:DB:103:THR:HA | 35:DB:180:LEU:HD11 | 1.83 | 0.60 |
| 34:BA:742:G:OP2 | 48:BO:35:ARG:NH2 | 2.32 | 0.60 |
| 34:DA:924:C:O2' | 34:DA:1502:A:N6 | 2.35 | 0.60 |
| 56:BW:51:U:H2' | 56:BW:52:G:C8 | 2.35 | 0.60 |
| 34:DA:427:U:OP1 | 37:DD:13:ARG:NH2 | 2.34 | 0.60 |
| 6:CF:34:TRP:CZ2 | 13:CP:8:PRO:HG3 | 2.35 | 0.60 |
| 49:DP:51:VAL:HG12 | 49:DP:53:VAL:H | 1.66 | 0.60 |
| 34:DA:630:G:H2' | 34:DA:631:G:H8 | 1.65 | 0.60 |
| 1:CA:289:A:H2' | 1:CA:290:G:O4' | 2.01 | 0.60 |
| 21:AX:35:THR:HG22 | 21:AX:38:GLU:HB2 | 1.83 | 0.60 |
| 1:CA:1493:C:N4 | 1:CA:2206:G:O2' | 2.34 | 0.60 |
| 1:AA:1093:G:N2 | 1:AA:1156:G:O2' | 2.33 | 0.60 |
| 1:AA:2303:U:H2' | 1:AA:2304:C:C6 | 2.36 | 0.60 |
| 1:AA:2331:G:H22 | 16:AS:3:ARG:NE | 1.99 | 0.60 |
| 1:AA:2130:C:H2' | 1:AA:2131:U:H6 | 1.66 | 0.60 |
| 1:CA:636:G:O2' | 1:CA:638:G:O2' | 2.19 | 0.60 |
| 30:C6:8:LYS:HD3 | 32:C8:34:TRP:CD2 | 2.36 | 0.60 |
| 34:DA:1055:A:N3 | 36:DC:156:ARG:NH1 | 2.49 | 0.60 |
| 1:CA:2875:C:OP1 | 17:CT:3:ARG:NH2 | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:986:A:N3 | 52:DS:52:TYR:OH | 2.33 | 0.60 |
| 36:BC:19:GLU:HB3 | 36:BC:40:ARG:NH2 | 2.16 | 0.60 |
| 59:BZ:-64:VAL:HG12 | 59:BZ:-29:LEU:HA | 1.82 | 0.60 |
| 58:BY:67:C:H2' | 58:BY:68:C:C6 | 2.36 | 0.60 |
| 11:AN:42:TRP:CH2 | 11:AN:44:PRO:HB3 | 2.36 | 0.60 |
| 35:BB:200:ILE:HB | 35:BB:202:PRO:HD3 | 1.82 | 0.60 |
| 1:AA:232:U:OP1 | 32:A8:6:THR:OG1 | 2.16 | 0.60 |
| 7:CG:15:VAL:HA | 7:CG:175:LEU:HD23 | 1.83 | 0.60 |
| 36:DC:8:ILE:HD13 | 36:DC:184:TYR:HB3 | 1.82 | 0.60 |
| 34:BA:524:G:H2' | 34:BA:525:C:C6 | 2.36 | 0.60 |
| 59:BZ:20:HIS:HA | 59:BZ:117:GLN:HB2 | 1.81 | 0.60 |
| 28:C4:59:PHE:HA | 28:C4:61:ARG:N | 2.17 | 0.60 |
| 1:AA:2044:U:O2' | 1:AA:2629:C:H5' | 2.02 | 0.60 |
| 3:AC:194:ILE:HD11 | 3:AC:227:PRO:CB | 2.32 | 0.60 |
| 1:CA:271(M):G:H4' | 1:CA:271(N):U:OP1 | 2.01 | 0.60 |
| 1:CA:400:G:N7 | 65:CA:4345:HOH:O | 2.32 | 0.60 |
| 3:AC:214:TYR:CE2 | 3:AC:224:ARG:HG2 | 2.36 | 0.60 |
| 59:DZ:363:ARG:HG2 | 59:DZ:363:ARG:NH1 | 2.11 | 0.60 |
| 1:AA:553:A:H3' | 1:AA:553:A:H8 | 1.66 | 0.60 |
| 1:AA:2585:C:H3' | 65:AA:4113:HOH:O | 2.00 | 0.60 |
| 34:DA:630:G:H2' | 34:DA:631:G:C8 | 2.37 | 0.60 |
| 4:CD:146:GLU:HB2 | 4:CD:189:CYS:HB3 | 1.84 | 0.60 |
| 42:DI:23:ASN:H | 42:DI:23:ASN:HD22 | 1.49 | 0.60 |
| 8:CH:101:ARG:HH22 | 8:CH:122:THR:HG23 | 1.67 | 0.60 |
| 1:AA:2262:G:OP1 | 14:AQ:85:LYS:HE3 | 2.01 | 0.60 |
| 5:AE:105:THR:OG1 | 5:AE:199:ARG:NH2 | 2.35 | 0.60 |
| 59:BZ:99:ARG:CB | 59:BZ:99:ARG:HH11 | 2.09 | 0.60 |
| 13:AP:39:LYS:HD2 | 13:AP:45:LEU:HD11 | 1.82 | 0.60 |
| 59:BZ:12:LEU:HD12 | 59:BZ:78:ARG:HD2 | 1.83 | 0.60 |
| 34:DA:982:U:O2 | 34:DA:1222:G:N1 | 2.31 | 0.60 |
| 41:BH:112:LEU:HA | 41:BH:134:ILE:HG12 | 1.81 | 0.60 |
| 51:DR:58:LEU:HD12 | 51:DR:62:GLU:HB3 | 1.84 | 0.60 |
| 34:DA:390:C:O3' | 49:DP:28:ARG:NH2 | 2.34 | 0.60 |
| 1:AA:2697:G:H5' | 12:AO:68:GLU:OE1 | 2.02 | 0.60 |
| 1:AA:1766:G:H3' | 1:AA:1767:A:H5'' | 1.81 | 0.60 |
| 20:CW:88:ARG:NH1 | 20:CW:94:ASP:OD2 | 2.34 | 0.60 |
| 41:DH:49:GLU:OE2 | 41:DH:62:TYR:OH | 2.15 | 0.60 |
| 34:DA:1189:C:OP1 | 43:DJ:51:ARG:NH2 | 2.34 | 0.60 |
| 1:CA:1021:A:C8 | 1:CA:1021:A:H3' | 2.37 | 0.60 |
| 3:CC:214:TYR:CE2 | 3:CC:224:ARG:HG2 | 2.36 | 0.60 |
| 3:CC:68:GLY:H | 3:CC:189:ASN:HD21 | 1.47 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:BX:61:C:H2' | 57:BX:62:C:C6 | 2.36 | 0.60 |
| 35:BB:187:LEU:HA | 35:BB:201:ILE:HB | 1.82 | 0.60 |
| 5:CE:56:PRO:HG3 | 5:CE:74:PRO:HG2 | 1.84 | 0.60 |
| 1:AA:2504:U:H2' | 1:AA:2505:U:C6 | 2.37 | 0.60 |
| 59:DZ:13:ARG:NE | 59:DZ:280:LEU:O | 2.30 | 0.60 |
| 25:C1:72:GLU:OE1 | 25:C1:76:ARG:NH2 | 2.35 | 0.60 |
| 35:DB:74:LYS:HD2 | 35:DB:165:VAL:HG11 | 1.84 | 0.60 |
| 14:CQ:26:TYR:CE1 | 14:CQ:28:ALA:HB2 | 2.37 | 0.60 |
| 34:DA:975:A:N6 | 43:DJ:60:ARG:HH12 | 2.00 | 0.60 |
| 45:DL:83:VAL:HG23 | 45:DL:107:ALA:HB2 | 1.82 | 0.60 |
| 34:BA:1251:A:H2' | 34:BA:1252:A:C8 | 2.37 | 0.60 |
| 3:AC:11:LEU:HD12 | 3:AC:33:LEU:HA | 1.82 | 0.60 |
| 18:AU:76:TYR:CE1 | 18:AU:80:ILE:HG13 | 2.36 | 0.60 |
| 41:DH:37:ARG:HH21 | 41:DH:38:ILE:HD11 | 1.66 | 0.60 |
| 1:AA:1312:G:O5' | 20:AW:15:ARG:NH2 | 2.35 | 0.60 |
| 38:DE:81:GLU:HG2 | 38:DE:90:VAL:HG13 | 1.82 | 0.60 |
| 1:AA:2075:G:OP1 | 5:AE:144:ARG:HG2 | 2.02 | 0.60 |
| 16:AS:14:VAL:O | 16:AS:18:ILE:HG12 | 2.01 | 0.60 |
| 59:BZ:276:VAL:HG13 | 59:BZ:280:LEU:HD12 | 1.82 | 0.60 |
| 4:CD:17:THR:O | 4:CD:211:ARG:NH2 | 2.34 | 0.60 |
| 36:BC:43:LEU:HD22 | 36:BC:47:LEU:HD11 | 1.83 | 0.60 |
| 42:DI:53:VAL:O | 42:DI:55:ALA:N | 2.34 | 0.60 |
| 34:BA:1305:G:H22 | 34:BA:1331:G:H1' | 1.65 | 0.59 |
| 34:DA:1003:G:N2 | 34:DA:1025:U:O4 | 2.35 | 0.59 |
| 1:CA:1153:C:OP1 | 18:CU:92:ARG:NH1 | 2.35 | 0.59 |
| 36:BC:6:HIS:HD2 | 36:BC:8:ILE:H | 1.50 | 0.59 |
| 59:DZ:438:PHE:HE2 | 59:DZ:440:VAL:HG23 | 1.65 | 0.59 |
| 4:CD:131:LEU:HB2 | 4:CD:136:ILE:HD11 | 1.83 | 0.59 |
| 55:DV:20:U:H2' | 55:DV:21:C:H6 | 1.67 | 0.59 |
| 59:DZ:35:TYR:HE2 | 59:DZ:269:VAL:HB | 1.66 | 0.59 |
| 7:AG:3:LEU:HD12 | 7:AG:5:VAL:HG12 | 1.84 | 0.59 |
| 1:CA:793:A:O2' | 65:CA:4198:HOH:O | 2.14 | 0.59 |
| 34:DA:664:G:N2 | 34:DA:741:G:H1 | 1.99 | 0.59 |
| 4:CD:96:HIS:CD2 | 4:CD:102:LYS:HG2 | 2.34 | 0.59 |
| 34:DA:1118:C:H2' | 34:DA:1119:C:H6 | 1.66 | 0.59 |
| 28:A4:26:SER:OG | 28:A4:27:THR:N | 2.35 | 0.59 |
| 13:CP:85:LEU:HA | 13:CP:88:LEU:HD12 | 1.84 | 0.59 |
| 23:CZ:19:ARG:NH1 | 23:CZ:84:GLU:O | 2.35 | 0.59 |
| 1:CA:854:G:O6 | 65:CA:4561:HOH:O | 2.13 | 0.59 |
| 47:BN:4:LYS:HA | 47:BN:7:ILE:HG23 | 1.83 | 0.59 |
| 1:CA:918:A:N3 | 2:CB:80:U:O2' | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:878:G:H5' | 41:DH:89:PRO:HG2 | 1.82 | 0.59 |
| 1:AA:2008:A:OP1 | 65:AA:4321:HOH:O | 2.16 | 0.59 |
| 1:AA:2201:C:O4' | 3:AC:169:THR:CG2 | 2.48 | 0.59 |
| 34:DA:920:U:H2' | 34:DA:921:U:H6 | 1.67 | 0.59 |
| 34:DA:1073:U:H2' | 34:DA:1074:G:C8 | 2.37 | 0.59 |
| 36:BC:53:ALA:HB2 | 36:BC:115:LEU:HD13 | 1.84 | 0.59 |
| 14:AQ:56:ARG:NH1 | 56:BW:52:G:H4' | 2.17 | 0.59 |
| 34:BA:193:C:H2' | 34:BA:194:C:C6 | 2.36 | 0.59 |
| 59:BZ:179:ASP:N | 59:BZ:184:LYS:O | 2.29 | 0.59 |
| 34:BA:555:C:H2' | 34:BA:556:C:C6 | 2.37 | 0.59 |
| 39:DF:2:ARG:NE | 39:DF:69:GLU:HG2 | 2.17 | 0.59 |
| 7:CG:113:ARG:NH1 | 7:CG:139:LEU:O | 2.34 | 0.59 |
| 10:AL:77:LEU:HD21 | 10:AL:111:LYS:HD2 | 1.84 | 0.59 |
| 1:CA:2781:A:H5'' | 1:CA:2782:G:H5' | 1.84 | 0.59 |
| 5:CE:78:LEU:O | 5:CE:79:ARG:HG2 | 2.01 | 0.59 |
| 1:CA:2273:A:O2' | 1:CA:2274:A:H5' | 2.02 | 0.59 |
| 1:CA:1053:C:C4 | 1:CA:1107:G:N2 | 2.68 | 0.59 |
| 1:CA:2132:U:C2 | 3:CC:6:LYS:HE3 | 2.37 | 0.59 |
| 23:CZ:108:PRO:HG2 | 23:CZ:117:LEU:HD13 | 1.85 | 0.59 |
| 10:AL:77:LEU:HD12 | 10:AL:107:ILE:HG23 | 1.85 | 0.59 |
| 3:CC:194:ILE:HD11 | 3:CC:227:PRO:CB | 2.32 | 0.59 |
| 1:CA:2485:G:H5'' | 14:CQ:46:GLN:HE21 | 1.67 | 0.59 |
| 59:DZ:407:PRO:HB3 | 59:DZ:452:SER:HB3 | 1.85 | 0.59 |
| 49:DP:43:LYS:HG2 | 49:DP:48:TRP:CG | 2.38 | 0.59 |
| 1:CA:908:C:OP2 | 14:CQ:22:LYS:NZ | 2.35 | 0.59 |
| 14:CQ:110:THR:HG23 | 14:CQ:113:GLN:HB2 | 1.83 | 0.59 |
| 1:AA:2255:U:H2' | 1:AA:2256:U:C6 | 2.37 | 0.59 |
| 1:CA:1589:C:H2' | 1:CA:1590:U:C6 | 2.37 | 0.59 |
| 8:AH:164:TYR:HB2 | 8:AH:167:GLU:HB2 | 1.83 | 0.59 |
| 34:BA:1240:U:OP2 | 40:BG:116:ALA:N | 2.27 | 0.59 |
| 12:AO:35:VAL:HG21 | 12:AO:69:ILE:HD13 | 1.84 | 0.59 |
| 35:DB:189:ASP:N | 35:DB:189:ASP:OD1 | 2.27 | 0.59 |
| 34:DA:1123:A:H4' | 43:DJ:37:PRO:HD2 | 1.85 | 0.59 |
| 34:DA:1030:C:H42 | 34:DA:1031:G:H1 | 1.50 | 0.59 |
| 1:CA:1108:U:H6 | 1:CA:1108:U:O5' | 1.85 | 0.59 |
| 42:BI:3:GLN:HG3 | 42:BI:20:ARG:HE | 1.67 | 0.59 |
| 1:CA:2166:G:H3' | 1:CA:2167:U:H5'' | 1.84 | 0.59 |
| 8:AH:88:LEU:HD13 | 8:AH:130:ARG:HG2 | 1.84 | 0.59 |
| 44:DK:22:HIS:HB3 | 44:DK:29:ILE:HB | 1.85 | 0.59 |
| 1:AA:1338:U:H2' | 1:AA:1339:C:C6 | 2.37 | 0.59 |
| 35:BB:178:ARG:NH2 | 41:BH:74:PRO:HB3 | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:331:G:H21 | 1:AA:354:A:H62 | 1.50 | 0.59 |
| 34:BA:736:C:H2' | 34:BA:737:A:C8 | 2.37 | 0.59 |
| 37:BD:60:GLU:OE1 | 37:BD:198:VAL:HA | 2.01 | 0.59 |
| 1:AA:2013:U:H2' | 1:AA:2014:G:H5'' | 1.84 | 0.59 |
| 1:CA:2165:G:H22 | 1:CA:2172:U:H5 | 1.51 | 0.59 |
| 3:CC:41:THR:HG22 | 3:CC:42:VAL:N | 2.17 | 0.59 |
| 35:DB:16:HIS:O | 35:DB:18:GLY:N | 2.36 | 0.59 |
| 37:DD:13:ARG:NH1 | 37:DD:38:TYR:O | 2.36 | 0.59 |
| 16:AS:3:ARG:HD3 | 16:AS:3:ARG:C | 2.22 | 0.59 |
| 49:DP:43:LYS:HG2 | 49:DP:48:TRP:CD2 | 2.37 | 0.59 |
| 34:BA:103:C:P | 53:BT:17:ARG:HH21 | 2.25 | 0.59 |
| 1:CA:2148:G:H2' | 1:CA:2149:G:C8 | 2.37 | 0.59 |
| 1:CA:2320:A:N3 | 1:CA:2320:A:H2' | 2.17 | 0.59 |
| 34:BA:1326:C:OP1 | 54:BU:12:LYS:NZ | 2.23 | 0.59 |
| 59:BZ:20:HIS:ND1 | 59:BZ:117:GLN:HG2 | 2.18 | 0.59 |
| 52:DS:63:THR:OG1 | 52:DS:64:GLU:N | 2.35 | 0.59 |
| 42:DI:14:VAL:HG23 | 42:DI:66:ARG:HB3 | 1.83 | 0.59 |
| 35:BB:201:ILE:HG21 | 35:BB:214:ILE:HG21 | 1.83 | 0.59 |
| 36:BC:13:GLY:HA3 | 47:BN:57:ARG:HH21 | 1.66 | 0.59 |
| 1:CA:2139:C:H42 | 1:CA:2152:G:H1 | 1.51 | 0.59 |
| 41:DH:73:ASP:OD1 | 41:DH:75:ARG:NH1 | 2.36 | 0.59 |
| 1:CA:1792:G:O2' | 1:CA:1830:C:OP1 | 2.20 | 0.59 |
| 27:C3:8:LEU:HD13 | 27:C3:31:LEU:HD23 | 1.84 | 0.59 |
| 53:DT:9:ASN:O | 53:DT:10:LEU:HB2 | 2.02 | 0.59 |
| 1:CA:309:G:N3 | 1:CA:329:G:O2' | 2.35 | 0.59 |
| 1:AA:1159:U:H2' | 1:AA:1160:G:C8 | 2.38 | 0.59 |
| 59:DZ:346:LYS:HZ1 | 59:DZ:384:ILE:HG23 | 1.68 | 0.59 |
| 41:BH:51:VAL:HG21 | 41:BH:60:ARG:HH11 | 1.67 | 0.59 |
| 1:CA:1108:U:C5 | 1:CA:1109:C:C4 | 2.91 | 0.59 |
| 34:DA:1330:U:H4' | 46:DM:23:TYR:CE1 | 2.37 | 0.59 |
| 42:BI:110:GLU:OE2 | 42:BI:113:LYS:NZ | 2.35 | 0.59 |
| 1:AA:1775:C:H5' | 1:AA:1776:G:OP2 | 2.03 | 0.59 |
| 59:BZ:146:LEU:HD12 | 59:BZ:167:PRO:HD3 | 1.85 | 0.59 |
| 36:BC:3:ASN:OD1 | 36:BC:3:ASN:N | 2.36 | 0.59 |
| 18:CU:86:ALA:HB2 | 18:CU:116:ALA:HB2 | 1.84 | 0.59 |
| 1:AA:1154:U:H1' | 1:AA:1155:C:OP1 | 2.03 | 0.58 |
| 3:AC:214:TYR:CZ | 3:AC:224:ARG:HG2 | 2.37 | 0.58 |
| 34:DA:1202:G:O4' | 47:DN:29:ARG:NH1 | 2.34 | 0.58 |
| 12:CO:120:GLU:OE1 | 17:CT:67:SER:OG | 2.21 | 0.58 |
| 34:DA:839:U:H5'' | 34:DA:840:C:H5 | 1.68 | 0.58 |
| 16:CS:10:ARG:O | 16:CS:14:VAL:HG13 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BJ:38:ILE:HD11 | 43:BJ:71:LEU:HD23 | 1.84 | 0.58 |
| 4:AD:52:ARG:NH2 | 65:AD:412:HOH:O | 2.29 | 0.58 |
| 59:DZ:74:TRP:O | 59:DZ:76:ASP:N | 2.36 | 0.58 |
| 1:CA:90:U:H1' | 1:CA:92:A:C8 | 2.38 | 0.58 |
| 1:AA:278:G:H2' | 1:AA:279:G:H5'' | 1.85 | 0.58 |
| 1:CA:2183:C:H2' | 1:CA:2184:G:H8 | 1.68 | 0.58 |
| 3:CC:214:TYR:CZ | 3:CC:224:ARG:HG2 | 2.37 | 0.58 |
| 1:CA:307:G:N1 | 1:CA:310:A:OP2 | 2.32 | 0.58 |
| 3:AC:41:THR:HG22 | 3:AC:42:VAL:N | 2.17 | 0.58 |
| 35:DB:71:VAL:HG22 | 35:DB:164:VAL:HA | 1.84 | 0.58 |
| 39:DF:35:ALA:HA | 39:DF:67:MET:HB3 | 1.84 | 0.58 |
| 59:BZ:138:LYS:HG2 | 64:BZ:702:GDP:C6 | 2.38 | 0.58 |
| 50:BQ:66:SER:O | 50:BQ:70:ARG:NH1 | 2.36 | 0.58 |
| 1:AA:1688:A:H2' | 1:AA:1689:G:O4' | 2.03 | 0.58 |
| 58:DY:50:U:H3 | 58:DY:64:A:H61 | 1.51 | 0.58 |
| 25:A1:3:LYS:HB2 | 25:A1:61:ARG:NH1 | 2.18 | 0.58 |
| 34:BA:1125:U:H4' | 43:BJ:5:ARG:NH2 | 2.18 | 0.58 |
| 14:CQ:16:ARG:HG2 | 14:CQ:16:ARG:HH11 | 1.68 | 0.58 |
| 56:BW:7:A:H61 | 56:BW:66:U:H3 | 1.49 | 0.58 |
| 28:C4:34:GLU:HG2 | 46:DM:3:ARG:HB3 | 1.84 | 0.58 |
| 59:BZ:289:ILE:HD11 | 59:BZ:331:TYR:HB3 | 1.85 | 0.58 |
| 37:DD:173:TRP:HB2 | 37:DD:187:ARG:O | 2.02 | 0.58 |
| 34:DA:1022:G:H2' | 34:DA:1023:G:C8 | 2.38 | 0.58 |
| 1:AA:1232:G:H5'' | 19:AV:81:TYR:CE1 | 2.37 | 0.58 |
| 39:DF:8:ILE:HD11 | 39:DF:79:LEU:HD13 | 1.85 | 0.58 |
| 46:BM:11:ARG:HB2 | 46:BM:46:LYS:HB3 | 1.84 | 0.58 |
| 34:BA:653:A:OP1 | 41:BH:56:LYS:NZ | 2.36 | 0.58 |
| 8:CH:64:LEU:HD23 | 8:CH:67:LEU:HD23 | 1.86 | 0.58 |
| 47:DN:9:LYS:HG3 | 47:DN:12:ARG:HD3 | 1.85 | 0.58 |
| 1:CA:657:U:H2' | 1:CA:658:C:C6 | 2.38 | 0.58 |
| 1:CA:208:C:H2' | 1:CA:209:C:C6 | 2.39 | 0.58 |
| 14:AQ:2:LEU:HD22 | 65:AQ:3104:HOH:O | 2.02 | 0.58 |
| 34:BA:1325:C:H2' | 34:BA:1326:C:H6 | 1.69 | 0.58 |
| 12:AO:2:ILE:HG13 | 12:AO:8:LEU:HD11 | 1.86 | 0.58 |
| 1:CA:774:A:HO2' | 1:CA:775:G:H8 | 1.50 | 0.58 |
| 1:CA:244:A:C2 | 1:CA:255:A:C4 | 2.92 | 0.58 |
| 51:BR:56:THR:HB | 51:BR:58:LEU:HD23 | 1.85 | 0.58 |
| 9:AK:74:LEU:O | 9:AK:76:GLY:N | 2.35 | 0.58 |
| 48:DO:29:VAL:HG11 | 48:DO:81:LEU:HD21 | 1.85 | 0.58 |
| 1:CA:1427:A:H4' | 1:CA:1428:C:O5' | 2.02 | 0.58 |
| 59:BZ:247:ARG:O | 59:BZ:251:ILE:HG13 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:DI:9:ARG:HG2 | 42:DI:14:VAL:HG12 | 1.84 | 0.58 |
| 42:DI:80:GLY:HA2 | 42:DI:83:ARG:HB2 | 1.84 | 0.58 |
| 34:DA:1052:U:H5'' | 34:DA:1053:G:OP2 | 2.03 | 0.58 |
| 34:BA:974:A:OP2 | 47:BN:29:ARG:NH2 | 2.36 | 0.58 |
| 34:BA:347:G:H2' | 34:BA:348:G:O4' | 2.03 | 0.58 |
| 11:AN:128:HIS:O | 11:AN:131:GLN:NE2 | 2.37 | 0.58 |
| 46:BM:84:ILE:HG13 | 46:BM:86:CYS:H | 1.67 | 0.58 |
| 34:DA:1220:G:N2 | 52:DS:54:GLY:O | 2.36 | 0.58 |
| 59:BZ:217:VAL:HA | 59:BZ:220:ALA:HB3 | 1.86 | 0.58 |
| 1:AA:1898:A:H2' | 1:AA:1899:A:C8 | 2.37 | 0.58 |
| 6:CF:126:VAL:HG21 | 6:CF:129:PHE:CZ | 2.39 | 0.58 |
| 47:BN:23:ARG:NH1 | 47:BN:30:ALA:HB2 | 2.19 | 0.58 |
| 59:DZ:4:ILE:HG22 | 59:DZ:5:LEU:HD23 | 1.86 | 0.58 |
| 39:BF:44:GLY:O | 39:BF:60:PHE:N | 2.30 | 0.58 |
| 34:DA:998:G:N2 | 34:DA:1043:C:N3 | 2.47 | 0.58 |
| 59:BZ:-36:LEU:HD21 | 59:BZ:-29:LEU:HD22 | 1.84 | 0.58 |
| 59:DZ:357:ARG:HD2 | 59:DZ:366:VAL:HG11 | 1.85 | 0.58 |
| 59:DZ:404:VAL:H | 59:DZ:405:PRO:HD3 | 1.69 | 0.58 |
| 34:BA:149:A:H2' | 34:BA:150:C:C6 | 2.39 | 0.58 |
| 34:DA:978:A:O2' | 34:DA:1322:C:N3 | 2.33 | 0.58 |
| 47:DN:27:CYS:SG | 47:DN:29:ARG:HB2 | 2.44 | 0.58 |
| 1:CA:1430:C:H2' | 1:CA:1431:U:H6 | 1.69 | 0.58 |
| 34:DA:1001:A:H2' | 34:DA:1001(A):G:H8 | 1.68 | 0.58 |
| 1:AA:551:A:H5'' | 1:AA:552:C:OP1 | 2.03 | 0.58 |
| 59:BZ:-58:LEU:HD21 | 59:BZ:-32:LEU:HD22 | 1.85 | 0.58 |
| 4:CD:26:LYS:NZ | 4:CD:30:GLU:HG2 | 2.19 | 0.58 |
| 24:C0:2:ALA:N | 65:C0:202:HOH:O | 2.37 | 0.58 |
| 34:DA:834:C:H2' | 34:DA:835:U:C6 | 2.39 | 0.58 |
| 34:BA:142:G:H2' | 34:BA:143:A:H8 | 1.68 | 0.58 |
| 34:DA:64:G:H4' | 34:DA:65:U:H3' | 1.86 | 0.58 |
| 38:BE:71:LEU:HD21 | 38:BE:115:VAL:HG22 | 1.85 | 0.58 |
| 34:BA:232:G:H1' | 34:BA:262:A:N1 | 2.19 | 0.58 |
| 30:A6:14:THR:HB | 30:A6:48:VAL:O | 2.04 | 0.58 |
| 1:CA:2349:G:OP1 | 65:CA:3743:HOH:O | 2.17 | 0.58 |
| 34:DA:673:G:H2' | 34:DA:674:G:C8 | 2.38 | 0.58 |
| 1:CA:2815:C:H5' | 29:C5:29:THR:HG21 | 1.85 | 0.58 |
| 1:AA:173:C:H2' | 1:AA:174:U:C6 | 2.39 | 0.58 |
| 1:CA:2788:C:OP1 | 5:CE:61:ARG:NH2 | 2.37 | 0.58 |
| 21:AX:11:PRO:HB3 | 21:AX:92:LEU:HD11 | 1.86 | 0.58 |
| 25:C1:18:ILE:HG12 | 25:C1:37:ILE:HG23 | 1.86 | 0.58 |
| 17:CT:23:ARG:HG3 | 17:CT:120:ARG:NH1 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1123:A:O2' | 10:AL:132:ARG:O | 2.21 | 0.58 |
| 1:AA:1101:G:O2' | 1:AA:1131:A:N1 | 2.30 | 0.58 |
| 50:BQ:97:SER:OG | 50:BQ:97:SER:O | 2.21 | 0.58 |
| 1:AA:181:C:OP1 | 65:AA:3944:HOH:O | 2.17 | 0.58 |
| 1:AA:1891:G:H4' | 3:AC:206:LYS:HD2 | 1.25 | 0.57 |
| 59:BZ:13:ARG:NH1 | 59:BZ:280:LEU:O | 2.37 | 0.57 |
| 34:DA:344:A:H5' | 34:DA:345:C:C5 | 2.35 | 0.57 |
| 34:DA:1321:C:H4' | 46:DM:87:TYR:CE2 | 2.39 | 0.57 |
| 1:AA:2227:G:O2' | 1:AA:2228:G:OP1 | 2.22 | 0.57 |
| 11:AN:42:TRP:CE3 | 18:AU:63:VAL:HG11 | 2.39 | 0.57 |
| 59:DZ:-62:LEU:HD11 | 59:DZ:-48:VAL:HG22 | 1.86 | 0.57 |
| 1:AA:2787:C:H2' | 1:AA:2788:A:O4' | 2.03 | 0.57 |
| 34:BA:410:G:OP1 | 37:BD:30:LYS:NZ | 2.24 | 0.57 |
| 40:DG:72:ARG:N | 40:DG:142:GLU:OE2 | 2.36 | 0.57 |
| 59:BZ:246:ILE:HG23 | 59:BZ:255:ILE:HD11 | 1.85 | 0.57 |
| 1:CA:796:C:H2' | 1:CA:797:C:C6 | 2.39 | 0.57 |
| 34:BA:1323:G:H2' | 34:BA:1324:A:C8 | 2.39 | 0.57 |
| 1:AA:2585:C:OP1 | 65:AA:4112:HOH:O | 2.17 | 0.57 |
| 49:BP:56:ALA:O | 49:BP:60:LEU:HB2 | 2.04 | 0.57 |
| 51:BR:32:ARG:HA | 51:BR:69:THR:HG21 | 1.86 | 0.57 |
| 1:CA:1364:G:OP2 | 25:C1:3:LYS:HG3 | 2.04 | 0.57 |
| 1:AA:2141:A:O2' | 1:AA:2142:G:H5' | 2.04 | 0.57 |
| 16:CS:41:ASP:OD2 | 16:CS:44:LYS:HE2 | 2.04 | 0.57 |
| 1:AA:1296:G:N7 | 13:AP:18:ARG:NH2 | 2.52 | 0.57 |
| 34:DA:1126:U:H4' | 34:DA:1281:U:H1' | 1.85 | 0.57 |
| 35:DB:77:ALA:HA | 35:DB:80:ILE:HG22 | 1.84 | 0.57 |
| 59:DZ:114:VAL:HG21 | 59:DZ:156:ARG:HB2 | 1.86 | 0.57 |
| 1:CA:2179:C:O4' | 3:CC:169:THR:HG22 | 2.03 | 0.57 |
| 46:DM:16:ASP:OD1 | 46:DM:16:ASP:N | 2.38 | 0.57 |
| 37:DD:61:LYS:HB2 | 37:DD:203:VAL:HG22 | 1.85 | 0.57 |
| 42:BI:99:LEU:HB3 | 42:BI:101:PHE:CE1 | 2.38 | 0.57 |
| 35:DB:80:ILE:HD11 | 35:DB:212:GLN:HA | 1.87 | 0.57 |
| 47:DN:48:ALA:HB2 | 47:DN:53:LEU:HD12 | 1.86 | 0.57 |
| 1:AA:2417:G:P | 13:AP:77:ARG:HH22 | 2.26 | 0.57 |
| 8:CH:143:GLN:O | 8:CH:146:ALA:N | 2.38 | 0.57 |
| 1:CA:2749:A:H1' | 8:CH:63:SER:HB3 | 1.86 | 0.57 |
| 28:A4:61:ARG:HH21 | 52:BS:42:PRO:HD2 | 1.69 | 0.57 |
| 59:BZ:225:GLU:HA | 59:BZ:228:MET:HB3 | 1.86 | 0.57 |
| 1:AA:610:C:OP2 | 13:AP:21:ARG:NH2 | 2.36 | 0.57 |
| 1:AA:1077:G:H21 | 33:A9:36:GLN:HE22 | 1.52 | 0.57 |
| 1:CA:1021:A:H8 | 1:CA:1021:A:H3' | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:43:LEU:HD11 | 7:AG:153:ARG:HG2 | 1.87 | 0.57 |
| 35:DB:74:LYS:O | 35:DB:78:GLN:HB2 | 2.04 | 0.57 |
| 34:BA:131:C:O2' | 34:BA:262:A:N3 | 2.34 | 0.57 |
| 1:CA:1062:G:O2' | 10:CL:133:SER:O | 2.17 | 0.57 |
| 28:C4:62:ARG:O | 28:C4:64:GLY:N | 2.37 | 0.57 |
| 9:CK:69:PRO:O | 9:CK:71:LEU:N | 2.35 | 0.57 |
| 35:BB:185:ILE:HG23 | 35:BB:199:TYR:HB2 | 1.85 | 0.57 |
| 1:CA:1648:C:OP1 | 65:CA:4161:HOH:O | 2.17 | 0.57 |
| 1:AA:1201:A:OP1 | 18:AU:55:ARG:HD3 | 2.04 | 0.57 |
| 42:BI:70:LYS:O | 42:BI:74:ILE:HG13 | 2.04 | 0.57 |
| 34:DA:736:C:H2' | 34:DA:737:A:C8 | 2.39 | 0.57 |
| 1:AA:1112:U:N3 | 1:AA:1114:G:OP2 | 2.37 | 0.57 |
| 35:DB:16:HIS:HB2 | 35:DB:204:ASN:HB3 | 1.86 | 0.57 |
| 59:BZ:162:VAL:HG21 | 59:BZ:255:ILE:HD12 | 1.85 | 0.57 |
| 1:AA:2735:G:H2' | 1:AA:2736:C:C6 | 2.39 | 0.57 |
| 56:DW:51:U:H2' | 56:DW:52:G:C8 | 2.40 | 0.57 |
| 59:BZ:-53:ASP:H | 59:BZ:-50:GLN:NE2 | 2.02 | 0.57 |
| 34:DA:1171:G:H2' | 34:DA:1172:C:C6 | 2.40 | 0.57 |
| 59:DZ:294:PRO:HG3 | 59:DZ:396:ARG:HB2 | 1.85 | 0.57 |
| 1:CA:1568:G:N7 | 65:CA:4604:HOH:O | 2.32 | 0.57 |
| 25:A1:77:ALA:HB2 | 25:A1:94:LEU:HD21 | 1.85 | 0.57 |
| 49:BP:17:TYR:CE2 | 49:BP:41:PRO:HG3 | 2.40 | 0.57 |
| 1:CA:1338:G:N7 | 21:CX:62:LYS:NZ | 2.49 | 0.57 |
| 34:DA:834:C:H2' | 34:DA:835:U:H6 | 1.69 | 0.57 |
| 1:CA:2744:G:N2 | 8:CH:143:GLN:OE1 | 2.37 | 0.57 |
| 59:BZ:-53:ASP:H | 59:BZ:-50:GLN:HE21 | 1.53 | 0.57 |
| 1:AA:561:A:H2' | 1:AA:562:C:C6 | 2.40 | 0.57 |
| 37:BD:162:LEU:HD13 | 37:BD:181:MET:HG2 | 1.87 | 0.57 |
| 1:AA:2158:C:H42 | 1:AA:2177:G:H1 | 1.53 | 0.57 |
| 59:DZ:619:ASP:HB3 | 59:DZ:662:LYS:HD2 | 1.86 | 0.57 |
| 1:CA:955:C:OP1 | 14:CQ:87:LYS:NZ | 2.34 | 0.57 |
| 12:CO:24:VAL:HB | 12:CO:33:ALA:HB2 | 1.87 | 0.57 |
| 34:DA:962:C:O2' | 65:DA:1841:HOH:O | 2.15 | 0.57 |
| 1:AA:1067:A:H8 | 1:AA:1068:G:H5'' | 1.70 | 0.57 |
| 35:BB:111:ARG:NH1 | 35:BB:111:ARG:HG2 | 2.17 | 0.57 |
| 34:BA:167:G:H2' | 34:BA:168:G:C8 | 2.37 | 0.57 |
| 59:DZ:16:GLY:HA3 | 59:DZ:101:LEU:HD22 | 1.85 | 0.57 |
| 1:CA:882:G:N2 | 1:CA:894:C:O2 | 2.34 | 0.57 |
| 37:BD:154:ASN:HA | 37:BD:159:ARG:HH21 | 1.69 | 0.57 |
| 26:C2:35:LEU:HD22 | 26:C2:44:LEU:HD11 | 1.84 | 0.57 |
| 34:DA:1256:A:H61 | 34:DA:1278:U:H1' | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BA:395:C:O3' | 59:BZ:349:LYS:NZ | 2.37 | 0.57 |
| 43:BJ:8:LEU:HD12 | 43:BJ:20:ALA:HB2 | 1.87 | 0.57 |
| 34:DA:646:U:H2' | 34:DA:647:C:C6 | 2.40 | 0.57 |
| 40:BG:18:TYR:CE2 | 40:BG:59:LEU:HB2 | 2.40 | 0.57 |
| 35:BB:77:ALA:HB2 | 35:BB:211:ILE:HD13 | 1.87 | 0.57 |
| 5:AE:111:ARG:HG3 | 5:AE:160:TYR:CD2 | 2.40 | 0.57 |
| 46:BM:3:ARG:HD2 | 46:BM:9:ILE:HG12 | 1.86 | 0.57 |
| 6:CF:195:ASP:HB3 | 6:CF:198:ALA:H | 1.70 | 0.57 |
| 1:CA:1108:U:C6 | 1:CA:1109:C:C5 | 2.92 | 0.57 |
| 36:BC:40:ARG:O | 36:BC:44:GLU:HB2 | 2.05 | 0.57 |
| 48:DO:56:LEU:O | 48:DO:60:VAL:HG23 | 2.05 | 0.57 |
| 1:CA:1693:U:O2' | 4:CD:14:ARG:NH2 | 2.37 | 0.57 |
| 34:DA:1001:A:H2' | 34:DA:1001(A):G:C8 | 2.40 | 0.57 |
| 34:BA:1239:A:H4' | 34:BA:1240:U:H5'' | 1.85 | 0.57 |
| 34:DA:503:C:OP2 | 45:DL:116:SER:HB3 | 2.04 | 0.57 |
| 38:BE:152:ARG:HA | 41:BH:64:LYS:NZ | 2.19 | 0.57 |
| 15:CR:104:ARG:HD2 | 15:CR:109:ALA:HB3 | 1.85 | 0.57 |
| 34:DA:188:C:H2' | 34:DA:189:G:H8 | 1.69 | 0.57 |
| 35:DB:7:VAL:HG12 | 35:DB:8:LYS:HG2 | 1.86 | 0.57 |
| 59:BZ:74:TRP:CD1 | 59:BZ:273:LEU:HB3 | 2.39 | 0.57 |
| 34:DA:316:G:OP2 | 34:DA:351:G:O2' | 2.22 | 0.57 |
| 1:AA:469:A:H1' | 1:AA:1246:C:O4' | 2.04 | 0.57 |
| 33:A9:2:LYS:HE2 | 33:A9:31:LYS:O | 2.04 | 0.57 |
| 5:AE:101:ARG:NH1 | 5:AE:169:ASN:O | 2.34 | 0.57 |
| 8:CH:3:ARG:CZ | 8:CH:4:ILE:H | 2.17 | 0.57 |
| 38:DE:139:LEU:C | 38:DE:141:GLN:H | 2.08 | 0.57 |
| 19:CV:3:ALA:HB3 | 19:CV:14:VAL:HG23 | 1.86 | 0.57 |
| 1:CA:1899:G:H2' | 1:CA:1899:G:N3 | 2.20 | 0.57 |
| 35:BB:37:ASN:OD1 | 35:BB:37:ASN:N | 2.38 | 0.57 |
| 30:C6:10:LEU:HD23 | 30:C6:22:ALA:HB2 | 1.86 | 0.57 |
| 21:CX:41:ASN:O | 21:CX:45:THR:HG23 | 2.05 | 0.57 |
| 34:DA:1135:U:H2' | 34:DA:1137:C:C2 | 2.40 | 0.57 |
| 6:CF:184:TYR:CE1 | 13:CP:3:LEU:HD21 | 2.39 | 0.57 |
| 35:DB:184:VAL:HG12 | 35:DB:197:VAL:HG13 | 1.87 | 0.57 |
| 6:AF:184:TYR:O | 6:AF:188:ARG:HG3 | 2.05 | 0.57 |
| 34:DA:881:G:OP2 | 45:DL:12:ARG:NH2 | 2.38 | 0.57 |
| 46:DM:78:ILE:HD12 | 46:DM:92:HIS:CE1 | 2.40 | 0.57 |
| 1:CA:214:G:O2' | 1:CA:216:A:O2' | 2.19 | 0.57 |
| 34:DA:1353:G:OP1 | 54:DU:10:ARG:NH1 | 2.38 | 0.57 |
| 34:BA:731:G:H5' | 34:BA:766:A:H4' | 1.87 | 0.57 |
| 34:BA:673:G:H2' | 34:BA:674:G:C8 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:AG:38:VAL:HG22 | 7:AG:93:THR:HG23 | 1.87 | 0.57 |
| 1:AA:185:A:H62 | 13:AP:38:GLN:HE22 | 1.51 | 0.57 |
| 59:BZ:247:ARG:HE | 59:BZ:251:ILE:HD11 | 1.70 | 0.56 |
| 1:AA:990:A:H2 | 65:AA:4753:HOH:O | 1.87 | 0.56 |
| 59:DZ:138:LYS:HG2 | 64:DZ:702:GDP:C5 | 2.40 | 0.56 |
| 1:AA:1827:U:H2' | 1:AA:1828:C:C6 | 2.40 | 0.56 |
| 34:DA:1106:G:H5'' | 36:DC:172:ARG:HG2 | 1.87 | 0.56 |
| 14:AQ:110:THR:HG23 | 14:AQ:113:GLN:OE1 | 2.05 | 0.56 |
| 8:CH:7:LEU:HD23 | 8:CH:69:ARG:HH12 | 1.70 | 0.56 |
| 23:CZ:145:GLU:H | 23:CZ:148:ASP:HB2 | 1.70 | 0.56 |
| 59:BZ:75:LYS:H | 59:BZ:75:LYS:HZ3 | 1.51 | 0.56 |
| 9:CK:26:LEU:HA | 9:CK:84:GLU:HA | 1.86 | 0.56 |
| 35:BB:97:TRP:CH2 | 35:BB:101:MET:HB2 | 2.40 | 0.56 |
| 59:DZ:224:ASP:HB3 | 59:DZ:227:ILE:HG12 | 1.87 | 0.56 |
| 1:AA:1067:A:H3' | 1:AA:1067:A:C8 | 2.40 | 0.56 |
| 4:AD:2:ALA:O | 4:AD:3:VAL:HB | 2.05 | 0.56 |
| 46:DM:22:ILE:HG23 | 46:DM:67:GLU:HG2 | 1.86 | 0.56 |
| 35:DB:16:HIS:CD2 | 35:DB:204:ASN:HB3 | 2.40 | 0.56 |
| 13:CP:64:LYS:HA | 32:C8:13:ARG:HB3 | 1.87 | 0.56 |
| 1:AA:843:C:H2' | 1:AA:844:C:C6 | 2.40 | 0.56 |
| 1:CA:1721:G:N1 | 1:CA:1739:U:OP2 | 2.38 | 0.56 |
| 7:AG:61:ALA:O | 28:A4:7:PRO:HG2 | 2.05 | 0.56 |
| 34:DA:527:G:O2' | 34:DA:535:A:N1 | 2.37 | 0.56 |
| 35:BB:55:PHE:HA | 35:BB:58:ILE:HG13 | 1.87 | 0.56 |
| 1:CA:1688:U:O2 | 1:CA:1700:A:H5' | 2.06 | 0.56 |
| 1:CA:2132:U:C2 | 3:CC:6:LYS:CD | 2.88 | 0.56 |
| 59:BZ:403:GLU:HG2 | 59:BZ:404:VAL:HG22 | 1.86 | 0.56 |
| 59:BZ:20:HIS:CE1 | 59:BZ:117:GLN:HG2 | 2.40 | 0.56 |
| 29:C5:16:ARG:HG2 | 29:C5:16:ARG:HH11 | 1.70 | 0.56 |
| 3:AC:6:LYS:HG3 | 3:AC:7:ARG:H | 1.69 | 0.56 |
| 6:CF:34:TRP:CE2 | 13:CP:8:PRO:HG3 | 2.40 | 0.56 |
| 46:BM:11:ARG:HA | 46:BM:45:VAL:HB | 1.86 | 0.56 |
| 1:CA:535:C:O3' | 18:CU:53:ARG:NH1 | 2.38 | 0.56 |
| 37:BD:168:ARG:HB2 | 37:BD:168:ARG:HH11 | 1.69 | 0.56 |
| 5:CE:111:ARG:HG3 | 5:CE:160:TYR:CD2 | 2.40 | 0.56 |
| 1:CA:957:A:H5' | 14:CQ:76:LYS:HD2 | 1.87 | 0.56 |
| 1:AA:1785:C:OP1 | 17:AT:96:ARG:NH1 | 2.35 | 0.56 |
| 59:DZ:150:ILE:O | 59:DZ:154:GLN:HG2 | 2.05 | 0.56 |
| 1:CA:1149:G:H2' | 1:CA:1150:C:C6 | 2.41 | 0.56 |
| 38:DE:9:LYS:HB2 | 38:DE:112:LEU:HD11 | 1.87 | 0.56 |
| 49:BP:39:TYR:CD2 | 49:BP:73:LEU:HD11 | 2.40 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:BZ:129:LYS:HA | 59:BZ:253:LEU:HD21 | 1.88 | 0.56 |
| 1:CA:566:U:H5'' | 13:CP:29:LYS:HE3 | 1.86 | 0.56 |
| 1:CA:1794:U:H2' | 1:CA:1795:C:H6 | 1.71 | 0.56 |
| 59:DZ:138:LYS:HG2 | 64:DZ:702:GDP:C6 | 2.41 | 0.56 |
| 55:DV:20:U:H2' | 55:DV:21:C:C6 | 2.40 | 0.56 |
| 1:AA:2121:U:H3 | 1:AA:2212:G:H1 | 1.54 | 0.56 |
| 34:BA:179:A:H2' | 34:BA:180:U:C6 | 2.41 | 0.56 |
| 34:DA:1147:C:HO2' | 42:DI:5:TYR:HH | 1.52 | 0.56 |
| 39:DF:7:ASN:N | 39:DF:7:ASN:HD22 | 2.04 | 0.56 |
| 1:AA:1068:G:N2 | 1:AA:1188:A:C2 | 2.74 | 0.56 |
| 22:AY:55:TYR:N | 22:AY:55:TYR:CD1 | 2.74 | 0.56 |
| 43:BJ:37:PRO:HA | 43:BJ:72:VAL:HG12 | 1.86 | 0.56 |
| 34:BA:179:A:H2' | 34:BA:180:U:H6 | 1.70 | 0.56 |
| 34:DA:1348:U:H4' | 42:DI:120:ARG:HD3 | 1.85 | 0.56 |
| 34:DA:1441:G:H5'' | 34:DA:1442:G:H5' | 1.88 | 0.56 |
| 59:DZ:369:LEU:HD21 | 59:DZ:375:GLY:HA3 | 1.88 | 0.56 |
| 21:CX:26:TYR:O | 21:CX:81:VAL:HG22 | 2.06 | 0.56 |
| 37:BD:25:ARG:HA | 37:BD:28:SER:HB3 | 1.88 | 0.56 |
| 59:BZ:125:ALA:HB1 | 59:BZ:132:ARG:NH1 | 2.20 | 0.56 |
| 22:CY:90:LEU:HB3 | 22:CY:92:ASN:HB3 | 1.87 | 0.56 |
| 7:CG:145:THR:HG23 | 7:CG:147:ASP:H | 1.71 | 0.56 |
| 14:AQ:104:PHE:HE2 | 14:AQ:125:LEU:HD11 | 1.70 | 0.56 |
| 59:BZ:555:LEU:HD11 | 59:BZ:599:PRO:HG2 | 1.87 | 0.56 |
| 17:AT:56:GLY:O | 17:AT:59:THR:HG23 | 2.05 | 0.56 |
| 1:CA:1359:A:N6 | 1:CA:1372:U:H3 | 2.04 | 0.56 |
| 25:C1:3:LYS:HB2 | 25:C1:61:ARG:NH1 | 2.21 | 0.56 |
| 34:DA:748:C:H4' | 34:DA:749:C:O5' | 2.05 | 0.56 |
| 34:BA:1103:C:OP1 | 35:BB:96:ARG:NH2 | 2.38 | 0.56 |
| 30:C6:23:THR:OG1 | 30:C6:24:GLU:N | 2.34 | 0.56 |
| 1:CA:1518:U:H2' | 1:CA:1519:G:O4' | 2.06 | 0.56 |
| 1:AA:1218:G:O2' | 1:AA:1219:A:O5' | 2.24 | 0.56 |
| 19:CV:72:VAL:HG13 | 19:CV:85:LYS:HB3 | 1.86 | 0.56 |
| 34:DA:1016:A:O2' | 34:DA:1217:C:O2' | 2.21 | 0.56 |
| 23:CZ:5:LEU:HD22 | 23:CZ:6:LYS:H | 1.71 | 0.56 |
| 59:BZ:495:GLY:N | 59:BZ:510:VAL:O | 2.38 | 0.56 |
| 3:CC:49:GLY:N | 3:CC:209:PHE:O | 2.39 | 0.56 |
| 16:CS:84:GLN:H | 16:CS:111:GLU:HB2 | 1.71 | 0.56 |
| 36:DC:57:ILE:HG13 | 36:DC:66:VAL:HG22 | 1.88 | 0.56 |
| 1:CA:1803:A:O2' | 4:CD:259:THR:HG21 | 2.06 | 0.56 |
| 1:AA:1154:U:O2' | 1:AA:1155:C:H5'' | 2.06 | 0.56 |
| 3:CC:42:VAL:O | 3:CC:216:THR:O | 2.24 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:552:C:C5 | 1:AA:2792:U:H2' | 2.41 | 0.56 |
| 1:AA:1123:A:H4' | 10:AL:91:PRO:HB2 | 1.87 | 0.56 |
| 5:CE:111:ARG:HA | 15:CR:1:MET:HE3 | 1.88 | 0.56 |
| 1:CA:1782:C:H1' | 1:CA:2609:U:H5'' | 1.86 | 0.56 |
| 4:CD:121:PRO:HB3 | 4:CD:135:PHE:CE2 | 2.41 | 0.56 |
| 59:DZ:630:GLN:HG2 | 59:DZ:646:PHE:HB2 | 1.86 | 0.56 |
| 29:A5:35:GLU:HG3 | 29:A5:51:TYR:CD2 | 2.41 | 0.56 |
| 34:BA:159:G:N2 | 34:BA:161:A:O5' | 2.39 | 0.56 |
| 1:CA:1412:A:H2' | 1:CA:1413:G:C8 | 2.40 | 0.56 |
| 46:DM:40:ASN:HD22 | 46:DM:41:PRO:HD2 | 1.71 | 0.56 |
| 45:DL:71:PRO:O | 45:DL:102:ARG:HD3 | 2.05 | 0.56 |
| 1:AA:482:C:H4' | 65:AA:5243:HOH:O | 2.04 | 0.56 |
| 36:DC:12:LEU:HD23 | 36:DC:16:ARG:HB3 | 1.86 | 0.56 |
| 51:BR:56:THR:HB | 51:BR:58:LEU:CD2 | 2.36 | 0.56 |
| 18:AU:81:HIS:CE1 | 18:AU:85:LYS:HD2 | 2.41 | 0.56 |
| 10:CL:89:HIS:O | 10:CL:91:PRO:HD3 | 2.06 | 0.56 |
| 1:AA:1825:U:H2' | 1:AA:1826:C:C6 | 2.41 | 0.56 |
| 59:DZ:614:GLU:HA | 59:DZ:617:MET:HG3 | 1.86 | 0.56 |
| 10:CL:134:MET:HG3 | 10:CL:136:VAL:HG12 | 1.87 | 0.56 |
| 13:CP:63:PRO:HG2 | 32:C8:25:MET:HB2 | 1.86 | 0.56 |
| 18:CU:28:ARG:NH1 | 18:CU:38:THR:OG1 | 2.38 | 0.56 |
| 1:CA:1668:A:OP1 | 12:CO:5:GLN:HG2 | 2.04 | 0.56 |
| 1:CA:2074:U:H2' | 1:CA:2075:U:C6 | 2.41 | 0.56 |
| 44:DK:79:SER:HB2 | 44:DK:106:LYS:HE3 | 1.87 | 0.56 |
| 1:AA:670:C:H5'' | 1:AA:671:A:OP2 | 2.06 | 0.56 |
| 34:DA:1118:C:H2' | 34:DA:1119:C:C6 | 2.41 | 0.56 |
| 35:BB:201:ILE:O | 35:BB:203:GLY:N | 2.39 | 0.56 |
| 30:C6:6:ARG:NH2 | 65:C6:4001:HOH:O | 2.30 | 0.56 |
| 59:BZ:-38:TYR:HD2 | 59:BZ:-37:LEU:HD23 | 1.71 | 0.56 |
| 1:CA:897:C:H1' | 56:DW:56:C:H41 | 1.71 | 0.56 |
| 34:DA:1326:C:H2' | 34:DA:1327:C:C6 | 2.41 | 0.56 |
| 15:AR:57:ARG:HB3 | 15:AR:59:ASP:OD1 | 2.06 | 0.56 |
| 7:AG:77:ILE:HG22 | 7:AG:80:PHE:H | 1.71 | 0.56 |
| 35:BB:21:ARG:HB3 | 35:BB:39:ILE:HG12 | 1.88 | 0.56 |
| 48:BO:16:ALA:HB1 | 48:BO:21:ASP:HB3 | 1.87 | 0.56 |
| 3:AC:49:GLY:N | 3:AC:209:PHE:O | 2.39 | 0.56 |
| 3:CC:6:LYS:HG3 | 3:CC:7:ARG:H | 1.69 | 0.55 |
| 1:AA:1116:A:H5' | 1:AA:1118:C:OP2 | 2.06 | 0.55 |
| 1:AA:555:G:O4' | 1:AA:555:G:N3 | 2.34 | 0.55 |
| 1:CA:1794:U:H2' | 1:CA:1795:C:C6 | 2.41 | 0.55 |
| 34:BA:1356:G:H2' | 34:BA:1357:A:C8 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:1095:U:OP1 | 34:DA:1108:G:N2 | 2.29 | 0.55 |
| 48:DO:54:ARG:O | 48:DO:58:MET:HG3 | 2.06 | 0.55 |
| 16:CS:39:ILE:HB | 16:CS:49:VAL:HG12 | 1.88 | 0.55 |
| 1:CA:922:U:H2' | 1:CA:923:C:C6 | 2.40 | 0.55 |
| 44:BK:99:GLN:HG2 | 44:BK:105:VAL:HG21 | 1.88 | 0.55 |
| 25:A1:51:VAL:HG11 | 25:A1:74:VAL:HG21 | 1.87 | 0.55 |
| 34:BA:262:A:H2' | 34:BA:263:A:C8 | 2.41 | 0.55 |
| 6:CF:197:ASP:OD1 | 6:CF:198:ALA:N | 2.39 | 0.55 |
| 6:AF:132:VAL:HG22 | 6:AF:163:VAL:HG22 | 1.88 | 0.55 |
| 18:CU:91:ASP:O | 18:CU:95:LEU:HD13 | 2.05 | 0.55 |
| 41:BH:116:LYS:HD3 | 41:BH:127:LEU:HD23 | 1.88 | 0.55 |
| 34:BA:662:G:H2' | 34:BA:663:A:C8 | 2.41 | 0.55 |
| 24:C0:53:MET:HG3 | 24:C0:59:LEU:HD23 | 1.87 | 0.55 |
| 10:AL:105:LEU:HD23 | 10:AL:120:LEU:HD22 | 1.87 | 0.55 |
| 1:AA:1423:G:H2' | 65:AA:5230:HOH:O | 2.06 | 0.55 |
| 6:AF:120:GLU:HB2 | 6:AF:122:LYS:HG3 | 1.88 | 0.55 |
| 17:AT:39:ARG:NH2 | 34:BA:345:C:OP1 | 2.39 | 0.55 |
| 1:CA:1689:A:N6 | 1:CA:1698:A:H2 | 1.88 | 0.55 |
| 17:AT:16:ARG:NH1 | 17:AT:18:ASP:OD1 | 2.39 | 0.55 |
| 35:DB:91:PRO:HD3 | 35:DB:154:LEU:HD12 | 1.88 | 0.55 |
| 36:BC:113:ALA:HB2 | 36:BC:202:ILE:HG13 | 1.89 | 0.55 |
| 35:DB:16:HIS:CD2 | 35:DB:17:PHE:H | 2.24 | 0.55 |
| 59:BZ:126:GLU:OE2 | 59:BZ:132:ARG:NH2 | 2.40 | 0.55 |
| 10:CL:75:SER:OG | 10:CL:134:MET:SD | 2.65 | 0.55 |
| 34:BA:537:G:H5'' | 45:BL:113:ARG:NH1 | 2.21 | 0.55 |
| 8:CH:46:GLU:HB2 | 8:CH:49:VAL:HG12 | 1.88 | 0.55 |
| 1:CA:639:U:H2' | 1:CA:640:C:C6 | 2.40 | 0.55 |
| 1:CA:492:A:H2' | 1:CA:493:G:O4' | 2.06 | 0.55 |
| 34:DA:742:G:OP2 | 48:DO:35:ARG:NH2 | 2.39 | 0.55 |
| 1:AA:1539:C:H5'' | 1:AA:1539:C:O2 | 2.06 | 0.55 |
| 44:DK:15:ALA:HB1 | 44:DK:78:GLN:HG3 | 1.87 | 0.55 |
| 45:DL:24:VAL:CG1 | 45:DL:27:LEU:HD22 | 2.33 | 0.55 |
| 35:BB:69:LEU:HD13 | 35:BB:91:PRO:HB2 | 1.88 | 0.55 |
| 28:C4:16:CYS:HA | 28:C4:33:VAL:HB | 1.88 | 0.55 |
| 50:DQ:66:SER:OG | 50:DQ:67:LYS:N | 2.38 | 0.55 |
| 17:CT:2:ASN:O | 17:CT:6:LEU:HD22 | 2.06 | 0.55 |
| 46:BM:3:ARG:HG2 | 46:BM:8:GLU:HA | 1.87 | 0.55 |
| 22:CY:23:ARG:HG2 | 22:CY:42:VAL:HG22 | 1.88 | 0.55 |
| 1:CA:1709:U:H2' | 1:CA:1710:C:C6 | 2.41 | 0.55 |
| 1:CA:2653:U:O2' | 8:CH:110:SER:HB3 | 2.07 | 0.55 |
| 1:AA:2874:G:OP1 | 17:AT:119:LYS:HE3 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:BK:84:VAL:HG21 | 44:BK:95:ILE:HD11 | 1.87 | 0.55 |
| 50:BQ:6:LEU:HG | 50:BQ:23:VAL:HG11 | 1.87 | 0.55 |
| 54:DU:9:ARG:O | 54:DU:13:ILE:HG13 | 2.07 | 0.55 |
| 23:AZ:111:VAL:HG23 | 23:AZ:117:LEU:HD13 | 1.88 | 0.55 |
| 35:DB:55:PHE:CD1 | 35:DB:58:ILE:HD12 | 2.42 | 0.55 |
| 34:DA:1273:G:H3' | 34:DA:1274:G:H8 | 1.71 | 0.55 |
| 41:BH:73:ASP:OD1 | 41:BH:75:ARG:HD3 | 2.06 | 0.55 |
| 34:DA:957:U:H2' | 34:DA:959:A:OP2 | 2.07 | 0.55 |
| 24:A0:43:THR:HG23 | 24:A0:43:THR:O | 2.07 | 0.55 |
| 1:AA:2504:U:H2' | 1:AA:2505:U:H6 | 1.71 | 0.55 |
| 1:CA:954:G:H5'' | 14:CQ:13:GLN:HB3 | 1.88 | 0.55 |
| 36:BC:153:VAL:HG22 | 36:BC:198:VAL:HG22 | 1.88 | 0.55 |
| 3:AC:52:PRO:HB2 | 3:AC:168:LYS:O | 2.07 | 0.55 |
| 3:CC:52:PRO:HB2 | 3:CC:168:LYS:O | 2.07 | 0.55 |
| 59:BZ:114:VAL:HB | 59:BZ:156:ARG:HH12 | 1.71 | 0.55 |
| 1:AA:943:C:O4' | 56:BW:56:C:H5 | 1.89 | 0.55 |
| 6:CF:53:THR:HG23 | 6:CF:55:GLY:H | 1.70 | 0.55 |
| 59:DZ:22:ASP:HA | 64:DZ:702:GDP:H5' | 1.89 | 0.55 |
| 1:AA:2146:G:C5' | 3:AC:175:PRO:HG3 | 2.35 | 0.55 |
| 34:DA:1003:G:H2' | 34:DA:1004:A:O4' | 2.06 | 0.55 |
| 3:AC:42:VAL:O | 3:AC:216:THR:O | 2.24 | 0.55 |
| 1:CA:1412:A:H2' | 1:CA:1413:G:H8 | 1.72 | 0.55 |
| 1:CA:2572:A:C8 | 5:CE:144:ARG:HD2 | 2.42 | 0.55 |
| 37:BD:43:HIS:O | 37:BD:46:LYS:HB2 | 2.07 | 0.55 |
| 5:AE:7:VAL:HG12 | 5:AE:51:PHE:HE2 | 1.72 | 0.55 |
| 11:AN:58:ASP:N | 11:AN:58:ASP:OD1 | 2.33 | 0.55 |
| 35:BB:82:ARG:HG3 | 35:BB:92:TYR:CZ | 2.41 | 0.55 |
| 38:BE:75:THR:OG1 | 38:BE:76:ILE:N | 2.40 | 0.55 |
| 1:CA:1155:A:OP1 | 18:CU:55:ARG:HD2 | 2.05 | 0.55 |
| 1:CA:1359:A:H61 | 1:CA:1372:U:H3 | 1.54 | 0.55 |
| 38:BE:40:ARG:NH2 | 38:BE:68:GLU:HA | 2.22 | 0.55 |
| 12:AO:35:VAL:HG11 | 12:AO:103:ALA:HB3 | 1.89 | 0.55 |
| 34:DA:1218:C:H2' | 34:DA:1219:U:C6 | 2.41 | 0.55 |
| 1:AA:1825:U:H2' | 1:AA:1826:C:H6 | 1.71 | 0.55 |
| 49:BP:43:LYS:HA | 49:BP:48:TRP:HB3 | 1.89 | 0.55 |
| 36:DC:129:ALA:HB3 | 36:DC:132:ARG:HB3 | 1.89 | 0.55 |
| 34:DA:255:G:H2' | 34:DA:256:U:C6 | 2.41 | 0.55 |
| 40:DG:115:ARG:HG2 | 40:DG:118:VAL:HG23 | 1.87 | 0.55 |
| 16:CS:48:LEU:HD23 | 16:CS:82:ILE:HD11 | 1.89 | 0.55 |
| 46:BM:122:LYS:HD3 | 46:BM:123:ALA:H | 1.72 | 0.55 |
| 42:DI:28:VAL:HA | 42:DI:63:ILE:O | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DB:189:ASP:O | 35:DB:192:SER:OG | 2.24 | 0.55 |
| 59:DZ:303:PRO:O | 59:DZ:305:PRO:HD3 | 2.07 | 0.55 |
| 58:BY:6:G:O6 | 58:BY:7:A:N6 | 2.40 | 0.55 |
| 1:CA:2345:G:N3 | 1:CA:2381:C:H2' | 2.21 | 0.55 |
| 1:AA:2699:U:H2' | 1:AA:2700:U:O4' | 2.07 | 0.55 |
| 5:CE:120:TRP:CE3 | 5:CE:155:LYS:HD3 | 2.41 | 0.55 |
| 1:AA:2346:G:H4' | 1:AA:2347:A:OP2 | 2.06 | 0.55 |
| 53:DT:54:LYS:HA | 53:DT:57:ARG:NH2 | 2.22 | 0.55 |
| 36:BC:82:GLU:HA | 36:BC:85:ARG:HH21 | 1.71 | 0.55 |
| 37:BD:8:VAL:HG23 | 37:BD:11:LEU:HD22 | 1.88 | 0.55 |
| 59:BZ:99:ARG:HG3 | 59:BZ:128:TYR:HE1 | 1.71 | 0.55 |
| 34:DA:1000:U:H2' | 34:DA:1001:A:C8 | 2.42 | 0.55 |
| 7:CG:15:VAL:HG21 | 7:CG:176:LEU:HD23 | 1.88 | 0.55 |
| 1:CA:2292:C:OP1 | 16:CS:17:ARG:NH2 | 2.29 | 0.55 |
| 1:AA:2221:A:H5'' | 1:AA:2222:C:OP2 | 2.07 | 0.55 |
| 15:CR:38:VAL:HB | 15:CR:39:PRO:HD3 | 1.89 | 0.55 |
| 59:BZ:608:VAL:HG22 | 59:BZ:671:MET:HG3 | 1.89 | 0.55 |
| 38:BE:12:LEU:HD11 | 38:BE:14:ARG:HD3 | 1.89 | 0.55 |
| 36:BC:148:GLY:HA3 | 36:BC:172:ARG:O | 2.07 | 0.55 |
| 1:CA:1336:A:OP2 | 21:CX:64:LYS:HE3 | 2.07 | 0.55 |
| 59:BZ:363:ARG:CG | 59:BZ:363:ARG:HH11 | 2.17 | 0.55 |
| 34:DA:235:C:H2' | 34:DA:236:G:H8 | 1.72 | 0.55 |
| 34:DA:1239:A:H62 | 34:DA:1299:A:N6 | 2.05 | 0.55 |
| 1:AA:2442:A:H2' | 1:AA:2442:A:N3 | 2.22 | 0.55 |
| 18:AU:76:TYR:CZ | 18:AU:80:ILE:HG13 | 2.41 | 0.55 |
| 1:AA:354:A:H2 | 1:AA:1255:A:H2' | 1.72 | 0.55 |
| 46:BM:11:ARG:HG3 | 46:BM:12:ASN:ND2 | 2.22 | 0.55 |
| 59:BZ:-38:TYR:O | 59:BZ:-35:PRO:HD2 | 2.07 | 0.55 |
| 57:DX:75:C:H5'' | 57:DX:76:31H:OP1 | 2.07 | 0.55 |
| 34:DA:707:C:H4' | 44:DK:20:TYR:CD2 | 2.42 | 0.55 |
| 39:BF:19:LEU:HD11 | 39:BF:59:TYR:CE2 | 2.42 | 0.55 |
| 48:BO:24:SER:OG | 48:BO:25:THR:N | 2.40 | 0.55 |
| 1:AA:1473:A:H4' | 1:AA:1474:C:O5' | 2.07 | 0.55 |
| 40:BG:16:LEU:H | 40:BG:16:LEU:HD22 | 1.71 | 0.55 |
| 35:BB:134:GLU:O | 35:BB:138:LEU:HG | 2.07 | 0.55 |
| 34:BA:942:G:H21 | 42:BI:124:GLN:NE2 | 2.04 | 0.55 |
| 3:AC:54:ARG:CZ | 3:AC:56:ASP:HB3 | 2.38 | 0.54 |
| 34:DA:1240:U:OP2 | 40:DG:116:ALA:N | 2.39 | 0.54 |
| 42:DI:128:ARG:NH1 | 57:DX:35:A:OP2 | 2.40 | 0.54 |
| 1:CA:271(H):G:HO2' | 1:CA:271(I):G:H8 | 1.53 | 0.54 |
| 3:CC:194:ILE:HD11 | 3:CC:227:PRO:HB3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:A4:61:ARG:HG3 | 28:A4:62:ARG:N | 2.21 | 0.54 |
| 8:CH:3:ARG:NH2 | 8:CH:4:ILE:H | 2.05 | 0.54 |
| 18:AU:83:LEU:HD13 | 18:AU:113:ALA:HB2 | 1.89 | 0.54 |
| 32:A8:42:ARG:HD2 | 65:A8:6306:HOH:O | 2.06 | 0.54 |
| 34:DA:174:C:H2' | 34:DA:175:C:H6 | 1.72 | 0.54 |
| 1:AA:1109:G:H1 | 1:AA:1121:C:H42 | 1.55 | 0.54 |
| 50:DQ:4:LYS:HE2 | 50:DQ:6:LEU:HD11 | 1.88 | 0.54 |
| 1:CA:800:A:OP1 | 1:CA:800:A:H8 | 1.90 | 0.54 |
| 5:AE:116:VAL:HG13 | 5:AE:122:PHE:HB2 | 1.89 | 0.54 |
| 34:BA:406:G:H5' | 37:BD:5:ILE:HD11 | 1.87 | 0.54 |
| 1:AA:543:G:H2' | 1:AA:544:U:C6 | 2.42 | 0.54 |
| 59:BZ:639:ASN:HA | 59:BZ:640:ALA:O | 2.07 | 0.54 |
| 1:CA:1106:G:C6 | 1:CA:1107:G:C5 | 2.95 | 0.54 |
| 34:DA:1316:G:H22 | 34:DA:1319:A:H5'' | 1.72 | 0.54 |
| 13:AP:95:VAL:HG22 | 13:AP:125:VAL:HG12 | 1.88 | 0.54 |
| 34:BA:1123:A:O2' | 43:BJ:37:PRO:O | 2.22 | 0.54 |
| 35:DB:210:SER:OG | 35:DB:211:ILE:HG13 | 2.07 | 0.54 |
| 7:AG:77:ILE:HD12 | 7:AG:82:LEU:HD12 | 1.88 | 0.54 |
| 51:BR:40:LEU:O | 51:BR:42:ARG:N | 2.40 | 0.54 |
| 34:BA:189(K):U:H2' | 34:BA:189(L):G:C8 | 2.42 | 0.54 |
| 22:CY:30:VAL:HG22 | 22:CY:37:VAL:HG12 | 1.89 | 0.54 |
| 38:DE:84:PHE:HB3 | 38:DE:134:ALA:HB2 | 1.89 | 0.54 |
| 9:AK:118:THR:N | 9:AK:121:ASP:O | 2.38 | 0.54 |
| 1:AA:1261:G:P | 18:AU:12:ARG:HH21 | 2.29 | 0.54 |
| 34:DA:985:C:H2' | 34:DA:986:A:C8 | 2.43 | 0.54 |
| 34:DA:1053:G:O5' | 34:DA:1054:C:H5' | 2.07 | 0.54 |
| 1:AA:469:A:C5 | 6:AF:45:ARG:HD2 | 2.43 | 0.54 |
| 39:BF:10:LEU:HB2 | 39:BF:59:TYR:HB3 | 1.90 | 0.54 |
| 1:AA:776:G:C6 | 4:AD:208:LYS:HB2 | 2.43 | 0.54 |
| 49:BP:3:LYS:N | 49:BP:22:THR:O | 2.41 | 0.54 |
| 59:DZ:496:LYS:HE2 | 59:DZ:509:HIS:CE1 | 2.42 | 0.54 |
| 59:BZ:348:ARG:HG2 | 59:BZ:348:ARG:HH11 | 1.72 | 0.54 |
| 23:CZ:92:SER:O | 23:CZ:130:PRO:HG2 | 2.07 | 0.54 |
| 34:DA:1104:G:H4' | 35:DB:111:ARG:NH1 | 2.22 | 0.54 |
| 34:BA:1435:G:H2' | 34:BA:1436:U:C6 | 2.42 | 0.54 |
| 1:AA:2764:G:H4' | 8:AH:4:ILE:HD11 | 1.88 | 0.54 |
| 59:DZ:116:PRO:HA | 59:DZ:119:GLU:HG3 | 1.89 | 0.54 |
| 3:AC:52:PRO:HG2 | 3:AC:53:ARG:H | 1.73 | 0.54 |
| 34:DA:1316:G:H4' | 47:DN:18:VAL:HG13 | 1.90 | 0.54 |
| 34:BA:555:C:H2' | 34:BA:556:C:H6 | 1.73 | 0.54 |
| 32:C8:9:GLY:O | 32:C8:13:ARG:HG2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1149:G:H2' | 1:CA:1150:C:H6 | 1.71 | 0.54 |
| 37:BD:41:GLY:O | 37:BD:43:HIS:N | 2.41 | 0.54 |
| 16:CS:15:ARG:HB3 | 16:CS:19:LYS:NZ | 2.22 | 0.54 |
| 44:BK:48:ILE:O | 44:BK:48:ILE:HG12 | 2.05 | 0.54 |
| 50:BQ:41:LYS:NZ | 50:BQ:92:ARG:HH21 | 2.05 | 0.54 |
| 28:A4:33:VAL:HG12 | 28:A4:35:VAL:H | 1.71 | 0.54 |
| 1:AA:2653:G:H5'' | 1:AA:2653:G:H8 | 1.71 | 0.54 |
| 11:AN:121:LYS:HB3 | 11:AN:123:TYR:HE2 | 1.72 | 0.54 |
| 7:AG:109:VAL:C | 7:AG:112:PRO:HD2 | 2.28 | 0.54 |
| 34:BA:1505:G:O2' | 55:BV:13:A:O2' | 2.26 | 0.54 |
| 45:DL:83:VAL:HG21 | 45:DL:100:ILE:HD13 | 1.90 | 0.54 |
| 12:CO:64:ARG:HB2 | 12:CO:83:ALA:HB3 | 1.90 | 0.54 |
| 34:DA:1133:G:H2' | 34:DA:1134:G:C8 | 2.42 | 0.54 |
| 3:AC:194:ILE:HD11 | 3:AC:227:PRO:HB3 | 1.89 | 0.54 |
| 16:AS:10:ARG:O | 16:AS:14:VAL:HG13 | 2.07 | 0.54 |
| 7:CG:145:THR:HG22 | 7:CG:148:MET:HG2 | 1.89 | 0.54 |
| 4:CD:121:PRO:HB3 | 4:CD:135:PHE:CD2 | 2.42 | 0.54 |
| 59:DZ:603:GLU:OE2 | 59:DZ:628:ARG:NH2 | 2.28 | 0.54 |
| 1:AA:559:U:H2' | 1:AA:560:C:C6 | 2.43 | 0.54 |
| 1:CA:2882:A:OP1 | 15:CR:96:ARG:NE | 2.30 | 0.54 |
| 34:DA:1387:G:H2' | 34:DA:1388:C:C6 | 2.42 | 0.54 |
| 27:C3:46:ASN:O | 27:C3:50:VAL:HG22 | 2.08 | 0.54 |
| 43:BJ:11:PHE:HE1 | 43:BJ:67:THR:HG22 | 1.73 | 0.54 |
| 35:BB:16:HIS:CG | 35:BB:17:PHE:N | 2.76 | 0.54 |
| 1:AA:2576:A:C2 | 1:AA:2659:U:H4' | 2.43 | 0.54 |
| 34:BA:1191:A:H5'' | 36:BC:4:LYS:NZ | 2.22 | 0.54 |
| 3:CC:44:VAL:HG23 | 3:CC:176:VAL:HG21 | 1.89 | 0.54 |
| 52:DS:12:ASP:OD1 | 52:DS:37:ARG:NH1 | 2.40 | 0.54 |
| 49:DP:28:ARG:HG3 | 49:DP:29:ASP:OD1 | 2.07 | 0.54 |
| 46:BM:9:ILE:HB | 46:BM:18:ALA:HB1 | 1.88 | 0.54 |
| 34:DA:858:G:O6 | 34:DA:869:G:H3' | 2.07 | 0.54 |
| 38:DE:12:LEU:HD12 | 38:DE:128:PRO:HB2 | 1.90 | 0.54 |
| 14:CQ:21:THR:HG21 | 14:CQ:101:ARG:HD3 | 1.90 | 0.54 |
| 59:BZ:227:ILE:HD13 | 59:BZ:242:LEU:HD23 | 1.89 | 0.54 |
| 34:DA:353:A:H5' | 34:DA:353:A:C8 | 2.42 | 0.54 |
| 4:CD:206:LEU:HD22 | 4:CD:211:ARG:HG2 | 1.88 | 0.54 |
| 34:BA:1239:A:H62 | 34:BA:1299:A:N6 | 2.06 | 0.54 |
| 59:DZ:404:VAL:H | 59:DZ:405:PRO:CD | 2.21 | 0.54 |
| 1:AA:714:U:O2 | 32:A8:2:PRO:HD2 | 2.07 | 0.54 |
| 16:CS:31:SER:OG | 16:CS:32:LEU:N | 2.41 | 0.54 |
| 3:CC:6:LYS:HA | 3:CC:9:ARG:HH11 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:AY:92:ASN:N | 22:AY:93:GLY:HA2 | 2.23 | 0.54 |
| 34:DA:1321:C:H4' | 46:DM:87:TYR:HE2 | 1.72 | 0.54 |
| 1:CA:774:A:N3 | 1:CA:774:A:H2' | 2.22 | 0.54 |
| 59:DZ:264:LEU:HB2 | 64:DZ:702:GDP:C5 | 2.42 | 0.54 |
| 46:DM:25:ILE:HG13 | 46:DM:29:ARG:HG2 | 1.90 | 0.54 |
| 59:DZ:346:LYS:NZ | 59:DZ:384:ILE:HG23 | 2.22 | 0.54 |
| 34:DA:255:G:H2' | 34:DA:256:U:H6 | 1.73 | 0.54 |
| 1:AA:486:A:H2' | 1:AA:487:C:O4' | 2.08 | 0.54 |
| 50:BQ:77:VAL:HG12 | 50:BQ:78:GLU:HB2 | 1.89 | 0.54 |
| 41:BH:120:THR:H | 41:BH:123:GLU:HB3 | 1.72 | 0.54 |
| 34:BA:134:A:H61 | 49:BP:25:ARG:NH1 | 2.06 | 0.54 |
| 1:CA:584:C:OP2 | 18:CU:6:THR:OG1 | 2.23 | 0.54 |
| 34:BA:957:U:O2' | 34:BA:959:A:N7 | 2.30 | 0.54 |
| 59:BZ:239:GLU:O | 59:BZ:243:VAL:HG23 | 2.07 | 0.54 |
| 17:CT:108:ARG:NH2 | 34:DA:1465:C:OP2 | 2.41 | 0.54 |
| 59:BZ:-25:SER:O | 59:BZ:-22:LYS:HB2 | 2.07 | 0.54 |
| 1:CA:2132:U:C2 | 3:CC:6:LYS:HD2 | 2.42 | 0.54 |
| 47:DN:23:ARG:NH1 | 47:DN:30:ALA:HB2 | 2.22 | 0.54 |
| 59:DZ:276:VAL:HG13 | 59:DZ:280:LEU:HD12 | 1.90 | 0.54 |
| 14:CQ:76:LYS:HB3 | 14:CQ:91:GLU:HG3 | 1.89 | 0.54 |
| 1:CA:1063:G:H2' | 1:CA:1064:C:H6 | 1.72 | 0.54 |
| 1:AA:2023:A:H2' | 1:AA:2024:G:C8 | 2.43 | 0.54 |
| 34:BA:49:U:O4 | 34:BA:365:U:H5 | 1.90 | 0.54 |
| 39:BF:86:ARG:O | 39:BF:87:ARG:HG2 | 2.07 | 0.54 |
| 59:DZ:38:ARG:HH12 | 59:DZ:270:GLN:NE2 | 2.05 | 0.54 |
| 23:CZ:132:ASN:HD21 | 23:CZ:160:GLY:H | 1.54 | 0.54 |
| 1:AA:715:G:H5' | 1:AA:716:G:OP2 | 2.07 | 0.54 |
| 10:CL:112:MET:H | 10:CL:113:PRO:HD2 | 1.73 | 0.54 |
| 59:BZ:85:PRO:HD2 | 59:BZ:94:VAL:HG13 | 1.89 | 0.54 |
| 59:BZ:114:VAL:CB | 59:BZ:156:ARG:HH12 | 2.21 | 0.54 |
| 59:DZ:5:LEU:HD13 | 59:DZ:305:PRO:HG2 | 1.90 | 0.54 |
| 1:CA:1165:U:H2' | 1:CA:1166:C:C6 | 2.43 | 0.54 |
| 1:AA:1846:A:OP1 | 1:AA:1846:A:H8 | 1.91 | 0.54 |
| 1:AA:664:U:H2' | 1:AA:665:C:C6 | 2.43 | 0.54 |
| 41:DH:39:LEU:HD12 | 41:DH:44:PHE:HB2 | 1.90 | 0.54 |
| 1:CA:956:G:OP2 | 14:CQ:14:ARG:NH2 | 2.35 | 0.54 |
| 1:AA:2349:G:OP1 | 65:AA:4051:HOH:O | 2.18 | 0.54 |
| 51:DR:53:ARG:HD2 | 51:DR:59:SER:O | 2.07 | 0.54 |
| 34:BA:1238:A:OP2 | 65:BA:2031:HOH:O | 2.19 | 0.54 |
| 1:AA:1452:U:H2' | 1:AA:1453:C:C6 | 2.42 | 0.54 |
| 3:AC:30:VAL:HG23 | 3:AC:31:LYS:HG2 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:2658:C:H2' | 1:AA:2659:U:O4' | 2.08 | 0.53 |
| 59:DZ:129:LYS:HZ1 | 59:DZ:517:LEU:HG | 1.74 | 0.53 |
| 3:CC:48:LEU:CB | 3:CC:50:ILE:HD12 | 2.38 | 0.53 |
| 1:AA:553:A:H2' | 1:AA:554:A:H5' | 1.90 | 0.53 |
| 1:CA:1495:A:OP2 | 65:CA:3810:HOH:O | 2.19 | 0.53 |
| 1:AA:354:A:HO2' | 1:AA:355:A:H8 | 1.55 | 0.53 |
| 7:CG:13:GLU:O | 7:CG:15:VAL:N | 2.40 | 0.53 |
| 30:C6:9:LEU:HA | 30:C6:54:ILE:HB | 1.89 | 0.53 |
| 34:BA:159:G:H2' | 34:BA:161:A:OP2 | 2.07 | 0.53 |
| 1:AA:1102:G:H5'' | 1:AA:1103:A:O4' | 2.08 | 0.53 |
| 59:DZ:96:ARG:HB2 | 59:DZ:96:ARG:NH1 | 2.23 | 0.53 |
| 41:BH:121:ASP:OD2 | 41:BH:121:ASP:N | 2.37 | 0.53 |
| 22:AY:92:ASN:ND2 | 22:AY:92:ASN:H | 2.02 | 0.53 |
| 1:CA:880:G:N2 | 1:CA:898:C:H1' | 2.20 | 0.53 |
| 59:BZ:165:GLN:NE2 | 59:BZ:259:PHE:HB3 | 2.22 | 0.53 |
| 46:DM:5:ALA:HB3 | 46:DM:22:ILE:HD12 | 1.90 | 0.53 |
| 34:BA:1355:G:H2' | 34:BA:1356:G:C8 | 2.43 | 0.53 |
| 34:BA:1349:A:OP2 | 42:BI:118:LYS:HE3 | 2.08 | 0.53 |
| 22:CY:49:VAL:HG11 | 22:CY:55:TYR:CD2 | 2.44 | 0.53 |
| 59:DZ:639:ASN:N | 59:DZ:640:ALA:HB3 | 2.23 | 0.53 |
| 43:BJ:49:VAL:CG2 | 47:BN:41:ARG:HB2 | 2.38 | 0.53 |
| 1:CA:127:A:H5'' | 1:CA:128:C:C6 | 2.44 | 0.53 |
| 1:CA:856:C:H2' | 1:CA:857:C:C6 | 2.43 | 0.53 |
| 1:CA:910:A:H62 | 14:CQ:12:GLN:HA | 1.72 | 0.53 |
| 34:DA:688:G:H2' | 34:DA:689:C:H6 | 1.73 | 0.53 |
| 8:AH:3:ARG:HG2 | 8:AH:6:ARG:HD2 | 1.90 | 0.53 |
| 34:DA:1402:C:H2' | 34:DA:1403:C:O4' | 2.08 | 0.53 |
| 52:BS:11:VAL:HG11 | 52:BS:16:LEU:HB2 | 1.90 | 0.53 |
| 34:BA:1014:A:H4' | 52:BS:14:HIS:NE2 | 2.24 | 0.53 |
| 3:CC:30:VAL:HG23 | 3:CC:31:LYS:HG2 | 1.89 | 0.53 |
| 1:CA:2207:G:H3' | 1:CA:2208:A:H5'' | 1.90 | 0.53 |
| 59:DZ:165:GLN:HE21 | 59:DZ:260:LEU:N | 2.04 | 0.53 |
| 42:BI:43:ALA:C | 42:BI:45:ALA:H | 2.12 | 0.53 |
| 46:DM:20:THR:HA | 46:DM:25:ILE:HG22 | 1.89 | 0.53 |
| 42:DI:8:GLY:O | 42:DI:15:ALA:N | 2.27 | 0.53 |
| 1:CA:997:G:OP1 | 18:CU:92:ARG:HG2 | 2.09 | 0.53 |
| 52:BS:3:ARG:NH1 | 52:BS:8:GLY:O | 2.42 | 0.53 |
| 59:BZ:181:LEU:HD12 | 59:BZ:216:LEU:HD21 | 1.90 | 0.53 |
| 5:AE:143:ASN:HD22 | 5:AE:147:PRO:HD3 | 1.73 | 0.53 |
| 1:CA:184:C:H2' | 1:CA:185:U:C6 | 2.43 | 0.53 |
| 1:CA:2305:A:H5'' | 7:CG:134:GLY:HA3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:247:G:H4' | 1:CA:386:G:C5 | 2.43 | 0.53 |
| 40:DG:111:ARG:NH2 | 40:DG:126:ASP:OD2 | 2.41 | 0.53 |
| 6:AF:24:LEU:HB3 | 6:AF:115:ALA:HB2 | 1.90 | 0.53 |
| 1:AA:2289:G:P | 24:A0:10:THR:HG21 | 2.49 | 0.53 |
| 34:BA:1030(D):A:N6 | 34:BA:1031:G:H21 | 2.07 | 0.53 |
| 3:AC:171:ALA:HB1 | 3:AC:173:HIS:CE1 | 2.44 | 0.53 |
| 3:AC:6:LYS:HA | 3:AC:9:ARG:HH11 | 1.72 | 0.53 |
| 14:CQ:26:TYR:CD1 | 14:CQ:28:ALA:HB2 | 2.44 | 0.53 |
| 59:BZ:138:LYS:HE2 | 64:BZ:702:GDP:C4 | 2.44 | 0.53 |
| 1:CA:2277:G:H5'' | 14:CQ:87:LYS:HB3 | 1.90 | 0.53 |
| 34:BA:1367:C:H4' | 43:BJ:48:THR:HG21 | 1.89 | 0.53 |
| 34:BA:354:G:H2' | 34:BA:355:C:H5' | 1.90 | 0.53 |
| 4:CD:129:ASN:O | 4:CD:193:VAL:HG13 | 2.08 | 0.53 |
| 57:DX:50:U:H3 | 57:DX:64:G:H1 | 1.56 | 0.53 |
| 12:AO:104:ARG:HH12 | 17:AT:43:GLN:HE22 | 1.57 | 0.53 |
| 21:CX:29:TRP:CZ3 | 21:CX:78:LYS:HB3 | 2.44 | 0.53 |
| 36:DC:63:ASN:HB2 | 36:DC:98:ASN:HB2 | 1.91 | 0.53 |
| 24:A0:27:GLU:HG3 | 24:A0:68:GLU:HA | 1.89 | 0.53 |
| 59:BZ:213:HIS:O | 59:BZ:217:VAL:HG23 | 2.09 | 0.53 |
| 1:CA:2166:G:H3' | 1:CA:2167:U:C5' | 2.38 | 0.53 |
| 36:DC:137:ALA:HA | 36:DC:140:ARG:HH11 | 1.72 | 0.53 |
| 42:DI:26:VAL:HG13 | 42:DI:61:ALA:HB3 | 1.88 | 0.53 |
| 35:DB:119:GLU:OE2 | 35:DB:153:ARG:NH1 | 2.32 | 0.53 |
| 1:AA:2053:A:C6 | 1:AA:2510:C:H1' | 2.43 | 0.53 |
| 34:BA:381:C:H2' | 34:BA:382:A:O4' | 2.09 | 0.53 |
| 34:BA:507:C:OP2 | 34:BA:508:C:O2' | 2.20 | 0.53 |
| 41:BH:87:SER:HA | 41:BH:93:VAL:HG23 | 1.90 | 0.53 |
| 1:AA:704:U:H2' | 1:AA:705:C:C6 | 2.44 | 0.53 |
| 53:BT:26:ASN:ND2 | 53:BT:71:THR:OG1 | 2.41 | 0.53 |
| 1:AA:2296:C:OP1 | 30:A6:3:SER:OG | 2.15 | 0.53 |
| 34:BA:404:U:H5' | 37:BD:122:ARG:HD3 | 1.89 | 0.53 |
| 3:CC:42:VAL:HG13 | 3:CC:43:GLU:H | 1.73 | 0.53 |
| 3:AC:64:SER:HA | 3:AC:161:ARG:H | 1.74 | 0.53 |
| 4:AD:68:LYS:HD2 | 4:AD:70:TRP:CZ2 | 2.44 | 0.53 |
| 52:BS:22:LEU:HB3 | 52:BS:27:GLU:HG3 | 1.91 | 0.53 |
| 52:BS:27:GLU:HB3 | 52:BS:28:LYS:HB3 | 1.91 | 0.53 |
| 65:AA:5297:HOH:O | 25:A1:20:ARG:HD3 | 2.07 | 0.53 |
| 51:BR:37:VAL:O | 51:BR:41:LYS:HG2 | 2.09 | 0.53 |
| 5:CE:47:VAL:HG11 | 5:CE:86:PRO:HD2 | 1.89 | 0.53 |
| 1:AA:2798:C:OP1 | 5:AE:41:LYS:NZ | 2.35 | 0.53 |
| 34:BA:1024:G:H2' | 34:BA:1025:U:H5'' | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DB:28:PHE:CD1 | 35:DB:190:THR:HG22 | 2.44 | 0.53 |
| 34:DA:1286:A:C8 | 34:DA:1287:A:H4' | 2.44 | 0.53 |
| 7:CG:49:ASP:N | 7:CG:49:ASP:OD1 | 2.41 | 0.53 |
| 59:DZ:284:LEU:HD22 | 59:DZ:284:LEU:H | 1.74 | 0.53 |
| 1:AA:2389:A:H2' | 1:AA:2390:A:C8 | 2.43 | 0.53 |
| 8:CH:154:PRO:HB3 | 8:CH:163:TYR:CE2 | 2.44 | 0.53 |
| 3:CC:54:ARG:CZ | 3:CC:56:ASP:HB3 | 2.37 | 0.53 |
| 1:CA:1359:A:C2 | 1:CA:1372:U:O4 | 2.61 | 0.53 |
| 42:BI:9:ARG:HD3 | 42:BI:14:VAL:HG22 | 1.91 | 0.53 |
| 1:AA:2287:C:C2 | 14:AQ:85:LYS:HE2 | 2.44 | 0.53 |
| 35:DB:164:VAL:HB | 35:DB:186:ALA:HB2 | 1.90 | 0.53 |
| 16:CS:14:VAL:O | 16:CS:18:ILE:HG12 | 2.08 | 0.53 |
| 35:BB:97:TRP:CZ2 | 35:BB:102:LEU:HD13 | 2.43 | 0.53 |
| 34:DA:857:C:H2' | 34:DA:858:G:O4' | 2.09 | 0.53 |
| 16:CS:67:ARG:HH11 | 16:CS:67:ARG:HB2 | 1.73 | 0.53 |
| 1:AA:1381:U:H2' | 1:AA:1382:A:O4' | 2.09 | 0.53 |
| 1:CA:668:G:H5' | 1:CA:669:G:OP2 | 2.09 | 0.53 |
| 34:DA:45:U:H2' | 34:DA:46:G:C8 | 2.44 | 0.53 |
| 1:AA:1157:A:H8 | 1:AA:1158:G:H1' | 1.73 | 0.53 |
| 1:AA:2146:G:H5' | 3:AC:175:PRO:HG3 | 1.90 | 0.53 |
| 3:AC:44:VAL:HG23 | 3:AC:176:VAL:HG21 | 1.89 | 0.53 |
| 59:BZ:138:LYS:HG2 | 64:BZ:702:GDP:C5 | 2.43 | 0.53 |
| 49:BP:17:TYR:HE2 | 49:BP:41:PRO:HG3 | 1.72 | 0.53 |
| 1:CA:1065:U:O2 | 1:CA:1074:G:N2 | 2.42 | 0.53 |
| 34:DA:1388:C:H2' | 34:DA:1389:C:C6 | 2.44 | 0.53 |
| 59:DZ:435:ASP:OD2 | 59:DZ:437:THR:OG1 | 2.26 | 0.53 |
| 32:A8:61:LEU:O | 32:A8:63:PRO:HD3 | 2.09 | 0.53 |
| 1:CA:637:A:H8 | 13:CP:117:GLU:HG3 | 1.73 | 0.53 |
| 34:BA:790:A:OP1 | 57:BX:38:A:O2' | 2.25 | 0.53 |
| 6:AF:162:LEU:HA | 6:AF:165:ARG:HD3 | 1.91 | 0.53 |
| 10:AL:88:ALA:HB3 | 10:AL:135:GLY:HA3 | 1.90 | 0.53 |
| 1:CA:489:G:N7 | 20:CW:49:LYS:NZ | 2.57 | 0.53 |
| 34:BA:250:A:H4' | 34:BA:251:G:O5' | 2.08 | 0.53 |
| 6:CF:192:LEU:HD13 | 6:CF:194:MET:HE2 | 1.89 | 0.53 |
| 35:DB:72:GLY:O | 35:DB:94:ASN:HA | 2.09 | 0.53 |
| 34:BA:677:U:H3 | 34:BA:713:G:H22 | 1.55 | 0.53 |
| 3:AC:42:VAL:HG13 | 3:AC:43:GLU:H | 1.73 | 0.53 |
| 3:CC:65:LEU:HD22 | 3:CC:189:ASN:HB3 | 1.91 | 0.53 |
| 4:CD:130:ALA:C | 4:CD:131:LEU:HD12 | 2.29 | 0.53 |
| 1:CA:958:U:OP2 | 14:CQ:14:ARG:NH1 | 2.42 | 0.53 |
| 34:DA:972:C:O2' | 43:DJ:55:LYS:O | 2.27 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:BW:43:C:H2' | 56:BW:44:G:C8 | 2.44 | 0.53 |
| 1:AA:602:G:H2' | 1:AA:603:C:C6 | 2.44 | 0.53 |
| 44:BK:44:SER:OG | 44:BK:47:VAL:HG23 | 2.09 | 0.53 |
| 36:DC:152:ILE:HB | 36:DC:167:TRP:HB3 | 1.90 | 0.53 |
| 59:DZ:168:ILE:HG12 | 59:DZ:205:TYR:CE2 | 2.44 | 0.53 |
| 7:CG:79:ASN:N | 7:CG:79:ASN:OD1 | 2.40 | 0.53 |
| 43:DJ:78:ASN:O | 43:DJ:80:LYS:N | 2.41 | 0.53 |
| 1:AA:2204:G:H2' | 1:AA:2205:C:C6 | 2.44 | 0.53 |
| 3:AC:65:LEU:HD22 | 3:AC:189:ASN:HB3 | 1.91 | 0.53 |
| 59:BZ:264:LEU:HB2 | 64:BZ:702:GDP:C5 | 2.43 | 0.53 |
| 34:DA:1218:C:P | 47:DN:9:LYS:HZ3 | 2.31 | 0.53 |
| 34:BA:452:A:H62 | 34:BA:480:U:H3 | 1.56 | 0.53 |
| 22:CY:77:PRO:HD3 | 22:CY:106:LEU:HD23 | 1.90 | 0.53 |
| 1:CA:673:C:H5" | 6:CF:81:PRO:HD2 | 1.91 | 0.53 |
| 34:BA:67:C:H2' | 34:BA:68:G:C8 | 2.44 | 0.53 |
| 37:BD:57:ARG:HE | 37:BD:202:LEU:HD22 | 1.74 | 0.53 |
| 6:CF:165:ARG:HG2 | 6:CF:168:ARG:HH21 | 1.74 | 0.53 |
| 35:BB:175:ARG:O | 35:BB:179:LYS:N | 2.36 | 0.53 |
| 6:AF:123:LEU:HD13 | 6:AF:192:LEU:HD13 | 1.90 | 0.53 |
| 1:CA:1144:G:H2' | 1:CA:1145:C:C6 | 2.44 | 0.52 |
| 3:CC:52:PRO:HG2 | 3:CC:53:ARG:H | 1.73 | 0.52 |
| 1:CA:2287:A:N6 | 1:CA:2344:U:H3 | 2.02 | 0.52 |
| 42:BI:50:LEU:HB2 | 42:BI:81:ILE:HD11 | 1.89 | 0.52 |
| 53:BT:9:ASN:O | 53:BT:10:LEU:HB2 | 2.08 | 0.52 |
| 53:DT:57:ARG:HH12 | 53:DT:100:ILE:HD12 | 1.74 | 0.52 |
| 1:CA:2291:U:H2' | 1:CA:2292:C:C6 | 2.44 | 0.52 |
| 5:CE:116:VAL:HG13 | 5:CE:122:PHE:HB2 | 1.90 | 0.52 |
| 34:BA:1458:G:H5" | 53:BT:31:SER:HB2 | 1.91 | 0.52 |
| 40:DG:54:THR:O | 40:DG:56:GLN:N | 2.41 | 0.52 |
| 59:BZ:682:GLN:O | 59:BZ:686:LYS:HB3 | 2.09 | 0.52 |
| 28:A4:63:TYR:N | 28:A4:63:TYR:CD1 | 2.77 | 0.52 |
| 6:CF:24:LEU:HD21 | 6:CF:114:VAL:HG12 | 1.90 | 0.52 |
| 35:BB:231:GLU:HB3 | 35:BB:232:PRO:HD3 | 1.90 | 0.52 |
| 34:DA:201:C:H42 | 34:DA:216:G:H1 | 1.57 | 0.52 |
| 34:BA:976:G:N2 | 34:BA:1363:C:OP2 | 2.36 | 0.52 |
| 3:CC:51:ASP:OD2 | 3:CC:54:ARG:HB2 | 2.09 | 0.52 |
| 3:CC:171:ALA:HB1 | 3:CC:173:HIS:CE1 | 2.43 | 0.52 |
| 34:DA:1062:U:H2' | 34:DA:1063:C:C5 | 2.45 | 0.52 |
| 34:DA:1435:G:H2' | 34:DA:1436:U:C6 | 2.44 | 0.52 |
| 58:DY:55:PSU:HN1 | 58:DY:57:G:H5' | 1.75 | 0.52 |
| 45:DL:28:LYS:N | 45:DL:29:GLY:HA2 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1157:A:O2' | 1:AA:1158:G:H4' | 2.10 | 0.52 |
| 1:CA:1057:A:HO2' | 1:CA:1058:G:P | 2.32 | 0.52 |
| 34:DA:620:C:H2' | 34:DA:621:A:O4' | 2.10 | 0.52 |
| 34:BA:1125:U:H4' | 43:BJ:5:ARG:HH22 | 1.74 | 0.52 |
| 46:DM:3:ARG:O | 46:DM:3:ARG:NH1 | 2.42 | 0.52 |
| 1:CA:1721:G:H8 | 1:CA:1741:A:H62 | 1.55 | 0.52 |
| 33:C9:17:ILE:HG22 | 33:C9:24:TYR:HB2 | 1.92 | 0.52 |
| 1:CA:1068:G:H21 | 1:CA:1096:A:H5' | 1.74 | 0.52 |
| 34:BA:8:A:N6 | 37:BD:205:GLU:O | 2.43 | 0.52 |
| 23:AZ:151:HIS:O | 23:AZ:153:SER:N | 2.35 | 0.52 |
| 2:CB:46:A:H2' | 2:CB:47:C:C6 | 2.44 | 0.52 |
| 24:C0:70:GLN:NE2 | 24:C0:72:ARG:HD2 | 2.24 | 0.52 |
| 1:AA:2638:C:H2' | 1:AA:2639:G:O4' | 2.08 | 0.52 |
| 3:AC:48:LEU:CB | 3:AC:50:ILE:HD12 | 2.38 | 0.52 |
| 1:AA:1525:G:O2' | 1:AA:1605:A:C2 | 2.62 | 0.52 |
| 34:DA:1218:C:OP2 | 47:DN:9:LYS:NZ | 2.39 | 0.52 |
| 43:BJ:17:ASP:OD1 | 43:BJ:70:ARG:NH1 | 2.43 | 0.52 |
| 36:BC:11:ARG:NH2 | 36:BC:177:THR:O | 2.41 | 0.52 |
| 1:CA:1815:A:OP2 | 4:CD:54:ARG:NH2 | 2.40 | 0.52 |
| 1:CA:1453:U:O2' | 1:CA:1455:G:N7 | 2.40 | 0.52 |
| 25:A1:15:ALA:HB3 | 25:A1:40:ARG:HD3 | 1.91 | 0.52 |
| 1:CA:335:C:H4' | 22:CY:73:ARG:CZ | 2.40 | 0.52 |
| 14:CQ:32:TYR:CE1 | 14:CQ:133:ARG:HD3 | 2.45 | 0.52 |
| 59:BZ:428:LEU:O | 59:BZ:432:ALA:N | 2.42 | 0.52 |
| 1:AA:470:C:H4' | 6:AF:49:ALA:HB2 | 1.91 | 0.52 |
| 1:AA:1921:G:H2' | 1:AA:1921:G:N3 | 2.25 | 0.52 |
| 1:CA:1237:A:OP1 | 65:CA:4443:HOH:O | 2.19 | 0.52 |
| 59:BZ:405:PRO:HB2 | 59:BZ:406:GLU:HA | 1.92 | 0.52 |
| 34:DA:921:U:O2 | 38:DE:19:MET:HB2 | 2.09 | 0.52 |
| 3:AC:51:ASP:OD2 | 3:AC:54:ARG:HB2 | 2.09 | 0.52 |
| 40:BG:113:GLU:HG2 | 40:BG:119:ARG:HG2 | 1.92 | 0.52 |
| 3:CC:67:HIS:CG | 3:CC:185:LYS:HD2 | 2.45 | 0.52 |
| 1:CA:607:U:OP1 | 6:CF:102:PRO:HA | 2.10 | 0.52 |
| 4:AD:101:GLU:OE1 | 4:AD:103:ARG:HD3 | 2.10 | 0.52 |
| 35:DB:97:TRP:CZ3 | 35:DB:101:MET:HB2 | 2.45 | 0.52 |
| 1:CA:811:U:H2' | 13:CP:21:ARG:HA | 1.91 | 0.52 |
| 1:AA:1648:U:O4 | 65:AA:4154:HOH:O | 2.10 | 0.52 |
| 1:AA:939:C:H2' | 1:AA:940:C:C6 | 2.44 | 0.52 |
| 1:CA:2695:C:H2' | 1:CA:2696:U:H6 | 1.75 | 0.52 |
| 36:BC:77:ILE:O | 36:BC:84:ILE:N | 2.34 | 0.52 |
| 19:CV:40:LEU:HB2 | 19:CV:46:VAL:HG13 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:CK:74:LEU:O | 9:CK:76:GLY:N | 2.40 | 0.52 |
| 34:BA:1165:C:H2' | 34:BA:1166:G:O4' | 2.08 | 0.52 |
| 21:CX:11:PRO:HB3 | 21:CX:92:LEU:HD11 | 1.91 | 0.52 |
| 3:AC:29:LEU:O | 3:AC:30:VAL:C | 2.48 | 0.52 |
| 49:BP:18:ARG:O | 49:BP:20:VAL:HB | 2.09 | 0.52 |
| 36:BC:58:GLU:H | 36:BC:65:ALA:HB3 | 1.75 | 0.52 |
| 59:BZ:156:ARG:NH1 | 59:BZ:156:ARG:HB3 | 2.25 | 0.52 |
| 59:DZ:165:GLN:NE2 | 59:DZ:260:LEU:H | 2.04 | 0.52 |
| 4:AD:17:THR:O | 4:AD:211:ARG:NH2 | 2.40 | 0.52 |
| 34:DA:1317:C:OP1 | 47:DN:17:LYS:HG2 | 2.09 | 0.52 |
| 1:AA:2343:G:H4' | 24:A0:43:THR:H | 1.74 | 0.52 |
| 35:BB:197:VAL:HG12 | 35:BB:200:ILE:HD13 | 1.90 | 0.52 |
| 38:DE:139:LEU:O | 38:DE:141:GLN:N | 2.42 | 0.52 |
| 34:DA:1012:U:H2' | 34:DA:1013:G:C8 | 2.44 | 0.52 |
| 1:CA:491:G:H2' | 1:CA:492:A:C8 | 2.44 | 0.52 |
| 2:CB:105:A:H2' | 2:CB:106:G:O4' | 2.08 | 0.52 |
| 34:BA:186:C:H2' | 34:BA:187:C:C6 | 2.45 | 0.52 |
| 59:DZ:592:GLU:HA | 59:DZ:595:GLN:HB3 | 1.92 | 0.52 |
| 38:DE:152:ARG:HG3 | 41:DH:43:GLY:O | 2.09 | 0.52 |
| 9:CK:40:LEU:HA | 9:CK:43:ALA:HB3 | 1.91 | 0.52 |
| 6:CF:21:ALA:HB3 | 6:CF:22:ALA:HA | 1.92 | 0.52 |
| 1:AA:11:G:H2' | 1:AA:12:U:H5'' | 1.91 | 0.52 |
| 16:CS:27:SER:HA | 16:CS:88:ASP:HB3 | 1.92 | 0.52 |
| 37:DD:189:PRO:HB2 | 37:DD:194:LEU:HD11 | 1.92 | 0.52 |
| 34:BA:1399:C:C2 | 34:BA:1502:A:N6 | 2.77 | 0.52 |
| 35:DB:178:ARG:NH1 | 35:DB:196:LEU:O | 2.42 | 0.52 |
| 36:DC:7:PRO:HG3 | 36:DC:201:TYR:HE2 | 1.75 | 0.52 |
| 49:BP:3:LYS:O | 49:BP:21:VAL:HA | 2.09 | 0.52 |
| 49:DP:23:ASP:OD1 | 49:DP:25:ARG:HD3 | 2.10 | 0.52 |
| 36:BC:22:TRP:CE2 | 47:BN:54:PRO:HG3 | 2.45 | 0.52 |
| 46:DM:84:ILE:O | 46:DM:86:CYS:N | 2.40 | 0.52 |
| 34:DA:859:A:H2' | 34:DA:860:A:O4' | 2.09 | 0.52 |
| 45:DL:69:TYR:HB2 | 45:DL:96:VAL:HG11 | 1.91 | 0.52 |
| 1:CA:1059:G:H3' | 1:CA:1060:U:C6 | 2.45 | 0.52 |
| 1:AA:1834:A:O2' | 4:AD:259:THR:HG21 | 2.09 | 0.52 |
| 1:AA:1221:G:H1' | 1:AA:1222:A:C5' | 2.39 | 0.52 |
| 3:CC:64:SER:HA | 3:CC:161:ARG:H | 1.74 | 0.52 |
| 34:BA:600:C:H2' | 34:BA:601:C:H6 | 1.73 | 0.52 |
| 14:CQ:16:ARG:HG2 | 14:CQ:16:ARG:NH1 | 2.24 | 0.52 |
| 20:CW:59:VAL:HG12 | 20:CW:60:ASN:HD22 | 1.75 | 0.52 |
| 7:CG:43:LEU:HD12 | 7:CG:45:GLU:HG3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:C7:30:VAL:O | 31:C7:34:ARG:HG3 | 2.10 | 0.52 |
| 2:CB:20:C:H42 | 2:CB:63:G:H1 | 1.57 | 0.52 |
| 1:CA:1028:A:N6 | 1:CA:1125:G:H2' | 2.25 | 0.52 |
| 34:DA:539:A:H2' | 34:DA:540:G:H8 | 1.75 | 0.52 |
| 1:AA:2734:A:H5'' | 65:AA:4044:HOH:O | 2.10 | 0.52 |
| 34:BA:418:C:H1' | 34:BA:540:G:O2' | 2.09 | 0.52 |
| 34:DA:1008:C:H2' | 34:DA:1009:G:O4' | 2.10 | 0.52 |
| 44:DK:48:ILE:O | 44:DK:50:TYR:N | 2.43 | 0.52 |
| 8:CH:12:PRO:O | 8:CH:15:VAL:HG12 | 2.09 | 0.52 |
| 17:CT:19:LEU:HD13 | 17:CT:86:ILE:HD12 | 1.90 | 0.52 |
| 40:BG:46:ALA:O | 40:BG:50:ILE:HG23 | 2.10 | 0.52 |
| 6:CF:184:TYR:CE2 | 6:CF:188:ARG:HD2 | 2.45 | 0.52 |
| 1:CA:330:A:HO2' | 1:CA:331:A:H8 | 1.56 | 0.52 |
| 37:BD:190:ASP:OD1 | 37:BD:190:ASP:N | 2.42 | 0.52 |
| 1:AA:2331:G:N2 | 16:AS:3:ARG:HA | 2.25 | 0.52 |
| 35:BB:77:ALA:O | 35:BB:81:VAL:HG22 | 2.10 | 0.52 |
| 34:BA:1106:G:C6 | 34:BA:1107:C:C4 | 2.98 | 0.52 |
| 1:CA:1815:A:OP1 | 1:CA:1815:A:H8 | 1.92 | 0.52 |
| 18:CU:81:HIS:HB3 | 18:CU:117:GLN:HE22 | 1.73 | 0.52 |
| 25:C1:8:SER:HB3 | 25:C1:66:HIS:CD2 | 2.45 | 0.52 |
| 1:AA:2643:G:O2' | 1:AA:2820:A:N1 | 2.32 | 0.52 |
| 38:DE:11:ILE:HG21 | 38:DE:105:VAL:HG22 | 1.92 | 0.52 |
| 34:DA:278:G:OP2 | 50:DQ:41:LYS:NZ | 2.43 | 0.52 |
| 36:DC:18:TRP:CD1 | 47:DN:54:PRO:HA | 2.45 | 0.52 |
| 1:CA:2871:C:N4 | 65:CA:4204:HOH:O | 2.42 | 0.52 |
| 1:CA:1932:A:H2' | 1:CA:1933:G:O4' | 2.10 | 0.52 |
| 34:BA:1068:G:H8 | 34:BA:1068:G:OP2 | 1.92 | 0.52 |
| 1:CA:1110:G:N3 | 1:CA:1110:G:H2' | 2.25 | 0.52 |
| 34:BA:368:U:N3 | 59:BZ:354:ARG:NH1 | 2.58 | 0.52 |
| 14:CQ:85:LYS:HB2 | 24:C0:7:LEU:HD12 | 1.91 | 0.52 |
| 39:BF:60:PHE:CE2 | 51:BR:78:LEU:HD21 | 2.45 | 0.52 |
| 34:DA:1352:C:H2' | 34:DA:1353:G:C8 | 2.45 | 0.52 |
| 6:AF:129:PHE:HB3 | 6:AF:132:VAL:HG13 | 1.92 | 0.52 |
| 34:DA:539:A:H2' | 34:DA:540:G:C8 | 2.45 | 0.52 |
| 38:DE:110:LEU:HD13 | 38:DE:118:ILE:HG21 | 1.92 | 0.52 |
| 8:CH:96:ALA:HB2 | 8:CH:105:LEU:HD23 | 1.92 | 0.52 |
| 1:CA:2275:C:H6 | 1:CA:2275:C:H5' | 1.74 | 0.52 |
| 30:A6:40:CYS:SG | 30:A6:42:TRP:HB2 | 2.50 | 0.52 |
| 7:CG:23:PHE:HB2 | 7:CG:25:TYR:CZ | 2.44 | 0.52 |
| 59:BZ:78:ARG:HH21 | 59:BZ:357:ARG:CZ | 2.23 | 0.51 |
| 3:AC:67:HIS:CG | 3:AC:185:LYS:HD2 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DB:122:PHE:HA | 35:DB:127:ILE:HD12 | 1.92 | 0.51 |
| 34:DA:1316:G:N2 | 34:DA:1319:A:H5'' | 2.25 | 0.51 |
| 59:BZ:494:GLU:HG2 | 59:BZ:511:LYS:HG2 | 1.91 | 0.51 |
| 57:DX:75:C:H5'' | 57:DX:76:31H:P | 2.49 | 0.51 |
| 41:BH:87:SER:HB2 | 41:BH:93:VAL:H | 1.75 | 0.51 |
| 59:BZ:2:LYS:O | 59:BZ:6:GLU:N | 2.42 | 0.51 |
| 7:CG:44:GLY:O | 7:CG:47:LYS:HB2 | 2.10 | 0.51 |
| 1:CA:1101:U:H2' | 1:CA:1102:C:C6 | 2.45 | 0.51 |
| 1:AA:1882:U:H2' | 1:AA:1883:C:O4' | 2.10 | 0.51 |
| 1:CA:65:C:H2' | 1:CA:66:C:C6 | 2.45 | 0.51 |
| 34:BA:1047:G:HO2' | 34:BA:1215:G:HO2' | 1.58 | 0.51 |
| 59:DZ:238:THR:O | 59:DZ:241:GLU:HG2 | 2.10 | 0.51 |
| 34:DA:130:A:O2' | 34:DA:131:C:O5' | 2.23 | 0.51 |
| 3:CC:218:THR:HG22 | 3:CC:219:MET:SD | 2.50 | 0.51 |
| 59:BZ:247:ARG:HG3 | 59:BZ:247:ARG:HH11 | 1.75 | 0.51 |
| 59:BZ:114:VAL:HG11 | 59:BZ:156:ARG:HH12 | 1.75 | 0.51 |
| 1:CA:1359:A:N1 | 1:CA:1372:U:C4 | 2.78 | 0.51 |
| 4:AD:3:VAL:HG13 | 4:AD:17:THR:HB | 1.92 | 0.51 |
| 1:AA:1091:A:H4' | 1:AA:1092:A:H5' | 1.93 | 0.51 |
| 1:AA:2304:C:P | 16:AS:17:ARG:HH12 | 2.33 | 0.51 |
| 30:A6:18:ARG:HD2 | 30:A6:42:TRP:CD1 | 2.45 | 0.51 |
| 50:BQ:67:LYS:O | 50:BQ:68:ARG:HG2 | 2.10 | 0.51 |
| 34:BA:767:A:H2' | 34:BA:768:A:O4' | 2.11 | 0.51 |
| 50:BQ:12:SER:HB3 | 50:BQ:20:THR:HB | 1.91 | 0.51 |
| 34:BA:10:A:OP2 | 38:BE:126:ARG:HD2 | 2.09 | 0.51 |
| 34:BA:1305:G:H5'' | 54:BU:4:GLY:HA3 | 1.93 | 0.51 |
| 34:DA:1004:A:H8 | 34:DA:1005:A:H4' | 1.75 | 0.51 |
| 3:CC:65:LEU:HB3 | 3:CC:189:ASN:HD22 | 1.75 | 0.51 |
| 4:CD:71:ASP:HB3 | 4:CD:103:ARG:HH22 | 1.75 | 0.51 |
| 34:DA:437:U:O2' | 37:DD:123:HIS:HD2 | 1.94 | 0.51 |
| 5:AE:59:VAL:HG12 | 5:AE:64:LYS:HG3 | 1.91 | 0.51 |
| 2:AB:77:U:H4' | 23:AZ:84:GLU:OE2 | 2.10 | 0.51 |
| 26:A2:32:LEU:HD11 | 26:A2:54:LYS:HG3 | 1.93 | 0.51 |
| 34:BA:882:C:O2' | 34:BA:883:C:H5' | 2.11 | 0.51 |
| 1:AA:2564:U:C2 | 1:AA:2566:U:H5' | 2.45 | 0.51 |
| 20:CW:41:LYS:HE3 | 29:C5:25:LEU:HD21 | 1.91 | 0.51 |
| 34:BA:976:G:OP1 | 47:BN:32:SER:N | 2.44 | 0.51 |
| 34:DA:1305:G:H22 | 34:DA:1331:G:H1' | 1.74 | 0.51 |
| 1:AA:2123:G:H1 | 1:AA:2210:C:H42 | 1.58 | 0.51 |
| 36:DC:125:GLU:OE2 | 36:DC:125:GLU:N | 2.43 | 0.51 |
| 1:CA:208:C:H2' | 1:CA:209:C:H6 | 1.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:BJ:8:LEU:HB2 | 43:BJ:70:ARG:HB2 | 1.92 | 0.51 |
| 21:CX:12:VAL:HG22 | 21:CX:29:TRP:CE2 | 2.45 | 0.51 |
| 36:DC:140:ARG:HH12 | 36:DC:141:VAL:HG23 | 1.76 | 0.51 |
| 32:A8:61:LEU:C | 32:A8:63:PRO:HD3 | 2.30 | 0.51 |
| 34:BA:1353:G:OP1 | 54:BU:10:ARG:NH1 | 2.43 | 0.51 |
| 15:CR:37:THR:OG1 | 15:CR:40:LYS:HG3 | 2.09 | 0.51 |
| 35:DB:9:GLU:O | 35:DB:11:LEU:N | 2.44 | 0.51 |
| 34:DA:392:G:H2' | 34:DA:393:A:H8 | 1.76 | 0.51 |
| 1:CA:2312:U:H5' | 7:CG:88:ILE:HD11 | 1.92 | 0.51 |
| 53:DT:39:LYS:O | 53:DT:42:GLN:N | 2.42 | 0.51 |
| 1:AA:2149:G:H21 | 1:AA:2195:A:H1' | 1.76 | 0.51 |
| 40:DG:151:TYR:OH | 44:DK:54:ARG:HD2 | 2.11 | 0.51 |
| 1:AA:1072:U:H4' | 1:AA:1073:A:OP1 | 2.09 | 0.51 |
| 39:BF:1:MET:HA | 39:BF:67:MET:O | 2.10 | 0.51 |
| 1:CA:1796:U:H2' | 1:CA:1797:C:C6 | 2.45 | 0.51 |
| 57:DX:2:G:H2' | 57:DX:2:G:N3 | 2.25 | 0.51 |
| 1:CA:323:G:C8 | 6:CF:171:PRO:HG3 | 2.46 | 0.51 |
| 59:DZ:264:LEU:HD12 | 64:DZ:702:GDP:N3 | 2.25 | 0.51 |
| 3:AC:65:LEU:HB3 | 3:AC:189:ASN:HD22 | 1.74 | 0.51 |
| 3:AC:218:THR:HG22 | 3:AC:219:MET:SD | 2.50 | 0.51 |
| 2:AB:105:A:OP1 | 23:AZ:72:ARG:NH1 | 2.44 | 0.51 |
| 49:DP:28:ARG:NH1 | 49:DP:29:ASP:OD2 | 2.43 | 0.51 |
| 34:DA:1178:G:N2 | 34:DA:1181:G:OP2 | 2.42 | 0.51 |
| 34:BA:103:C:OP2 | 53:BT:17:ARG:NH2 | 2.43 | 0.51 |
| 38:DE:33:VAL:HG13 | 38:DE:112:LEU:HD12 | 1.92 | 0.51 |
| 17:AT:119:LYS:O | 17:AT:123:GLN:HG3 | 2.10 | 0.51 |
| 4:CD:77:ALA:HB2 | 4:CD:97:TYR:CD2 | 2.44 | 0.51 |
| 13:AP:89:ALA:HA | 13:AP:121:LYS:HE2 | 1.92 | 0.51 |
| 34:DA:1152:A:H2' | 34:DA:1153:C:H6 | 1.76 | 0.51 |
| 36:DC:136:GLN:C | 36:DC:138:VAL:H | 2.13 | 0.51 |
| 34:BA:45:U:H2' | 34:BA:46:G:C8 | 2.46 | 0.51 |
| 41:DH:4:ASP:OD2 | 41:DH:85:ARG:NH1 | 2.44 | 0.51 |
| 1:CA:2784:C:H1' | 5:CE:37:ARG:HH12 | 1.75 | 0.51 |
| 1:AA:509:A:O4' | 22:AY:48:ALA:HB1 | 2.10 | 0.51 |
| 4:CD:69:ARG:NH2 | 4:CD:128:GLY:O | 2.43 | 0.51 |
| 34:BA:1379:G:O6 | 40:BG:2:ALA:HB3 | 2.10 | 0.51 |
| 22:CY:99:CYS:SG | 22:CY:100:ALA:N | 2.84 | 0.51 |
| 59:BZ:145:ASP:HB3 | 59:BZ:148:LEU:HD23 | 1.92 | 0.51 |
| 3:AC:50:ILE:H | 3:AC:50:ILE:HD13 | 1.76 | 0.51 |
| 3:AC:6:LYS:N | 3:AC:9:ARG:NH1 | 2.58 | 0.51 |
| 8:CH:143:GLN:O | 8:CH:145:ALA:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 34:DA:828:A:H2' | 34:DA:829:G:O4' | 2.11 | 0.51 |
| 34:BA:110:C:O2' | 49:BP:25:ARG:O | 2.26 | 0.51 |
| 1:CA:1102:C:H2' | 1:CA:1103:A:C8 | 2.45 | 0.51 |
| 38:BE:135:THR:O | 38:BE:139:LEU:HG | 2.11 | 0.51 |
| 1:AA:1476:C:H2' | 1:AA:1477:U:C6 | 2.46 | 0.51 |
| 9:AK:56:ASN:HA | 9:AK:83:TYR:HA | 1.93 | 0.51 |
| 11:CN:94:HIS:O | 11:CN:97:ARG:HB2 | 2.11 | 0.51 |
| 1:CA:1653:G:H3' | 15:CR:2:ARG:HD3 | 1.93 | 0.51 |
| 34:DA:280:C:OP1 | 50:DQ:91:ARG:NH1 | 2.43 | 0.51 |
| 10:AL:98:ARG:HA | 10:AL:136:VAL:HG23 | 1.91 | 0.51 |
| 51:DR:32:ARG:HD2 | 51:DR:65:ILE:HG21 | 1.92 | 0.51 |
| 59:BZ:78:ARG:HE | 59:BZ:357:ARG:NH1 | 2.08 | 0.51 |
| 3:CC:50:ILE:HD13 | 3:CC:50:ILE:H | 1.76 | 0.51 |
| 4:AD:2:ALA:N | 4:AD:20:ASP:OD2 | 2.44 | 0.51 |
| 3:AC:68:GLY:H | 3:AC:189:ASN:ND2 | 2.09 | 0.51 |
| 4:AD:102:LYS:C | 4:AD:103:ARG:HG2 | 2.30 | 0.51 |
| 1:CA:2880:C:O3' | 15:CR:90:ARG:NH1 | 2.43 | 0.51 |
| 1:CA:2572:A:N7 | 5:CE:144:ARG:HD2 | 2.26 | 0.51 |
| 34:DA:1401:G:C2 | 34:DA:1402:C:H1' | 2.46 | 0.51 |
| 59:BZ:485:GLU:HB3 | 59:BZ:560:VAL:HG22 | 1.93 | 0.51 |
| 1:CA:221:A:O2' | 1:CA:266:G:N7 | 2.42 | 0.51 |
| 1:CA:863:A:H2' | 1:CA:864:G:C8 | 2.46 | 0.51 |
| 1:AA:95:G:OP1 | 26:A2:46:GLN:NE2 | 2.39 | 0.51 |
| 8:CH:86:GLU:OE2 | 8:CH:132:ARG:NH2 | 2.43 | 0.51 |
| 2:CB:7:G:H4' | 16:CS:29:PHE:CD2 | 2.46 | 0.51 |
| 1:CA:236:C:H2' | 1:CA:237:C:C6 | 2.44 | 0.51 |
| 3:CC:6:LYS:N | 3:CC:9:ARG:NH1 | 2.59 | 0.51 |
| 45:DL:24:VAL:HG13 | 45:DL:98:TYR:CE1 | 2.46 | 0.51 |
| 36:BC:52:LEU:HD23 | 36:BC:53:ALA:N | 2.25 | 0.51 |
| 37:DD:150:GLU:O | 37:DD:153:ARG:HG2 | 2.10 | 0.51 |
| 1:AA:1387:U:O2 | 21:AX:80:ILE:HD12 | 2.10 | 0.51 |
| 59:DZ:373:ASP:OD2 | 59:DZ:374:LEU:N | 2.44 | 0.51 |
| 1:CA:2815:C:H2' | 1:CA:2816:C:H6 | 1.75 | 0.51 |
| 1:CA:706:A:OP1 | 4:CD:7:LYS:NZ | 2.42 | 0.51 |
| 59:DZ:539:ILE:O | 59:DZ:542:VAL:HG12 | 2.11 | 0.51 |
| 1:AA:934:A:O2' | 1:AA:935:C:OP2 | 2.23 | 0.51 |
| 1:CA:2638:G:P | 5:CE:82:ARG:NH2 | 2.84 | 0.51 |
| 8:AH:89:ILE:CD1 | 8:AH:96:ALA:HB2 | 2.41 | 0.51 |
| 1:CA:1448:G:H4' | 1:CA:1542:A:OP1 | 2.11 | 0.51 |
| 1:AA:1496:A:H5' | 1:AA:1497:G:OP2 | 2.11 | 0.51 |
| 59:BZ:417:THR:HA | 59:BZ:418:LYS:HG2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:BF:8:ILE:HD13 | 39:BF:26:ILE:HD13 | 1.93 | 0.51 |
| 53:DT:63:ILE:HD13 | 53:DT:80:ARG:HB3 | 1.93 | 0.51 |
| 21:CX:36:LYS:HA | 21:CX:39:ILE:HD12 | 1.93 | 0.51 |
| 34:BA:17:U:H2' | 34:BA:18:C:C6 | 2.46 | 0.51 |
| 34:BA:976:G:H5' | 34:BA:1358:U:O2' | 2.11 | 0.51 |
| 34:DA:1166:G:H5' | 34:DA:1168:A:OP2 | 2.11 | 0.51 |
| 13:CP:39:LYS:HD2 | 13:CP:45:LEU:HD11 | 1.93 | 0.51 |
| 3:CC:54:ARG:HD2 | 3:CC:55:SER:H | 1.76 | 0.51 |
| 49:BP:20:VAL:HG21 | 49:BP:32:TYR:CD2 | 2.46 | 0.51 |
| 39:DF:87:ARG:HH11 | 39:DF:87:ARG:CG | 2.20 | 0.51 |
| 59:DZ:129:LYS:NZ | 59:DZ:517:LEU:HG | 2.26 | 0.51 |
| 59:DZ:169:GLY:N | 59:DZ:170:ARG:HH12 | 2.09 | 0.51 |
| 1:CA:1547:C:H2' | 1:CA:1548:C:C6 | 2.43 | 0.51 |
| 34:DA:979:C:H42 | 47:DN:18:VAL:HB | 1.76 | 0.51 |
| 1:CA:1877:A:H5' | 1:CA:1878:G:OP2 | 2.11 | 0.51 |
| 7:CG:18:GLU:HG2 | 7:CG:175:LEU:HD21 | 1.93 | 0.51 |
| 1:CA:2836:U:H2' | 1:CA:2837:G:C8 | 2.45 | 0.51 |
| 16:AS:58:LEU:HD22 | 16:AS:59:LYS:HG3 | 1.92 | 0.51 |
| 34:DA:1347:G:HO2' | 34:DA:1373:G:H1 | 1.58 | 0.51 |
| 11:AN:30:ILE:HG22 | 11:AN:34:LEU:HD22 | 1.93 | 0.51 |
| 4:CD:10:THR:OG1 | 4:CD:13:ARG:HB2 | 2.10 | 0.51 |
| 1:AA:1040:C:OP1 | 18:AU:53:ARG:NH2 | 2.44 | 0.51 |
| 1:CA:1786:A:H1' | 1:CA:1938:A:N6 | 2.25 | 0.51 |
| 1:CA:1247:A:OP1 | 6:CF:95:ARG:NH2 | 2.43 | 0.51 |
| 34:BA:523:A:H61 | 45:BL:92:ASP:HB2 | 1.75 | 0.51 |
| 59:DZ:18:ALA:HB1 | 59:DZ:121:VAL:HG21 | 1.93 | 0.51 |
| 15:AR:33:ARG:HD2 | 15:AR:113:LEU:HD13 | 1.91 | 0.51 |
| 1:AA:553:A:C2' | 1:AA:554:A:H5' | 2.41 | 0.51 |
| 1:CA:1429:G:H2' | 1:CA:1430:C:C6 | 2.46 | 0.51 |
| 37:BD:190:ASP:HB2 | 37:BD:193:ASP:HB2 | 1.93 | 0.51 |
| 59:DZ:610:VAL:HG22 | 59:DZ:669:PHE:HB3 | 1.92 | 0.51 |
| 35:DB:97:TRP:CH2 | 35:DB:101:MET:HB2 | 2.45 | 0.51 |
| 34:DA:427:U:H3' | 34:DA:428:G:H2' | 1.93 | 0.51 |
| 34:BA:134:A:H61 | 49:BP:25:ARG:HH12 | 1.58 | 0.51 |
| 34:BA:8:A:N6 | 37:BD:209:ARG:HB2 | 2.26 | 0.51 |
| 43:DJ:8:LEU:HD23 | 43:DJ:96:ILE:HG23 | 1.93 | 0.51 |
| 1:AA:1289:G:O2' | 13:AP:7:ARG:NH2 | 2.43 | 0.51 |
| 41:DH:28:ALA:HB3 | 41:DH:57:PRO:HB2 | 1.93 | 0.51 |
| 34:DA:892:A:O2' | 34:DA:1415:G:H4' | 2.11 | 0.51 |
| 34:BA:1278:U:H5' | 34:BA:1279:A:O4' | 2.11 | 0.51 |
| 1:CA:2365:G:N7 | 32:C8:39:LYS:NZ | 2.54 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:31:C:C2' | 2:CB:32:C:H5' | 2.41 | 0.51 |
| 6:AF:53:THR:CG2 | 6:AF:55:GLY:H | 2.24 | 0.51 |
| 1:AA:2434:A:O4' | 58:BY:76:A:N6 | 2.44 | 0.51 |
| 1:CA:1939:U:OP1 | 1:CA:2604:U:O2' | 2.26 | 0.51 |
| 35:DB:96:ARG:O | 35:DB:98:LEU:HD22 | 2.11 | 0.50 |
| 1:AA:553:A:H2 | 1:AA:2065:C:H5' | 1.75 | 0.50 |
| 3:CC:42:VAL:CG1 | 3:CC:43:GLU:N | 2.73 | 0.50 |
| 3:AC:42:VAL:CG1 | 3:AC:43:GLU:N | 2.73 | 0.50 |
| 36:DC:28:GLN:O | 36:DC:32:LEU:HD23 | 2.11 | 0.50 |
| 59:DZ:491:VAL:HG12 | 59:DZ:493:VAL:HG13 | 1.93 | 0.50 |
| 34:DA:1279:A:H5'' | 34:DA:1280:A:OP1 | 2.11 | 0.50 |
| 16:CS:66:ALA:O | 16:CS:69:VAL:HG13 | 2.11 | 0.50 |
| 35:DB:229:VAL:HG12 | 35:DB:230:VAL:H | 1.76 | 0.50 |
| 37:DD:117:ALA:O | 37:DD:121:VAL:HG23 | 2.10 | 0.50 |
| 34:BA:114:U:O2' | 34:BA:115:G:H5' | 2.10 | 0.50 |
| 1:CA:1778:U:H2' | 1:CA:1784:A:N6 | 2.26 | 0.50 |
| 1:AA:1686:U:O2' | 1:AA:1687:C:H5' | 2.11 | 0.50 |
| 35:BB:160:ASP:N | 35:BB:160:ASP:OD1 | 2.44 | 0.50 |
| 46:BM:60:VAL:HG13 | 46:BM:64:TRP:HZ3 | 1.76 | 0.50 |
| 18:AU:61:TRP:CH2 | 18:AU:93:LYS:HB2 | 2.46 | 0.50 |
| 59:BZ:177:ILE:HD12 | 59:BZ:188:TYR:CE2 | 2.46 | 0.50 |
| 35:DB:84:GLU:HB3 | 35:DB:219:VAL:HG21 | 1.93 | 0.50 |
| 1:CA:1204:A:H2 | 1:CA:1241:A:N6 | 1.97 | 0.50 |
| 34:DA:559:A:OP1 | 38:DE:126:ARG:NH2 | 2.44 | 0.50 |
| 1:CA:297:C:OP1 | 22:CY:95:LYS:NZ | 2.43 | 0.50 |
| 7:CG:98:ARG:HA | 7:CG:101:ILE:HD12 | 1.93 | 0.50 |
| 34:DA:23:C:OP2 | 34:DA:561:U:N3 | 2.34 | 0.50 |
| 34:DA:1118:C:H1' | 34:DA:1179:A:C4 | 2.46 | 0.50 |
| 1:AA:1553:A:O2' | 1:AA:1554:A:O4' | 2.29 | 0.50 |
| 14:CQ:109:VAL:HG22 | 14:CQ:113:GLN:OE1 | 2.11 | 0.50 |
| 59:DZ:302:HIS:CD2 | 59:DZ:303:PRO:HD2 | 2.45 | 0.50 |
| 11:AN:121:LYS:HB3 | 11:AN:123:TYR:CE2 | 2.47 | 0.50 |
| 40:BG:66:VAL:HG12 | 40:BG:70:LYS:HE3 | 1.93 | 0.50 |
| 1:CA:176:G:O2' | 1:CA:177:G:H5' | 2.11 | 0.50 |
| 1:AA:484:G:O2' | 1:AA:495:G:O6 | 2.24 | 0.50 |
| 23:AZ:70:LEU:HG | 23:AZ:91:LEU:HD21 | 1.92 | 0.50 |
| 10:AL:108:ALA:O | 10:AL:112:MET:HB3 | 2.11 | 0.50 |
| 1:CA:2061:G:OP2 | 65:CA:4063:HOH:O | 2.19 | 0.50 |
| 59:BZ:76:ASP:N | 59:BZ:76:ASP:OD2 | 2.42 | 0.50 |
| 1:CA:1052:C:N4 | 1:CA:1053:C:H41 | 2.09 | 0.50 |
| 3:AC:57:GLN:HB2 | 3:AC:202:PRO:HG2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:54:ARG:HD2 | 3:AC:55:SER:H | 1.76 | 0.50 |
| 23:AZ:111:VAL:HG12 | 23:AZ:112:ARG:H | 1.77 | 0.50 |
| 59:BZ:329:ARG:HD2 | 59:BZ:331:TYR:CE1 | 2.47 | 0.50 |
| 1:AA:943:C:H4' | 56:BW:55:PSU:O3' | 2.11 | 0.50 |
| 1:AA:139:A:H8 | 1:AA:1454:C:O2' | 1.91 | 0.50 |
| 35:DB:178:ARG:HH22 | 41:DH:68:ARG:NH2 | 2.05 | 0.50 |
| 3:CC:44:VAL:HG21 | 3:CC:176:VAL:HG21 | 1.92 | 0.50 |
| 1:CA:2805:G:H2' | 1:CA:2807:G:H8 | 1.74 | 0.50 |
| 34:DA:1346:A:H5'' | 42:DI:120:ARG:HH12 | 1.76 | 0.50 |
| 1:CA:86:C:OP1 | 22:CY:32:PRO:HG2 | 2.11 | 0.50 |
| 40:DG:111:ARG:NH1 | 40:DG:113:GLU:OE1 | 2.44 | 0.50 |
| 1:CA:2567:G:H2' | 1:CA:2568:C:C6 | 2.47 | 0.50 |
| 59:DZ:629:GLY:HA3 | 59:DZ:647:VAL:HG12 | 1.93 | 0.50 |
| 1:CA:1288:U:O4 | 15:CR:106:GLY:HA3 | 2.12 | 0.50 |
| 34:DA:665:A:H1' | 34:DA:733:A:O4' | 2.11 | 0.50 |
| 1:AA:515:G:N7 | 20:AW:49:LYS:NZ | 2.59 | 0.50 |
| 50:DQ:65:ILE:HB | 50:DQ:69:LYS:HB3 | 1.93 | 0.50 |
| 1:CA:34:C:H2' | 1:CA:34:C:O2 | 2.10 | 0.50 |
| 1:CA:1044:G:H21 | 1:CA:1111:A:H2 | 1.59 | 0.50 |
| 42:DI:88:TYR:CD2 | 42:DI:89:ASN:HB2 | 2.46 | 0.50 |
| 5:CE:9:VAL:HG13 | 5:CE:25:VAL:O | 2.11 | 0.50 |
| 1:CA:1798:U:H5' | 4:CD:259:THR:CG2 | 2.24 | 0.50 |
| 3:CC:29:LEU:O | 3:CC:30:VAL:C | 2.48 | 0.50 |
| 1:CA:1371:G:H2' | 1:CA:1372:U:H5 | 1.77 | 0.50 |
| 34:BA:353:A:C8 | 34:BA:353:A:H5' | 2.42 | 0.50 |
| 3:CC:68:GLY:H | 3:CC:189:ASN:ND2 | 2.08 | 0.50 |
| 34:BA:200:G:H1 | 34:BA:217:C:N4 | 2.10 | 0.50 |
| 34:BA:1179:A:H2' | 34:BA:1180:A:O4' | 2.12 | 0.50 |
| 1:AA:1410:G:P | 25:A1:3:LYS:HG3 | 2.51 | 0.50 |
| 28:A4:59:PHE:HB3 | 52:BS:67:VAL:HG11 | 1.94 | 0.50 |
| 59:DZ:154:GLN:O | 59:DZ:158:GLY:HA2 | 2.12 | 0.50 |
| 21:CX:25:LYS:HA | 21:CX:81:VAL:O | 2.12 | 0.50 |
| 5:AE:5:LEU:HD12 | 5:AE:51:PHE:HB2 | 1.92 | 0.50 |
| 58:DY:55:PSU:N3 | 58:DY:58:A:N7 | 2.49 | 0.50 |
| 36:DC:113:ALA:O | 36:DC:116:VAL:N | 2.44 | 0.50 |
| 34:DA:1412:C:H2' | 34:DA:1413:A:C8 | 2.47 | 0.50 |
| 1:AA:2860:A:OP2 | 1:AA:2876:U:H5 | 1.93 | 0.50 |
| 1:CA:11:G:H2' | 1:CA:12:U:H5'' | 1.93 | 0.50 |
| 32:A8:62:LEU:HB3 | 32:A8:65:GLU:HG2 | 1.93 | 0.50 |
| 34:DA:1070:U:H2' | 34:DA:1071:C:H6 | 1.75 | 0.50 |
| 1:CA:2031:A:C6 | 1:CA:2498:C:H1' | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1211:U:H2' | 1:AA:1212:C:C6 | 2.46 | 0.50 |
| 1:CA:1482:G:H2' | 1:CA:1484:G:H8 | 1.76 | 0.50 |
| 19:CV:24:LYS:HA | 19:CV:92:THR:OG1 | 2.11 | 0.50 |
| 34:BA:955:U:O2' | 52:BS:83:HIS:HD2 | 1.94 | 0.50 |
| 48:DO:15:PHE:CZ | 48:DO:85:LEU:HD21 | 2.47 | 0.50 |
| 25:C1:89:GLU:O | 25:C1:93:GLU:HG2 | 2.11 | 0.50 |
| 35:BB:153:ARG:NH1 | 35:BB:153:ARG:HB3 | 2.26 | 0.50 |
| 59:BZ:21:ILE:HD13 | 59:BZ:21:ILE:N | 2.25 | 0.50 |
| 1:CA:298:G:H5'' | 1:CA:299:A:OP1 | 2.10 | 0.50 |
| 1:AA:721:G:H1' | 6:AF:74:ARG:HD3 | 1.92 | 0.50 |
| 1:CA:2126:A:N6 | 1:CA:2172:U:H5' | 2.27 | 0.50 |
| 1:CA:2113:U:H3 | 1:CA:2170:A:H61 | 1.59 | 0.50 |
| 1:CA:2876:G:H4' | 17:CT:2:ASN:ND2 | 2.26 | 0.50 |
| 3:CC:191:ARG:O | 3:CC:195:ARG:HG2 | 2.11 | 0.50 |
| 34:DA:1095:U:P | 34:DA:1108:G:H1 | 2.35 | 0.50 |
| 34:DA:728:A:N7 | 48:DO:54:ARG:HD2 | 2.26 | 0.50 |
| 1:CA:2572:A:N7 | 5:CE:145:LYS:HB2 | 2.27 | 0.50 |
| 34:DA:1509:C:H2' | 34:DA:1510:U:O4' | 2.12 | 0.50 |
| 59:BZ:623:ASP:CG | 59:BZ:662:LYS:HE3 | 2.31 | 0.50 |
| 44:BK:41:THR:OG1 | 44:BK:42:TRP:N | 2.43 | 0.50 |
| 1:CA:733:G:OP2 | 65:CA:3724:HOH:O | 2.20 | 0.50 |
| 13:CP:111:ARG:HD3 | 13:CP:128:HIS:CD2 | 2.47 | 0.50 |
| 1:CA:987:G:O2' | 1:CA:1000:A:N3 | 2.41 | 0.50 |
| 50:DQ:48:GLU:OE2 | 50:DQ:50:LYS:HE3 | 2.12 | 0.50 |
| 48:BO:81:LEU:O | 48:BO:85:LEU:HB2 | 2.11 | 0.50 |
| 1:AA:2843:G:H8 | 1:AA:2843:G:OP1 | 1.95 | 0.50 |
| 38:BE:51:VAL:O | 38:BE:55:VAL:HG23 | 2.11 | 0.50 |
| 34:BA:1511:G:H2' | 34:BA:1512:U:O4' | 2.10 | 0.50 |
| 12:AO:48:PRO:HB3 | 34:BA:1422:G:H5' | 1.94 | 0.50 |
| 59:BZ:554:PRO:HG3 | 59:BZ:594:VAL:HG12 | 1.93 | 0.50 |
| 3:CC:57:GLN:HB2 | 3:CC:202:PRO:HG2 | 1.93 | 0.50 |
| 3:CC:54:ARG:HH22 | 3:CC:56:ASP:HB3 | 1.75 | 0.50 |
| 34:BA:765:G:H5'' | 34:BA:766:A:OP1 | 2.12 | 0.50 |
| 4:AD:155:LEU:HD23 | 4:AD:177:LEU:HD22 | 1.94 | 0.50 |
| 1:CA:2150:U:H2' | 1:CA:2151:G:C8 | 2.47 | 0.50 |
| 1:CA:1098:A:H2' | 1:CA:1099:G:O4' | 2.11 | 0.50 |
| 34:BA:52:G:H2' | 34:BA:53:A:H8 | 1.75 | 0.50 |
| 38:BE:20:GLN:HG2 | 38:BE:25:ARG:HD2 | 1.93 | 0.50 |
| 23:CZ:96:VAL:N | 23:CZ:128:VAL:O | 2.44 | 0.50 |
| 6:AF:64:ILE:HD12 | 6:AF:65:TRP:CD2 | 2.47 | 0.50 |
| 1:AA:2574:U:O2' | 12:AO:23:ARG:HD3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:44:VAL:HG21 | 3:AC:176:VAL:HG21 | 1.92 | 0.50 |
| 18:CU:79:PHE:CZ | 18:CU:83:LEU:HD21 | 2.46 | 0.50 |
| 1:AA:1553:A:O2' | 1:AA:1554:A:O5' | 2.29 | 0.50 |
| 35:DB:102:LEU:HB3 | 35:DB:180:LEU:HD12 | 1.93 | 0.50 |
| 3:AC:191:ARG:O | 3:AC:195:ARG:HG2 | 2.11 | 0.50 |
| 1:AA:2287:C:O2 | 14:AQ:85:LYS:HG3 | 2.12 | 0.50 |
| 34:BA:109:A:H2' | 34:BA:326:G:N2 | 2.27 | 0.50 |
| 1:AA:1846:A:O3' | 65:AA:4736:HOH:O | 2.18 | 0.50 |
| 34:DA:1152:A:H2' | 34:DA:1153:C:C6 | 2.47 | 0.50 |
| 53:DT:64:ASP:OD2 | 53:DT:81:LYS:NZ | 2.38 | 0.50 |
| 1:CA:2365:G:O6 | 32:C8:39:LYS:NZ | 2.45 | 0.50 |
| 59:DZ:127:LYS:HG3 | 59:DZ:520:GLY:HA3 | 1.93 | 0.50 |
| 1:AA:1284:G:OP2 | 65:AA:4926:HOH:O | 2.19 | 0.50 |
| 16:CS:12:PHE:O | 16:CS:16:ASN:ND2 | 2.44 | 0.50 |
| 35:DB:142:LEU:HA | 35:DB:145:LEU:HB2 | 1.94 | 0.50 |
| 36:DC:97:LYS:O | 36:DC:99:VAL:N | 2.45 | 0.50 |
| 34:DA:17:U:H2' | 34:DA:18:C:C6 | 2.47 | 0.50 |
| 1:CA:271(E):U:H2' | 1:CA:271(F):C:C6 | 2.46 | 0.50 |
| 34:BA:1312:G:N7 | 52:BS:2:PRO:HD2 | 2.27 | 0.50 |
| 54:BU:3:LYS:HB3 | 54:BU:14:TRP:CG | 2.47 | 0.50 |
| 59:BZ:517:LEU:HD13 | 59:BZ:564:LYS:HB2 | 1.94 | 0.50 |
| 11:AN:5:VAL:HG23 | 11:AN:6:PRO:HD2 | 1.94 | 0.50 |
| 10:AL:99:ILE:O | 10:AL:139:VAL:N | 2.39 | 0.50 |
| 37:BD:134:ASP:O | 37:BD:136:PRO:HD3 | 2.11 | 0.50 |
| 1:CA:2506:U:O2 | 56:DW:76:F3N:HD2 | 2.11 | 0.50 |
| 1:CA:1070:A:H2' | 1:CA:1097:U:OP1 | 2.11 | 0.50 |
| 3:AC:183:PRO:C | 3:AC:185:LYS:H | 2.16 | 0.50 |
| 1:AA:553:A:C8 | 1:AA:553:A:C3' | 2.94 | 0.50 |
| 3:CC:183:PRO:C | 3:CC:185:LYS:H | 2.16 | 0.50 |
| 34:BA:1255:G:C2 | 34:BA:1283:G:C2 | 3.00 | 0.50 |
| 35:DB:16:HIS:CG | 35:DB:17:PHE:N | 2.80 | 0.50 |
| 1:AA:2152:U:H1' | 1:AA:2180:A:N1 | 2.27 | 0.50 |
| 7:AG:114:ILE:HA | 7:AG:140:ILE:HD11 | 1.93 | 0.50 |
| 59:BZ:216:LEU:HD11 | 59:BZ:246:ILE:HD11 | 1.93 | 0.50 |
| 34:BA:1436:U:OP1 | 53:BT:23:ARG:NH2 | 2.44 | 0.50 |
| 1:CA:627:A:C6 | 1:CA:637:A:C8 | 3.00 | 0.50 |
| 51:DR:32:ARG:HA | 51:DR:69:THR:HG21 | 1.93 | 0.50 |
| 34:BA:1509:C:H2' | 34:BA:1510:U:O4' | 2.12 | 0.50 |
| 59:BZ:-62:LEU:HD11 | 59:BZ:-48:VAL:HG22 | 1.93 | 0.50 |
| 38:DE:69:VAL:HG22 | 38:DE:71:LEU:HD13 | 1.94 | 0.50 |
| 34:BA:1260:C:OP1 | 34:BA:1284:C:O2' | 2.24 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 34:DA:20:U:H2' | 34:DA:21:G:O4' | 2.12 | 0.50 |
| 48:DO:71:GLN:HB2 | 48:DO:78:TYR:CD2 | 2.47 | 0.50 |
| 1:CA:2131:G:N7 | 1:CA:2133:G:N2 | 2.59 | 0.50 |
| 25:A1:80:LEU:HB3 | 25:A1:82:LEU:HG | 1.93 | 0.50 |
| 34:DA:1203:C:H2' | 34:DA:1204:A:C8 | 2.47 | 0.50 |
| 23:CZ:69:THR:HG22 | 23:CZ:90:VAL:HA | 1.94 | 0.50 |
| 9:CK:85:ASP:O | 9:CK:87:VAL:N | 2.45 | 0.50 |
| 59:BZ:438:PHE:HB3 | 59:BZ:458:HIS:HE1 | 1.77 | 0.50 |
| 1:AA:70:A:N7 | 21:AX:31:HIS:HE1 | 2.09 | 0.50 |
| 29:C5:16:ARG:HD2 | 29:C5:20:ARG:NH1 | 2.27 | 0.50 |
| 10:AL:106:GLU:O | 10:AL:109:LYS:HB2 | 2.12 | 0.50 |
| 5:CE:77:ILE:HD11 | 5:CE:79:ARG:NH1 | 2.27 | 0.50 |
| 55:BV:14:A:C6 | 58:BY:34:G:C6 | 3.00 | 0.50 |
| 34:BA:406:G:C2 | 34:BA:407:G:C8 | 3.00 | 0.50 |
| 1:CA:1237:A:OP1 | 65:CA:4442:HOH:O | 2.19 | 0.50 |
| 1:CA:2364:C:OP1 | 24:C0:55:ARG:HD3 | 2.11 | 0.50 |
| 53:DT:43:LEU:O | 53:DT:47:GLY:N | 2.45 | 0.50 |
| 34:BA:1456:G:O3' | 53:BT:39:LYS:NZ | 2.41 | 0.50 |
| 1:CA:1300:U:H4' | 1:CA:1301:A:C5' | 2.42 | 0.50 |
| 4:AD:79:VAL:HG12 | 4:AD:113:VAL:HA | 1.94 | 0.50 |
| 1:CA:2298:A:H2' | 1:CA:2299:G:O4' | 2.12 | 0.50 |
| 34:DA:572:A:OP1 | 65:DA:1836:HOH:O | 2.18 | 0.50 |
| 1:CA:30:G:H2' | 1:CA:31:C:C6 | 2.46 | 0.50 |
| 34:DA:1355:G:H2' | 34:DA:1356:G:C8 | 2.46 | 0.50 |
| 34:BA:1010:G:N2 | 34:BA:1020:U:H1' | 2.26 | 0.50 |
| 35:DB:112:VAL:O | 35:DB:116:GLU:HB3 | 2.12 | 0.50 |
| 34:BA:714:G:H2' | 34:BA:715:A:C8 | 2.47 | 0.50 |
| 34:BA:560:U:H5' | 34:BA:566:G:N2 | 2.26 | 0.49 |
| 14:AQ:14:ARG:HG2 | 14:AQ:41:TRP:CH2 | 2.41 | 0.49 |
| 35:DB:54:THR:O | 35:DB:58:ILE:HG13 | 2.12 | 0.49 |
| 1:AA:1387:U:O4' | 21:AX:57:LEU:HD12 | 2.12 | 0.49 |
| 12:CO:23:ARG:HG3 | 12:CO:24:VAL:N | 2.27 | 0.49 |
| 59:DZ:526:VAL:HG23 | 59:DZ:566:THR:HA | 1.94 | 0.49 |
| 34:BA:645:C:H2' | 34:BA:646:U:C6 | 2.46 | 0.49 |
| 1:AA:2518:U:C2 | 1:AA:2597:U:O4 | 2.65 | 0.49 |
| 59:DZ:388:THR:HG21 | 59:DZ:397:VAL:O | 2.12 | 0.49 |
| 18:CU:49:HIS:HA | 18:CU:52:ARG:HB3 | 1.94 | 0.49 |
| 36:DC:15:THR:HG21 | 36:DC:181:ASN:HA | 1.94 | 0.49 |
| 2:AB:1:U:O2 | 2:AB:1:U:H2' | 2.11 | 0.49 |
| 34:DA:583:A:H2' | 34:DA:584:G:O4' | 2.12 | 0.49 |
| 19:AV:14:VAL:HB | 19:AV:96:ILE:HG13 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:2787:C:HO2' | 1:CA:2810:A:HO2' | 1.60 | 0.49 |
| 1:AA:1249:A:N1 | 1:AA:1287:A:N7 | 2.59 | 0.49 |
| 22:AY:54:LYS:H | 22:AY:56:PRO:HG3 | 1.77 | 0.49 |
| 4:CD:148:GLU:CB | 4:CD:151:LYS:HD2 | 2.40 | 0.49 |
| 1:CA:1026:U:H4' | 1:CA:1027:A:OP1 | 2.11 | 0.49 |
| 59:BZ:396:ARG:HH21 | 59:BZ:396:ARG:CG | 2.23 | 0.49 |
| 1:CA:2815:C:H2' | 1:CA:2816:C:C6 | 2.47 | 0.49 |
| 56:DW:21:A:N6 | 56:DW:46:7MG:N3 | 2.60 | 0.49 |
| 35:DB:150:SER:O | 35:DB:153:ARG:HG2 | 2.12 | 0.49 |
| 43:DJ:47:PHE:HB2 | 43:DJ:63:PHE:HB2 | 1.93 | 0.49 |
| 34:BA:129:U:H5' | 50:BQ:3:LYS:NZ | 2.27 | 0.49 |
| 59:DZ:36:THR:HB | 59:DZ:72:CYS:HB2 | 1.93 | 0.49 |
| 34:BA:1228:C:P | 46:BM:108:ARG:HH22 | 2.35 | 0.49 |
| 8:CH:75:ALA:O | 8:CH:79:VAL:HG22 | 2.12 | 0.49 |
| 1:AA:346:A:H5' | 1:AA:364:A:H1' | 1.93 | 0.49 |
| 1:CA:1637:A:H4' | 1:CA:2711:A:O2' | 2.11 | 0.49 |
| 1:CA:2600:A:H2' | 1:CA:2601:C:C6 | 2.48 | 0.49 |
| 14:AQ:24:GLY:O | 14:AQ:102:VAL:HG23 | 2.12 | 0.49 |
| 59:DZ:119:GLU:HB3 | 59:DZ:123:ARG:HH21 | 1.77 | 0.49 |
| 34:DA:1084:G:H5' | 34:DA:1102:A:OP2 | 2.12 | 0.49 |
| 1:CA:2116:G:H5' | 1:CA:2117:A:OP2 | 2.11 | 0.49 |
| 43:DJ:38:ILE:CG1 | 43:DJ:71:LEU:HB3 | 2.42 | 0.49 |
| 13:AP:62:LEU:O | 32:A8:13:ARG:HD3 | 2.11 | 0.49 |
| 3:AC:191:ARG:O | 3:AC:194:ILE:HG22 | 2.12 | 0.49 |
| 53:BT:13:LEU:O | 53:BT:17:ARG:HG3 | 2.12 | 0.49 |
| 34:BA:539:A:H2' | 34:BA:540:G:C8 | 2.47 | 0.49 |
| 17:CT:83:ILE:HD13 | 17:CT:86:ILE:HD11 | 1.94 | 0.49 |
| 36:DC:131:ARG:NH1 | 38:DE:50:GLU:HG3 | 2.27 | 0.49 |
| 17:AT:65:LYS:HE2 | 17:AT:67:SER:HB2 | 1.94 | 0.49 |
| 1:CA:1188:U:H4' | 19:CV:79:VAL:HG22 | 1.94 | 0.49 |
| 1:AA:225:C:H2' | 1:AA:226:C:C6 | 2.47 | 0.49 |
| 38:BE:7:GLU:N | 38:BE:35:GLY:O | 2.45 | 0.49 |
| 53:DT:40:ALA:HB2 | 53:DT:55:ILE:HG22 | 1.93 | 0.49 |
| 35:BB:218:ALA:O | 35:BB:222:ILE:HG13 | 2.13 | 0.49 |
| 1:CA:1418:G:N7 | 65:CA:4067:HOH:O | 2.35 | 0.49 |
| 12:CO:48:PRO:HB3 | 34:DA:1422:G:H5' | 1.95 | 0.49 |
| 59:BZ:328:ILE:HD12 | 59:BZ:377:VAL:HG12 | 1.93 | 0.49 |
| 4:CD:96:HIS:NE2 | 4:CD:102:LYS:HE2 | 2.27 | 0.49 |
| 59:DZ:160:ARG:NH1 | 59:DZ:256:THR:OG1 | 2.37 | 0.49 |
| 34:DA:254:G:P | 50:DQ:66:SER:HG | 2.34 | 0.49 |
| 34:DA:1299:A:H2' | 34:DA:1299:A:N3 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 43:DJ:30:SER:O | 43:DJ:30:SER:OG | 2.29 | 0.49 |
| 36:DC:47:LEU:HG | 36:DC:68:VAL:HG11 | 1.93 | 0.49 |
| 42:DI:46:ALA:HB2 | 42:DI:74:ILE:HG23 | 1.94 | 0.49 |
| 37:DD:13:ARG:HD3 | 37:DD:32:ALA:HB1 | 1.95 | 0.49 |
| 35:DB:77:ALA:HB2 | 35:DB:211:ILE:HD13 | 1.95 | 0.49 |
| 34:BA:674:G:H2' | 34:BA:675:A:H8 | 1.76 | 0.49 |
| 23:CZ:110:GLY:HA3 | 23:CZ:145:GLU:HA | 1.93 | 0.49 |
| 34:BA:1171:G:H2' | 34:BA:1172:C:C6 | 2.47 | 0.49 |
| 32:A8:37:SER:OG | 32:A8:38:GLY:N | 2.45 | 0.49 |
| 1:AA:841:G:H2' | 1:AA:842:C:C6 | 2.47 | 0.49 |
| 45:DL:88:GLY:O | 45:DL:99:HIS:HD2 | 1.96 | 0.49 |
| 1:CA:1480:G:C6 | 1:CA:1481:U:N3 | 2.80 | 0.49 |
| 13:AP:27:HIS:HB2 | 65:AP:315:HOH:O | 2.11 | 0.49 |
| 34:BA:688:G:H2' | 34:BA:689:C:H6 | 1.77 | 0.49 |
| 1:AA:1074:A:N6 | 1:AA:1171:G:H2' | 2.27 | 0.49 |
| 1:AA:1095:C:H2' | 1:AA:1096:A:H5' | 1.95 | 0.49 |
| 13:CP:38:GLN:O | 13:CP:39:LYS:HB3 | 2.12 | 0.49 |
| 59:DZ:511:LYS:HB2 | 59:DZ:569:ASP:HB3 | 1.94 | 0.49 |
| 35:BB:178:ARG:HH22 | 41:BH:68:ARG:NH1 | 2.11 | 0.49 |
| 3:CC:191:ARG:O | 3:CC:194:ILE:HG22 | 2.12 | 0.49 |
| 58:BY:34:G:O5' | 58:BY:34:G:H8 | 1.96 | 0.49 |
| 59:BZ:75:LYS:O | 59:BZ:77:HIS:HD2 | 1.95 | 0.49 |
| 1:CA:1782:C:H1' | 1:CA:2609:U:C5' | 2.43 | 0.49 |
| 34:DA:1107:C:C4 | 34:DA:1108:G:C8 | 3.00 | 0.49 |
| 4:AD:12:SER:HB3 | 4:AD:208:LYS:HB3 | 1.95 | 0.49 |
| 1:AA:1466:U:O2' | 1:AA:1467:G:OP1 | 2.28 | 0.49 |
| 1:CA:18:C:H2' | 1:CA:19:C:C6 | 2.48 | 0.49 |
| 22:AY:79:CYS:SG | 22:AY:81:LYS:HG3 | 2.52 | 0.49 |
| 1:CA:2758:A:C2 | 1:CA:2759:G:H1' | 2.46 | 0.49 |
| 34:DA:259:G:H2' | 34:DA:260:G:O4' | 2.13 | 0.49 |
| 50:DQ:45:HIS:CD2 | 50:DQ:47:PRO:HD3 | 2.47 | 0.49 |
| 53:BT:40:ALA:HB2 | 53:BT:55:ILE:HG22 | 1.95 | 0.49 |
| 1:AA:1712:A:N3 | 12:AO:1:MET:HE2 | 2.28 | 0.49 |
| 37:DD:59:ARG:O | 37:DD:63:LYS:HD3 | 2.12 | 0.49 |
| 11:AN:96:GLU:CD | 11:AN:96:GLU:H | 2.16 | 0.49 |
| 35:DB:46:LYS:O | 35:DB:50:GLU:HB2 | 2.13 | 0.49 |
| 1:AA:1834:A:H4' | 4:AD:259:THR:CG2 | 2.41 | 0.49 |
| 1:AA:2200:C:O2' | 3:AC:169:THR:CB | 2.59 | 0.49 |
| 39:DF:87:ARG:NH1 | 39:DF:87:ARG:HG3 | 2.18 | 0.49 |
| 1:CA:300:A:P | 22:CY:86:ARG:NH2 | 2.84 | 0.49 |
| 35:DB:178:ARG:HH21 | 41:DH:74:PRO:HB3 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:2171:A:H1' | 1:CA:2172:U:C6 | 2.47 | 0.49 |
| 42:DI:3:GLN:CG | 42:DI:20:ARG:HE | 2.26 | 0.49 |
| 51:BR:26:LEU:HD21 | 51:BR:39:VAL:HG13 | 1.94 | 0.49 |
| 43:BJ:11:PHE:CE1 | 43:BJ:67:THR:HG22 | 2.47 | 0.49 |
| 48:BO:33:THR:HG21 | 48:BO:85:LEU:HD22 | 1.93 | 0.49 |
| 34:DA:1148:U:H2' | 34:DA:1149:C:O4' | 2.13 | 0.49 |
| 13:AP:52:GLU:HG2 | 32:A8:57:ARG:HH22 | 1.77 | 0.49 |
| 46:DM:70:LEU:O | 46:DM:74:VAL:HG23 | 2.12 | 0.49 |
| 1:CA:819:A:C4 | 1:CA:1189:A:C2 | 3.00 | 0.49 |
| 1:AA:826:U:OP1 | 4:AD:49:ILE:HD12 | 2.13 | 0.49 |
| 1:CA:2849:U:H4' | 1:CA:2868:A:C2 | 2.47 | 0.49 |
| 1:CA:2773:C:H5'' | 5:CE:164:ARG:HG2 | 1.93 | 0.49 |
| 34:DA:9:G:OP1 | 38:DE:122:GLU:HG3 | 2.13 | 0.49 |
| 1:AA:1220:U:O3' | 1:AA:1221:G:H4' | 2.13 | 0.49 |
| 59:DZ:244:ALA:HA | 59:DZ:247:ARG:HB3 | 1.94 | 0.49 |
| 34:DA:1073:U:O2 | 35:DB:104:ASN:ND2 | 2.39 | 0.49 |
| 17:AT:77:PRO:HB2 | 17:AT:80:SER:HB2 | 1.94 | 0.49 |
| 34:DA:977:A:O2' | 34:DA:979:C:OP2 | 2.22 | 0.49 |
| 34:BA:92:C:H2' | 34:BA:93:G:C8 | 2.48 | 0.49 |
| 59:DZ:302:HIS:HD2 | 59:DZ:303:PRO:HD2 | 1.77 | 0.49 |
| 46:BM:3:ARG:HG3 | 46:BM:4:ILE:H | 1.77 | 0.49 |
| 34:BA:1342:C:O2' | 42:BI:124:GLN:HG3 | 2.12 | 0.49 |
| 34:DA:91:C:H2' | 34:DA:92:C:C6 | 2.48 | 0.49 |
| 34:BA:21:G:H2' | 34:BA:22:G:C8 | 2.47 | 0.49 |
| 34:BA:903:G:OP1 | 65:BA:1925:HOH:O | 2.19 | 0.49 |
| 13:AP:84:ASN:HB3 | 13:AP:117:GLU:O | 2.13 | 0.49 |
| 23:AZ:73:GLN:HB3 | 23:AZ:87:ASP:HB2 | 1.95 | 0.49 |
| 1:CA:2396:G:OP1 | 25:C1:25:LYS:NZ | 2.29 | 0.49 |
| 1:CA:1498:C:O4' | 1:CA:1577:C:H4' | 2.13 | 0.49 |
| 44:BK:73:MET:HG2 | 44:BK:103:LEU:HD21 | 1.94 | 0.49 |
| 9:CK:27:VAL:HA | 9:CK:113:GLN:HA | 1.95 | 0.49 |
| 1:CA:1130:U:O2 | 5:CE:149:ARG:NH2 | 2.40 | 0.49 |
| 1:AA:2830:A:C8 | 5:AE:109:LYS:HE2 | 2.47 | 0.49 |
| 59:BZ:140:ASP:HA | 59:BZ:172:ASP:H | 1.78 | 0.49 |
| 34:BA:693:G:H2' | 34:BA:694:A:C8 | 2.48 | 0.49 |
| 17:AT:15:VAL:HG13 | 17:AT:79:HIS:CE1 | 2.48 | 0.49 |
| 15:CR:33:ARG:HG3 | 15:CR:115:GLU:HB3 | 1.95 | 0.49 |
| 34:DA:983:A:N3 | 34:DA:983:A:H3' | 2.28 | 0.49 |
| 51:DR:52:PRO:O | 51:DR:56:THR:HG23 | 2.12 | 0.49 |
| 34:BA:1128:C:H4' | 34:BA:1148:U:O2 | 2.13 | 0.49 |
| 20:CW:19:LEU:HB3 | 29:C5:25:LEU:HD11 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1169:G:H1 | 1:CA:1180:C:H42 | 1.61 | 0.49 |
| 4:CD:24:ILE:HD13 | 4:CD:84:TYR:HB2 | 1.95 | 0.49 |
| 36:DC:120:VAL:HA | 36:DC:123:GLN:HE21 | 1.78 | 0.49 |
| 15:CR:30:THR:HG22 | 15:CR:31:HIS:CD2 | 2.48 | 0.49 |
| 18:AU:36:ARG:HD2 | 18:AU:40:PHE:CZ | 2.48 | 0.49 |
| 59:DZ:634:MET:HE3 | 59:DZ:643:ILE:HG12 | 1.94 | 0.49 |
| 34:BA:757:U:H2' | 34:BA:758:G:O4' | 2.13 | 0.49 |
| 1:CA:2405:G:OP1 | 13:CP:77:ARG:NH2 | 2.44 | 0.49 |
| 53:BT:76:ALA:O | 53:BT:80:ARG:HG2 | 2.13 | 0.49 |
| 22:AY:86:ARG:HH11 | 22:AY:100:ALA:HA | 1.76 | 0.49 |
| 23:CZ:93:ASP:HA | 23:CZ:131:ARG:NH2 | 2.28 | 0.49 |
| 18:CU:34:LYS:HE2 | 18:CU:34:LYS:HA | 1.94 | 0.49 |
| 34:DA:767:A:H2' | 34:DA:768:A:O4' | 2.12 | 0.49 |
| 1:AA:2181:G:H2' | 1:AA:2182:G:C8 | 2.48 | 0.49 |
| 34:BA:707:C:H2' | 34:BA:708:C:C6 | 2.48 | 0.49 |
| 1:AA:2660:C:H2' | 1:AA:2661:U:C6 | 2.48 | 0.49 |
| 1:AA:2096:U:H2' | 1:AA:2097:U:C6 | 2.47 | 0.49 |
| 1:AA:1067:A:H3' | 1:AA:1067:A:H8 | 1.76 | 0.49 |
| 59:BZ:78:ARG:HH21 | 59:BZ:357:ARG:NH2 | 2.10 | 0.49 |
| 1:CA:1031:G:H21 | 33:C9:36:GLN:NE2 | 2.06 | 0.49 |
| 35:DB:96:ARG:HD2 | 35:DB:98:LEU:HD13 | 1.94 | 0.49 |
| 37:BD:107:ARG:HH12 | 37:BD:194:LEU:HD21 | 1.77 | 0.49 |
| 36:DC:32:LEU:HD12 | 36:DC:59:ARG:NH1 | 2.27 | 0.49 |
| 1:AA:239:G:P | 32:A8:13:ARG:HH22 | 2.35 | 0.49 |
| 34:DA:1121:U:C2' | 34:DA:1122:U:H5' | 2.43 | 0.49 |
| 45:DL:102:ARG:HE | 45:DL:102:ARG:HB3 | 1.49 | 0.49 |
| 35:BB:20:GLU:HA | 35:BB:21:ARG:NH2 | 2.27 | 0.49 |
| 1:AA:1594:C:H2' | 1:AA:1595:C:C6 | 2.47 | 0.49 |
| 44:BK:48:ILE:O | 44:BK:50:TYR:N | 2.45 | 0.49 |
| 34:DA:522:C:OP2 | 45:DL:69:TYR:OH | 2.22 | 0.49 |
| 34:BA:559:A:OP1 | 38:BE:126:ARG:NH2 | 2.45 | 0.49 |
| 1:AA:346:A:H3' | 6:AF:169:ASN:HD21 | 1.77 | 0.49 |
| 34:BA:443:C:H2' | 34:BA:444:C:C6 | 2.48 | 0.49 |
| 40:DG:26:PHE:O | 40:DG:30:ILE:HG13 | 2.13 | 0.49 |
| 1:CA:613:G:N2 | 1:CA:614(C):A:O2' | 2.46 | 0.49 |
| 34:DA:790:A:H2' | 34:DA:791:G:C8 | 2.48 | 0.49 |
| 34:BA:814:A:N7 | 34:BA:816:A:C4 | 2.81 | 0.49 |
| 34:DA:8:A:N6 | 37:DD:209:ARG:HB2 | 2.27 | 0.49 |
| 2:CB:61:G:C6 | 2:CB:62:C:C4 | 3.01 | 0.49 |
| 34:DA:909:A:H2' | 34:DA:910:C:O4' | 2.13 | 0.49 |
| 59:BZ:147:TRP:O | 59:BZ:151:ARG:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:2250:G:N3 | 1:AA:2250:G:H2' | 2.26 | 0.49 |
| 1:AA:2285:A:H2' | 1:AA:2286:A:C8 | 2.48 | 0.49 |
| 1:AA:868:A:H2' | 1:AA:991:G:H5'' | 1.94 | 0.49 |
| 1:CA:81:G:HO2' | 1:CA:295:G:HO2' | 1.57 | 0.49 |
| 1:CA:500:G:N2 | 1:CA:502:A:H3' | 2.28 | 0.49 |
| 1:AA:1468:G:H1' | 1:AA:1542:A:N1 | 2.27 | 0.49 |
| 1:CA:608:A:H2' | 1:CA:609:A:C8 | 2.48 | 0.49 |
| 34:BA:222:U:H2' | 34:BA:223:U:C6 | 2.48 | 0.49 |
| 4:CD:273:ARG:HG2 | 4:CD:274:ARG:N | 2.28 | 0.49 |
| 34:DA:1101:A:H4' | 34:DA:1102:A:O5' | 2.12 | 0.49 |
| 59:DZ:169:GLY:H | 59:DZ:170:ARG:NH1 | 2.09 | 0.49 |
| 3:CC:184:GLU:O | 3:CC:188:ASP:OD2 | 2.31 | 0.49 |
| 3:AC:42:VAL:HA | 3:AC:216:THR:O | 2.13 | 0.49 |
| 4:AD:71:ASP:CB | 4:AD:103:ARG:HH22 | 2.26 | 0.49 |
| 17:CT:6:LEU:O | 17:CT:10:VAL:HG23 | 2.12 | 0.49 |
| 13:CP:59:LEU:O | 32:C8:13:ARG:HD2 | 2.13 | 0.49 |
| 34:DA:707:C:H2' | 34:DA:708:C:H6 | 1.78 | 0.49 |
| 1:AA:1846:A:P | 4:AD:54:ARG:HH22 | 2.36 | 0.49 |
| 43:DJ:63:PHE:HE2 | 47:DN:45:ARG:HA | 1.78 | 0.49 |
| 1:AA:794:U:O2 | 1:AA:2036:A:H1' | 2.12 | 0.49 |
| 13:CP:101:VAL:HA | 13:CP:106:LEU:O | 2.13 | 0.49 |
| 34:DA:1251:A:H2' | 34:DA:1252:A:C8 | 2.47 | 0.49 |
| 1:CA:647:G:H8 | 1:CA:647:G:O5' | 1.96 | 0.49 |
| 51:DR:33:ASP:OD2 | 51:DR:36:ASN:HB2 | 2.13 | 0.49 |
| 59:BZ:519:ARG:HH22 | 59:BZ:678:GLU:H | 1.59 | 0.49 |
| 1:AA:801:C:H2' | 1:AA:802:C:C6 | 2.48 | 0.49 |
| 41:BH:29:SER:OG | 41:BH:32:LYS:HG3 | 2.13 | 0.49 |
| 14:CQ:18:LYS:O | 14:CQ:98:LYS:NZ | 2.35 | 0.49 |
| 1:AA:656:A:OP1 | 13:AP:65:ARG:NH1 | 2.44 | 0.49 |
| 47:DN:27:CYS:SG | 47:DN:28:GLY:N | 2.86 | 0.48 |
| 37:DD:98:GLU:OE1 | 37:DD:103:ASN:ND2 | 2.46 | 0.48 |
| 38:BE:36:ASP:OD2 | 38:BE:40:ARG:HB2 | 2.13 | 0.48 |
| 35:DB:103:THR:HG23 | 35:DB:176:GLU:OE1 | 2.13 | 0.48 |
| 1:AA:2021:C:H4' | 1:AA:2736:C:O2 | 2.13 | 0.48 |
| 34:BA:674:G:H2' | 34:BA:675:A:C8 | 2.48 | 0.48 |
| 1:CA:1434:A:H61 | 1:CA:1558:A:N6 | 2.10 | 0.48 |
| 34:DA:687:A:N3 | 34:DA:688:G:H1' | 2.28 | 0.48 |
| 18:AU:61:TRP:CZ2 | 18:AU:93:LYS:HB2 | 2.48 | 0.48 |
| 37:BD:88:VAL:HG12 | 37:BD:91:SER:H | 1.78 | 0.48 |
| 7:AG:126:ASP:HB3 | 7:AG:130:ASN:H | 1.78 | 0.48 |
| 1:CA:1628:G:H2' | 1:CA:1629:U:C6 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:12:C:O5' | 2:CB:12:C:H6 | 1.96 | 0.48 |
| 1:CA:272:G:H4' | 1:CA:272(A):U:H5'' | 1.95 | 0.48 |
| 52:DS:11:VAL:O | 52:DS:13:ASP:N | 2.46 | 0.48 |
| 1:AA:898:U:O2' | 27:A3:42:ALA:O | 2.29 | 0.48 |
| 34:BA:429:U:H3' | 37:BD:9:CYS:SG | 2.53 | 0.48 |
| 1:AA:1890:A:N6 | 1:AA:1905:G:O2' | 2.45 | 0.48 |
| 1:AA:537:G:N7 | 65:AA:4769:HOH:O | 2.34 | 0.48 |
| 1:AA:1117:G:H1' | 1:AA:1135:G:C8 | 2.48 | 0.48 |
| 1:CA:1091:G:H2' | 1:CA:1092:C:C6 | 2.49 | 0.48 |
| 14:AQ:56:ARG:HH12 | 56:BW:52:G:H4' | 1.78 | 0.48 |
| 34:DA:1051:C:H2' | 34:DA:1052:U:H6 | 1.78 | 0.48 |
| 34:DA:1001(A):G:O6 | 34:DA:1039:C:N4 | 2.37 | 0.48 |
| 59:BZ:-29:LEU:H | 59:BZ:-29:LEU:CD2 | 2.26 | 0.48 |
| 4:CD:2:ALA:O | 4:CD:3:VAL:HB | 2.13 | 0.48 |
| 34:BA:1014:A:H4' | 52:BS:14:HIS:CE1 | 2.48 | 0.48 |
| 6:AF:53:THR:HG22 | 6:AF:56:GLU:HG3 | 1.95 | 0.48 |
| 35:DB:219:VAL:O | 35:DB:222:ILE:HG12 | 2.13 | 0.48 |
| 10:AL:112:MET:HG2 | 10:AL:113:PRO:HD3 | 1.94 | 0.48 |
| 1:AA:556:C:OP1 | 1:AA:584:G:N1 | 2.45 | 0.48 |
| 15:AR:86:ARG:NH2 | 15:AR:87:TYR:OH | 2.44 | 0.48 |
| 40:DG:93:PRO:HA | 40:DG:96:GLN:HE21 | 1.78 | 0.48 |
| 1:AA:1492:C:H2' | 1:AA:1493:C:H6 | 1.78 | 0.48 |
| 1:AA:311:C:H2' | 1:AA:312:C:C6 | 2.48 | 0.48 |
| 58:BY:28:G:H2' | 58:BY:29:G:H8 | 1.78 | 0.48 |
| 36:DC:39:ILE:O | 36:DC:43:LEU:HG | 2.13 | 0.48 |
| 1:AA:1425:A:H4' | 1:AA:1426:G:OP2 | 2.12 | 0.48 |
| 5:AE:120:TRP:CD2 | 5:AE:155:LYS:HG2 | 2.48 | 0.48 |
| 35:BB:229:VAL:HG12 | 35:BB:230:VAL:H | 1.77 | 0.48 |
| 13:AP:83:VAL:HG13 | 13:AP:112:LEU:HD21 | 1.94 | 0.48 |
| 1:CA:2132:U:C4 | 3:CC:6:LYS:CE | 2.94 | 0.48 |
| 1:AA:1068:G:N7 | 11:AN:66:LYS:HE2 | 2.28 | 0.48 |
| 48:DO:24:SER:O | 48:DO:28:GLN:HG3 | 2.12 | 0.48 |
| 1:AA:1098:C:H2' | 1:AA:1099:C:C6 | 2.48 | 0.48 |
| 1:CA:2356:C:H2' | 1:CA:2357:U:O4' | 2.14 | 0.48 |
| 34:DA:363:A:C5 | 45:DL:31:PRO:HD2 | 2.47 | 0.48 |
| 1:AA:1117:G:H21 | 1:AA:1135:G:HO2' | 1.61 | 0.48 |
| 37:BD:98:GLU:OE1 | 37:BD:107:ARG:NH1 | 2.46 | 0.48 |
| 34:BA:91:C:H5' | 34:BA:92:C:OP2 | 2.14 | 0.48 |
| 34:DA:428:G:OP2 | 37:DD:10:ARG:NH1 | 2.47 | 0.48 |
| 1:AA:2331:G:C2 | 16:AS:3:ARG:HA | 2.47 | 0.48 |
| 34:BA:1239:A:C4 | 34:BA:1298:C:N4 | 2.81 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DB:111:ARG:HG2 | 35:DB:111:ARG:HH11 | 1.78 | 0.48 |
| 20:CW:60:ASN:N | 20:CW:60:ASN:HD22 | 2.11 | 0.48 |
| 1:CA:2364:C:H2' | 1:CA:2365:G:O4' | 2.13 | 0.48 |
| 34:DA:1355:G:H2' | 34:DA:1356:G:H8 | 1.78 | 0.48 |
| 1:CA:2522:U:O2' | 1:CA:2647:U:OP1 | 2.24 | 0.48 |
| 59:DZ:103:GLY:H | 59:DZ:130:VAL:HG23 | 1.77 | 0.48 |
| 11:CN:128:HIS:CE1 | 11:CN:135:PRO:HG2 | 2.48 | 0.48 |
| 32:C8:33:ASN:HA | 32:C8:36:LYS:HD3 | 1.95 | 0.48 |
| 27:A3:23:LEU:HD13 | 27:A3:50:VAL:HG11 | 1.95 | 0.48 |
| 4:AD:35:LYS:HB2 | 4:AD:36:PRO:HD2 | 1.95 | 0.48 |
| 35:BB:27:LYS:O | 35:BB:194:PRO:HG2 | 2.12 | 0.48 |
| 52:BS:51:VAL:O | 52:BS:58:VAL:N | 2.44 | 0.48 |
| 4:AD:124:PRO:O | 4:AD:126:GLN:N | 2.46 | 0.48 |
| 42:BI:93:ARG:HB2 | 42:BI:93:ARG:NH1 | 2.29 | 0.48 |
| 34:BA:1325:C:H2' | 34:BA:1326:C:C6 | 2.48 | 0.48 |
| 1:CA:2163:C:C5 | 1:CA:2164:C:H1' | 2.49 | 0.48 |
| 37:BD:187:ARG:HG2 | 37:BD:188:LEU:N | 2.29 | 0.48 |
| 37:BD:98:GLU:OE1 | 37:BD:103:ASN:ND2 | 2.35 | 0.48 |
| 34:DA:1208:C:H2' | 34:DA:1209:C:H6 | 1.79 | 0.48 |
| 35:BB:178:ARG:HH22 | 41:BH:68:ARG:HH12 | 1.60 | 0.48 |
| 1:CA:848:G:N9 | 1:CA:933:A:H8 | 2.11 | 0.48 |
| 35:DB:16:HIS:HD2 | 35:DB:204:ASN:HB3 | 1.79 | 0.48 |
| 1:AA:2584:A:N7 | 5:AE:144:ARG:HD2 | 2.27 | 0.48 |
| 59:BZ:150:ILE:O | 59:BZ:154:GLN:HG3 | 2.13 | 0.48 |
| 59:DZ:606:MET:O | 59:DZ:646:PHE:HA | 2.14 | 0.48 |
| 34:BA:109:A:H4' | 34:BA:110:C:OP2 | 2.13 | 0.48 |
| 40:BG:50:ILE:HD11 | 40:BG:58:PRO:HA | 1.95 | 0.48 |
| 6:CF:51:THR:O | 6:CF:93:LYS:HE2 | 2.13 | 0.48 |
| 12:CO:2:ILE:HD12 | 12:CO:6:THR:HG21 | 1.95 | 0.48 |
| 14:AQ:54:MET:HG3 | 14:AQ:117:ALA:HB1 | 1.96 | 0.48 |
| 1:AA:662:A:H4' | 1:AA:663:G:O5' | 2.14 | 0.48 |
| 25:A1:8:SER:OG | 25:A1:10:LYS:HG3 | 2.13 | 0.48 |
| 1:AA:2686:G:H5' | 12:AO:26:LYS:HE2 | 1.95 | 0.48 |
| 25:A1:5:CYS:SG | 25:A1:62:VAL:HG23 | 2.53 | 0.48 |
| 14:CQ:75:THR:HA | 14:CQ:89:ASN:O | 2.12 | 0.48 |
| 40:BG:152:ALA:O | 40:BG:155:ARG:HB3 | 2.13 | 0.48 |
| 6:AF:8:GLN:HE22 | 6:AF:21:ALA:HB2 | 1.78 | 0.48 |
| 2:AB:48:A:H4' | 16:AS:95:HIS:HD2 | 1.79 | 0.48 |
| 1:AA:504:A:N1 | 1:AA:525:G:H4' | 2.27 | 0.48 |
| 34:DA:769:G:O2' | 34:DA:770:C:H5' | 2.13 | 0.48 |
| 44:BK:62:GLN:HB2 | 44:BK:93:GLN:HG3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:AR:38:VAL:HG22 | 15:AR:112:ALA:HB2 | 1.95 | 0.48 |
| 45:DL:24:VAL:HG12 | 45:DL:27:LEU:HB2 | 1.95 | 0.48 |
| 34:BA:153:C:N4 | 34:BA:168:G:H1 | 2.11 | 0.48 |
| 59:BZ:221:ALA:HB2 | 59:BZ:227:ILE:HG22 | 1.95 | 0.48 |
| 1:AA:945:A:O2' | 1:AA:946:A:H8 | 1.96 | 0.48 |
| 1:CA:848:G:C4 | 1:CA:933:A:H8 | 2.32 | 0.48 |
| 56:BW:9:A:H1' | 56:BW:45:U:O2' | 2.14 | 0.48 |
| 35:DB:210:SER:OG | 35:DB:211:ILE:N | 2.46 | 0.48 |
| 1:CA:2695:C:H2' | 1:CA:2696:U:C6 | 2.49 | 0.48 |
| 59:BZ:2:LYS:HA | 59:BZ:5:LEU:HD12 | 1.95 | 0.48 |
| 34:DA:1347:G:H5'' | 42:DI:107:ARG:HB3 | 1.94 | 0.48 |
| 24:A0:32:ARG:H | 24:A0:35:ASN:ND2 | 2.11 | 0.48 |
| 14:CQ:38:GLU:HA | 14:CQ:99:PRO:HG3 | 1.96 | 0.48 |
| 38:BE:84:PHE:HB3 | 38:BE:134:ALA:HB2 | 1.95 | 0.48 |
| 4:AD:10:THR:OG1 | 4:AD:13:ARG:HB2 | 2.13 | 0.48 |
| 1:AA:746:A:H2' | 1:AA:747:G:O4' | 2.13 | 0.48 |
| 6:CF:120:GLU:HB2 | 6:CF:122:LYS:HG2 | 1.95 | 0.48 |
| 52:DS:27:GLU:HB3 | 52:DS:28:LYS:HD3 | 1.96 | 0.48 |
| 1:CA:1274:A:N3 | 1:CA:1297:C:H1' | 2.28 | 0.48 |
| 2:CB:3:C:H2' | 2:CB:4:C:H6 | 1.78 | 0.48 |
| 1:CA:2235:G:H2' | 1:CA:2236:C:C6 | 2.48 | 0.48 |
| 59:BZ:336:THR:O | 59:BZ:339:SER:OG | 2.24 | 0.48 |
| 35:BB:189:ASP:N | 35:BB:189:ASP:OD1 | 2.33 | 0.48 |
| 1:AA:2372:A:H2' | 1:AA:2373:A:O4' | 2.14 | 0.48 |
| 59:DZ:149:VAL:O | 59:DZ:153:MET:HB2 | 2.12 | 0.48 |
| 1:AA:908:A:C2 | 1:AA:963:A:C4 | 3.01 | 0.48 |
| 34:DA:690:G:H2' | 34:DA:691:G:C8 | 2.49 | 0.48 |
| 1:CA:1860:G:H5' | 3:CC:206:LYS:HE2 | 1.87 | 0.48 |
| 4:AD:273:ARG:HG2 | 4:AD:274:ARG:H | 1.79 | 0.48 |
| 59:DZ:169:GLY:N | 59:DZ:170:ARG:NH1 | 2.61 | 0.48 |
| 1:CA:2163:C:H5 | 1:CA:2164:C:H1' | 1.78 | 0.48 |
| 34:DA:586:C:O2' | 34:DA:878:G:H4' | 2.12 | 0.48 |
| 34:BA:736:C:H2' | 34:BA:737:A:H8 | 1.78 | 0.48 |
| 46:BM:86:CYS:HB2 | 52:BS:73:GLU:HB3 | 1.96 | 0.48 |
| 28:C4:62:ARG:H | 28:C4:62:ARG:NE | 2.11 | 0.48 |
| 1:AA:878:G:O2' | 13:AP:38:GLN:NE2 | 2.47 | 0.48 |
| 35:BB:101:MET:HA | 35:BB:108:ILE:HD12 | 1.94 | 0.48 |
| 53:DT:54:LYS:HA | 53:DT:57:ARG:CZ | 2.44 | 0.48 |
| 6:AF:118:ALA:HB2 | 6:AF:123:LEU:HD23 | 1.95 | 0.48 |
| 1:CA:65:C:H2' | 1:CA:66:C:H6 | 1.79 | 0.48 |
| 4:CD:94:LEU:HD22 | 4:CD:95:LEU:H | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:2107:C:H42 | 1:CA:2182:G:H1 | 1.61 | 0.48 |
| 5:AE:174:ASP:OD1 | 5:AE:175:VAL:N | 2.47 | 0.48 |
| 25:A1:50:ARG:HG2 | 25:A1:59:THR:HB | 1.95 | 0.48 |
| 34:DA:448:A:P | 34:DA:485:G:H22 | 2.36 | 0.48 |
| 34:BA:1053:G:N7 | 34:BA:1200:C:H5'' | 2.28 | 0.48 |
| 34:BA:1233:G:H2' | 34:BA:1234:C:C6 | 2.49 | 0.48 |
| 14:AQ:31:ASP:HB2 | 14:AQ:32:TYR:CD2 | 2.49 | 0.48 |
| 1:CA:1025:G:C4 | 1:CA:1135:C:H1' | 2.48 | 0.48 |
| 9:CK:118:THR:N | 9:CK:121:ASP:O | 2.47 | 0.48 |
| 1:AA:518:G:O6 | 65:AA:4472:HOH:O | 2.18 | 0.48 |
| 57:BX:19:G:H5'' | 57:BX:60:U:O4 | 2.12 | 0.48 |
| 1:CA:2359:C:H2' | 1:CA:2360:A:O4' | 2.13 | 0.48 |
| 34:DA:1238:A:N3 | 34:DA:1241:G:O2' | 2.42 | 0.48 |
| 41:BH:114:THR:HG22 | 41:BH:130:GLY:O | 2.13 | 0.48 |
| 44:BK:20:TYR:HB2 | 44:BK:31:THR:HG23 | 1.94 | 0.48 |
| 7:AG:48:GLU:HA | 7:AG:51:ARG:NE | 2.27 | 0.48 |
| 43:DJ:5:ARG:N | 43:DJ:73:ASP:HA | 2.29 | 0.48 |
| 34:DA:1318:A:H5'' | 52:DS:3:ARG:NH2 | 2.29 | 0.48 |
| 6:CF:192:LEU:HD22 | 6:CF:194:MET:HG3 | 1.96 | 0.48 |
| 37:DD:8:VAL:HG23 | 37:DD:11:LEU:HD22 | 1.96 | 0.48 |
| 1:AA:908:A:H2' | 1:AA:909:G:O4' | 2.14 | 0.48 |
| 41:DH:20:TYR:HD2 | 41:DH:65:TYR:CD2 | 2.32 | 0.48 |
| 34:DA:1499:A:H1' | 34:DA:1520:G:H5' | 1.95 | 0.48 |
| 59:DZ:556:ILE:HD13 | 59:DZ:558:PHE:HD2 | 1.78 | 0.48 |
| 1:CA:1005:C:H2' | 1:CA:1006:C:C6 | 2.49 | 0.48 |
| 34:BA:1205:U:O2' | 36:BC:195:VAL:HG23 | 2.14 | 0.48 |
| 23:AZ:152:ALA:O | 23:AZ:155:LEU:HB2 | 2.14 | 0.48 |
| 1:CA:2507:C:H2' | 1:CA:2508:G:O4' | 2.14 | 0.48 |
| 23:AZ:41:LEU:O | 23:AZ:41:LEU:HD22 | 2.13 | 0.48 |
| 15:CR:97:VAL:HG22 | 15:CR:114:VAL:HG13 | 1.96 | 0.48 |
| 34:BA:1144:G:N2 | 34:BA:1146:A:H62 | 2.12 | 0.48 |
| 1:CA:697:C:H2' | 1:CA:698:C:C6 | 2.48 | 0.48 |
| 1:CA:919:G:N2 | 1:CA:2269:A:OP2 | 2.47 | 0.48 |
| 35:DB:121:LEU:H | 35:DB:125:PRO:HG2 | 1.78 | 0.48 |
| 1:CA:1142(A):A:C4 | 1:CA:1144:G:C8 | 3.02 | 0.48 |
| 59:DZ:514:VAL:HA | 59:DZ:564:LYS:O | 2.13 | 0.48 |
| 1:AA:597:C:N3 | 5:AE:145:LYS:NZ | 2.53 | 0.48 |
| 36:BC:8:ILE:HD13 | 36:BC:184:TYR:HB3 | 1.94 | 0.48 |
| 34:BA:1299:A:H5'' | 34:BA:1299:A:N3 | 2.29 | 0.48 |
| 34:BA:437:U:O2' | 37:BD:123:HIS:HD2 | 1.97 | 0.48 |
| 1:AA:1210:G:H2' | 1:AA:1211:U:C6 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:2181:G:H2' | 1:AA:2182:G:H8 | 1.78 | 0.48 |
| 1:AA:311:C:H2' | 1:AA:312:C:H6 | 1.78 | 0.48 |
| 39:BF:82:ARG:HB3 | 39:BF:85:VAL:HG23 | 1.96 | 0.48 |
| 40:DG:94:ARG:O | 40:DG:97:GLN:HB3 | 2.14 | 0.48 |
| 43:BJ:44:VAL:HG13 | 43:BJ:66:ARG:HG2 | 1.95 | 0.48 |
| 1:CA:38:A:H2' | 1:CA:39:C:C6 | 2.49 | 0.48 |
| 1:AA:1769:G:H2' | 1:AA:1770:A:H8 | 1.79 | 0.48 |
| 38:DE:16:THR:OG1 | 38:DE:17:ALA:N | 2.45 | 0.48 |
| 1:AA:313:A:H61 | 1:AA:375:G:H1' | 1.79 | 0.48 |
| 11:AN:112:LEU:HD12 | 11:AN:112:LEU:O | 2.14 | 0.48 |
| 1:AA:997:G:OP1 | 14:AQ:16:ARG:NH2 | 2.47 | 0.48 |
| 1:CA:1384:A:N3 | 1:CA:1405:U:H1' | 2.29 | 0.48 |
| 8:CH:164:TYR:HB2 | 8:CH:167:GLU:HB2 | 1.96 | 0.48 |
| 1:AA:1071:G:C4 | 1:AA:1180:C:H1' | 2.49 | 0.48 |
| 21:AX:31:HIS:CD2 | 21:AX:32:PRO:HD2 | 2.48 | 0.48 |
| 59:BZ:21:ILE:HD11 | 59:BZ:117:GLN:NE2 | 2.29 | 0.48 |
| 12:CO:102:VAL:HB | 12:CO:106:LEU:HD12 | 1.94 | 0.48 |
| 58:BY:58:A:C2 | 58:BY:60:U:H2' | 2.48 | 0.48 |
| 59:BZ:132:ARG:HD3 | 59:BZ:132:ARG:N | 2.28 | 0.48 |
| 34:BA:49:U:C2 | 34:BA:361:G:N2 | 2.82 | 0.48 |
| 1:AA:2567:U:H5'' | 1:AA:2568:C:OP2 | 2.14 | 0.48 |
| 34:BA:1279:A:H5'' | 34:BA:1280:A:OP1 | 2.14 | 0.48 |
| 34:DA:70:G:H1 | 34:DA:99:U:H3 | 1.60 | 0.48 |
| 34:BA:1189:C:H5'' | 34:BA:1190:G:OP2 | 2.14 | 0.48 |
| 57:DX:49:G:N2 | 57:DX:66:C:C2 | 2.82 | 0.48 |
| 38:DE:92:LYS:HB3 | 38:DE:119:LEU:HB2 | 1.96 | 0.48 |
| 1:AA:116:A:C8 | 1:AA:117:A:C8 | 3.02 | 0.48 |
| 37:BD:31:CYS:SG | 37:BD:33:MET:N | 2.87 | 0.48 |
| 50:DQ:95:TYR:HA | 50:DQ:98:LEU:HD12 | 1.96 | 0.48 |
| 52:BS:15:LEU:O | 52:BS:19:VAL:HG23 | 2.14 | 0.48 |
| 23:AZ:29:TYR:HB3 | 23:AZ:34:ASN:ND2 | 2.17 | 0.48 |
| 34:BA:1226:C:H4' | 52:BS:80:TYR:CZ | 2.49 | 0.48 |
| 59:DZ:170:ARG:HA | 59:DZ:170:ARG:HD3 | 1.62 | 0.48 |
| 1:CA:1830:C:OP2 | 65:CA:4300:HOH:O | 2.20 | 0.48 |
| 28:A4:61:ARG:HH21 | 52:BS:42:PRO:CD | 2.26 | 0.48 |
| 50:DQ:5:VAL:O | 50:DQ:6:LEU:HD13 | 2.14 | 0.48 |
| 34:DA:689:C:P | 44:DK:46:GLY:HA3 | 2.54 | 0.48 |
| 34:DA:392:G:H2' | 34:DA:393:A:C8 | 2.49 | 0.48 |
| 15:CR:17:ARG:O | 15:CR:20:LEU:HB3 | 2.14 | 0.48 |
| 1:AA:1566:U:H2' | 1:AA:1567:G:O4' | 2.14 | 0.48 |
| 38:DE:10:MET:HB3 | 38:DE:13:ILE:HD11 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:AA:2339:A:H2' | 1:AA:2340:A:C8 | 2.48 | 0.48 |
| 18:CU:32:PHE:HZ | 18:CU:36:ARG:HH21 | 1.61 | 0.48 |
| 4:AD:108:PRO:HB3 | 4:AD:143:HIS:CE1 | 2.49 | 0.48 |
| 4:CD:134:ARG:NH1 | 4:CD:188:GLU:OE2 | 2.47 | 0.48 |
| 1:CA:1220:A:OP2 | 18:CU:19:LYS:NZ | 2.47 | 0.48 |
| 34:DA:300:A:H2' | 34:DA:301:G:O4' | 2.14 | 0.48 |
| 59:DZ:328:ILE:HD12 | 59:DZ:377:VAL:HG12 | 1.96 | 0.48 |
| 1:CA:660:G:O3' | 6:CF:38:ARG:NH2 | 2.47 | 0.48 |
| 58:BY:9:A:H1' | 58:BY:45:U:H2' | 1.96 | 0.48 |
| 35:DB:76:GLN:NE2 | 35:DB:206:ASP:O | 2.47 | 0.48 |
| 14:AQ:57:HIS:CE1 | 14:AQ:116:GLU:HG2 | 2.49 | 0.48 |
| 30:C6:25:LYS:HE3 | 30:C6:30:THR:O | 2.13 | 0.48 |
| 34:DA:993:G:O6 | 34:DA:1045:C:N4 | 2.41 | 0.47 |
| 38:BE:10:MET:HA | 38:BE:32:VAL:HG22 | 1.95 | 0.47 |
| 34:DA:1273:G:H3' | 34:DA:1274:G:C8 | 2.48 | 0.47 |
| 7:CG:18:GLU:HG3 | 7:CG:18:GLU:O | 2.12 | 0.47 |
| 39:DF:30:LEU:HD23 | 39:DF:75:LEU:HD21 | 1.96 | 0.47 |
| 34:BA:411:A:C8 | 34:BA:413:G:C8 | 3.01 | 0.47 |
| 1:CA:1514:U:H2' | 1:CA:1515:G:C8 | 2.49 | 0.47 |
| 35:BB:20:GLU:HB3 | 35:BB:190:THR:OG1 | 2.14 | 0.47 |
| 22:CY:13:VAL:HB | 22:CY:72:VAL:HG13 | 1.95 | 0.47 |
| 1:CA:218:A:C2 | 1:CA:235:U:H4' | 2.49 | 0.47 |
| 1:CA:2395:C:O2' | 25:C1:30:VAL:HG22 | 2.14 | 0.47 |
| 5:AE:141:ILE:HD12 | 5:AE:150:VAL:HG21 | 1.96 | 0.47 |
| 21:AX:88:LYS:NZ | 21:AX:90:GLU:OE1 | 2.47 | 0.47 |
| 53:BT:21:LYS:O | 53:BT:25:ARG:HG3 | 2.15 | 0.47 |
| 24:C0:23:VAL:HG22 | 24:C0:38:VAL:HG22 | 1.96 | 0.47 |
| 4:AD:146:GLU:HB2 | 4:AD:189:CYS:HB3 | 1.96 | 0.47 |
| 34:DA:1375:A:O2' | 40:DG:29:LYS:NZ | 2.47 | 0.47 |
| 8:CH:54:ARG:HD3 | 8:CH:65:HIS:ND1 | 2.29 | 0.47 |
| 19:AV:5:VAL:HG21 | 19:AV:35:LEU:HD23 | 1.96 | 0.47 |
| 34:DA:563:A:H2' | 34:DA:567:G:C8 | 2.49 | 0.47 |
| 34:DA:1342:C:H4' | 42:DI:125:TYR:HB3 | 1.95 | 0.47 |
| 1:CA:2712(A):A:H5'' | 1:CA:2713:A:OP2 | 2.13 | 0.47 |
| 34:DA:920:U:C2 | 34:DA:921:U:C5 | 3.02 | 0.47 |
| 34:DA:714:G:H2' | 34:DA:715:A:C8 | 2.49 | 0.47 |
| 34:DA:1239:A:N6 | 34:DA:1299:A:H62 | 2.11 | 0.47 |
| 1:CA:2611:U:H3' | 1:CA:2611:U:OP2 | 2.14 | 0.47 |
| 1:AA:354:A:H2 | 1:AA:1255:A:C2' | 2.26 | 0.47 |
| 59:BZ:146:LEU:HD12 | 59:BZ:167:PRO:CD | 2.44 | 0.47 |
| 22:CY:37:VAL:HG21 | 22:CY:72:VAL:HG21 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:BP:22:THR:HA | 49:BP:33:ILE:HG12 | 1.96 | 0.47 |
| 59:BZ:348:ARG:HG2 | 59:BZ:348:ARG:NH1 | 2.29 | 0.47 |
| 59:BZ:168:ILE:HD11 | 59:BZ:178:ILE:HG13 | 1.96 | 0.47 |
| 35:DB:141:GLU:HG2 | 35:DB:145:LEU:HD12 | 1.97 | 0.47 |
| 34:DA:149:A:H2' | 34:DA:150:C:C6 | 2.49 | 0.47 |
| 34:BA:708:C:H2' | 34:BA:709:G:H8 | 1.79 | 0.47 |
| 34:BA:814:A:H2' | 34:BA:816:A:H5'' | 1.96 | 0.47 |
| 59:BZ:416:LYS:HB2 | 59:BZ:474:ALA:HA | 1.96 | 0.47 |
| 35:DB:82:ARG:HG3 | 35:DB:92:TYR:OH | 2.14 | 0.47 |
| 35:BB:170:GLU:O | 35:BB:174:VAL:HG23 | 2.14 | 0.47 |
| 1:AA:2317:A:H5'' | 7:AG:134:GLY:HA3 | 1.96 | 0.47 |
| 6:AF:161:GLU:HG2 | 6:AF:164:ARG:NH2 | 2.29 | 0.47 |
| 1:CA:1641:A:H2' | 1:CA:1642:G:O4' | 2.14 | 0.47 |
| 51:DR:26:LEU:HD21 | 51:DR:42:ARG:HE | 1.79 | 0.47 |
| 1:CA:930:U:H4' | 1:CA:931:G:O5' | 2.14 | 0.47 |
| 1:CA:2693:A:H2' | 1:CA:2694:G:H8 | 1.78 | 0.47 |
| 34:DA:927:G:H4' | 34:DA:927:G:OP2 | 2.12 | 0.47 |
| 34:BA:164:U:H2' | 34:BA:165:C:C6 | 2.49 | 0.47 |
| 36:BC:52:LEU:HD23 | 36:BC:54:ARG:H | 1.79 | 0.47 |
| 34:DA:1041:A:C6 | 34:DA:1042:G:C6 | 3.02 | 0.47 |
| 34:DA:1301:U:O2' | 34:DA:1302:U:H5' | 2.14 | 0.47 |
| 1:AA:2074:G:H4' | 5:AE:143:ASN:O | 2.14 | 0.47 |
| 1:CA:185:U:H4' | 1:CA:218:A:H4' | 1.95 | 0.47 |
| 36:BC:22:TRP:CH2 | 36:BC:32:LEU:HB2 | 2.49 | 0.47 |
| 8:AH:89:ILE:HD12 | 8:AH:96:ALA:HB2 | 1.95 | 0.47 |
| 34:BA:1020:U:H2' | 34:BA:1021:G:C8 | 2.49 | 0.47 |
| 1:CA:500:G:N1 | 1:CA:503:A:OP2 | 2.47 | 0.47 |
| 12:AO:87:ILE:HD12 | 12:AO:91:LEU:HA | 1.96 | 0.47 |
| 37:DD:68:TYR:CE1 | 37:DD:97:LEU:HB3 | 2.49 | 0.47 |
| 34:DA:429:U:H3' | 37:DD:9:CYS:SG | 2.54 | 0.47 |
| 34:DA:1338:G:C6 | 34:DA:1339:A:C6 | 3.02 | 0.47 |
| 52:BS:52:TYR:HA | 52:BS:56:GLN:O | 2.14 | 0.47 |
| 34:DA:636:U:H2' | 34:DA:637:G:C8 | 2.49 | 0.47 |
| 1:AA:142:G:H1' | 21:AX:37:THR:HG21 | 1.96 | 0.47 |
| 34:BA:927:G:OP2 | 34:BA:927:G:H4' | 2.13 | 0.47 |
| 34:BA:1229:A:OP2 | 46:BM:114:ARG:HD3 | 2.14 | 0.47 |
| 59:BZ:534:ILE:HD11 | 59:BZ:570:GLY:HA3 | 1.96 | 0.47 |
| 1:AA:1358:U:H4' | 1:AA:1359:U:O5' | 2.14 | 0.47 |
| 1:CA:2203:U:O4' | 4:CD:151:LYS:HE2 | 2.14 | 0.47 |
| 1:CA:2356:C:O3' | 24:C0:20:ARG:HD3 | 2.14 | 0.47 |
| 10:CL:103:GLN:HA | 10:CL:106:GLU:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:C8:10:ALA:CB | 32:C8:62:LEU:HD21 | 2.43 | 0.47 |
| 59:BZ:217:VAL:HG13 | 59:BZ:242:LEU:HD21 | 1.95 | 0.47 |
| 34:BA:1255:G:N7 | 43:BJ:43:ARG:NH2 | 2.62 | 0.47 |
| 1:AA:354:A:O2' | 1:AA:355:A:H8 | 1.96 | 0.47 |
| 34:BA:436:C:H2' | 34:BA:437:U:C6 | 2.49 | 0.47 |
| 34:BA:354:G:C2' | 34:BA:355:C:H5' | 2.44 | 0.47 |
| 1:AA:225:C:H2' | 1:AA:226:C:H6 | 1.78 | 0.47 |
| 1:AA:826:U:P | 4:AD:49:ILE:HD12 | 2.55 | 0.47 |
| 34:DA:1342:C:H1' | 42:DI:124:GLN:HE21 | 1.79 | 0.47 |
| 35:DB:134:GLU:O | 35:DB:138:LEU:HG | 2.15 | 0.47 |
| 1:CA:2391:G:OP2 | 32:C8:32:LEU:HD23 | 2.13 | 0.47 |
| 59:BZ:542:VAL:HG23 | 59:BZ:582:PHE:O | 2.14 | 0.47 |
| 1:AA:955:A:H2' | 1:AA:958:C:C5 | 2.49 | 0.47 |
| 16:AS:83:LYS:HB2 | 16:AS:83:LYS:HE2 | 1.60 | 0.47 |
| 34:DA:374:A:C6 | 34:DA:375:U:C4 | 3.02 | 0.47 |
| 34:DA:194:C:H2' | 34:DA:195:A:H5'' | 1.97 | 0.47 |
| 1:CA:1266:G:O4' | 20:CW:15:ARG:NH2 | 2.47 | 0.47 |
| 7:AG:79:ASN:OD1 | 7:AG:79:ASN:N | 2.48 | 0.47 |
| 35:BB:212:GLN:NE2 | 35:BB:234:PRO:O | 2.47 | 0.47 |
| 3:CC:180:SER:O | 3:CC:181:PHE:O | 2.33 | 0.47 |
| 3:AC:30:VAL:CG2 | 3:AC:31:LYS:H | 2.27 | 0.47 |
| 49:BP:74:LEU:O | 49:BP:79:VAL:HG23 | 2.13 | 0.47 |
| 3:AC:184:GLU:O | 3:AC:188:ASP:OD2 | 2.31 | 0.47 |
| 1:CA:2166:G:N7 | 1:CA:2168:G:N2 | 2.62 | 0.47 |
| 1:CA:2171:A:N3 | 1:CA:2172:U:N3 | 2.62 | 0.47 |
| 52:BS:65:ASN:HD22 | 52:BS:65:ASN:N | 2.12 | 0.47 |
| 1:CA:870:A:C2 | 1:CA:908:C:C2 | 3.02 | 0.47 |
| 34:DA:321:A:N7 | 34:DA:328:C:O2' | 2.35 | 0.47 |
| 58:BY:19:G:H4' | 58:BY:20:U:OP2 | 2.12 | 0.47 |
| 1:AA:1105:G:H1 | 1:AA:1125:C:H42 | 1.61 | 0.47 |
| 52:BS:36:ARG:HB3 | 52:BS:72:GLY:CA | 2.44 | 0.47 |
| 1:CA:1847:A:H3' | 1:CA:1848:A:H5' | 1.97 | 0.47 |
| 1:CA:757:U:H2' | 1:CA:758:C:O4' | 2.15 | 0.47 |
| 1:CA:1486:A:O2' | 1:CA:1487:G:H5' | 2.14 | 0.47 |
| 34:BA:586:C:O2' | 34:BA:878:G:H4' | 2.14 | 0.47 |
| 1:CA:2440:C:OP2 | 65:CA:4113:HOH:O | 2.20 | 0.47 |
| 19:CV:29:PRO:HA | 19:CV:61:VAL:HG22 | 1.95 | 0.47 |
| 14:CQ:24:GLY:HA2 | 14:CQ:67:ARG:NH2 | 2.29 | 0.47 |
| 1:CA:1054:A:N6 | 1:CA:1055:G:C6 | 2.82 | 0.47 |
| 34:DA:1264:C:H2' | 34:DA:1265:G:C8 | 2.49 | 0.47 |
| 13:AP:134:ALA:O | 13:AP:138:LEU:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|----------------------|--------------------------|-------------------|
| 12:AO:35:VAL:HG11 | 12:AO:103:ALA:CB | 2.44 | 0.47 |
| 1:CA:1477:A:H2' | 1:CA:1478:G:O4' | 2.13 | 0.47 |
| 23:AZ:153:SER:HB3 | 23:AZ:167:PRO:HB3 | 1.97 | 0.47 |
| 48:BO:29:VAL:HG11 | 48:BO:81:LEU:HD21 | 1.97 | 0.47 |
| 36:DC:123:GLN:O | 36:DC:128:PHE:HB2 | 2.15 | 0.47 |
| 1:CA:2469:A:H2' | 1:CA:2470:G:O4' | 2.15 | 0.47 |
| 23:CZ:105:VAL:N | 23:CZ:139:VAL:O | 2.48 | 0.47 |
| 40:DG:50:ILE:HD11 | 40:DG:58:PRO:HB3 | 1.95 | 0.47 |
| 1:AA:592:U:C4 | 1:AA:593:G:C6 | 3.03 | 0.47 |
| 34:DA:633:G:H2' | 34:DA:634:C:C6 | 2.50 | 0.47 |
| 6:AF:150:GLY:HA2 | 6:AF:172:TRP:CD2 | 2.49 | 0.47 |
| 40:DG:75:VAL:HA | 40:DG:87:VAL:O | 2.15 | 0.47 |
| 1:CA:839:U:H2' | 1:CA:840:C:C6 | 2.50 | 0.47 |
| 16:CS:61:ASN:O | 16:CS:65:VAL:HG23 | 2.14 | 0.47 |
| 12:AO:17:ARG:HA | 12:AO:17:ARG:HD2 | 1.62 | 0.47 |
| 59:BZ:286:ILE:H | 59:BZ:286:ILE:HD13 | 1.79 | 0.47 |
| 59:BZ:325:LEU:HA | 59:BZ:325:LEU:HD23 | 1.75 | 0.47 |
| 1:CA:1319:G:C6 | 1:CA:1320:C:N4 | 2.82 | 0.47 |
| 11:CN:102:ALA:O | 11:CN:106:MET:HG3 | 2.15 | 0.47 |
| 33:A9:27:CYS:SG | 33:A9:28:GLU:N | 2.87 | 0.47 |
| 3:AC:180:SER:O | 3:AC:181:PHE:O | 2.32 | 0.47 |
| 43:DJ:49:VAL:HG12 | 43:DJ:61:GLU:O | 2.14 | 0.47 |
| 59:BZ:20:HIS:CE1 | 59:BZ:115:GLU:HB3 | 2.49 | 0.47 |
| 1:AA:2228:G:H2' | 1:AA:2229:A:C2 | 2.50 | 0.47 |
| 34:DA:1030(A):G:H2' | 34:DA:1030(B):C:H5'' | 1.97 | 0.47 |
| 1:CA:674:G:H1' | 6:CF:74:ARG:HD3 | 1.96 | 0.47 |
| 4:AD:206:LEU:HD23 | 4:AD:206:LEU:HA | 1.69 | 0.47 |
| 34:DA:1305:G:O2' | 34:DA:1331:G:N2 | 2.47 | 0.47 |
| 1:CA:2126:A:H61 | 1:CA:2172:U:H5' | 1.80 | 0.47 |
| 3:CC:42:VAL:HA | 3:CC:216:THR:O | 2.13 | 0.47 |
| 34:BA:1316:G:N2 | 34:BA:1318:A:H3' | 2.30 | 0.47 |
| 6:AF:101:LEU:HD12 | 6:AF:102:PRO:HD2 | 1.96 | 0.47 |
| 1:AA:1525:G:H2' | 1:AA:1526:G:H8 | 1.78 | 0.47 |
| 7:AG:63:ILE:HD13 | 7:AG:141:PHE:CG | 2.50 | 0.47 |
| 42:DI:23:ASN:OD1 | 42:DI:25:LYS:HE2 | 2.15 | 0.47 |
| 59:DZ:272:LEU:O | 59:DZ:276:VAL:HG23 | 2.14 | 0.47 |
| 36:BC:6:HIS:CD2 | 36:BC:7:PRO:HD2 | 2.49 | 0.47 |
| 34:DA:1278:U:H5' | 34:DA:1279:A:C5' | 2.44 | 0.47 |
| 36:DC:129:ALA:O | 36:DC:133:ALA:N | 2.41 | 0.47 |
| 1:AA:1109:G:N2 | 1:AA:1122:C:O2 | 2.48 | 0.47 |
| 7:CG:23:PHE:HB2 | 7:CG:25:TYR:CE1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:DX:67:C:C2' | 57:DX:68:C:H5' | 2.44 | 0.47 |
| 4:CD:72:LYS:HG3 | 4:CD:103:ARG:NH2 | 2.30 | 0.47 |
| 34:DA:1203:C:H2' | 34:DA:1204:A:H8 | 1.80 | 0.47 |
| 59:DZ:15:ILE:HA | 59:DZ:103:GLY:O | 2.14 | 0.47 |
| 34:BA:1233:G:H2' | 34:BA:1234:C:H6 | 1.80 | 0.47 |
| 38:DE:101:ILE:HG13 | 38:DE:119:LEU:HD23 | 1.96 | 0.47 |
| 59:BZ:484:ARG:NH1 | 59:BZ:559:PRO:HG2 | 2.30 | 0.47 |
| 49:BP:58:TYR:O | 49:BP:61:SER:OG | 2.22 | 0.47 |
| 2:CB:66:A:H61 | 2:CB:109:C:H5'' | 1.79 | 0.47 |
| 51:BR:51:LEU:HD23 | 51:BR:52:PRO:HD2 | 1.96 | 0.47 |
| 1:CA:2108:C:H2' | 1:CA:2109:U:C6 | 2.50 | 0.47 |
| 34:DA:1076:C:C2 | 34:DA:1082:G:N2 | 2.82 | 0.47 |
| 59:BZ:399:LEU:O | 59:BZ:401:SER:N | 2.48 | 0.47 |
| 59:BZ:399:LEU:C | 59:BZ:401:SER:H | 2.17 | 0.47 |
| 39:BF:15:ASP:OD1 | 39:BF:18:GLN:N | 2.39 | 0.47 |
| 1:CA:750:A:H2' | 1:CA:751:A:H5'' | 1.97 | 0.47 |
| 1:CA:479:A:N3 | 1:CA:481:G:H5'' | 2.29 | 0.47 |
| 14:CQ:11:LYS:NZ | 14:CQ:88:GLY:O | 2.32 | 0.47 |
| 1:AA:821:A:H2' | 1:AA:821:A:N3 | 2.29 | 0.47 |
| 7:AG:21:ARG:O | 7:AG:21:ARG:HG2 | 2.13 | 0.47 |
| 9:CK:70:GLU:O | 9:CK:72:ASP:N | 2.48 | 0.47 |
| 41:DH:109:ILE:HB | 41:DH:120:THR:HG22 | 1.97 | 0.47 |
| 22:AY:38:ILE:HD11 | 22:AY:66:PRO:HG3 | 1.97 | 0.47 |
| 57:DX:23:C:H2' | 57:DX:24:U:C6 | 2.50 | 0.47 |
| 29:C5:35:GLU:HG2 | 29:C5:51:TYR:CG | 2.49 | 0.47 |
| 47:DN:32:SER:O | 47:DN:40:CYS:HA | 2.15 | 0.47 |
| 2:CB:13:A:N1 | 2:CB:69:G:O2' | 2.40 | 0.47 |
| 34:DA:518:C:H5'' | 34:DA:519:C:C6 | 2.49 | 0.47 |
| 1:CA:747:U:O2 | 1:CA:2014:A:H1' | 2.15 | 0.47 |
| 1:AA:762:G:C2 | 48:BO:56:LEU:HD21 | 2.49 | 0.47 |
| 59:DZ:490:PRO:HG3 | 59:DZ:516:PRO:HD2 | 1.96 | 0.47 |
| 47:BN:3:ARG:HH21 | 47:BN:3:ARG:HB3 | 1.79 | 0.47 |
| 59:BZ:359:HIS:ND1 | 59:BZ:362:HIS:CE1 | 2.83 | 0.47 |
| 20:CW:29:LEU:O | 20:CW:33:ARG:HG3 | 2.15 | 0.47 |
| 3:CC:6:LYS:HA | 3:CC:9:ARG:NH1 | 2.30 | 0.47 |
| 59:BZ:405:PRO:CB | 59:BZ:406:GLU:HA | 2.45 | 0.47 |
| 59:BZ:114:VAL:O | 59:BZ:115:GLU:HB2 | 2.15 | 0.47 |
| 1:AA:894:U:H5 | 1:AA:978:A:H62 | 1.58 | 0.47 |
| 34:DA:713:G:H2' | 34:DA:714:G:C8 | 2.50 | 0.47 |
| 28:C4:48:ARG:HA | 28:C4:48:ARG:HD3 | 1.76 | 0.47 |
| 3:AC:68:GLY:N | 3:AC:189:ASN:ND2 | 2.62 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DA:1121:U:H2' | 34:DA:1122:U:H5' | 1.97 | 0.47 |
| 1:CA:1478:G:HO2' | 1:CA:1558:A:H2 | 1.60 | 0.47 |
| 52:BS:27:GLU:HG2 | 52:BS:47:HIS:NE2 | 2.29 | 0.47 |
| 1:CA:1059:G:H5' | 1:CA:1060:U:O5' | 2.15 | 0.47 |
| 1:AA:2147:G:OP1 | 3:AC:71:LYS:HE2 | 2.15 | 0.47 |
| 12:AO:23:ARG:HG3 | 12:AO:24:VAL:N | 2.29 | 0.47 |
| 1:CA:1340:U:OP1 | 21:CX:16:LYS:NZ | 2.43 | 0.47 |
| 20:CW:14:PRO:HG2 | 20:CW:78:GLU:HG2 | 1.96 | 0.47 |
| 5:AE:12:THR:HG22 | 5:AE:13:ARG:H | 1.80 | 0.47 |
| 34:DA:364:A:H2' | 34:DA:365:U:C6 | 2.50 | 0.47 |
| 59:DZ:408:VAL:O | 59:DZ:482:ALA:HB3 | 2.15 | 0.47 |
| 6:CF:150:GLY:HA2 | 6:CF:172:TRP:CE3 | 2.49 | 0.47 |
| 1:CA:196:A:H2' | 1:CA:196:A:N3 | 2.30 | 0.47 |
| 49:DP:60:LEU:HD13 | 49:DP:60:LEU:HA | 1.70 | 0.47 |
| 1:AA:2623:U:H6 | 1:AA:2623:U:H5' | 1.80 | 0.47 |
| 18:AU:74:LEU:HD12 | 18:AU:74:LEU:H | 1.79 | 0.47 |
| 1:AA:440:C:OP2 | 65:AA:4986:HOH:O | 2.21 | 0.47 |
| 45:DL:7:ILE:HA | 45:DL:7:ILE:HD13 | 1.78 | 0.47 |
| 34:BA:1070:U:H2' | 34:BA:1071:C:H6 | 1.80 | 0.47 |
| 5:CE:52:LEU:O | 5:CE:76:ARG:N | 2.38 | 0.47 |
| 34:DA:404:U:H2' | 34:DA:405:U:H6 | 1.80 | 0.47 |
| 21:CX:44:GLU:OE2 | 21:CX:51:VAL:N | 2.48 | 0.47 |
| 1:CA:1891:G:O6 | 65:CA:4398:HOH:O | 2.20 | 0.47 |
| 36:DC:50:ALA:HB1 | 36:DC:70:VAL:HG21 | 1.96 | 0.47 |
| 38:BE:32:VAL:O | 38:BE:43:LEU:HD12 | 2.15 | 0.47 |
| 3:CC:17:PRO:HG2 | 3:CC:18:ASN:H | 1.79 | 0.47 |
| 1:CA:2119:A:H2 | 1:CA:2171:A:H5' | 1.79 | 0.47 |
| 3:CC:42:VAL:CG1 | 3:CC:43:GLU:H | 2.28 | 0.47 |
| 35:DB:167:PRO:HD3 | 35:DB:187:LEU:O | 2.15 | 0.47 |
| 36:BC:6:HIS:CD2 | 36:BC:8:ILE:H | 2.32 | 0.47 |
| 1:CA:1590:U:H2' | 1:CA:1591:G:C8 | 2.49 | 0.47 |
| 34:BA:974:A:P | 47:BN:29:ARG:HH21 | 2.37 | 0.47 |
| 34:DA:1126:U:C4' | 34:DA:1281:U:H1' | 2.44 | 0.47 |
| 36:DC:137:ALA:HA | 36:DC:140:ARG:NH1 | 2.30 | 0.47 |
| 1:CA:660:G:H5' | 6:CF:99:TYR:CE2 | 2.50 | 0.47 |
| 8:CH:139:GLN:HG3 | 8:CH:140:LYS:N | 2.30 | 0.47 |
| 1:CA:2427:C:H5" | 1:CA:2428:G:OP1 | 2.14 | 0.47 |
| 34:BA:189(D):C:O2 | 34:BA:189(H):G:C6 | 2.68 | 0.47 |
| 59:DZ:262:SER:HB3 | 59:DZ:267:LYS:HB2 | 1.96 | 0.47 |
| 53:DT:50:GLU:H | 53:DT:99:LEU:HD12 | 1.79 | 0.47 |
| 39:BF:37:VAL:HG12 | 39:BF:38:GLU:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CN:67:LEU:HD13 | 11:CN:87:LEU:HD13 | 1.97 | 0.47 |
| 59:DZ:182:ARG:O | 59:DZ:184:LYS:N | 2.48 | 0.47 |
| 1:AA:2720:G:H1' | 15:AR:71:GLN:HE22 | 1.79 | 0.47 |
| 28:A4:57:GLU:HB2 | 28:A4:58:ARG:HE | 1.80 | 0.47 |
| 1:CA:193:U:OP2 | 65:CA:4435:HOH:O | 2.20 | 0.47 |
| 7:CG:121:ASN:O | 7:CG:124:SER:HB3 | 2.15 | 0.47 |
| 28:A4:36:CYS:SG | 28:A4:37:SER:N | 2.88 | 0.47 |
| 34:BA:1037:C:H2' | 34:BA:1038:C:C6 | 2.50 | 0.47 |
| 18:AU:104:GLN:H | 18:AU:104:GLN:CD | 2.16 | 0.47 |
| 34:DA:1049:U:C5 | 34:DA:1201:A:H5' | 2.50 | 0.47 |
| 34:BA:1391:U:H2' | 34:BA:1392:G:C8 | 2.50 | 0.47 |
| 47:DN:24:CYS:HB3 | 47:DN:27:CYS:SG | 2.55 | 0.47 |
| 3:AC:46:ALA:O | 3:AC:47:LYS:HB2 | 2.15 | 0.47 |
| 1:CA:2167:U:OP1 | 1:CA:2167:U:H4' | 2.15 | 0.47 |
| 59:BZ:226:ASN:HB3 | 59:BZ:241:GLU:OE2 | 2.15 | 0.47 |
| 4:AD:52:ARG:HB2 | 4:AD:53:PHE:CD2 | 2.50 | 0.47 |
| 8:CH:7:LEU:HA | 8:CH:8:PRO:HD3 | 1.80 | 0.47 |
| 34:DA:828:A:N6 | 34:DA:858:G:O2' | 2.47 | 0.47 |
| 9:AK:54:ALA:HB1 | 9:AK:83:TYR:O | 2.14 | 0.47 |
| 46:BM:33:ALA:HB2 | 46:BM:64:TRP:HH2 | 1.80 | 0.47 |
| 34:BA:1456:G:H1' | 53:BT:39:LYS:NZ | 2.30 | 0.47 |
| 1:AA:1095:C:C2' | 1:AA:1096:A:H5' | 2.45 | 0.47 |
| 34:DA:936:C:H2' | 34:DA:937:A:O4' | 2.15 | 0.47 |
| 1:CA:1713:U:H2' | 1:CA:1714:G:H8 | 1.80 | 0.47 |
| 34:BA:738:C:H2' | 34:BA:739:C:C6 | 2.50 | 0.47 |
| 42:BI:53:VAL:O | 42:BI:55:ALA:N | 2.48 | 0.47 |
| 1:CA:328:U:H4' | 22:CY:68:HIS:CE1 | 2.50 | 0.47 |
| 13:CP:97:PRO:HD3 | 13:CP:126:VAL:O | 2.15 | 0.47 |
| 27:A3:43:ILE:O | 27:A3:47:VAL:HG23 | 2.15 | 0.47 |
| 49:DP:57:ARG:NH2 | 49:DP:79:VAL:O | 2.48 | 0.47 |
| 27:A3:18:ASP:N | 27:A3:18:ASP:OD1 | 2.48 | 0.47 |
| 34:BA:696:A:N1 | 34:BA:797:C:O2' | 2.39 | 0.47 |
| 20:CW:58:ALA:HB1 | 20:CW:64:MET:HB2 | 1.96 | 0.47 |
| 49:BP:20:VAL:HG21 | 49:BP:32:TYR:CG | 2.50 | 0.46 |
| 1:CA:882:G:H2' | 1:CA:883:G:C8 | 2.46 | 0.46 |
| 22:AY:23:ARG:HG2 | 22:AY:42:VAL:HG22 | 1.96 | 0.46 |
| 43:DJ:35:SER:HB3 | 43:DJ:73:ASP:HB2 | 1.97 | 0.46 |
| 34:BA:1284:C:H3' | 34:BA:1285:A:H8 | 1.80 | 0.46 |
| 36:DC:114:PRO:HA | 36:DC:185:GLY:HA3 | 1.96 | 0.46 |
| 3:AC:17:PRO:HG2 | 3:AC:18:ASN:H | 1.79 | 0.46 |
| 58:BY:72:C:H2' | 58:BY:73:A:O4' | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 57:DX:55:PSU:O2' | 57:DX:57:A:N7 | 2.31 | 0.46 |
| 34:DA:900:A:H2' | 34:DA:901:A:C8 | 2.50 | 0.46 |
| 34:DA:1289:A:C8 | 34:DA:1290:G:C8 | 3.03 | 0.46 |
| 3:AC:223:VAL:HG23 | 3:AC:223:VAL:O | 2.15 | 0.46 |
| 4:AD:242:ARG:HD3 | 4:AD:242:ARG:N | 2.29 | 0.46 |
| 19:CV:71:LEU:HA | 19:CV:71:LEU:HD23 | 1.72 | 0.46 |
| 1:CA:620:G:H5' | 1:CA:620:G:N3 | 2.30 | 0.46 |
| 9:CK:23:SER:HA | 9:CK:117:LEU:O | 2.15 | 0.46 |
| 34:BA:1346:A:N1 | 34:BA:1374:A:H5'' | 2.30 | 0.46 |
| 27:C3:6:VAL:HG13 | 27:C3:56:VAL:HG22 | 1.97 | 0.46 |
| 12:AO:2:ILE:HB | 12:AO:33:ALA:HB3 | 1.97 | 0.46 |
| 34:DA:992:U:O2' | 34:DA:993:G:OP2 | 2.27 | 0.46 |
| 1:CA:740:U:H2' | 1:CA:741:G:C8 | 2.51 | 0.46 |
| 3:CC:176:VAL:O | 3:CC:176:VAL:HG12 | 2.15 | 0.46 |
| 20:AW:14:PRO:HG2 | 20:AW:78:GLU:CG | 2.44 | 0.46 |
| 1:CA:993:G:N2 | 19:CV:23:GLU:OE2 | 2.45 | 0.46 |
| 34:DA:1347:G:N2 | 34:DA:1373:G:H2' | 2.29 | 0.46 |
| 32:A8:39:LYS:O | 32:A8:43:GLN:HG3 | 2.14 | 0.46 |
| 57:BX:55:PSU:O2' | 57:BX:57:A:N7 | 2.37 | 0.46 |
| 1:CA:2014:A:H2' | 1:CA:2015:A:C8 | 2.50 | 0.46 |
| 8:AH:40:GLU:OE2 | 8:AH:60:ARG:NH1 | 2.47 | 0.46 |
| 34:DA:543:C:O2' | 34:DA:544:G:H5' | 2.14 | 0.46 |
| 8:CH:113:VAL:HG11 | 8:CH:151:ILE:HD13 | 1.96 | 0.46 |
| 34:DA:1159:U:O4' | 34:DA:1182:G:N2 | 2.47 | 0.46 |
| 1:CA:2336:A:H61 | 24:C0:43:THR:HG21 | 1.79 | 0.46 |
| 59:BZ:233:GLU:HB3 | 59:BZ:234:GLY:H | 1.54 | 0.46 |
| 1:CA:579:G:H2' | 1:CA:580:C:C6 | 2.50 | 0.46 |
| 4:CD:175:LEU:HD12 | 4:CD:185:VAL:HG21 | 1.97 | 0.46 |
| 10:CL:78:ILE:O | 10:CL:78:ILE:HG12 | 2.15 | 0.46 |
| 15:CR:29:LEU:HA | 15:CR:29:LEU:HD12 | 1.83 | 0.46 |
| 1:CA:2615:U:H2' | 1:CA:2616:C:H6 | 1.80 | 0.46 |
| 11:AN:75:TYR:CE2 | 11:AN:77:GLY:HA2 | 2.50 | 0.46 |
| 26:C2:9:GLN:OE1 | 26:C2:56:GLN:HG2 | 2.15 | 0.46 |
| 19:CV:6:LYS:HB2 | 19:CV:38:LEU:HD21 | 1.97 | 0.46 |
| 1:AA:1907:A:H2' | 1:AA:1908:C:O4' | 2.14 | 0.46 |
| 18:AU:112:ARG:CG | 18:AU:112:ARG:HH11 | 2.28 | 0.46 |
| 1:CA:2178:C:O2' | 3:CC:169:THR:CB | 2.56 | 0.46 |
| 14:AQ:48:GLU:HB2 | 65:AQ:3104:HOH:O | 2.14 | 0.46 |
| 46:BM:84:ILE:HG13 | 46:BM:86:CYS:N | 2.29 | 0.46 |
| 43:BJ:16:LEU:HD21 | 43:BJ:70:ARG:HG2 | 1.97 | 0.46 |
| 34:DA:147:G:H1 | 34:DA:175:C:H42 | 1.64 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:CQ:21:THR:CG2 | 14:CQ:101:ARG:HH11 | 2.28 | 0.46 |
| 1:AA:1769:G:H2' | 1:AA:1770:A:C8 | 2.51 | 0.46 |
| 34:DA:364:A:H2' | 34:DA:365:U:H6 | 1.80 | 0.46 |
| 58:DY:25:C:H2' | 58:DY:26:A:H8 | 1.80 | 0.46 |
| 59:DZ:620:VAL:O | 59:DZ:624:LEU:HB2 | 2.16 | 0.46 |
| 41:BH:20:TYR:HD2 | 41:BH:65:TYR:CE2 | 2.32 | 0.46 |
| 1:AA:397:G:H4' | 1:AA:398:A:OP2 | 2.15 | 0.46 |
| 1:CA:32:C:O2' | 1:CA:33:U:H5' | 2.16 | 0.46 |
| 1:CA:861:A:C2 | 1:CA:917:A:C4 | 3.03 | 0.46 |
| 34:DA:179:A:H2' | 34:DA:180:U:C6 | 2.50 | 0.46 |
| 34:DA:724:G:C2 | 34:DA:725:G:C8 | 3.03 | 0.46 |
| 1:CA:1042:G:H1 | 1:CA:1113:U:H3 | 1.63 | 0.46 |
| 5:AE:9:VAL:HB | 17:AT:3:ARG:HG2 | 1.97 | 0.46 |
| 1:CA:2454:G:H1' | 65:CA:3889:HOH:O | 2.15 | 0.46 |
| 34:BA:160:A:H2' | 34:BA:160:A:N3 | 2.31 | 0.46 |
| 35:BB:18:GLY:O | 35:BB:19:HIS:HB3 | 2.16 | 0.46 |
| 1:CA:2430:A:OP2 | 65:CA:4250:HOH:O | 2.20 | 0.46 |
| 59:BZ:165:GLN:HA | 59:BZ:180:VAL:HG13 | 1.95 | 0.46 |
| 35:DB:167:PRO:HG3 | 35:DB:188:ALA:HB2 | 1.98 | 0.46 |
| 3:AC:6:LYS:HA | 3:AC:9:ARG:NH1 | 2.30 | 0.46 |
| 34:BA:1148:U:O3' | 42:BI:14:VAL:HG11 | 2.15 | 0.46 |
| 65:AA:5273:HOH:O | 5:AE:147:PRO:HD2 | 2.15 | 0.46 |
| 16:CS:88:ASP:C | 16:CS:90:GLY:H | 2.19 | 0.46 |
| 1:AA:934:A:HO2' | 1:AA:935:C:P | 2.37 | 0.46 |
| 35:DB:218:ALA:O | 35:DB:222:ILE:HG23 | 2.16 | 0.46 |
| 1:CA:580:C:H2' | 1:CA:581:C:C6 | 2.51 | 0.46 |
| 1:AA:1913:G:C6 | 1:AA:1914:C:C4 | 3.03 | 0.46 |
| 51:BR:33:ASP:OD2 | 51:BR:36:ASN:HB2 | 2.16 | 0.46 |
| 12:CO:1:MET:HG2 | 12:CO:67:LYS:HG2 | 1.96 | 0.46 |
| 34:DA:426:G:OP1 | 37:DD:36:ARG:HD2 | 2.16 | 0.46 |
| 44:BK:27:ASN:OD1 | 44:BK:55:LYS:HB3 | 2.15 | 0.46 |
| 1:CA:2483:C:OP1 | 56:DW:64:A:H4' | 2.16 | 0.46 |
| 38:DE:68:GLU:OE1 | 38:DE:70:PRO:HG3 | 2.15 | 0.46 |
| 1:CA:2493:U:H2' | 1:CA:2494:G:O4' | 2.15 | 0.46 |
| 34:BA:487:A:H2' | 34:BA:488:C:O4' | 2.16 | 0.46 |
| 33:C9:25:VAL:HB | 33:C9:34:GLN:HB2 | 1.97 | 0.46 |
| 1:CA:1001:A:H2' | 1:CA:1002:G:O4' | 2.14 | 0.46 |
| 1:CA:2685:G:N7 | 65:CA:3903:HOH:O | 2.36 | 0.46 |
| 1:AA:2430:A:H2' | 1:AA:2431:U:C6 | 2.50 | 0.46 |
| 34:DA:186:C:H2' | 34:DA:187:C:H6 | 1.80 | 0.46 |
| 34:BA:923:A:OP1 | 38:BE:21:ALA:HB2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:CH:147:ASN:OD1 | 8:CH:147:ASN:N | 2.47 | 0.46 |
| 7:CG:39:ILE:N | 7:CG:39:ILE:HD12 | 2.31 | 0.46 |
| 34:DA:509:A:C8 | 34:DA:509:A:H3' | 2.50 | 0.46 |
| 26:A2:35:LEU:HA | 26:A2:35:LEU:HD23 | 1.63 | 0.46 |
| 1:AA:2332:A:H2' | 1:AA:2332:A:N3 | 2.31 | 0.46 |
| 59:BZ:19:ALA:HB1 | 59:BZ:23:ALA:HB3 | 1.97 | 0.46 |
| 1:CA:2261:C:O2' | 1:CA:2262:U:H5' | 2.15 | 0.46 |
| 8:CH:13:LYS:HA | 8:CH:14:GLY:HA2 | 1.70 | 0.46 |
| 10:CL:76:TYR:CD2 | 10:CL:77:LEU:HD23 | 2.50 | 0.46 |
| 1:CA:2683:C:O2 | 12:CO:70:LYS:NZ | 2.42 | 0.46 |
| 6:CF:184:TYR:HE1 | 13:CP:3:LEU:HD21 | 1.80 | 0.46 |
| 59:BZ:145:ASP:HB3 | 59:BZ:148:LEU:HB3 | 1.98 | 0.46 |
| 5:CE:12:THR:HG22 | 17:CT:58:ASN:HD21 | 1.81 | 0.46 |
| 3:AC:42:VAL:CG1 | 3:AC:43:GLU:H | 2.27 | 0.46 |
| 59:DZ:183:MET:SD | 59:DZ:213:HIS:HB2 | 2.56 | 0.46 |
| 1:CA:908:C:O2' | 1:CA:909:A:H5' | 2.16 | 0.46 |
| 1:CA:1075:C:H5' | 14:CQ:59:ARG:HH21 | 1.79 | 0.46 |
| 51:DR:32:ARG:HD2 | 51:DR:65:ILE:CG2 | 2.45 | 0.46 |
| 34:BA:52:G:H2' | 34:BA:53:A:C8 | 2.50 | 0.46 |
| 1:CA:1300:U:H4' | 1:CA:1301:A:H5'' | 1.96 | 0.46 |
| 36:DC:5:ILE:HD11 | 47:DN:49:HIS:HE1 | 1.79 | 0.46 |
| 7:AG:83:ARG:O | 7:AG:86:MET:HB2 | 2.16 | 0.46 |
| 7:AG:72:ARG:NH1 | 7:AG:87:PRO:HG3 | 2.31 | 0.46 |
| 1:CA:621:A:OP2 | 13:CP:108:LYS:NZ | 2.43 | 0.46 |
| 38:BE:148:VAL:HG21 | 41:BH:107:LEU:HB3 | 1.98 | 0.46 |
| 34:DA:165:C:H2' | 34:DA:166:G:C8 | 2.50 | 0.46 |
| 59:BZ:670:VAL:HB | 59:BZ:672:PHE:CZ | 2.51 | 0.46 |
| 59:BZ:687:LEU:O | 59:BZ:689:LYS:N | 2.49 | 0.46 |
| 53:BT:57:ARG:HH12 | 53:BT:100:ILE:HG13 | 1.79 | 0.46 |
| 34:DA:1288:A:N1 | 34:DA:1371:G:H1' | 2.30 | 0.46 |
| 14:CQ:135:ASP:HB3 | 14:CQ:137:TYR:H | 1.79 | 0.46 |
| 43:DJ:65:LEU:HD13 | 47:DN:56:VAL:HG22 | 1.97 | 0.46 |
| 1:AA:1343:C:OP1 | 1:AA:2722:C:H4' | 2.16 | 0.46 |
| 40:BG:26:PHE:CE2 | 40:BG:30:ILE:HD11 | 2.50 | 0.46 |
| 1:AA:449:A:H2' | 1:AA:450:A:C8 | 2.50 | 0.46 |
| 1:CA:1232:G:C6 | 1:CA:1233:C:C4 | 3.03 | 0.46 |
| 46:BM:80:ARG:NH2 | 52:BS:69:HIS:HE1 | 2.14 | 0.46 |
| 13:CP:37:GLY:C | 13:CP:38:GLN:O | 2.49 | 0.46 |
| 5:AE:176:ILE:HB | 5:AE:181:LEU:HB2 | 1.97 | 0.46 |
| 59:BZ:20:HIS:HA | 59:BZ:117:GLN:CB | 2.45 | 0.46 |
| 3:AC:176:VAL:O | 3:AC:176:VAL:HG12 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:996:A:C2 | 1:CA:997:G:C8 | 3.03 | 0.46 |
| 17:AT:96:ARG:CZ | 17:AT:96:ARG:HB3 | 2.46 | 0.46 |
| 1:CA:1063:G:O2' | 10:CL:89:HIS:O | 2.33 | 0.46 |
| 1:CA:2061:G:H5'' | 1:CA:2503:A:C2 | 2.51 | 0.46 |
| 34:BA:954:G:H2' | 34:BA:955:U:C6 | 2.51 | 0.46 |
| 1:AA:2274:U:H4' | 1:AA:2340:A:C2 | 2.50 | 0.46 |
| 34:BA:1036:G:H3' | 34:BA:1037:C:H6 | 1.81 | 0.46 |
| 38:BE:83:GLU:HG2 | 38:BE:88:LYS:HD2 | 1.98 | 0.46 |
| 1:CA:1449:A:H5' | 1:CA:1450:G:OP2 | 2.15 | 0.46 |
| 57:BX:31:G:N7 | 57:BX:32:5MC:HM52 | 2.30 | 0.46 |
| 34:BA:836:G:C6 | 34:BA:851:G:C6 | 3.04 | 0.46 |
| 2:AB:66:A:H61 | 2:AB:108:U:H2' | 1.79 | 0.46 |
| 34:DA:622:A:C8 | 34:DA:623:C:C6 | 3.04 | 0.46 |
| 1:CA:125:G:OP1 | 31:C7:14:LYS:HE2 | 2.15 | 0.46 |
| 56:BW:18:G:O2' | 56:BW:57:G:N2 | 2.44 | 0.46 |
| 7:AG:171:ALA:O | 7:AG:175:LEU:HD22 | 2.14 | 0.46 |
| 1:AA:2086:C:H2' | 1:AA:2087:C:C6 | 2.50 | 0.46 |
| 37:BD:97:LEU:HD23 | 37:BD:97:LEU:HA | 1.70 | 0.46 |
| 59:DZ:409:ILE:HG12 | 59:DZ:459:LEU:HD12 | 1.97 | 0.46 |
| 19:CV:43:GLU:N | 19:CV:43:GLU:OE2 | 2.49 | 0.46 |
| 1:CA:1889:A:H2' | 1:CA:1890:A:C8 | 2.51 | 0.46 |
| 59:BZ:280:LEU:HA | 59:BZ:281:PRO:HD3 | 1.76 | 0.46 |
| 34:DA:921:U:H2' | 34:DA:922:G:O4' | 2.16 | 0.46 |
| 3:AC:20:VAL:O | 3:AC:224:ARG:O | 2.34 | 0.46 |
| 1:CA:2173:A:H2' | 1:CA:2174:C:O4' | 2.16 | 0.46 |
| 34:DA:1241:G:H2' | 34:DA:1242:C:C6 | 2.51 | 0.46 |
| 36:BC:181:ASN:ND2 | 36:BC:204:LEU:HD12 | 2.30 | 0.46 |
| 56:DW:44:G:H2' | 56:DW:45:U:H5' | 1.97 | 0.46 |
| 41:BH:132:GLU:O | 41:BH:134:ILE:N | 2.48 | 0.46 |
| 1:CA:1210:A:H5'' | 1:CA:1212:G:O4' | 2.16 | 0.46 |
| 12:CO:64:ARG:HG2 | 12:CO:79:PHE:CD1 | 2.50 | 0.46 |
| 34:BA:1318:A:OP1 | 52:BS:3:ARG:NH2 | 2.49 | 0.46 |
| 34:DA:1318:A:H5'' | 52:DS:3:ARG:HH22 | 1.80 | 0.46 |
| 1:CA:2113:U:H3 | 1:CA:2170:A:N6 | 2.13 | 0.46 |
| 39:DF:30:LEU:HB3 | 39:DF:35:ALA:HB3 | 1.98 | 0.46 |
| 40:BG:18:TYR:CD2 | 40:BG:59:LEU:HD13 | 2.51 | 0.46 |
| 1:CA:491:G:H2' | 1:CA:492:A:H8 | 1.81 | 0.46 |
| 34:BA:452:A:O2' | 34:BA:453:A:OP2 | 2.28 | 0.46 |
| 37:BD:8:VAL:O | 37:BD:11:LEU:HB2 | 2.15 | 0.46 |
| 1:AA:1451:U:H2' | 1:AA:1452:U:C6 | 2.51 | 0.46 |
| 8:CH:90:LYS:HD2 | 8:CH:163:TYR:CD1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DB:90:MET:SD | 35:DB:222:ILE:HD12 | 2.55 | 0.46 |
| 15:AR:56:LYS:HE3 | 15:AR:87:TYR:O | 2.16 | 0.46 |
| 4:AD:145:VAL:HG12 | 4:AD:146:GLU:O | 2.15 | 0.46 |
| 36:DC:77:ILE:HG13 | 36:DC:78:GLY:H | 1.79 | 0.46 |
| 8:AH:69:ARG:HG3 | 8:AH:70:THR:N | 2.28 | 0.46 |
| 59:BZ:9:LEU:HD22 | 59:BZ:284:LEU:HD13 | 1.96 | 0.46 |
| 34:DA:109:A:H2' | 34:DA:326:G:N2 | 2.29 | 0.46 |
| 59:BZ:342:TYR:N | 59:BZ:390:VAL:O | 2.47 | 0.46 |
| 7:CG:103:LEU:HD23 | 7:CG:106:LEU:HD23 | 1.98 | 0.46 |
| 26:A2:41:ILE:HG13 | 26:A2:43:GLN:HG3 | 1.97 | 0.46 |
| 1:AA:1817:A:H8 | 65:AA:5175:HOH:O | 1.98 | 0.46 |
| 1:CA:2079:U:O3' | 25:C1:35:THR:OG1 | 2.32 | 0.46 |
| 1:CA:2422:A:H5' | 58:DY:76:A:H62 | 1.80 | 0.46 |
| 1:AA:1057:G:OP1 | 18:AU:77:SER:OG | 2.33 | 0.46 |
| 38:DE:5:ASP:N | 38:DE:5:ASP:OD1 | 2.49 | 0.46 |
| 3:AC:211:ARG:HH11 | 3:AC:211:ARG:HG2 | 1.81 | 0.46 |
| 7:CG:109:VAL:HG21 | 28:C4:14:ILE:HD13 | 1.96 | 0.46 |
| 17:CT:106:SER:O | 17:CT:110:ILE:HG13 | 2.15 | 0.46 |
| 59:BZ:87:HIS:O | 59:BZ:90:PHE:N | 2.45 | 0.46 |
| 3:CC:48:LEU:HD23 | 3:CC:59:VAL:HG21 | 1.98 | 0.46 |
| 15:CR:33:ARG:HE | 15:CR:113:LEU:HD22 | 1.80 | 0.46 |
| 45:DL:85:ILE:HG22 | 45:DL:100:ILE:HG12 | 1.97 | 0.46 |
| 1:AA:553:A:C2 | 1:AA:2065:C:H4' | 2.49 | 0.46 |
| 34:DA:1305:G:H5' | 54:DU:4:GLY:HA3 | 1.97 | 0.46 |
| 1:CA:271(O):C:H2' | 1:CA:271(P):C:C6 | 2.51 | 0.46 |
| 40:DG:113:GLU:HB2 | 40:DG:119:ARG:HG2 | 1.97 | 0.46 |
| 34:BA:1260:C:O5' | 34:BA:1284:C:H4' | 2.16 | 0.46 |
| 1:CA:2395:C:H2' | 1:CA:2396:G:O4' | 2.15 | 0.46 |
| 22:CY:44:ILE:HA | 22:CY:63:LYS:O | 2.16 | 0.46 |
| 1:AA:834:U:H5'' | 1:AA:835:A:H5' | 1.98 | 0.46 |
| 5:CE:176:ILE:HB | 5:CE:181:LEU:HB2 | 1.97 | 0.46 |
| 12:CO:111:PHE:O | 12:CO:115:VAL:HG23 | 2.15 | 0.46 |
| 23:AZ:128:VAL:HG23 | 23:AZ:161:VAL:HA | 1.97 | 0.46 |
| 1:CA:27:G:C2 | 1:CA:512:G:N3 | 2.83 | 0.46 |
| 34:BA:1104:G:H2' | 34:BA:1105:A:H8 | 1.81 | 0.46 |
| 3:CC:211:ARG:HG2 | 3:CC:211:ARG:HH11 | 1.81 | 0.46 |
| 1:AA:1993:A:OP1 | 65:AA:4251:HOH:O | 2.20 | 0.46 |
| 22:CY:9:LYS:HA | 22:CY:10:GLY:HA2 | 1.59 | 0.46 |
| 1:CA:1584:C:H2' | 1:CA:1586:A:H5' | 1.97 | 0.46 |
| 34:DA:955:U:H2' | 34:DA:956:U:O4' | 2.16 | 0.46 |
| 3:CC:46:ALA:O | 3:CC:47:LYS:HB2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CB:76:G:H2' | 2:CB:77:U:O4' | 2.16 | 0.46 |
| 34:DA:1216:G:H5'' | 47:DN:5:ALA:HB2 | 1.97 | 0.46 |
| 34:DA:1095:U:H2' | 34:DA:1096:C:O4' | 2.16 | 0.46 |
| 59:BZ:177:ILE:HD12 | 59:BZ:188:TYR:HE2 | 1.80 | 0.46 |
| 23:AZ:139:VAL:HG22 | 23:AZ:155:LEU:HD11 | 1.96 | 0.46 |
| 1:AA:1550:C:H2' | 1:AA:1551:C:C6 | 2.51 | 0.46 |
| 34:BA:189(B):C:N3 | 34:BA:189(J):G:C2 | 2.84 | 0.46 |
| 43:BJ:31:GLY:HA2 | 43:BJ:32:ALA:HA | 1.44 | 0.46 |
| 59:BZ:617:MET:HG2 | 59:BZ:643:ILE:HD11 | 1.96 | 0.46 |
| 1:CA:1902:C:H5' | 4:CD:246:PRO:HD3 | 1.98 | 0.46 |
| 48:DO:25:THR:HG21 | 48:DO:70:LEU:HB2 | 1.98 | 0.46 |
| 59:DZ:236:GLU:H | 59:DZ:236:GLU:HG3 | 1.40 | 0.46 |
| 36:DC:54:ARG:NH1 | 36:DC:54:ARG:HB3 | 2.30 | 0.46 |
| 34:BA:1161:C:H2' | 34:BA:1162:C:C6 | 2.51 | 0.46 |
| 15:AR:44:LEU:HD22 | 15:AR:48:VAL:HG23 | 1.98 | 0.46 |
| 5:CE:108:SER:HB3 | 5:CE:165:VAL:HG21 | 1.97 | 0.46 |
| 1:CA:1053:C:H2' | 1:CA:1054:A:O5' | 2.16 | 0.46 |
| 1:AA:1067:A:H62 | 1:AA:1186:U:H3 | 1.63 | 0.46 |
| 35:DB:96:ARG:O | 35:DB:98:LEU:N | 2.49 | 0.46 |
| 37:BD:120:LEU:HB3 | 37:BD:126:ILE:HD11 | 1.97 | 0.46 |
| 2:AB:7:G:H5' | 16:AS:29:PHE:CE2 | 2.51 | 0.46 |
| 37:DD:4:TYR:O | 37:DD:5:ILE:HG22 | 2.16 | 0.46 |
| 1:CA:1589:C:H2' | 1:CA:1590:U:H6 | 1.78 | 0.46 |
| 34:BA:973:G:H3' | 34:BA:974:A:H5'' | 1.98 | 0.46 |
| 59:BZ:-38:TYR:CD2 | 59:BZ:-37:LEU:HD23 | 2.51 | 0.46 |
| 34:BA:1350:A:C6 | 34:BA:1351:U:N3 | 2.84 | 0.46 |
| 1:AA:801:C:H2' | 1:AA:802:C:H6 | 1.81 | 0.46 |
| 1:AA:2087:C:H2' | 1:AA:2088:C:C6 | 2.51 | 0.46 |
| 1:AA:2365:G:H1' | 24:A0:34:GLY:HA3 | 1.97 | 0.46 |
| 31:C7:24:THR:O | 31:C7:28:ARG:HG3 | 2.16 | 0.46 |
| 34:DA:1014:A:OP1 | 52:DS:18:LYS:NZ | 2.49 | 0.46 |
| 1:CA:2741:A:H2' | 1:CA:2742:C:O4' | 2.16 | 0.46 |
| 59:DZ:546:ILE:HD13 | 59:DZ:565:VAL:HG11 | 1.98 | 0.46 |
| 1:CA:1545:A:H2' | 1:CA:1546:C:O4' | 2.16 | 0.46 |
| 1:CA:2677:G:H2' | 1:CA:2678:C:C6 | 2.51 | 0.46 |
| 39:DF:10:LEU:HD12 | 39:DF:85:VAL:HA | 1.98 | 0.46 |
| 59:DZ:-41:ALA:O | 59:DZ:-36:LEU:HB2 | 2.16 | 0.46 |
| 57:BX:23:C:H2' | 57:BX:24:U:C6 | 2.51 | 0.46 |
| 40:BG:104:LEU:HA | 40:BG:104:LEU:HD13 | 1.55 | 0.46 |
| 46:BM:65:LYS:O | 46:BM:70:LEU:HG | 2.16 | 0.46 |
| 1:CA:2630:G:H2' | 1:CA:2631:G:C8 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:A8:29:LYS:HB2 | 32:A8:33:ASN:HD21 | 1.81 | 0.46 |
| 1:AA:2128:G:H1 | 1:AA:2205:C:N4 | 2.05 | 0.45 |
| 34:DA:1254:C:O5' | 34:DA:1254:C:H6 | 1.99 | 0.45 |
| 46:BM:94:ARG:NH1 | 52:BS:80:TYR:HD2 | 2.14 | 0.45 |
| 4:CD:275:LYS:HA | 4:CD:276:LYS:C | 2.36 | 0.45 |
| 34:DA:1023:G:H3' | 34:DA:1024:G:H8 | 1.81 | 0.45 |
| 2:AB:7:G:H5' | 16:AS:29:PHE:CD2 | 2.51 | 0.45 |
| 8:AH:90:LYS:HD2 | 8:AH:163:TYR:CD1 | 2.52 | 0.45 |
| 52:BS:63:THR:HG23 | 52:BS:66:MET:HE3 | 1.98 | 0.45 |
| 1:AA:1529:G:C6 | 1:AA:1553:A:C6 | 3.04 | 0.45 |
| 34:BA:1298:C:H4' | 34:BA:1299:A:C4 | 2.51 | 0.45 |
| 14:AQ:2:LEU:HB2 | 14:AQ:70:PRO:CG | 2.46 | 0.45 |
| 1:CA:1063:G:H2' | 1:CA:1064:C:C6 | 2.50 | 0.45 |
| 35:BB:21:ARG:HH21 | 35:BB:21:ARG:H | 1.65 | 0.45 |
| 34:DA:860:A:N6 | 34:DA:861:G:C2 | 2.84 | 0.45 |
| 16:CS:29:PHE:HD1 | 16:CS:92:TYR:HH | 1.61 | 0.45 |
| 49:DP:74:LEU:HG | 49:DP:79:VAL:HG21 | 1.97 | 0.45 |
| 21:AX:13:LEU:HD11 | 26:A2:41:ILE:HG22 | 1.97 | 0.45 |
| 1:AA:1462:G:O2' | 1:AA:1463:C:H5 | 1.99 | 0.45 |
| 34:DA:242:C:H2' | 34:DA:243:A:H5' | 1.96 | 0.45 |
| 34:DA:1431:C:H2' | 34:DA:1432:G:O4' | 2.16 | 0.45 |
| 5:CE:21:VAL:HA | 5:CE:22:PRO:HD3 | 1.72 | 0.45 |
| 1:AA:1314:A:H2' | 1:AA:1315:A:O4' | 2.16 | 0.45 |
| 3:CC:37:LYS:O | 3:CC:38:PHE:HB3 | 2.17 | 0.45 |
| 1:AA:1153:G:H4' | 9:AK:81:VAL:HA | 1.98 | 0.45 |
| 59:DZ:75:LYS:NZ | 59:DZ:75:LYS:HA | 2.31 | 0.45 |
| 41:DH:127:LEU:HA | 41:DH:127:LEU:HD13 | 1.73 | 0.45 |
| 34:BA:236:G:OP1 | 50:BQ:40:LYS:NZ | 2.49 | 0.45 |
| 1:AA:1345:G:H5' | 1:AA:1347:A:O4' | 2.16 | 0.45 |
| 34:BA:228:A:H2' | 34:BA:229:U:O4' | 2.16 | 0.45 |
| 1:CA:784:A:H5' | 1:CA:785:G:OP1 | 2.16 | 0.45 |
| 12:AO:115:VAL:HG13 | 12:AO:121:VAL:HG21 | 1.98 | 0.45 |
| 45:DL:6:THR:HG23 | 45:DL:9:GLN:OE1 | 2.16 | 0.45 |
| 1:CA:1803:A:H4' | 4:CD:259:THR:HG23 | 1.99 | 0.45 |
| 1:CA:1022:G:C5 | 1:CA:1140:C:C4 | 3.04 | 0.45 |
| 1:AA:1097:G:H1 | 1:AA:1154:U:H5 | 1.64 | 0.45 |
| 1:AA:2299:A:N6 | 1:AA:2356:U:H3 | 2.05 | 0.45 |
| 28:C4:33:VAL:HG12 | 28:C4:35:VAL:H | 1.81 | 0.45 |
| 59:DZ:166:LEU:O | 59:DZ:178:ILE:N | 2.41 | 0.45 |
| 1:CA:2123:G:H2' | 1:CA:2124:G:C8 | 2.51 | 0.45 |
| 34:DA:980:C:HO2' | 47:DN:21:TYR:HE2 | 1.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:669:A:H4' | 1:AA:670:C:H5 | 1.81 | 0.45 |
| 37:DD:153:ARG:HB2 | 37:DD:181:MET:SD | 2.57 | 0.45 |
| 57:DX:72:A:C6 | 57:DX:73:A:C6 | 3.04 | 0.45 |
| 59:DZ:609:GLU:O | 59:DZ:669:PHE:HA | 2.15 | 0.45 |
| 44:BK:120:ARG:HA | 44:BK:121:PRO:HD3 | 1.79 | 0.45 |
| 1:CA:1477:A:C2 | 1:CA:1515:G:C2 | 3.05 | 0.45 |
| 1:AA:1261:G:OP2 | 18:AU:12:ARG:NH2 | 2.42 | 0.45 |
| 53:DT:36:LEU:HD12 | 53:DT:55:ILE:HG23 | 1.97 | 0.45 |
| 2:CB:21:G:H2' | 2:CB:22:U:O4' | 2.16 | 0.45 |
| 1:CA:1406:U:H2' | 1:CA:1407:C:C6 | 2.50 | 0.45 |
| 8:CH:144:VAL:O | 8:CH:148:ILE:HG12 | 2.16 | 0.45 |
| 8:AH:41:MET:CE | 8:AH:65:HIS:HA | 2.46 | 0.45 |
| 34:DA:601:C:H2' | 34:DA:602:A:C8 | 2.51 | 0.45 |
| 58:DY:30:G:H2' | 58:DY:31:A:H8 | 1.81 | 0.45 |
| 40:BG:78:ARG:NH1 | 40:BG:79:ARG:HD2 | 2.31 | 0.45 |
| 34:DA:160:A:H2' | 34:DA:161:A:O4' | 2.16 | 0.45 |
| 21:AX:43:VAL:HG13 | 21:AX:47:PHE:HD2 | 1.81 | 0.45 |
| 1:AA:67:G:H2' | 1:AA:68:C:O4' | 2.16 | 0.45 |
| 5:AE:167:VAL:HG23 | 5:AE:170:LEU:HD11 | 1.98 | 0.45 |
| 28:A4:14:ILE:HB | 28:A4:22:ILE:HB | 1.97 | 0.45 |
| 46:DM:90:LEU:HD22 | 46:DM:93:ARG:HE | 1.81 | 0.45 |
| 34:DA:731:G:H5' | 34:DA:766:A:H4' | 1.97 | 0.45 |
| 1:AA:2812:A:H1' | 1:AA:2904:U:H1' | 1.97 | 0.45 |
| 1:AA:2451:A:C8 | 1:AA:2451:A:C5' | 3.00 | 0.45 |
| 35:DB:44:LEU:HD22 | 35:DB:44:LEU:H | 1.81 | 0.45 |
| 36:BC:45:LYS:HB2 | 36:BC:45:LYS:HE3 | 1.78 | 0.45 |
| 58:BY:40:C:H2' | 58:BY:41:C:H6 | 1.82 | 0.45 |
| 1:CA:2722:G:H2' | 1:CA:2723:C:C6 | 2.51 | 0.45 |
| 22:CY:83:THR:OG1 | 22:CY:84:ARG:N | 2.50 | 0.45 |
| 1:CA:2135:A:H2' | 1:CA:2136:C:C6 | 2.51 | 0.45 |
| 23:CZ:45:ASP:O | 23:CZ:49:ARG:HG3 | 2.16 | 0.45 |
| 34:BA:255:G:H2' | 34:BA:256:U:C6 | 2.52 | 0.45 |
| 34:DA:1024:G:C2' | 34:DA:1025:U:H5'' | 2.45 | 0.45 |
| 54:DU:2:GLY:O | 54:DU:4:GLY:N | 2.49 | 0.45 |
| 44:BK:20:TYR:HB2 | 44:BK:31:THR:CG2 | 2.46 | 0.45 |
| 37:BD:194:LEU:HD12 | 37:BD:195:ALA:H | 1.81 | 0.45 |
| 1:AA:2199:C:O2 | 3:AC:173:HIS:HE1 | 1.99 | 0.45 |
| 34:DA:1216:G:H5'' | 47:DN:5:ALA:CB | 2.46 | 0.45 |
| 1:AA:354:A:H2 | 1:AA:1255:A:O2' | 1.99 | 0.45 |
| 59:BZ:264:LEU:HD12 | 64:BZ:702:GDP:N3 | 2.31 | 0.45 |
| 49:BP:40:ASP:HA | 49:BP:41:PRO:HD2 | 1.76 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:1104:G:C4 | 34:DA:1105:A:C8 | 3.04 | 0.45 |
| 59:BZ:10:LYS:O | 59:BZ:282:SER:HB2 | 2.16 | 0.45 |
| 1:CA:2029:G:H2' | 1:CA:2031:A:OP1 | 2.16 | 0.45 |
| 4:AD:106:ILE:O | 4:AD:108:PRO:HD3 | 2.16 | 0.45 |
| 57:BX:67:C:C2' | 57:BX:68:C:H5' | 2.46 | 0.45 |
| 1:CA:1342:A:O2' | 1:CA:1344:G:OP2 | 2.26 | 0.45 |
| 59:DZ:560:VAL:HG11 | 59:DZ:594:VAL:HG11 | 1.99 | 0.45 |
| 34:DA:757:U:H2' | 34:DA:758:G:O4' | 2.15 | 0.45 |
| 1:AA:2500:A:H2' | 1:AA:2501:G:O4' | 2.16 | 0.45 |
| 23:AZ:54:HIS:O | 23:AZ:98:MET:HE1 | 2.16 | 0.45 |
| 53:BT:42:GLN:HG3 | 53:BT:43:LEU:HD23 | 1.99 | 0.45 |
| 34:BA:1417:G:N2 | 34:BA:1482:G:H2' | 2.32 | 0.45 |
| 11:AN:4:TYR:CD2 | 18:AU:100:VAL:HG11 | 2.52 | 0.45 |
| 34:DA:369:C:OP2 | 34:DA:388:G:N2 | 2.37 | 0.45 |
| 44:BK:59:TYR:CE2 | 44:BK:63:LEU:HD12 | 2.51 | 0.45 |
| 34:DA:1205:U:H4' | 36:DC:195:VAL:HG23 | 1.97 | 0.45 |
| 4:AD:85:ASP:OD2 | 4:AD:88:ARG:HD2 | 2.15 | 0.45 |
| 21:AX:61:GLY:HA3 | 21:AX:73:ARG:O | 2.17 | 0.45 |
| 34:DA:302:G:N3 | 34:DA:556:C:H4' | 2.30 | 0.45 |
| 36:DC:104:GLN:HE21 | 36:DC:105:GLU:N | 2.13 | 0.45 |
| 34:BA:13:U:OP1 | 65:BA:2020:HOH:O | 2.21 | 0.45 |
| 1:CA:602:G:O2' | 1:CA:655:A:N6 | 2.49 | 0.45 |
| 6:CF:184:TYR:O | 6:CF:188:ARG:HG3 | 2.15 | 0.45 |
| 59:BZ:170:ARG:O | 59:BZ:173:THR:OG1 | 2.33 | 0.45 |
| 28:C4:16:CYS:SG | 28:C4:36:CYS:HB3 | 2.57 | 0.45 |
| 59:BZ:14:ASN:OD1 | 59:BZ:80:ASN:HB2 | 2.16 | 0.45 |
| 1:CA:2135:A:OP1 | 1:CA:2160:G:H1' | 2.16 | 0.45 |
| 7:AG:120:LEU:HD12 | 7:AG:179:PRO:HD2 | 1.99 | 0.45 |
| 1:AA:611:U:O4 | 1:AA:717:A:H1' | 2.15 | 0.45 |
| 59:DZ:74:TRP:CE3 | 59:DZ:74:TRP:HA | 2.49 | 0.45 |
| 47:BN:23:ARG:HD2 | 47:BN:28:GLY:O | 2.16 | 0.45 |
| 1:CA:1364:G:P | 25:C1:3:LYS:HG3 | 2.56 | 0.45 |
| 28:A4:59:PHE:HA | 28:A4:61:ARG:HG2 | 1.98 | 0.45 |
| 34:BA:435:C:H2' | 34:BA:436:C:C6 | 2.51 | 0.45 |
| 1:CA:2881:C:H2' | 1:CA:2882:A:O4' | 2.16 | 0.45 |
| 43:BJ:67:THR:O | 43:BJ:67:THR:OG1 | 2.34 | 0.45 |
| 4:CD:71:ASP:HB3 | 4:CD:103:ARG:NH2 | 2.32 | 0.45 |
| 34:BA:695:A:H2' | 34:BA:696:A:O4' | 2.17 | 0.45 |
| 1:AA:2804:C:H2' | 1:AA:2805:G:H8 | 1.82 | 0.45 |
| 49:DP:22:THR:HA | 49:DP:33:ILE:HG13 | 1.99 | 0.45 |
| 34:DA:604:G:H2' | 34:DA:605:U:O4' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1773:A:H5'' | 65:CA:4317:HOH:O | 2.15 | 0.45 |
| 34:BA:580:U:H2' | 34:BA:581:G:O4' | 2.16 | 0.45 |
| 34:DA:641:U:O2 | 34:DA:642:A:N6 | 2.25 | 0.45 |
| 1:CA:1488:G:C6 | 1:CA:1489:U:N3 | 2.85 | 0.45 |
| 34:BA:718:G:C8 | 44:BK:116:HIS:HB3 | 2.51 | 0.45 |
| 43:BJ:64:GLU:HB3 | 47:BN:59:ALA:HB2 | 1.99 | 0.45 |
| 59:DZ:215:LYS:O | 59:DZ:219:VAL:HG23 | 2.16 | 0.45 |
| 1:CA:1109:C:H2' | 1:CA:1110:G:N7 | 2.31 | 0.45 |
| 59:DZ:20:HIS:CE1 | 59:DZ:117:GLN:HG3 | 2.52 | 0.45 |
| 35:BB:16:HIS:CD2 | 35:BB:17:PHE:N | 2.85 | 0.45 |
| 35:BB:16:HIS:C | 35:BB:18:GLY:H | 2.18 | 0.45 |
| 34:BA:1392:G:H21 | 34:BA:1502:A:H8 | 1.63 | 0.45 |
| 3:CC:20:VAL:O | 3:CC:224:ARG:O | 2.34 | 0.45 |
| 1:AA:2556:G:H1' | 1:AA:2658:C:H4' | 1.99 | 0.45 |
| 3:AC:48:LEU:HD23 | 3:AC:59:VAL:HG21 | 1.98 | 0.45 |
| 37:BD:126:ILE:HG22 | 37:BD:127:THR:H | 1.82 | 0.45 |
| 28:A4:40:HIS:CE1 | 28:A4:42:PHE:HB3 | 2.52 | 0.45 |
| 1:AA:555:G:C5 | 1:AA:2044:U:H5'' | 2.51 | 0.45 |
| 34:BA:1118:C:OP1 | 42:BI:104:ARG:NH1 | 2.49 | 0.45 |
| 1:CA:271(H):G:O2' | 1:CA:271(I):G:H8 | 2.00 | 0.45 |
| 8:CH:3:ARG:NH2 | 8:CH:5:GLY:H | 2.14 | 0.45 |
| 48:BO:25:THR:HG21 | 48:BO:70:LEU:HB2 | 1.96 | 0.45 |
| 1:CA:2275:C:C6 | 1:CA:2275:C:H5' | 2.51 | 0.45 |
| 1:AA:1848:G:H2' | 1:AA:1849:U:H5' | 1.98 | 0.45 |
| 52:DS:15:LEU:HD12 | 52:DS:18:LYS:HD2 | 1.98 | 0.45 |
| 23:AZ:28:MET:HA | 23:AZ:88:PHE:O | 2.17 | 0.45 |
| 34:DA:97:G:O2' | 34:DA:98:G:H5'' | 2.16 | 0.45 |
| 1:AA:303:C:H42 | 1:AA:385:G:H1 | 1.63 | 0.45 |
| 1:AA:386:U:O2' | 1:AA:387:G:H5'' | 2.16 | 0.45 |
| 59:BZ:660:ARG:HE | 59:BZ:665:GLY:HA2 | 1.82 | 0.45 |
| 3:AC:37:LYS:O | 3:AC:38:PHE:HB3 | 2.17 | 0.45 |
| 2:AB:32:C:C2 | 2:AB:51:G:N2 | 2.85 | 0.45 |
| 1:AA:2891:C:H2' | 1:AA:2892:A:O4' | 2.17 | 0.45 |
| 16:CS:3:ARG:HE | 16:CS:4:LEU:N | 2.14 | 0.45 |
| 18:CU:27:LEU:HB3 | 18:CU:31:SER:HB3 | 1.98 | 0.45 |
| 1:AA:2702:C:OP2 | 1:AA:2702:C:H6 | 1.99 | 0.45 |
| 35:BB:208:ILE:HD12 | 35:BB:208:ILE:H | 1.82 | 0.45 |
| 40:BG:12:LEU:HD12 | 40:BG:12:LEU:H | 1.80 | 0.45 |
| 37:BD:65:ARG:HG2 | 37:BD:75:PHE:CD1 | 2.52 | 0.45 |
| 1:AA:1336:C:H2' | 1:AA:1337:C:C6 | 2.52 | 0.45 |
| 11:CN:4:TYR:CD2 | 18:CU:100:VAL:HG11 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:72:U:OP2 | 26:C2:29:LYS:NZ | 2.44 | 0.45 |
| 22:AY:92:ASN:N | 22:AY:92:ASN:HD22 | 2.07 | 0.45 |
| 29:C5:20:ARG:HG2 | 29:C5:23:HIS:CE1 | 2.51 | 0.45 |
| 35:DB:51:LEU:O | 35:DB:55:PHE:N | 2.25 | 0.45 |
| 37:DD:31:CYS:O | 37:DD:35:ARG:HG3 | 2.17 | 0.45 |
| 59:BZ:182:ARG:O | 59:BZ:184:LYS:N | 2.50 | 0.45 |
| 39:DF:2:ARG:HE | 39:DF:69:GLU:HG2 | 1.80 | 0.45 |
| 3:CC:194:ILE:HD11 | 3:CC:227:PRO:HB2 | 1.99 | 0.45 |
| 59:DZ:357:ARG:NH1 | 59:DZ:373:ASP:OD1 | 2.49 | 0.45 |
| 1:AA:2792:U:H5' | 1:AA:2794:A:O4' | 2.16 | 0.45 |
| 34:BA:262:A:C6 | 34:BA:263:A:C6 | 3.04 | 0.45 |
| 25:A1:94:LEU:HD23 | 25:A1:94:LEU:HA | 1.72 | 0.45 |
| 34:DA:503:C:H2' | 34:DA:504:C:H6 | 1.81 | 0.45 |
| 1:CA:1064:C:H3' | 1:CA:1065:U:C6 | 2.51 | 0.45 |
| 1:AA:2051:G:H2' | 1:AA:2053:A:OP1 | 2.16 | 0.45 |
| 1:AA:2564:U:O2 | 1:AA:2566:U:H5' | 2.17 | 0.45 |
| 1:CA:2318:G:O2' | 1:CA:2318:G:N3 | 2.48 | 0.45 |
| 1:AA:517:A:H2' | 1:AA:518:G:O4' | 2.17 | 0.45 |
| 36:DC:105:GLU:OE1 | 36:DC:107:GLN:N | 2.50 | 0.45 |
| 42:BI:46:ALA:HB1 | 42:BI:77:ILE:HG22 | 1.98 | 0.45 |
| 33:A9:7:VAL:HG12 | 33:A9:34:GLN:HB3 | 1.97 | 0.45 |
| 40:BG:91:VAL:HB | 40:BG:96:GLN:HG2 | 1.99 | 0.45 |
| 59:BZ:93:GLU:HA | 59:BZ:96:ARG:HG3 | 1.99 | 0.45 |
| 34:BA:865:A:H2' | 34:BA:866:C:C6 | 2.52 | 0.45 |
| 37:DD:163:GLU:O | 37:DD:166:LYS:HG3 | 2.16 | 0.45 |
| 26:C2:37:PHE:O | 26:C2:40:SER:OG | 2.31 | 0.45 |
| 3:CC:203:GLU:CD | 3:CC:203:GLU:N | 2.70 | 0.45 |
| 3:CC:223:VAL:HG23 | 3:CC:223:VAL:O | 2.15 | 0.45 |
| 32:A8:54:GLU:HA | 32:A8:54:GLU:OE1 | 2.17 | 0.45 |
| 59:BZ:-9:LEU:HD12 | 59:BZ:-9:LEU:HA | 1.71 | 0.45 |
| 37:BD:108:LEU:HB3 | 37:BD:110:PHE:CE1 | 2.52 | 0.45 |
| 20:AW:10:VAL:HG21 | 20:AW:103:ILE:HD12 | 1.98 | 0.45 |
| 13:AP:63:PRO:HG2 | 32:A8:25:MET:HB2 | 1.97 | 0.45 |
| 34:BA:667:G:H4' | 48:BO:51:HIS:ND1 | 2.32 | 0.45 |
| 16:CS:94:TYR:CE1 | 16:CS:99:LYS:HG3 | 2.52 | 0.45 |
| 50:BQ:32:TYR:O | 50:BQ:34:LYS:N | 2.41 | 0.45 |
| 59:BZ:82:ILE:HD13 | 59:BZ:100:VAL:HG12 | 1.98 | 0.45 |
| 59:BZ:78:ARG:HE | 59:BZ:357:ARG:CZ | 2.29 | 0.45 |
| 5:AE:110:GLY:O | 65:AR:5101:HOH:O | 2.21 | 0.45 |
| 59:DZ:225:GLU:H | 59:DZ:225:GLU:CD | 2.18 | 0.45 |
| 3:AC:16:ASP:OD2 | 3:AC:19:LYS:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:7:ARG:HH22 | 3:AC:219:MET:HB2 | 1.82 | 0.45 |
| 1:AA:2343:G:O2' | 24:A0:43:THR:HG22 | 2.17 | 0.45 |
| 8:CH:7:LEU:HD23 | 8:CH:69:ARG:NH1 | 2.31 | 0.45 |
| 2:CB:106:G:H5' | 23:CZ:31:ARG:HG2 | 1.97 | 0.45 |
| 59:DZ:535:PRO:O | 59:DZ:539:ILE:HG12 | 2.17 | 0.45 |
| 1:CA:1043:C:H2' | 1:CA:1044:G:H8 | 1.82 | 0.45 |
| 57:BX:19:G:C5 | 57:BX:57:A:C2 | 3.05 | 0.45 |
| 34:DA:429:U:H5' | 37:DD:9:CYS:SG | 2.56 | 0.45 |
| 1:AA:1817:A:H1' | 1:AA:1960:A:N6 | 2.32 | 0.45 |
| 1:AA:471:C:H2' | 1:AA:472:G:O4' | 2.16 | 0.45 |
| 39:BF:33:TYR:HE2 | 39:BF:78:GLU:HG2 | 1.81 | 0.45 |
| 1:CA:263:C:H2' | 1:CA:264:C:O4' | 2.17 | 0.45 |
| 22:CY:35:TYR:CD2 | 22:CY:69:ALA:HB3 | 2.51 | 0.45 |
| 1:CA:1030:G:N2 | 33:C9:5:ALA:O | 2.50 | 0.45 |
| 34:DA:1097:C:H2' | 34:DA:1098:C:H6 | 1.81 | 0.45 |
| 34:BA:949:A:H2' | 34:BA:950:U:O4' | 2.17 | 0.45 |
| 34:BA:1402:C:H2' | 34:BA:1403:C:O4' | 2.17 | 0.45 |
| 1:AA:2105:G:H8 | 1:AA:2105:G:O5' | 2.00 | 0.45 |
| 6:CF:196:LEU:HD23 | 6:CF:196:LEU:HA | 1.54 | 0.45 |
| 35:BB:172:ILE:HG13 | 35:BB:172:ILE:H | 1.56 | 0.45 |
| 1:AA:269:G:N7 | 1:AA:270:C:N4 | 2.65 | 0.45 |
| 1:AA:2575:U:O2 | 1:AA:2577:A:H8 | 2.00 | 0.45 |
| 49:DP:14:ASN:N | 49:DP:15:PRO:HD3 | 2.31 | 0.45 |
| 3:AC:54:ARG:HH22 | 3:AC:56:ASP:HB3 | 1.76 | 0.45 |
| 59:BZ:14:ASN:HD22 | 59:BZ:329:ARG:HH21 | 1.64 | 0.45 |
| 59:BZ:87:HIS:CB | 59:BZ:90:PHE:HB3 | 2.46 | 0.45 |
| 34:DA:926:G:C6 | 34:DA:1505:G:C5 | 3.05 | 0.45 |
| 59:BZ:-32:LEU:HA | 59:BZ:-32:LEU:HD23 | 1.82 | 0.45 |
| 1:CA:2751:G:H4' | 8:CH:4:ILE:HD11 | 1.99 | 0.45 |
| 36:DC:148:GLY:HA3 | 36:DC:172:ARG:O | 2.16 | 0.45 |
| 1:AA:1476:C:H2' | 1:AA:1477:U:H6 | 1.81 | 0.45 |
| 1:AA:1378:G:OP1 | 65:AA:4576:HOH:O | 2.21 | 0.45 |
| 1:AA:1478:C:H2' | 1:AA:1479:U:O4' | 2.16 | 0.45 |
| 1:CA:533:G:H5' | 18:CU:24:TYR:CE1 | 2.52 | 0.45 |
| 23:CZ:40:ASP:HB3 | 23:CZ:43:GLU:HG3 | 1.98 | 0.45 |
| 1:CA:362:U:O2' | 1:CA:363:G:H5' | 2.17 | 0.45 |
| 1:AA:1671:C:H2' | 1:AA:1672:G:O4' | 2.17 | 0.45 |
| 59:BZ:304:ASP:HA | 59:BZ:305:PRO:HD2 | 1.81 | 0.45 |
| 34:DA:644:G:H4' | 41:DH:92:ARG:NH2 | 2.31 | 0.45 |
| 7:CG:115:ARG:HH11 | 7:CG:115:ARG:H | 1.63 | 0.45 |
| 59:BZ:98:MET:HG2 | 59:BZ:101:LEU:HD12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:DZ:517:LEU:HD13 | 59:DZ:564:LYS:HB2 | 1.99 | 0.45 |
| 59:DZ:358:MET:HE1 | 59:DZ:363:ARG:HH12 | 1.82 | 0.45 |
| 1:AA:669:A:H4' | 1:AA:670:C:C5 | 2.52 | 0.45 |
| 59:DZ:181:LEU:O | 59:DZ:183:MET:N | 2.50 | 0.45 |
| 42:DI:9:ARG:O | 42:DI:104:ARG:HG3 | 2.17 | 0.45 |
| 13:AP:125:VAL:HG23 | 13:AP:125:VAL:O | 2.17 | 0.45 |
| 29:A5:35:GLU:HG3 | 29:A5:51:TYR:CG | 2.52 | 0.45 |
| 34:DA:1151:A:O2' | 34:DA:1152:A:H8 | 2.00 | 0.45 |
| 34:DA:297:G:N2 | 34:DA:300:A:OP2 | 2.45 | 0.45 |
| 34:DA:49:U:O4 | 34:DA:365:U:H5 | 2.00 | 0.45 |
| 1:CA:2727:G:O2' | 12:CO:70:LYS:NZ | 2.48 | 0.45 |
| 53:BT:100:ILE:H | 53:BT:100:ILE:HG12 | 1.43 | 0.45 |
| 34:DA:1058:G:H2' | 34:DA:1059:C:C6 | 2.52 | 0.45 |
| 34:DA:1157:A:H5' | 34:DA:1158:C:C6 | 2.52 | 0.45 |
| 1:CA:271(A):A:N7 | 1:CA:271(W):G:N2 | 2.60 | 0.45 |
| 34:DA:176:C:H2' | 34:DA:177:C:H6 | 1.81 | 0.45 |
| 51:BR:66:LEU:O | 51:BR:70:ILE:HG13 | 2.17 | 0.45 |
| 34:DA:600:C:C2 | 34:DA:639:G:C2 | 3.05 | 0.45 |
| 5:AE:47:VAL:HG22 | 5:AE:84:PHE:O | 2.17 | 0.45 |
| 8:AH:13:LYS:HA | 8:AH:14:GLY:HA2 | 1.71 | 0.45 |
| 8:AH:71:LEU:HA | 8:AH:71:LEU:HD12 | 1.81 | 0.45 |
| 3:AC:203:GLU:N | 3:AC:203:GLU:CD | 2.70 | 0.45 |
| 34:DA:111:G:O6 | 34:DA:330:C:N4 | 2.44 | 0.45 |
| 25:C1:77:ALA:HB1 | 25:C1:82:LEU:HD11 | 1.99 | 0.45 |
| 3:CC:179:ALA:O | 3:CC:180:SER:O | 2.35 | 0.45 |
| 3:CC:30:VAL:CG2 | 3:CC:31:LYS:H | 2.27 | 0.45 |
| 3:AC:179:ALA:O | 3:AC:180:SER:O | 2.35 | 0.45 |
| 34:DA:10:A:OP2 | 38:DE:126:ARG:HD2 | 2.17 | 0.45 |
| 1:AA:2228:G:O2' | 1:AA:2229:A:OP1 | 2.31 | 0.45 |
| 34:DA:1254:C:OP1 | 43:DJ:45:ARG:HA | 2.16 | 0.45 |
| 49:BP:74:LEU:HG | 49:BP:79:VAL:HG21 | 1.99 | 0.45 |
| 59:DZ:462:ILE:O | 59:DZ:466:LEU:HB2 | 2.17 | 0.45 |
| 10:AL:103:GLN:HA | 10:AL:106:GLU:HG2 | 1.98 | 0.45 |
| 1:CA:1494:A:H2' | 1:CA:1495:A:C8 | 2.52 | 0.45 |
| 1:CA:89:G:H3' | 1:CA:90:U:H5" | 1.98 | 0.45 |
| 25:C1:3:LYS:HB2 | 25:C1:61:ARG:HH11 | 1.79 | 0.45 |
| 34:BA:453:A:C6 | 34:BA:454:C:C4 | 3.05 | 0.45 |
| 56:DW:21:A:N6 | 56:DW:46:7MG:C4 | 2.85 | 0.45 |
| 1:CA:1059:G:O2' | 10:CL:126:MET:O | 2.28 | 0.45 |
| 59:BZ:178:ILE:HA | 59:BZ:185:ALA:HB2 | 1.99 | 0.45 |
| 1:CA:2298:A:N6 | 1:CA:2318:G:C8 | 2.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:91:C:OP1 | 14:AQ:16:ARG:HG3 | 2.17 | 0.45 |
| 23:CZ:104:PHE:HA | 23:CZ:139:VAL:HB | 1.99 | 0.45 |
| 57:BX:31:G:C8 | 57:BX:32:5MC:HM52 | 2.52 | 0.45 |
| 46:DM:59:TYR:CE1 | 46:DM:63:THR:HG21 | 2.52 | 0.45 |
| 59:DZ:257:PRO:HB2 | 59:DZ:259:PHE:HE1 | 1.82 | 0.45 |
| 45:DL:70:ILE:HD13 | 45:DL:75:HIS:CD2 | 2.51 | 0.45 |
| 59:BZ:-66:MET:N | 59:BZ:-46:VAL:O | 2.49 | 0.45 |
| 36:DC:130:VAL:O | 36:DC:134:ILE:HG12 | 2.17 | 0.45 |
| 34:BA:838:G:N2 | 34:BA:849:C:C2 | 2.85 | 0.45 |
| 50:DQ:40:LYS:HD3 | 50:DQ:42:TYR:CZ | 2.52 | 0.45 |
| 38:DE:144:THR:OG1 | 38:DE:147:ASP:OD2 | 2.24 | 0.45 |
| 5:CE:31:CYS:HA | 5:CE:32:PRO:HD2 | 1.83 | 0.45 |
| 15:AR:54:LEU:HD12 | 15:AR:54:LEU:HA | 1.66 | 0.45 |
| 48:BO:14:GLU:HG3 | 48:BO:14:GLU:O | 2.17 | 0.45 |
| 4:AD:93:ALA:HB3 | 4:AD:105:ILE:HG13 | 1.99 | 0.45 |
| 11:CN:58:ASP:OD1 | 11:CN:125:GLY:N | 2.32 | 0.45 |
| 59:DZ:246:ILE:HG23 | 59:DZ:255:ILE:HD11 | 1.99 | 0.45 |
| 24:A0:24:LYS:O | 24:A0:25:ARG:HD3 | 2.16 | 0.45 |
| 34:BA:620:C:H2' | 34:BA:621:A:O4' | 2.16 | 0.45 |
| 3:CC:7:ARG:HH22 | 3:CC:219:MET:HB2 | 1.82 | 0.44 |
| 35:BB:162:ILE:HD11 | 35:BB:184:VAL:HG22 | 1.99 | 0.44 |
| 34:DA:1320:C:OP1 | 52:DS:70:LYS:HE2 | 2.18 | 0.44 |
| 34:DA:838:G:H1 | 34:DA:848:C:N4 | 2.09 | 0.44 |
| 35:DB:54:THR:HG21 | 35:DB:201:ILE:HD11 | 1.98 | 0.44 |
| 47:DN:22:THR:HB | 47:DN:33:VAL:CB | 2.47 | 0.44 |
| 58:DY:35:A:H2' | 58:DY:36:A:O4' | 2.17 | 0.44 |
| 58:DY:37:MIA:H2' | 58:DY:38:A:O4' | 2.17 | 0.44 |
| 8:CH:3:ARG:HB3 | 8:CH:6:ARG:HG2 | 1.99 | 0.44 |
| 1:CA:1517:G:C6 | 1:CA:1518:U:N3 | 2.85 | 0.44 |
| 1:AA:1108:G:H1 | 1:AA:1122:C:H42 | 1.65 | 0.44 |
| 34:BA:1014:A:H4' | 52:BS:14:HIS:CD2 | 2.52 | 0.44 |
| 1:CA:2305:A:H2' | 1:CA:2306:C:O4' | 2.17 | 0.44 |
| 34:BA:506:G:C5 | 34:BA:507:C:C4 | 3.05 | 0.44 |
| 5:AE:120:TRP:CE2 | 5:AE:155:LYS:HG2 | 2.52 | 0.44 |
| 2:CB:3:C:H2' | 2:CB:4:C:C6 | 2.52 | 0.44 |
| 34:BA:1005:A:H1' | 34:BA:1036:G:H22 | 1.82 | 0.44 |
| 1:AA:987:G:O2' | 1:AA:988:U:H5' | 2.17 | 0.44 |
| 1:AA:1002:A:N1 | 1:AA:2470:G:H4' | 2.32 | 0.44 |
| 59:DZ:552:SER:HB3 | 59:DZ:591:LYS:NZ | 2.32 | 0.44 |
| 34:BA:551:U:H2' | 34:BA:552:U:C6 | 2.52 | 0.44 |
| 7:AG:145:THR:H | 7:AG:148:MET:HE2 | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:DA:15:G:H2' | 34:DA:16:A:H8 | 1.81 | 0.44 |
| 1:AA:864:C:O2' | 1:AA:886:U:H5'' | 2.17 | 0.44 |
| 56:BW:13:C:HO2' | 56:BW:14:A:P | 2.39 | 0.44 |
| 34:BA:43:C:H42 | 34:BA:399:G:H1 | 1.65 | 0.44 |
| 28:A4:15:ILE:HD13 | 28:A4:21:VAL:HG13 | 1.99 | 0.44 |
| 34:DA:1270:C:H2' | 34:DA:1271:G:C8 | 2.51 | 0.44 |
| 11:AN:39:ARG:HA | 11:AN:40:PRO:HD3 | 1.80 | 0.44 |
| 43:BJ:78:ASN:O | 43:BJ:80:LYS:N | 2.50 | 0.44 |
| 37:DD:12:CYS:HB3 | 37:DD:17:VAL:O | 2.17 | 0.44 |
| 1:AA:2650:G:P | 5:AE:82:ARG:NH2 | 2.90 | 0.44 |
| 34:DA:423:G:H3' | 34:DA:423:G:N3 | 2.32 | 0.44 |
| 53:DT:92:LEU:HA | 53:DT:92:LEU:HD23 | 1.81 | 0.44 |
| 1:CA:530:G:N3 | 1:CA:530:G:O4' | 2.49 | 0.44 |
| 34:BA:1152:A:OP1 | 43:BJ:68:HIS:ND1 | 2.49 | 0.44 |
| 59:BZ:94:VAL:HA | 59:BZ:97:SER:HB2 | 1.99 | 0.44 |
| 1:AA:1355:G:P | 31:A7:9:ARG:HD3 | 2.58 | 0.44 |
| 3:AC:55:SER:C | 3:AC:57:GLN:N | 2.71 | 0.44 |
| 1:AA:1099:C:H2' | 1:AA:1100:A:H5'' | 1.99 | 0.44 |
| 1:CA:300:A:H3' | 22:CY:84:ARG:NH2 | 2.32 | 0.44 |
| 28:C4:59:PHE:CE1 | 52:DS:64:GLU:HB2 | 2.52 | 0.44 |
| 59:DZ:169:GLY:O | 59:DZ:173:THR:OG1 | 2.28 | 0.44 |
| 35:DB:16:HIS:HB2 | 35:DB:204:ASN:ND2 | 2.32 | 0.44 |
| 58:BY:48:C:H2' | 58:BY:48:C:OP1 | 2.17 | 0.44 |
| 42:BI:49:PRO:HG3 | 42:BI:101:PHE:CD2 | 2.52 | 0.44 |
| 36:DC:7:PRO:HG3 | 36:DC:201:TYR:CE2 | 2.51 | 0.44 |
| 1:CA:2139:C:N4 | 1:CA:2152:G:H1 | 2.15 | 0.44 |
| 34:BA:142:G:H2' | 34:BA:143:A:C8 | 2.48 | 0.44 |
| 34:BA:1356:G:N2 | 34:BA:1367:C:O2 | 2.50 | 0.44 |
| 1:CA:1336:A:H2' | 1:CA:1337:G:C8 | 2.53 | 0.44 |
| 38:DE:12:LEU:O | 38:DE:30:ALA:HA | 2.18 | 0.44 |
| 34:DA:1252:A:H2' | 34:DA:1253:G:O4' | 2.17 | 0.44 |
| 1:CA:647:G:H2' | 1:CA:648:G:O4' | 2.17 | 0.44 |
| 1:AA:116:A:H3' | 1:AA:117:A:C5' | 2.48 | 0.44 |
| 34:BA:1036:G:H3' | 34:BA:1037:C:C6 | 2.53 | 0.44 |
| 1:CA:2336:A:H61 | 24:C0:43:THR:CG2 | 2.30 | 0.44 |
| 7:CG:67:LYS:H | 28:C4:6:HIS:CE1 | 2.35 | 0.44 |
| 4:CD:124:PRO:O | 4:CD:126:GLN:N | 2.51 | 0.44 |
| 59:DZ:632:LEU:HG | 59:DZ:645:ALA:HA | 1.99 | 0.44 |
| 1:CA:2303:G:O2' | 7:CG:132:ASN:HB2 | 2.17 | 0.44 |
| 50:DQ:7:THR:HA | 50:DQ:57:VAL:O | 2.17 | 0.44 |
| 42:BI:4:TYR:CE1 | 42:BI:88:TYR:HA | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:320:C:H2' | 1:AA:321:C:H6 | 1.81 | 0.44 |
| 1:AA:795:G:C8 | 20:AW:89:ALA:HB1 | 2.51 | 0.44 |
| 1:CA:851:U:H5' | 27:C3:49:LYS:HD2 | 1.98 | 0.44 |
| 1:CA:118:A:O5' | 1:CA:119:A:H5'' | 2.16 | 0.44 |
| 53:BT:45:GLN:HB3 | 53:BT:45:GLN:HE21 | 1.66 | 0.44 |
| 34:BA:841:U:OP2 | 34:BA:841:U:H6 | 2.00 | 0.44 |
| 1:AA:866:A:H8 | 1:AA:866:A:H5' | 1.82 | 0.44 |
| 43:DJ:42:THR:CG2 | 43:DJ:68:HIS:HD2 | 2.30 | 0.44 |
| 35:BB:223:ILE:HA | 35:BB:226:ARG:HB2 | 2.00 | 0.44 |
| 1:AA:1177:G:H21 | 11:AN:73:THR:CG2 | 2.30 | 0.44 |
| 1:AA:1809:U:H2' | 1:AA:1815:A:N6 | 2.33 | 0.44 |
| 42:BI:26:VAL:HG22 | 42:BI:61:ALA:HB3 | 1.97 | 0.44 |
| 10:CL:119:ASP:HB3 | 10:CL:120:LEU:H | 1.66 | 0.44 |
| 1:CA:601:C:OP1 | 6:CF:108:LYS:NZ | 2.37 | 0.44 |
| 1:AA:990:A:C4 | 1:AA:2460:A:C2 | 3.06 | 0.44 |
| 34:BA:1323:G:H4' | 34:BA:1363:C:N3 | 2.33 | 0.44 |
| 34:BA:664:G:N2 | 34:BA:741:G:H1 | 2.03 | 0.44 |
| 59:DZ:247:ARG:NH2 | 59:DZ:285:ASP:OD1 | 2.50 | 0.44 |
| 41:BH:86:ILE:HG21 | 41:BH:133:LEU:HD13 | 1.99 | 0.44 |
| 58:BY:60:U:H5'' | 58:BY:61:C:C5 | 2.45 | 0.44 |
| 34:DA:1119:C:OP1 | 42:DI:83:ARG:NH2 | 2.47 | 0.44 |
| 34:DA:1281:U:H5'' | 34:DA:1282:C:H5 | 1.81 | 0.44 |
| 1:CA:1434:A:H61 | 1:CA:1558:A:H62 | 1.64 | 0.44 |
| 34:BA:1075:C:H5'' | 35:BB:179:LYS:HE2 | 1.98 | 0.44 |
| 1:AA:310:C:H2' | 1:AA:311:C:C6 | 2.52 | 0.44 |
| 34:DA:1082:G:H2' | 34:DA:1083:U:O4' | 2.17 | 0.44 |
| 1:AA:886:U:H1' | 1:AA:1236:G:H1' | 1.99 | 0.44 |
| 4:AD:246:PRO:O | 4:AD:254:THR:HG22 | 2.17 | 0.44 |
| 50:BQ:9:VAL:O | 50:BQ:21:VAL:HA | 2.17 | 0.44 |
| 1:AA:2102:G:OP1 | 25:A1:35:THR:HG21 | 2.18 | 0.44 |
| 1:AA:395:C:H2' | 1:AA:396:C:O4' | 2.18 | 0.44 |
| 34:BA:1478:C:H2' | 34:BA:1479:C:C6 | 2.52 | 0.44 |
| 1:CA:1289:C:H2' | 1:CA:1290:C:H6 | 1.80 | 0.44 |
| 1:CA:661:C:H4' | 13:CP:13:ASN:OD1 | 2.18 | 0.44 |
| 34:BA:1218:C:H2' | 34:BA:1219:U:C6 | 2.51 | 0.44 |
| 38:BE:33:VAL:HG21 | 38:BE:109:ILE:HA | 2.00 | 0.44 |
| 13:AP:82:GLY:HA2 | 13:AP:113:LYS:O | 2.17 | 0.44 |
| 1:CA:2607:G:H2' | 1:CA:2608:G:O4' | 2.17 | 0.44 |
| 59:DZ:115:GLU:O | 59:DZ:118:SER:HB2 | 2.17 | 0.44 |
| 1:CA:1021:A:C8 | 1:CA:1021:A:C3' | 3.00 | 0.44 |
| 34:DA:1323:G:H2' | 34:DA:1324:A:C8 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BA:1129:C:H5'' | 42:BI:16:ARG:NH1 | 2.23 | 0.44 |
| 34:DA:235:C:H5' | 50:DQ:70:ARG:HG2 | 1.98 | 0.44 |
| 3:CC:174:ALA:HA | 3:CC:175:PRO:HD3 | 1.82 | 0.44 |
| 41:BH:6:ILE:O | 41:BH:10:LEU:HG | 2.18 | 0.44 |
| 3:CC:16:ASP:OD2 | 3:CC:19:LYS:HB2 | 2.17 | 0.44 |
| 1:CA:1434:A:O2' | 1:CA:1435:G:H5' | 2.17 | 0.44 |
| 34:DA:1013:G:N2 | 34:DA:1016:A:OP2 | 2.44 | 0.44 |
| 34:DA:1286:A:H8 | 34:DA:1287:A:H4' | 1.81 | 0.44 |
| 59:BZ:418:LYS:HD3 | 59:BZ:418:LYS:HA | 1.77 | 0.44 |
| 6:AF:64:ILE:HD11 | 6:AF:75:HIS:HB2 | 2.00 | 0.44 |
| 59:DZ:127:LYS:HE2 | 59:DZ:128:TYR:HE2 | 1.81 | 0.44 |
| 2:CB:8:U:O3' | 16:CS:25:ARG:NH2 | 2.38 | 0.44 |
| 16:CS:25:ARG:NH1 | 16:CS:42:ASP:OD1 | 2.50 | 0.44 |
| 13:AP:112:LEU:HD13 | 13:AP:127:ALA:HB2 | 1.99 | 0.44 |
| 4:CD:94:LEU:O | 4:CD:95:LEU:HD23 | 2.18 | 0.44 |
| 34:BA:667:G:OP1 | 34:BA:732:C:O2' | 2.21 | 0.44 |
| 1:CA:2466:C:H5' | 33:C9:5:ALA:HB3 | 1.98 | 0.44 |
| 5:CE:96:PHE:O | 5:CE:175:VAL:HG11 | 2.18 | 0.44 |
| 35:BB:166:ASP:HB3 | 35:BB:169:LYS:HB2 | 1.99 | 0.44 |
| 7:AG:121:ASN:HA | 7:AG:122:PRO:HD3 | 1.81 | 0.44 |
| 14:AQ:62:GLY:HA2 | 23:AZ:116:VAL:HG21 | 2.00 | 0.44 |
| 44:BK:30:VAL:HG21 | 44:BK:65:ALA:HA | 1.98 | 0.44 |
| 34:BA:1412:C:H2' | 34:BA:1413:A:C8 | 2.53 | 0.44 |
| 5:AE:31:CYS:HA | 5:AE:32:PRO:HD2 | 1.76 | 0.44 |
| 4:CD:29:PRO:HA | 4:CD:83:GLU:OE1 | 2.18 | 0.44 |
| 1:CA:858:U:O2 | 1:CA:2268:A:H2' | 2.18 | 0.44 |
| 35:BB:80:ILE:O | 35:BB:80:ILE:HG13 | 2.17 | 0.44 |
| 38:BE:79:GLU:HG3 | 38:BE:79:GLU:H | 1.61 | 0.44 |
| 26:A2:61:LEU:HD23 | 26:A2:61:LEU:HA | 1.62 | 0.44 |
| 6:CF:36:VAL:HG11 | 6:CF:183:VAL:CG1 | 2.48 | 0.44 |
| 23:AZ:111:VAL:C | 23:AZ:113:ALA:H | 2.21 | 0.44 |
| 3:AC:24:ASP:C | 3:AC:24:ASP:OD1 | 2.55 | 0.44 |
| 34:DA:235:C:H2' | 34:DA:236:G:C8 | 2.52 | 0.44 |
| 3:CC:68:GLY:N | 3:CC:189:ASN:ND2 | 2.62 | 0.44 |
| 1:AA:2130:C:H2' | 1:AA:2131:U:C6 | 2.51 | 0.44 |
| 1:CA:2148:G:H2' | 1:CA:2149:G:H8 | 1.81 | 0.44 |
| 34:DA:833:U:H2' | 34:DA:834:C:H6 | 1.83 | 0.44 |
| 34:BA:410:G:H5'' | 34:BA:411:A:OP1 | 2.18 | 0.44 |
| 1:AA:2417:G:OP1 | 13:AP:77:ARG:NH2 | 2.51 | 0.44 |
| 1:CA:1074:G:H2' | 1:CA:1075:C:C6 | 2.53 | 0.44 |
| 59:DZ:168:ILE:N | 59:DZ:176:GLY:O | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:2638:G:P | 5:CE:82:ARG:HH21 | 2.39 | 0.44 |
| 32:C8:31:HIS:O | 32:C8:32:LEU:HB2 | 2.18 | 0.44 |
| 1:AA:2804:C:H2' | 1:AA:2805:G:C8 | 2.53 | 0.44 |
| 1:CA:1894:C:O2' | 1:CA:1895:C:H5' | 2.16 | 0.44 |
| 34:BA:1445:C:H2' | 34:BA:1446:U:O4' | 2.17 | 0.44 |
| 1:CA:359:A:H2' | 1:CA:360:G:O4' | 2.18 | 0.44 |
| 1:AA:1495:G:H1' | 1:AA:1574:A:N1 | 2.33 | 0.44 |
| 1:CA:459:U:H5'' | 31:C7:40:TRP:CD2 | 2.53 | 0.44 |
| 59:DZ:604:PRO:HG2 | 59:DZ:649:LEU:HB3 | 1.98 | 0.44 |
| 13:CP:123:LEU:HA | 13:CP:123:LEU:HD23 | 1.79 | 0.44 |
| 8:CH:73:ALA:O | 8:CH:76:VAL:HB | 2.18 | 0.44 |
| 16:CS:105:ALA:O | 16:CS:110:LEU:HB2 | 2.17 | 0.44 |
| 27:A3:4:LEU:HA | 27:A3:4:LEU:HD23 | 1.75 | 0.44 |
| 35:BB:71:VAL:HA | 35:BB:93:VAL:HG23 | 2.00 | 0.44 |
| 1:AA:212:A:O2' | 1:AA:447:C:O2 | 2.28 | 0.44 |
| 44:DK:43:SER:OG | 44:DK:44:SER:N | 2.51 | 0.44 |
| 34:BA:1326:C:H5'' | 54:BU:12:LYS:HE3 | 1.99 | 0.44 |
| 3:CC:30:VAL:CG2 | 3:CC:31:LYS:N | 2.78 | 0.44 |
| 52:DS:36:ARG:HD2 | 52:DS:52:TYR:O | 2.18 | 0.44 |
| 3:AC:22:THR:HG23 | 3:AC:25:GLU:OE1 | 2.17 | 0.44 |
| 3:CC:22:THR:HG23 | 3:CC:25:GLU:OE1 | 2.17 | 0.44 |
| 41:BH:112:LEU:HD13 | 41:BH:114:THR:HG23 | 1.98 | 0.44 |
| 34:DA:1262:C:H2' | 34:DA:1263:C:H6 | 1.83 | 0.44 |
| 34:DA:1272:G:C2 | 34:DA:1273:G:H1' | 2.52 | 0.44 |
| 1:CA:2238:G:N3 | 1:CA:2238:G:H2' | 2.32 | 0.44 |
| 36:DC:7:PRO:O | 36:DC:11:ARG:NH1 | 2.50 | 0.44 |
| 12:AO:69:ILE:HG13 | 12:AO:69:ILE:O | 2.16 | 0.44 |
| 46:DM:40:ASN:ND2 | 46:DM:41:PRO:HD2 | 2.32 | 0.44 |
| 35:BB:28:PHE:CD1 | 35:BB:190:THR:HA | 2.52 | 0.44 |
| 34:BA:418:C:H2' | 34:BA:419:C:H6 | 1.83 | 0.44 |
| 1:CA:646:A:H2' | 1:CA:647:G:O4' | 2.17 | 0.44 |
| 1:CA:1847:A:H4' | 1:CA:1848:A:OP2 | 2.17 | 0.44 |
| 1:CA:515:A:H1' | 1:CA:581:C:H1' | 1.99 | 0.44 |
| 34:BA:358:U:P | 59:BZ:381:LYS:HZ2 | 2.40 | 0.44 |
| 10:CL:88:ALA:O | 10:CL:90:LYS:N | 2.50 | 0.44 |
| 8:AH:29:PRO:HD2 | 8:AH:79:VAL:O | 2.18 | 0.44 |
| 54:BU:5:ASP:O | 54:BU:11:GLY:HA3 | 2.17 | 0.44 |
| 1:AA:1941:A:H5'' | 1:AA:1942:C:OP2 | 2.17 | 0.44 |
| 1:CA:752:A:P | 31:C7:3:ARG:HH22 | 2.41 | 0.44 |
| 34:BA:685:G:O2' | 34:BA:686:U:H5' | 2.18 | 0.44 |
| 59:DZ:681:LYS:HE2 | 59:DZ:681:LYS:HB3 | 1.72 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BA:1530:G:H4' | 34:BA:1530:G:OP1 | 2.17 | 0.44 |
| 39:DF:49:ALA:HB2 | 51:DR:78:LEU:O | 2.18 | 0.44 |
| 41:DH:97:VAL:HA | 41:DH:100:ILE:HG13 | 1.98 | 0.44 |
| 59:BZ:553:GLY:H | 59:BZ:557:GLY:HA2 | 1.82 | 0.44 |
| 21:CX:35:THR:HG22 | 21:CX:38:GLU:N | 2.14 | 0.44 |
| 35:BB:44:LEU:H | 35:BB:44:LEU:HD22 | 1.82 | 0.44 |
| 1:CA:1019:U:O2' | 1:CA:1021:A:H2 | 1.99 | 0.44 |
| 1:AA:1188:A:C4 | 1:AA:1190:G:C8 | 3.06 | 0.44 |
| 34:DA:1165:C:H2' | 34:DA:1166:G:O4' | 2.18 | 0.44 |
| 20:AW:18:ARG:HG2 | 20:AW:76:VAL:HB | 2.00 | 0.44 |
| 59:DZ:610:VAL:HG21 | 59:DZ:655:TYR:OH | 2.18 | 0.44 |
| 3:AC:39:ASP:O | 3:AC:178:LYS:HE3 | 2.17 | 0.44 |
| 34:DA:839:U:H5'' | 34:DA:840:C:C5 | 2.51 | 0.44 |
| 59:BZ:-38:TYR:O | 59:BZ:-34:ARG:HG2 | 2.18 | 0.44 |
| 1:CA:1479:G:O2' | 1:CA:1558:A:H5' | 2.18 | 0.44 |
| 23:CZ:5:LEU:HD13 | 23:CZ:6:LYS:O | 2.18 | 0.44 |
| 1:CA:2063:C:H1' | 57:DX:76:31H:HCN | 2.00 | 0.44 |
| 58:DY:55:PSU:HN1 | 58:DY:57:G:C5' | 2.29 | 0.44 |
| 1:CA:1653:G:C6 | 15:CR:9:LYS:HG3 | 2.53 | 0.44 |
| 53:DT:81:LYS:O | 53:DT:85:MET:HG3 | 2.17 | 0.44 |
| 6:AF:53:THR:HG23 | 6:AF:55:GLY:H | 1.81 | 0.44 |
| 59:BZ:177:ILE:O | 59:BZ:185:ALA:HA | 2.17 | 0.44 |
| 59:BZ:524:GLU:HB3 | 59:BZ:564:LYS:HG3 | 2.00 | 0.44 |
| 1:AA:1889:G:N2 | 1:AA:1905:G:H2' | 2.33 | 0.44 |
| 37:DD:67:ILE:HG22 | 37:DD:68:TYR:CD2 | 2.52 | 0.44 |
| 34:BA:1268:A:H2' | 34:BA:1269:A:C8 | 2.52 | 0.44 |
| 15:AR:55:ALA:HB2 | 15:AR:79:LEU:HD13 | 1.99 | 0.44 |
| 34:BA:630:G:H2' | 34:BA:631:G:H8 | 1.82 | 0.44 |
| 1:CA:1076:C:H2' | 1:CA:1077:A:C8 | 2.53 | 0.44 |
| 28:A4:53:GLU:HB3 | 28:A4:54:GLY:HA2 | 2.00 | 0.44 |
| 39:BF:99:ALA:O | 39:BF:100:ASN:HB2 | 2.16 | 0.44 |
| 1:CA:271(X):G:C2 | 1:CA:271(Y):U:O4 | 2.70 | 0.44 |
| 7:AG:34:LEU:HD23 | 7:AG:34:LEU:HA | 1.70 | 0.44 |
| 8:AH:111:HIS:H | 8:AH:111:HIS:CD2 | 2.35 | 0.44 |
| 34:BA:977:A:O2' | 34:BA:981:U:N3 | 2.47 | 0.44 |
| 21:AX:60:ARG:NH1 | 31:A7:47:ARG:HH21 | 2.15 | 0.44 |
| 34:BA:1159:U:OP1 | 35:BB:133:LYS:NZ | 2.48 | 0.44 |
| 17:CT:85:LYS:NZ | 17:CT:87:ASP:OD2 | 2.46 | 0.44 |
| 11:CN:103:VAL:O | 11:CN:107:LEU:HG | 2.17 | 0.44 |
| 59:BZ:94:VAL:HG12 | 59:BZ:97:SER:HB2 | 1.99 | 0.44 |
| 17:CT:53:ARG:O | 17:CT:59:THR:HB | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:DZ:129:LYS:O | 59:DZ:253:LEU:HD11 | 2.18 | 0.44 |
| 1:CA:1359:A:N1 | 1:CA:1372:U:O4 | 2.51 | 0.44 |
| 34:DA:1239:A:H4' | 34:DA:1240:U:C5' | 2.44 | 0.44 |
| 34:BA:1226:C:H4' | 52:BS:80:TYR:OH | 2.18 | 0.44 |
| 42:DI:17:VAL:HG11 | 42:DI:80:GLY:C | 2.38 | 0.44 |
| 34:BA:200:G:N2 | 34:BA:218:C:C2 | 2.85 | 0.44 |
| 3:CC:39:ASP:O | 3:CC:178:LYS:HE3 | 2.18 | 0.44 |
| 59:DZ:-53:ASP:H | 59:DZ:-50:GLN:HE22 | 1.66 | 0.44 |
| 18:AU:76:TYR:OH | 18:AU:92:ARG:NH1 | 2.43 | 0.44 |
| 13:CP:88:LEU:HD11 | 13:CP:114:ILE:HD12 | 1.99 | 0.44 |
| 43:BJ:6:ILE:O | 43:BJ:71:LEU:HD12 | 2.18 | 0.44 |
| 14:CQ:16:ARG:HH11 | 14:CQ:16:ARG:CG | 2.29 | 0.44 |
| 1:CA:657:U:H2' | 1:CA:658:C:H6 | 1.83 | 0.44 |
| 46:BM:84:ILE:N | 46:BM:85:GLY:HA2 | 2.33 | 0.44 |
| 28:A4:59:PHE:HD2 | 52:BS:42:PRO:HG3 | 1.83 | 0.44 |
| 1:AA:2653:G:H5'' | 1:AA:2653:G:C8 | 2.52 | 0.44 |
| 59:BZ:243:VAL:HG13 | 59:BZ:279:TYR:CE1 | 2.53 | 0.44 |
| 1:AA:2710:U:H2' | 1:AA:2711:C:C6 | 2.53 | 0.44 |
| 35:DB:88:ALA:HB2 | 35:DB:219:VAL:HG13 | 1.99 | 0.44 |
| 4:AD:147:LEU:HD13 | 4:AD:155:LEU:HD11 | 1.99 | 0.44 |
| 47:DN:45:ARG:O | 47:DN:49:HIS:HD2 | 2.01 | 0.44 |
| 34:DA:25:C:O2' | 34:DA:26:A:H5' | 2.17 | 0.44 |
| 1:AA:905:U:O2 | 1:AA:2280:A:H2' | 2.17 | 0.44 |
| 34:DA:502:G:C2 | 34:DA:544:G:C2 | 3.06 | 0.44 |
| 34:BA:1077:G:N2 | 34:BA:1080:A:OP2 | 2.46 | 0.44 |
| 34:DA:1328:C:OP1 | 54:DU:21:TYR:OH | 2.28 | 0.44 |
| 1:CA:2282:G:H4' | 1:CA:2389:G:O2' | 2.16 | 0.44 |
| 1:CA:251:A:C5 | 1:CA:252:G:H1' | 2.53 | 0.44 |
| 1:AA:2034:G:OP1 | 20:AW:11:ARG:NH2 | 2.44 | 0.44 |
| 34:DA:309:G:H1' | 34:DA:608:A:C2 | 2.52 | 0.44 |
| 1:AA:1576:G:H2' | 1:AA:1577:C:O4' | 2.18 | 0.44 |
| 41:DH:33:GLU:O | 41:DH:36:LEU:N | 2.46 | 0.44 |
| 34:BA:96:U:O2' | 34:BA:97:G:H5' | 2.18 | 0.44 |
| 22:CY:38:ILE:HD13 | 22:CY:66:PRO:HA | 2.00 | 0.44 |
| 23:CZ:53:ILE:HG22 | 23:CZ:71:VAL:HB | 2.00 | 0.44 |
| 1:AA:2421:G:H2' | 1:AA:2422:G:O4' | 2.18 | 0.44 |
| 47:DN:15:LYS:HE2 | 47:DN:16:PHE:CZ | 2.52 | 0.44 |
| 1:CA:569:U:C4 | 1:CA:570:G:C6 | 3.06 | 0.44 |
| 59:BZ:508:GLY:HA3 | 59:BZ:581:ALA:O | 2.18 | 0.44 |
| 41:DH:125:ARG:HE | 41:DH:125:ARG:HB2 | 1.37 | 0.44 |
| 11:CN:39:ARG:HE | 11:CN:39:ARG:HB3 | 1.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AL:93:ARG:NH1 | 10:AL:94:GLU:HB2 | 2.33 | 0.44 |
| 27:C3:5:LYS:NZ | 27:C3:57:GLU:OE2 | 2.51 | 0.44 |
| 1:CA:1607:C:H4' | 1:CA:1608:A:O5' | 2.17 | 0.44 |
| 1:AA:34:C:H5'' | 1:AA:35:G:OP2 | 2.18 | 0.44 |
| 1:CA:771:G:OP1 | 31:C7:10:ARG:NH1 | 2.50 | 0.44 |
| 1:AA:1249:A:N6 | 1:AA:1286:U:H2' | 2.32 | 0.44 |
| 34:BA:1324:A:H2' | 34:BA:1325:C:C6 | 2.52 | 0.44 |
| 35:DB:162:ILE:O | 35:DB:185:ILE:HG12 | 2.18 | 0.44 |
| 34:DA:1320:C:H5' | 52:DS:70:LYS:HG3 | 2.00 | 0.44 |
| 3:CC:24:ASP:OD1 | 3:CC:24:ASP:C | 2.55 | 0.44 |
| 1:AA:553:A:C2 | 1:AA:2065:C:H5' | 2.52 | 0.44 |
| 1:CA:1495:A:H2' | 1:CA:1496:A:H8 | 1.82 | 0.44 |
| 1:CA:848:G:O6 | 1:CA:928:G:H2' | 2.17 | 0.44 |
| 47:BN:23:ARG:CZ | 47:BN:30:ALA:HB2 | 2.48 | 0.44 |
| 59:BZ:125:ALA:C | 59:BZ:132:ARG:HH12 | 2.21 | 0.44 |
| 1:CA:493:G:H2' | 1:CA:494:G:O4' | 2.18 | 0.44 |
| 20:CW:59:VAL:HG12 | 20:CW:60:ASN:ND2 | 2.33 | 0.44 |
| 23:CZ:67:LEU:HD22 | 23:CZ:90:VAL:HG11 | 1.99 | 0.44 |
| 1:AA:324:A:P | 22:AY:86:ARG:HH22 | 2.40 | 0.44 |
| 1:AA:504:A:C6 | 1:AA:506:A:C6 | 3.06 | 0.44 |
| 52:DS:27:GLU:HB2 | 52:DS:28:LYS:NZ | 2.33 | 0.44 |
| 22:CY:35:TYR:CE2 | 22:CY:69:ALA:HB3 | 2.52 | 0.44 |
| 34:DA:537:G:H5'' | 45:DL:113:ARG:NH1 | 2.33 | 0.44 |
| 41:DH:14:ARG:O | 41:DH:18:ARG:HD3 | 2.18 | 0.44 |
| 1:CA:1996:C:H4' | 1:CA:1997:G:OP1 | 2.17 | 0.44 |
| 1:AA:243:G:O6 | 32:A8:5:LYS:HG2 | 2.17 | 0.44 |
| 1:AA:104:C:H2' | 1:AA:105:C:H6 | 1.83 | 0.44 |
| 1:AA:1575:A:N6 | 1:AA:1588:G:O2' | 2.45 | 0.44 |
| 20:AW:61:ASN:HB2 | 20:AW:62:HIS:CD2 | 2.52 | 0.44 |
| 34:DA:513:C:H42 | 34:DA:538:G:H1 | 1.66 | 0.44 |
| 4:AD:132:PRO:HD3 | 4:AD:190:TYR:CZ | 2.53 | 0.44 |
| 59:DZ:654:GLY:O | 59:DZ:658:ASP:HB2 | 2.18 | 0.44 |
| 1:CA:651:G:OP2 | 32:C8:21:LYS:HE3 | 2.18 | 0.44 |
| 59:BZ:107:VAL:HG13 | 59:BZ:135:PHE:HD2 | 1.83 | 0.44 |
| 52:DS:40:ILE:HB | 52:DS:67:VAL:O | 2.17 | 0.44 |
| 9:AK:85:ASP:O | 9:AK:87:VAL:N | 2.51 | 0.44 |
| 40:BG:8:GLU:H | 40:BG:8:GLU:CD | 2.21 | 0.44 |
| 13:AP:135:LEU:HD23 | 13:AP:135:LEU:HA | 1.75 | 0.44 |
| 15:AR:118:GLU:H | 15:AR:118:GLU:CD | 2.21 | 0.44 |
| 1:AA:808:A:OP1 | 65:AA:4735:HOH:O | 2.21 | 0.44 |
| 1:CA:1235:G:C6 | 1:CA:1236:G:N1 | 2.85 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:1900:G:H2' | 1:AA:1901:C:C6 | 2.52 | 0.44 |
| 53:DT:79:ARG:HD2 | 53:DT:83:ARG:NH1 | 2.33 | 0.44 |
| 1:AA:1891:G:H5' | 3:AC:206:LYS:CE | 2.48 | 0.43 |
| 1:AA:1065:U:O2' | 1:AA:1067:A:H2 | 1.90 | 0.43 |
| 34:DA:1324:A:O4' | 34:DA:1362:C:H4' | 2.18 | 0.43 |
| 1:CA:2124:G:O6 | 1:CA:2174:C:N4 | 2.48 | 0.43 |
| 37:BD:13:ARG:HB3 | 37:BD:38:TYR:O | 2.18 | 0.43 |
| 34:BA:1066:C:O2' | 34:BA:1067:A:H5' | 2.18 | 0.43 |
| 56:DW:43:C:H2' | 56:DW:44:G:C8 | 2.53 | 0.43 |
| 58:BY:58:A:O2' | 58:BY:60:U:H5 | 2.01 | 0.43 |
| 1:CA:2892:A:C8 | 1:CA:2893:G:N7 | 2.86 | 0.43 |
| 35:DB:158:LEU:HA | 35:DB:159:PRO:HD2 | 1.86 | 0.43 |
| 34:BA:1251:A:H2' | 34:BA:1252:A:H8 | 1.81 | 0.43 |
| 7:AG:43:LEU:HB3 | 7:AG:44:GLY:H | 1.46 | 0.43 |
| 34:DA:1228:C:OP2 | 46:DM:111:LYS:HD3 | 2.18 | 0.43 |
| 3:AC:194:ILE:HD11 | 3:AC:227:PRO:HB2 | 1.99 | 0.43 |
| 34:DA:881:G:P | 45:DL:12:ARG:HH22 | 2.42 | 0.43 |
| 57:DX:67:C:H2' | 57:DX:68:C:H5' | 1.99 | 0.43 |
| 34:DA:437:U:H5' | 37:DD:155:LEU:HD21 | 2.00 | 0.43 |
| 36:DC:113:ALA:HA | 36:DC:116:VAL:HG23 | 2.00 | 0.43 |
| 34:DA:1510:U:H2' | 34:DA:1511:G:C8 | 2.52 | 0.43 |
| 37:BD:121:VAL:O | 37:BD:134:ASP:HA | 2.18 | 0.43 |
| 59:BZ:401:SER:O | 59:BZ:402:ILE:HG12 | 2.18 | 0.43 |
| 36:DC:77:ILE:HG13 | 36:DC:78:GLY:N | 2.33 | 0.43 |
| 1:AA:386:U:H6 | 1:AA:386:U:H2' | 1.60 | 0.43 |
| 23:CZ:10:ARG:NH2 | 23:CZ:26:GLY:O | 2.49 | 0.43 |
| 1:CA:1158:C:H4' | 27:C3:32:GLN:HB2 | 1.99 | 0.43 |
| 34:DA:1410:G:H2' | 34:DA:1411:C:H6 | 1.83 | 0.43 |
| 44:DK:85:ARG:HG2 | 44:DK:111:ASP:O | 2.18 | 0.43 |
| 1:CA:322:A:C5 | 1:CA:340:A:C2 | 3.06 | 0.43 |
| 23:CZ:39:VAL:HG21 | 23:CZ:44:PHE:HB2 | 2.00 | 0.43 |
| 1:AA:1014:U:H2' | 1:AA:1015:C:C6 | 2.52 | 0.43 |
| 51:BR:59:SER:OG | 51:BR:62:GLU:HG2 | 2.18 | 0.43 |
| 7:CG:61:ALA:HA | 7:CG:66:GLN:O | 2.17 | 0.43 |
| 38:DE:31:LEU:HD11 | 38:DE:132:ALA:HB2 | 1.99 | 0.43 |
| 3:AC:60:ARG:HG3 | 3:AC:165:ARG:HB2 | 2.00 | 0.43 |
| 7:CG:96:ARG:O | 7:CG:99:MET:HB3 | 2.18 | 0.43 |
| 27:C3:7:LYS:HB2 | 27:C3:34:GLU:HG3 | 1.99 | 0.43 |
| 34:DA:652:U:O4 | 34:DA:752:G:O2' | 2.22 | 0.43 |
| 4:CD:5:LYS:HB3 | 4:CD:5:LYS:HE3 | 1.63 | 0.43 |
| 48:BO:5:LYS:HD2 | 48:BO:5:LYS:H | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:BE:24:ARG:HG2 | 38:BE:24:ARG:HH11 | 1.83 | 0.43 |
| 11:CN:34:LEU:O | 11:CN:49:GLY:HA3 | 2.17 | 0.43 |
| 34:DA:685:G:N2 | 34:DA:686:U:C4 | 2.86 | 0.43 |
| 1:CA:2175:C:H1' | 3:CC:218:THR:O | 2.18 | 0.43 |
| 49:DP:5:ARG:HB3 | 49:DP:67:THR:CG2 | 2.48 | 0.43 |
| 34:BA:926:G:C6 | 34:BA:1505:G:C6 | 3.06 | 0.43 |
| 3:CC:55:SER:C | 3:CC:57:GLN:N | 2.71 | 0.43 |
| 1:CA:300:A:H1' | 1:CA:319:C:H1' | 1.99 | 0.43 |
| 17:AT:80:SER:HA | 17:AT:81:PRO:HD3 | 1.85 | 0.43 |
| 28:C4:46:GLN:HG2 | 28:C4:48:ARG:HH21 | 1.83 | 0.43 |
| 35:DB:187:LEU:HA | 35:DB:201:ILE:HB | 1.99 | 0.43 |
| 59:DZ:-53:ASP:O | 59:DZ:-50:GLN:HB3 | 2.17 | 0.43 |
| 59:DZ:493:VAL:HG21 | 59:DZ:593:ALA:HB2 | 2.00 | 0.43 |
| 41:DH:34:GLU:O | 41:DH:38:ILE:HG12 | 2.18 | 0.43 |
| 34:DA:1029:C:H2' | 34:DA:1030:C:H5'' | 2.00 | 0.43 |
| 55:BV:14:A:N6 | 55:BV:15:A:C6 | 2.87 | 0.43 |
| 34:DA:1434:A:H2' | 34:DA:1435:G:O4' | 2.18 | 0.43 |
| 30:A6:18:ARG:HD2 | 30:A6:42:TRP:CG | 2.53 | 0.43 |
| 1:CA:2461:C:H2' | 1:CA:2462:U:C6 | 2.54 | 0.43 |
| 46:DM:57:ARG:O | 46:DM:61:GLU:HB2 | 2.18 | 0.43 |
| 1:AA:2867:G:N2 | 1:AA:2870:A:OP2 | 2.45 | 0.43 |
| 1:AA:1485:A:H2' | 1:AA:1486:G:O4' | 2.18 | 0.43 |
| 35:BB:45:GLN:O | 35:BB:49:GLU:HG3 | 2.18 | 0.43 |
| 59:BZ:-7:GLU:HA | 59:BZ:-4:ALA:HB3 | 1.98 | 0.43 |
| 34:BA:1136:U:H5'' | 34:BA:1137:C:N3 | 2.33 | 0.43 |
| 1:AA:1127:U:O3' | 10:AL:117:THR:HB | 2.18 | 0.43 |
| 41:DH:121:ASP:N | 41:DH:121:ASP:OD1 | 2.49 | 0.43 |
| 7:CG:116:ASP:OD1 | 7:CG:116:ASP:N | 2.51 | 0.43 |
| 40:DG:149:ARG:HG2 | 44:DK:59:TYR:CE1 | 2.54 | 0.43 |
| 43:DJ:52:GLY:HA2 | 43:DJ:53:PRO:HD3 | 1.82 | 0.43 |
| 21:CX:32:PRO:HA | 21:CX:77:LYS:HD2 | 2.00 | 0.43 |
| 1:CA:2132:U:C2 | 3:CC:6:LYS:CE | 3.01 | 0.43 |
| 34:BA:925:G:H1' | 34:BA:1502:A:C4 | 2.53 | 0.43 |
| 58:DY:65:G:H2' | 58:DY:66:U:C6 | 2.53 | 0.43 |
| 59:BZ:289:ILE:HG13 | 59:BZ:289:ILE:H | 1.50 | 0.43 |
| 45:DL:31:PRO:HB2 | 45:DL:32:PHE:CD2 | 2.53 | 0.43 |
| 46:BM:14:ARG:HB2 | 46:BM:17:VAL:HG23 | 2.00 | 0.43 |
| 46:DM:25:ILE:HD11 | 46:DM:66:LEU:HD23 | 1.99 | 0.43 |
| 37:BD:120:LEU:HA | 37:BD:120:LEU:HD23 | 1.70 | 0.43 |
| 34:DA:1051:C:H2' | 34:DA:1052:U:C6 | 2.53 | 0.43 |
| 34:DA:620:C:C2 | 37:DD:135:LEU:HG | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1557:C:H5'' | 1:CA:1558:A:OP2 | 2.17 | 0.43 |
| 38:BE:76:ILE:HB | 38:BE:77:PRO:HD2 | 2.01 | 0.43 |
| 34:BA:406:G:N2 | 34:BA:437:U:O2 | 2.51 | 0.43 |
| 9:AK:118:THR:O | 9:AK:120:LYS:N | 2.47 | 0.43 |
| 8:CH:154:PRO:HB3 | 8:CH:163:TYR:CZ | 2.53 | 0.43 |
| 34:BA:1020:U:H2' | 34:BA:1021:G:H8 | 1.83 | 0.43 |
| 34:BA:688:G:H2' | 34:BA:689:C:C6 | 2.54 | 0.43 |
| 34:DA:1342:C:O2' | 42:DI:124:GLN:HG2 | 2.17 | 0.43 |
| 5:AE:12:THR:HG22 | 5:AE:13:ARG:N | 2.32 | 0.43 |
| 1:AA:2219:U:C5 | 1:AA:2236:G:C6 | 3.06 | 0.43 |
| 58:DY:39:PSU:C2 | 58:DY:40:C:C4 | 3.07 | 0.43 |
| 1:CA:724:U:H2' | 1:CA:725:G:O4' | 2.18 | 0.43 |
| 4:AD:275:LYS:HB3 | 4:AD:276:LYS:H | 1.52 | 0.43 |
| 34:BA:299:G:H2' | 34:BA:300:A:C8 | 2.54 | 0.43 |
| 1:CA:2110:G:H4' | 1:CA:2111:C:OP2 | 2.17 | 0.43 |
| 34:BA:1058:G:N2 | 43:BJ:53:PRO:HG3 | 2.33 | 0.43 |
| 35:BB:121:LEU:HA | 35:BB:121:LEU:HD13 | 1.85 | 0.43 |
| 34:DA:60:A:H4' | 34:DA:61:G:O5' | 2.19 | 0.43 |
| 36:DC:178:LEU:HD13 | 36:DC:178:LEU:HA | 1.85 | 0.43 |
| 46:BM:73:GLU:O | 46:BM:77:ASN:ND2 | 2.48 | 0.43 |
| 1:CA:945:A:C4 | 1:CA:2448:A:C2 | 3.06 | 0.43 |
| 25:A1:86:SER:OG | 25:A1:89:GLU:HG2 | 2.18 | 0.43 |
| 1:CA:2086:U:H2' | 1:CA:2087:G:C8 | 2.52 | 0.43 |
| 12:AO:122:LEU:HD13 | 17:AT:72:VAL:HG11 | 1.98 | 0.43 |
| 1:CA:1144:G:H2' | 1:CA:1145:C:H6 | 1.81 | 0.43 |
| 36:BC:58:GLU:HB2 | 36:BC:65:ALA:CB | 2.48 | 0.43 |
| 34:DA:1321:C:H5'' | 34:DA:1322:C:H2' | 2.00 | 0.43 |
| 59:DZ:169:GLY:HA3 | 59:DZ:173:THR:O | 2.18 | 0.43 |
| 52:BS:50:ALA:HB1 | 52:BS:57:HIS:HB3 | 1.99 | 0.43 |
| 12:CO:120:GLU:HG2 | 12:CO:122:LEU:HG | 1.99 | 0.43 |
| 58:BY:53:G:H1 | 58:BY:61:C:H42 | 1.64 | 0.43 |
| 43:DJ:39:PRO:HA | 43:DJ:70:ARG:HD3 | 2.00 | 0.43 |
| 7:AG:137:GLU:HB3 | 7:AG:139:LEU:HD12 | 2.01 | 0.43 |
| 59:DZ:74:TRP:HE1 | 59:DZ:274:ASP:N | 2.17 | 0.43 |
| 1:AA:278:G:OP1 | 25:A1:76:ARG:HD2 | 2.18 | 0.43 |
| 34:BA:235:C:H5' | 50:BQ:70:ARG:HG2 | 2.00 | 0.43 |
| 56:BW:7:A:H5' | 56:BW:8:4SU:H5 | 1.99 | 0.43 |
| 17:CT:120:ARG:HA | 17:CT:123:GLN:HG3 | 2.00 | 0.43 |
| 34:DA:961:U:H2' | 34:DA:962:C:O4' | 2.19 | 0.43 |
| 28:A4:6:HIS:HA | 28:A4:7:PRO:HD3 | 1.79 | 0.43 |
| 7:CG:145:THR:HG22 | 7:CG:148:MET:CG | 2.47 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:1617:A:H2' | 1:AA:1618:A:C8 | 2.53 | 0.43 |
| 34:BA:1434:A:H2' | 34:BA:1435:G:O4' | 2.18 | 0.43 |
| 2:CB:8:U:H6 | 2:CB:8:U:H5'' | 1.83 | 0.43 |
| 46:BM:70:LEU:O | 46:BM:74:VAL:HG23 | 2.19 | 0.43 |
| 1:CA:652(C):G:H5'' | 1:CA:652(D):C:OP2 | 2.19 | 0.43 |
| 17:AT:24:PRO:HA | 17:AT:49:VAL:HG22 | 2.01 | 0.43 |
| 56:BW:39:PSU:H2' | 56:BW:40:C:C6 | 2.53 | 0.43 |
| 1:AA:1922:A:N1 | 1:AA:1992:A:C6 | 2.87 | 0.43 |
| 6:CF:60:SER:OG | 6:CF:61:GLY:N | 2.51 | 0.43 |
| 1:CA:1719:G:C6 | 1:CA:1720:U:C4 | 3.07 | 0.43 |
| 1:AA:2453:C:OP2 | 1:AA:2598:C:O2' | 2.36 | 0.43 |
| 34:BA:1116:C:O2' | 42:BI:108:VAL:HG21 | 2.18 | 0.43 |
| 44:BK:43:SER:HB3 | 44:BK:68:ALA:HB2 | 2.00 | 0.43 |
| 1:AA:85:C:O2' | 1:AA:86:C:H5' | 2.18 | 0.43 |
| 34:DA:1187:G:H4' | 42:DI:111:ARG:HH11 | 1.84 | 0.43 |
| 34:DA:35:G:H2' | 34:DA:36:C:C6 | 2.53 | 0.43 |
| 34:BA:761:G:C6 | 34:BA:762:C:C4 | 3.06 | 0.43 |
| 35:DB:25:ASN:HA | 35:DB:26:PRO:HD3 | 1.82 | 0.43 |
| 35:BB:68:ILE:HG12 | 35:BB:161:ALA:HB3 | 2.00 | 0.43 |
| 29:A5:38:ALA:CB | 29:A5:48:GLU:HG3 | 2.49 | 0.43 |
| 36:BC:100:ALA:O | 36:BC:101:LEU:HB2 | 2.19 | 0.43 |
| 16:AS:36:TYR:N | 16:AS:36:TYR:CD1 | 2.86 | 0.43 |
| 22:AY:20:TYR:CE1 | 22:AY:43:ASN:HA | 2.53 | 0.43 |
| 39:BF:55:ASP:HA | 39:BF:56:PRO:HD3 | 1.85 | 0.43 |
| 2:AB:28:C:H2' | 2:AB:29:A:O4' | 2.18 | 0.43 |
| 13:CP:100:LEU:HA | 13:CP:100:LEU:HD23 | 1.77 | 0.43 |
| 3:CC:54:ARG:HE | 3:CC:57:GLN:HG2 | 1.83 | 0.43 |
| 22:AY:90:LEU:HB2 | 22:AY:94:LYS:O | 2.18 | 0.43 |
| 34:DA:1074:G:C6 | 34:DA:1075:C:C4 | 3.07 | 0.43 |
| 34:DA:1399:C:C2 | 34:DA:1502:A:N6 | 2.87 | 0.43 |
| 34:DA:1316:G:H22 | 34:DA:1319:A:C5' | 2.31 | 0.43 |
| 1:AA:1604:C:H5'' | 1:AA:1605:A:OP2 | 2.19 | 0.43 |
| 4:CD:146:GLU:HB2 | 4:CD:189:CYS:CB | 2.49 | 0.43 |
| 4:CD:3:VAL:HG13 | 4:CD:17:THR:HB | 2.00 | 0.43 |
| 59:DZ:428:LEU:HD13 | 59:DZ:440:VAL:HG11 | 2.01 | 0.43 |
| 59:DZ:438:PHE:CE2 | 59:DZ:440:VAL:HG23 | 2.50 | 0.43 |
| 23:CZ:75:ASN:O | 23:CZ:84:GLU:HG2 | 2.18 | 0.43 |
| 28:C4:34:GLU:HG2 | 46:DM:3:ARG:CB | 2.48 | 0.43 |
| 34:DA:189:G:H2' | 34:DA:189(A):C:C6 | 2.54 | 0.43 |
| 50:DQ:6:LEU:O | 50:DQ:58:GLU:HA | 2.19 | 0.43 |
| 34:DA:1465:C:H2' | 34:DA:1466:C:O4' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BB:192:SER:O | 35:BB:194:PRO:HD3 | 2.18 | 0.43 |
| 34:BA:1189:C:OP1 | 43:BJ:51:ARG:NH2 | 2.51 | 0.43 |
| 19:CV:1:MET:HG3 | 19:CV:43:GLU:OE2 | 2.18 | 0.43 |
| 34:BA:950:U:H2' | 34:BA:951:G:C8 | 2.53 | 0.43 |
| 31:A7:5:TRP:CD1 | 31:A7:7:PRO:HD3 | 2.53 | 0.43 |
| 32:A8:36:LYS:HB2 | 32:A8:41:ILE:HD11 | 1.99 | 0.43 |
| 38:DE:42:GLY:HA2 | 38:DE:65:ASN:O | 2.19 | 0.43 |
| 1:AA:2784:C:H2' | 1:AA:2785:C:C6 | 2.53 | 0.43 |
| 1:CA:1071:G:H1' | 1:CA:1089:G:H2' | 2.00 | 0.43 |
| 2:CB:24:G:N7 | 2:CB:56:G:H2' | 2.33 | 0.43 |
| 23:AZ:146:ILE:HA | 23:AZ:147:GLY:HA2 | 1.65 | 0.43 |
| 1:CA:1837:C:O2' | 1:CA:1927:A:N3 | 2.42 | 0.43 |
| 34:DA:394:G:H2' | 34:DA:395:C:C6 | 2.54 | 0.43 |
| 34:BA:1029:C:N4 | 34:BA:1030(A):G:N3 | 2.66 | 0.43 |
| 8:CH:126:PRO:HB2 | 8:CH:127:GLU:H | 1.64 | 0.43 |
| 34:BA:1131:G:H8 | 34:BA:1131:G:O5' | 2.01 | 0.43 |
| 1:AA:438:G:C5 | 13:AP:72:PRO:HB3 | 2.53 | 0.43 |
| 43:DJ:50:ILE:HD11 | 43:DJ:57:LYS:HE2 | 1.99 | 0.43 |
| 1:CA:141:A:C8 | 1:CA:1408:C:O2' | 2.69 | 0.43 |
| 5:AE:131:ALA:HB1 | 5:AE:134:ILE:HD11 | 2.00 | 0.43 |
| 59:BZ:131:PRO:HG2 | 59:BZ:281:PRO:HG2 | 2.00 | 0.43 |
| 34:BA:1324:A:O4' | 34:BA:1362:C:H4' | 2.18 | 0.43 |
| 1:AA:2316:G:H22 | 1:AA:2324:U:H3 | 1.66 | 0.43 |
| 36:BC:44:GLU:HA | 36:BC:52:LEU:HD13 | 1.99 | 0.43 |
| 1:CA:1754:C:H5'' | 17:CT:113:LYS:HE3 | 1.99 | 0.43 |
| 47:DN:23:ARG:HD2 | 47:DN:28:GLY:O | 2.19 | 0.43 |
| 1:CA:1056:G:H5'' | 1:CA:1057:A:O4' | 2.17 | 0.43 |
| 13:CP:55:ARG:HA | 65:CP:308:HOH:O | 2.19 | 0.43 |
| 36:DC:16:ARG:HD2 | 36:DC:16:ARG:HA | 1.66 | 0.43 |
| 39:DF:79:LEU:HA | 39:DF:79:LEU:HD23 | 1.83 | 0.43 |
| 43:BJ:70:ARG:HD3 | 43:BJ:70:ARG:HA | 1.88 | 0.43 |
| 24:C0:53:MET:HG3 | 24:C0:59:LEU:CD2 | 2.46 | 0.43 |
| 59:BZ:637:ARG:C | 59:BZ:639:ASN:H | 2.21 | 0.43 |
| 50:BQ:92:ARG:HD3 | 50:BQ:92:ARG:HA | 1.83 | 0.43 |
| 23:AZ:120:ILE:HG13 | 23:AZ:171:ILE:C | 2.39 | 0.43 |
| 23:AZ:150:LEU:HB3 | 23:AZ:171:ILE:HD11 | 2.01 | 0.43 |
| 59:BZ:7:ASN:HB3 | 59:BZ:10:LYS:HE2 | 1.99 | 0.43 |
| 32:A8:37:SER:OG | 32:A8:39:LYS:N | 2.52 | 0.43 |
| 2:CB:22:U:H3 | 2:CB:61:G:H1 | 1.66 | 0.43 |
| 23:AZ:155:LEU:HA | 23:AZ:155:LEU:HD12 | 1.76 | 0.43 |
| 34:BA:486:U:H2' | 34:BA:487:A:H8 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:DZ:459:LEU:HA | 59:DZ:459:LEU:HD23 | 1.83 | 0.43 |
| 1:AA:1549:U:H2' | 1:AA:1550:C:C6 | 2.53 | 0.43 |
| 1:AA:2649:U:H5'' | 5:AE:82:ARG:HH21 | 1.83 | 0.43 |
| 34:DA:89:C:H2' | 34:DA:90:U:O4' | 2.18 | 0.43 |
| 7:CG:52:ILE:O | 7:CG:53:LEU:HD23 | 2.18 | 0.43 |
| 1:CA:729:G:C6 | 4:CD:208:LYS:HB2 | 2.52 | 0.43 |
| 1:CA:2218:U:O4' | 25:C1:52:ARG:NH2 | 2.51 | 0.43 |
| 43:DJ:46:ARG:NH2 | 43:DJ:64:GLU:OE1 | 2.52 | 0.43 |
| 6:AF:124:LEU:O | 6:AF:193:VAL:HA | 2.19 | 0.43 |
| 34:DA:1291:G:OP1 | 40:DG:37:ASN:ND2 | 2.51 | 0.43 |
| 1:AA:2724:U:O2' | 1:AA:2726:A:H5' | 2.19 | 0.43 |
| 1:AA:2724:U:OP1 | 1:AA:2727:G:H4' | 2.18 | 0.43 |
| 1:CA:671:C:H2' | 1:CA:672:C:C6 | 2.54 | 0.43 |
| 23:CZ:18:LEU:HA | 23:CZ:18:LEU:HD13 | 1.78 | 0.43 |
| 59:DZ:319:ASP:HA | 59:DZ:320:PRO:HD3 | 1.84 | 0.43 |
| 59:BZ:411:VAL:HB | 59:BZ:459:LEU:HD13 | 2.01 | 0.43 |
| 1:AA:861:C:H4' | 1:AA:1270:C:O2 | 2.19 | 0.43 |
| 1:CA:1110:G:N3 | 1:CA:1110:G:C2' | 2.82 | 0.43 |
| 59:DZ:123:ARG:HD2 | 59:DZ:675:HIS:ND1 | 2.34 | 0.43 |
| 36:BC:59:ARG:O | 43:BJ:92:THR:HG22 | 2.18 | 0.43 |
| 59:BZ:114:VAL:HG12 | 59:BZ:115:GLU:N | 2.32 | 0.43 |
| 56:DW:76:F3N:O | 56:DW:76:F3N:H5'' | 2.17 | 0.43 |
| 59:DZ:160:ARG:HH21 | 59:DZ:253:LEU:HA | 1.84 | 0.43 |
| 46:DM:14:ARG:HB3 | 46:DM:16:ASP:OD1 | 2.18 | 0.43 |
| 34:BA:194:C:H2' | 34:BA:195:A:H5'' | 2.01 | 0.43 |
| 58:BY:25:C:C2 | 58:BY:26:A:C8 | 3.07 | 0.43 |
| 34:DA:735:C:O2' | 34:DA:736:C:H5' | 2.18 | 0.43 |
| 36:DC:110:ASN:HB3 | 36:DC:141:VAL:HA | 2.01 | 0.43 |
| 1:CA:1452:A:O2' | 1:CA:1453:U:H2' | 2.19 | 0.43 |
| 34:DA:539:A:OP2 | 45:DL:115:LYS:NZ | 2.48 | 0.43 |
| 34:BA:1284:C:H3' | 34:BA:1285:A:C8 | 2.53 | 0.43 |
| 34:BA:757:U:O2' | 34:BA:879:C:O2 | 2.28 | 0.43 |
| 59:BZ:519:ARG:NH2 | 59:BZ:678:GLU:H | 2.16 | 0.43 |
| 1:CA:1628:G:H2' | 1:CA:1629:U:H6 | 1.84 | 0.43 |
| 1:AA:310:C:H2' | 1:AA:311:C:H6 | 1.83 | 0.43 |
| 27:A3:23:LEU:HA | 27:A3:23:LEU:HD12 | 1.81 | 0.43 |
| 1:CA:2692:C:O2' | 1:CA:2693:A:H5' | 2.19 | 0.43 |
| 45:DL:7:ILE:O | 45:DL:11:VAL:HG23 | 2.18 | 0.43 |
| 8:CH:148:ILE:O | 8:CH:151:ILE:HB | 2.19 | 0.43 |
| 34:BA:448:A:C4 | 34:BA:487:A:C2 | 3.07 | 0.43 |
| 59:DZ:552:SER:HB3 | 59:DZ:591:LYS:HZ2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:CD:16:MET:HE1 | 4:CD:208:LYS:HD3 | 2.01 | 0.43 |
| 59:BZ:330:VAL:HB | 59:BZ:371:ALA:HA | 2.01 | 0.43 |
| 34:BA:548:G:C6 | 34:BA:549:C:C4 | 3.06 | 0.43 |
| 38:BE:143:ARG:NH1 | 41:BH:77:GLU:OE2 | 2.52 | 0.43 |
| 11:AN:15:LEU:HD22 | 11:AN:16:ILE:N | 2.33 | 0.43 |
| 1:AA:2478:C:OP1 | 33:A9:4:ARG:HB3 | 2.19 | 0.43 |
| 8:AH:98:LEU:HA | 8:AH:98:LEU:HD12 | 1.84 | 0.43 |
| 1:CA:41:C:H2' | 1:CA:42:G:O4' | 2.19 | 0.43 |
| 1:CA:57:C:H2' | 1:CA:58:G:O4' | 2.19 | 0.43 |
| 36:DC:173:VAL:O | 36:DC:175:LEU:HD12 | 2.18 | 0.43 |
| 6:AF:199:TRP:O | 6:AF:203:GLN:HG2 | 2.18 | 0.43 |
| 1:CA:1857:G:C6 | 1:CA:1858:G:N1 | 2.87 | 0.43 |
| 34:DA:632:A:OP2 | 34:DA:632:A:H8 | 2.02 | 0.43 |
| 1:CA:597:U:H2' | 1:CA:598:G:C8 | 2.54 | 0.43 |
| 23:CZ:70:LEU:HA | 23:CZ:70:LEU:HD23 | 1.79 | 0.43 |
| 22:AY:28:LYS:HE3 | 22:AY:28:LYS:HB3 | 1.79 | 0.43 |
| 20:AW:1:MET:HE3 | 20:AW:1:MET:HA | 2.01 | 0.43 |
| 53:BT:97:ALA:N | 53:BT:98:PRO:HD3 | 2.33 | 0.43 |
| 34:BA:1437:C:H2' | 34:BA:1438:G:C8 | 2.54 | 0.43 |
| 59:DZ:309:LEU:HA | 59:DZ:333:GLY:HA3 | 2.01 | 0.43 |
| 59:BZ:69:VAL:HG11 | 59:BZ:374:LEU:HD22 | 2.01 | 0.43 |
| 34:BA:377:G:OP1 | 49:BP:5:ARG:HD2 | 2.19 | 0.43 |
| 4:AD:8:PRO:HB3 | 4:AD:14:ARG:HB2 | 1.99 | 0.43 |
| 28:C4:59:PHE:HA | 28:C4:60:GLN:C | 2.39 | 0.43 |
| 59:DZ:228:MET:O | 59:DZ:232:LEU:HD22 | 2.18 | 0.43 |
| 47:DN:24:CYS:HA | 47:DN:38:GLY:O | 2.18 | 0.43 |
| 1:CA:2328:A:H2' | 1:CA:2329:G:H8 | 1.83 | 0.43 |
| 34:BA:872:A:C5 | 34:BA:874:G:C8 | 3.06 | 0.43 |
| 28:A4:10:VAL:N | 28:A4:26:SER:O | 2.37 | 0.43 |
| 35:DB:71:VAL:O | 35:DB:165:VAL:HG23 | 2.19 | 0.43 |
| 3:CC:195:ARG:HH11 | 3:CC:195:ARG:HG3 | 1.83 | 0.43 |
| 59:BZ:486:THR:O | 59:BZ:599:PRO:HA | 2.18 | 0.43 |
| 1:CA:574:C:N3 | 5:CE:145:LYS:NZ | 2.61 | 0.43 |
| 34:DA:707:C:H2' | 34:DA:708:C:C6 | 2.52 | 0.43 |
| 16:CS:67:ARG:O | 16:CS:71:ARG:HG3 | 2.18 | 0.43 |
| 34:BA:1279:A:N1 | 36:BC:26:LYS:NZ | 2.67 | 0.43 |
| 16:CS:69:VAL:O | 16:CS:72:ALA:HB3 | 2.19 | 0.43 |
| 1:AA:313:A:H2' | 1:AA:314:G:O4' | 2.18 | 0.43 |
| 40:DG:29:LYS:HB3 | 40:DG:105:VAL:HG21 | 2.00 | 0.43 |
| 1:CA:443:A:H5'' | 1:CA:444:C:OP1 | 2.19 | 0.43 |
| 1:AA:142:G:H1' | 21:AX:37:THR:CG2 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:733:G:N2 | 1:AA:835:A:H61 | 2.17 | 0.43 |
| 34:DA:1097:C:H2' | 34:DA:1098:C:C6 | 2.54 | 0.43 |
| 25:C1:50:ARG:HG2 | 25:C1:59:THR:HB | 2.01 | 0.43 |
| 34:DA:152:A:N6 | 34:DA:170:U:C2 | 2.86 | 0.43 |
| 8:AH:86:GLU:OE2 | 8:AH:132:ARG:NH2 | 2.52 | 0.43 |
| 6:CF:140:LEU:HD13 | 6:CF:170:LEU:HD21 | 2.00 | 0.43 |
| 59:DZ:87:HIS:O | 59:DZ:89:ASP:N | 2.47 | 0.43 |
| 39:DF:82:ARG:HD2 | 39:DF:82:ARG:HA | 1.70 | 0.43 |
| 22:AY:49:VAL:HG11 | 22:AY:61:ILE:HD13 | 1.99 | 0.43 |
| 18:CU:104:GLN:NE2 | 18:CU:105:VAL:HG23 | 2.34 | 0.43 |
| 11:CN:43:THR:HB | 11:CN:46:VAL:CG2 | 2.49 | 0.43 |
| 5:AE:49:LEU:HA | 5:AE:49:LEU:HD12 | 1.78 | 0.43 |
| 46:DM:50:GLU:O | 46:DM:54:VAL:HG22 | 2.19 | 0.43 |
| 23:CZ:45:ASP:CG | 23:CZ:49:ARG:HH11 | 2.22 | 0.43 |
| 14:AQ:56:ARG:HD2 | 14:AQ:56:ARG:HA | 1.45 | 0.43 |
| 34:DA:1206:G:C6 | 34:DA:1207:G:C5 | 3.07 | 0.43 |
| 34:BA:872:A:C4 | 34:BA:874:G:N7 | 2.87 | 0.43 |
| 35:DB:102:LEU:HD23 | 35:DB:182:ILE:HD12 | 2.00 | 0.43 |
| 12:AO:69:ILE:HD11 | 12:AO:105:GLU:OE1 | 2.18 | 0.43 |
| 34:DA:735:C:H2' | 34:DA:736:C:H6 | 1.84 | 0.43 |
| 37:BD:166:LYS:N | 37:BD:168:ARG:HH12 | 2.17 | 0.43 |
| 1:CA:1668:A:H4' | 1:CA:1669:A:O5' | 2.18 | 0.43 |
| 39:BF:19:LEU:HD11 | 39:BF:59:TYR:CZ | 2.54 | 0.43 |
| 59:DZ:38:ARG:HH12 | 59:DZ:270:GLN:HE22 | 1.66 | 0.43 |
| 35:DB:94:ASN:HA | 35:DB:94:ASN:HD22 | 1.56 | 0.43 |
| 1:CA:1095:A:H2' | 1:CA:1096:A:C8 | 2.54 | 0.43 |
| 34:DA:1356:G:N2 | 34:DA:1367:C:O2 | 2.51 | 0.43 |
| 12:AO:1:MET:HE3 | 12:AO:32:TYR:CD1 | 2.54 | 0.43 |
| 1:AA:2163:G:N7 | 1:AA:2173:G:N2 | 2.67 | 0.43 |
| 1:AA:313:A:N6 | 1:AA:375:G:H1' | 2.33 | 0.43 |
| 6:CF:57:VAL:HG13 | 6:CF:59:TYR:CD2 | 2.53 | 0.43 |
| 1:CA:2468:G:C6 | 1:CA:2481:G:C4 | 3.07 | 0.43 |
| 39:DF:96:PRO:HB3 | 51:DR:30:ASP:OD2 | 2.19 | 0.43 |
| 1:AA:694:G:N2 | 1:AA:696:C:O2 | 2.31 | 0.43 |
| 59:DZ:-58:LEU:HB3 | 59:DZ:-55:LEU:HB2 | 2.01 | 0.43 |
| 59:BZ:536:LYS:HD2 | 59:BZ:536:LYS:H | 1.83 | 0.43 |
| 5:AE:79:ARG:HA | 5:AE:79:ARG:HD3 | 1.84 | 0.43 |
| 1:CA:982:C:O5' | 1:CA:982:C:H6 | 2.02 | 0.43 |
| 3:CC:60:ARG:HG3 | 3:CC:165:ARG:HB2 | 2.01 | 0.43 |
| 59:DZ:324:ARG:HD3 | 59:DZ:380:LEU:O | 2.19 | 0.43 |
| 1:AA:275:C:H2' | 1:AA:276:C:C6 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:AE:28:ALA:HB3 | 5:AE:93:VAL:HG13 | 2.00 | 0.43 |
| 3:CC:31:LYS:HG2 | 3:CC:31:LYS:H | 1.57 | 0.43 |
| 48:BO:32:LEU:O | 48:BO:35:ARG:N | 2.51 | 0.43 |
| 13:CP:39:LYS:HB2 | 13:CP:45:LEU:CG | 2.40 | 0.43 |
| 42:BI:81:ILE:HA | 42:BI:84:ALA:HB3 | 2.00 | 0.43 |
| 1:AA:933:C:H4' | 1:AA:933:C:OP1 | 2.18 | 0.43 |
| 34:DA:1004:A:N6 | 34:DA:1037:C:C2 | 2.87 | 0.43 |
| 37:BD:173:TRP:HB2 | 37:BD:187:ARG:O | 2.19 | 0.43 |
| 3:AC:6:LYS:N | 3:AC:9:ARG:HH12 | 2.17 | 0.43 |
| 1:CA:289:A:N6 | 1:CA:351:G:O2' | 2.49 | 0.43 |
| 1:CA:171:G:H2' | 1:CA:172:C:C6 | 2.54 | 0.43 |
| 59:BZ:146:LEU:HD22 | 59:BZ:150:ILE:HD11 | 2.00 | 0.43 |
| 14:AQ:2:LEU:HB2 | 14:AQ:70:PRO:HG3 | 2.01 | 0.43 |
| 34:DA:833:U:H2' | 34:DA:834:C:C6 | 2.54 | 0.43 |
| 59:DZ:-62:LEU:HD12 | 59:DZ:-62:LEU:N | 2.34 | 0.43 |
| 1:CA:1064:C:H4' | 10:CL:89:HIS:HB3 | 2.00 | 0.43 |
| 7:AG:77:ILE:O | 7:AG:82:LEU:N | 2.49 | 0.43 |
| 46:DM:80:ARG:O | 46:DM:84:ILE:HG12 | 2.19 | 0.43 |
| 4:CD:94:LEU:HD22 | 4:CD:95:LEU:N | 2.33 | 0.43 |
| 57:DX:23:C:H2' | 57:DX:24:U:H6 | 1.83 | 0.43 |
| 34:BA:1437:C:H2' | 34:BA:1438:G:H8 | 1.84 | 0.43 |
| 49:BP:8:ARG:C | 49:BP:9:PHE:HD1 | 2.22 | 0.43 |
| 1:CA:571:A:O2' | 19:CV:78:LYS:HE2 | 2.18 | 0.43 |
| 52:BS:20:LEU:HD21 | 52:BS:43:GLU:HG2 | 2.00 | 0.43 |
| 1:AA:1384:G:N7 | 21:AX:62:LYS:NZ | 2.59 | 0.43 |
| 53:DT:44:ALA:HB1 | 53:DT:91:LEU:HB2 | 2.00 | 0.43 |
| 1:CA:25:U:H2' | 1:CA:26:G:O4' | 2.19 | 0.43 |
| 34:DA:612:C:O2 | 34:DA:629:G:N2 | 2.52 | 0.43 |
| 12:AO:10:VAL:HG21 | 12:AO:16:ALA:HB3 | 2.01 | 0.43 |
| 1:CA:2489:G:C6 | 1:CA:2490:G:N1 | 2.87 | 0.43 |
| 53:BT:56:MET:HE1 | 53:BT:85:MET:HG2 | 2.01 | 0.43 |
| 1:CA:867:C:N4 | 1:CA:868:U:O4 | 2.52 | 0.43 |
| 1:CA:760:G:H2' | 1:CA:761:A:O4' | 2.19 | 0.43 |
| 38:BE:64:ARG:HE | 38:BE:64:ARG:HB3 | 1.70 | 0.43 |
| 30:A6:50:ARG:HB2 | 30:A6:50:ARG:HE | 1.65 | 0.43 |
| 1:AA:613:A:H2' | 1:AA:614:C:O4' | 2.19 | 0.43 |
| 14:AQ:39:PRO:HA | 14:AQ:97:VAL:O | 2.19 | 0.43 |
| 1:CA:2290:G:C2 | 1:CA:2343:C:O2 | 2.72 | 0.43 |
| 1:AA:1975:A:H2 | 1:AA:2561:G:N3 | 2.17 | 0.43 |
| 5:CE:195:LEU:HD21 | 65:CE:3111:HOH:O | 2.19 | 0.43 |
| 36:BC:78:GLY:HA3 | 36:BC:83:ARG:H | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:699:A:C2 | 1:CA:1633:G:N3 | 2.86 | 0.43 |
| 1:CA:699:A:H2' | 1:CA:700:G:O4' | 2.19 | 0.43 |
| 34:DA:73:G:C6 | 34:DA:76:C:C4 | 3.07 | 0.43 |
| 1:AA:2569:G:H2' | 1:AA:2570:C:C6 | 2.54 | 0.43 |
| 59:DZ:420:ASP:OD1 | 59:DZ:423:LYS:HB2 | 2.19 | 0.43 |
| 3:CC:11:LEU:HD11 | 3:CC:35:THR:HG23 | 2.01 | 0.42 |
| 1:AA:2203:G:O2' | 1:AA:2204:G:OP1 | 2.30 | 0.42 |
| 1:CA:528:A:OP2 | 11:CN:114:ARG:NH1 | 2.51 | 0.42 |
| 59:BZ:88:VAL:HG22 | 59:BZ:120:THR:HG21 | 2.01 | 0.42 |
| 1:CA:1027:A:C2 | 1:CA:2488:A:H5' | 2.54 | 0.42 |
| 1:AA:1003:U:OP2 | 14:AQ:14:ARG:HD3 | 2.19 | 0.42 |
| 34:DA:253:U:H2' | 34:DA:254:G:C8 | 2.54 | 0.42 |
| 1:AA:553:A:N1 | 1:AA:2064:A:H2' | 2.33 | 0.42 |
| 3:AC:11:LEU:HD11 | 3:AC:35:THR:HG23 | 2.01 | 0.42 |
| 3:AC:195:ARG:NH1 | 3:AC:195:ARG:HG3 | 2.34 | 0.42 |
| 1:CA:639:U:H2' | 1:CA:640:C:H6 | 1.81 | 0.42 |
| 50:BQ:41:LYS:HZ3 | 50:BQ:92:ARG:HH21 | 1.66 | 0.42 |
| 12:AO:104:ARG:HH12 | 17:AT:43:GLN:NE2 | 2.17 | 0.42 |
| 34:BA:445:G:C6 | 34:BA:490:G:C6 | 3.07 | 0.42 |
| 1:AA:866:A:H8 | 1:AA:866:A:C5' | 2.31 | 0.42 |
| 34:BA:908:A:H2' | 34:BA:909:A:C8 | 2.54 | 0.42 |
| 35:BB:173:ALA:O | 35:BB:176:GLU:N | 2.52 | 0.42 |
| 35:BB:24:TRP:CE3 | 35:BB:26:PRO:HA | 2.54 | 0.42 |
| 34:DA:1438:G:H2' | 34:DA:1439:C:C6 | 2.53 | 0.42 |
| 50:DQ:31:LEU:HD23 | 50:DQ:32:TYR:CZ | 2.54 | 0.42 |
| 1:AA:589:U:H2' | 1:AA:590:A:O4' | 2.19 | 0.42 |
| 23:AZ:89:PHE:HE2 | 23:AZ:96:VAL:HG23 | 1.84 | 0.42 |
| 35:DB:70:PHE:CE1 | 35:DB:163:PHE:HD2 | 2.37 | 0.42 |
| 1:CA:830:G:H4' | 1:CA:831:G:OP2 | 2.17 | 0.42 |
| 32:C8:57:ARG:O | 32:C8:60:LEU:N | 2.49 | 0.42 |
| 1:AA:1692:G:H5'' | 1:AA:1693:C:H5' | 2.01 | 0.42 |
| 1:CA:1570:A:H2' | 1:CA:1571:A:C8 | 2.54 | 0.42 |
| 4:CD:106:ILE:HG21 | 4:CD:106:ILE:HD13 | 1.80 | 0.42 |
| 59:BZ:201:ILE:H | 59:BZ:201:ILE:HG13 | 1.67 | 0.42 |
| 59:DZ:295:GLU:HG3 | 59:DZ:295:GLU:H | 1.48 | 0.42 |
| 34:BA:1513:A:H2' | 34:BA:1514:C:C6 | 2.53 | 0.42 |
| 1:AA:2589:A:H5' | 29:A5:3:LYS:HD2 | 2.00 | 0.42 |
| 57:BX:2:G:H2' | 57:BX:3:C:C6 | 2.54 | 0.42 |
| 34:DA:7:G:H5' | 34:DA:298:A:O4' | 2.19 | 0.42 |
| 46:DM:17:VAL:O | 46:DM:20:THR:OG1 | 2.35 | 0.42 |
| 36:DC:47:LEU:HB3 | 36:DC:52:LEU:HB3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:CP:55:ARG:HG2 | 13:CP:56:SER:N | 2.34 | 0.42 |
| 41:BH:88:LYS:O | 41:BH:92:ARG:HD3 | 2.19 | 0.42 |
| 34:BA:1123:A:H61 | 34:BA:1149:C:N4 | 2.14 | 0.42 |
| 34:BA:1149:C:H2' | 34:BA:1150:U:H6 | 1.84 | 0.42 |
| 34:DA:1221:G:H4' | 52:DS:53:ASN:O | 2.19 | 0.42 |
| 1:AA:180:A:H2' | 1:AA:181:C:C6 | 2.54 | 0.42 |
| 59:BZ:639:ASN:N | 59:BZ:640:ALA:HB3 | 2.33 | 0.42 |
| 52:BS:27:GLU:HA | 52:BS:28:LYS:HA | 1.91 | 0.42 |
| 34:DA:872:A:C4 | 34:DA:874:G:N7 | 2.87 | 0.42 |
| 34:DA:67:C:H4' | 34:DA:172:A:O4' | 2.18 | 0.42 |
| 41:DH:21:LYS:O | 41:DH:65:TYR:OH | 2.30 | 0.42 |
| 16:AS:78:LEU:HD21 | 16:AS:83:LYS:HG3 | 2.01 | 0.42 |
| 1:AA:733:G:P | 31:A7:11:LYS:HZ3 | 2.41 | 0.42 |
| 16:CS:3:ARG:O | 16:CS:4:LEU:HD23 | 2.19 | 0.42 |
| 34:DA:1048:G:OP1 | 47:DN:3:ARG:NH2 | 2.52 | 0.42 |
| 56:DW:54:5MU:C4 | 56:DW:55:PSU:C2 | 3.07 | 0.42 |
| 1:CA:1805:U:O2 | 4:CD:50:THR:HB | 2.18 | 0.42 |
| 7:AG:101:ILE:HG22 | 7:AG:105:LYS:HE2 | 2.01 | 0.42 |
| 34:BA:1504:G:OP1 | 34:BA:1507:A:H4' | 2.19 | 0.42 |
| 22:CY:76:CYS:SG | 22:CY:78:ALA:HB3 | 2.59 | 0.42 |
| 1:CA:2529:G:O6 | 33:C9:31:LYS:NZ | 2.52 | 0.42 |
| 34:DA:814:A:N7 | 34:DA:816:A:C4 | 2.87 | 0.42 |
| 34:BA:1492:A:H4' | 45:BL:47:LYS:HE3 | 2.01 | 0.42 |
| 34:BA:991:U:C4 | 34:BA:1212:U:H1' | 2.54 | 0.42 |
| 17:CT:99:LEU:HD22 | 17:CT:101:PHE:HE1 | 1.84 | 0.42 |
| 23:CZ:97:GLU:H | 23:CZ:97:GLU:HG2 | 1.55 | 0.42 |
| 1:CA:1154:G:O5' | 1:CA:1154:G:H8 | 2.02 | 0.42 |
| 40:DG:52:GLU:H | 40:DG:52:GLU:HG2 | 1.60 | 0.42 |
| 43:DJ:23:ILE:HD13 | 43:DJ:23:ILE:HA | 1.84 | 0.42 |
| 1:CA:746:A:H2' | 1:CA:2612:C:H5'' | 2.00 | 0.42 |
| 35:DB:47:THR:HG23 | 35:DB:202:PRO:HG2 | 2.01 | 0.42 |
| 35:BB:215:LEU:HD23 | 35:BB:215:LEU:HA | 1.79 | 0.42 |
| 59:BZ:13:ARG:NH1 | 59:BZ:247:ARG:NH2 | 2.55 | 0.42 |
| 59:DZ:114:VAL:HG23 | 59:DZ:152:THR:HB | 2.01 | 0.42 |
| 1:CA:1141:U:H4' | 1:CA:1142(A):A:O4' | 2.19 | 0.42 |
| 59:DZ:160:ARG:HD3 | 59:DZ:256:THR:OG1 | 2.20 | 0.42 |
| 37:BD:194:LEU:HD12 | 37:BD:195:ALA:N | 2.34 | 0.42 |
| 19:AV:49:THR:O | 19:AV:49:THR:CG2 | 2.67 | 0.42 |
| 34:BA:1148:U:H2' | 34:BA:1149:C:O4' | 2.19 | 0.42 |
| 59:BZ:509:HIS:NE2 | 59:BZ:511:LYS:HE2 | 2.35 | 0.42 |
| 3:AC:195:ARG:HH11 | 3:AC:195:ARG:HG3 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:C3:8:LEU:HD23 | 27:C3:8:LEU:HA | 1.79 | 0.42 |
| 34:BA:1072:G:C6 | 34:BA:1073:U:C4 | 3.08 | 0.42 |
| 36:DC:56:ASP:C | 36:DC:57:ILE:HD12 | 2.40 | 0.42 |
| 34:DA:1326:C:H2' | 34:DA:1327:C:H6 | 1.84 | 0.42 |
| 39:BF:10:LEU:HD23 | 39:BF:61:LEU:HD23 | 2.01 | 0.42 |
| 57:DX:47:U:H3' | 57:DX:48:C:C5' | 2.50 | 0.42 |
| 1:CA:637:A:H5'' | 13:CP:117:GLU:HG2 | 2.01 | 0.42 |
| 8:CH:15:VAL:HG23 | 8:CH:28:GLY:HA3 | 2.00 | 0.42 |
| 17:CT:30:VAL:HG13 | 17:CT:86:ILE:HG12 | 2.02 | 0.42 |
| 1:AA:2566:U:H2' | 1:AA:2567:U:C6 | 2.54 | 0.42 |
| 59:BZ:438:PHE:HB3 | 59:BZ:458:HIS:CE1 | 2.54 | 0.42 |
| 37:DD:11:LEU:O | 37:DD:15:GLU:HG2 | 2.18 | 0.42 |
| 1:AA:2284:U:H5'' | 1:AA:2285:A:OP1 | 2.19 | 0.42 |
| 1:AA:268:G:O2' | 1:AA:269:G:H8 | 2.02 | 0.42 |
| 41:BH:8:ASP:O | 41:BH:11:THR:N | 2.46 | 0.42 |
| 53:DT:90:GLN:O | 53:DT:93:GLU:HG3 | 2.19 | 0.42 |
| 34:BA:1002:G:H2' | 34:BA:1003:G:O4' | 2.20 | 0.42 |
| 11:CN:91:LEU:HD23 | 11:CN:91:LEU:HA | 1.74 | 0.42 |
| 59:DZ:193:GLY:O | 59:DZ:196:ILE:HG22 | 2.18 | 0.42 |
| 30:A6:12:GLU:HA | 30:A6:19:ARG:HA | 2.00 | 0.42 |
| 39:DF:94:GLN:HE22 | 51:DR:72:ARG:HH12 | 1.67 | 0.42 |
| 1:CA:2439:A:H5' | 1:CA:2439:A:C8 | 2.55 | 0.42 |
| 6:CF:33:LEU:HD12 | 6:CF:33:LEU:HA | 1.61 | 0.42 |
| 7:CG:33:ARG:NH1 | 7:CG:33:ARG:HB2 | 2.34 | 0.42 |
| 50:BQ:89:LEU:HA | 50:BQ:89:LEU:HD23 | 1.61 | 0.42 |
| 7:CG:31:VAL:HG22 | 7:CG:32:PRO:HD2 | 2.01 | 0.42 |
| 1:CA:1239:G:H2' | 1:CA:1240:U:O4' | 2.19 | 0.42 |
| 1:CA:2130:U:OP1 | 3:CC:6:LYS:HG2 | 2.20 | 0.42 |
| 17:AT:39:ARG:HH22 | 34:BA:345:C:H5 | 1.66 | 0.42 |
| 1:CA:1022:G:H22 | 1:CA:1142(A):A:H2 | 1.62 | 0.42 |
| 3:CC:27:ALA:O | 3:CC:30:VAL:CG2 | 2.64 | 0.42 |
| 34:DA:991:U:H3' | 34:DA:1212:U:C4 | 2.54 | 0.42 |
| 42:BI:127:LYS:O | 42:BI:128:ARG:HG2 | 2.19 | 0.42 |
| 1:AA:1137:G:C6 | 1:AA:1147:U:C2 | 3.07 | 0.42 |
| 46:DM:29:ARG:HG3 | 46:DM:64:TRP:CH2 | 2.54 | 0.42 |
| 42:DI:17:VAL:HA | 42:DI:63:ILE:HG12 | 2.02 | 0.42 |
| 35:BB:50:GLU:O | 35:BB:54:THR:N | 2.50 | 0.42 |
| 1:CA:2243:U:H2' | 1:CA:2244:U:H6 | 1.83 | 0.42 |
| 59:BZ:-29:LEU:H | 59:BZ:-29:LEU:HD23 | 1.84 | 0.42 |
| 34:BA:1272:G:H2' | 34:BA:1273:G:O4' | 2.18 | 0.42 |
| 35:BB:200:ILE:H | 35:BB:200:ILE:HG12 | 1.47 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:189(L):G:H2' | 34:DA:190:U:C6 | 2.54 | 0.42 |
| 1:CA:1514:U:H2' | 1:CA:1515:G:H8 | 1.84 | 0.42 |
| 34:BA:1100:C:O2' | 34:BA:1102:A:OP1 | 2.38 | 0.42 |
| 34:BA:254:G:OP1 | 50:BQ:67:LYS:O | 2.37 | 0.42 |
| 59:BZ:417:THR:HA | 59:BZ:418:LYS:CB | 2.49 | 0.42 |
| 1:AA:1346:U:H4' | 1:AA:1347:A:H5'' | 2.01 | 0.42 |
| 10:CL:90:LYS:HD3 | 10:CL:93:ARG:NH2 | 2.33 | 0.42 |
| 1:AA:734:C:H5'' | 31:A7:2:LYS:HE2 | 2.02 | 0.42 |
| 37:BD:147:ALA:HA | 37:BD:182:LYS:HA | 2.01 | 0.42 |
| 1:AA:2402:U:O2' | 1:AA:2403:G:H5' | 2.19 | 0.42 |
| 1:AA:2407:C:H2' | 1:AA:2408:G:O4' | 2.19 | 0.42 |
| 1:CA:1354:A:H2' | 1:CA:1355:G:O4' | 2.19 | 0.42 |
| 65:CA:4673:HOH:O | 5:CE:135:HIS:NE2 | 2.30 | 0.42 |
| 34:BA:1292:U:H2' | 34:BA:1293:G:C8 | 2.55 | 0.42 |
| 34:DA:575:G:C6 | 34:DA:821:G:N7 | 2.87 | 0.42 |
| 37:DD:191:ARG:HD2 | 37:DD:191:ARG:HA | 1.73 | 0.42 |
| 7:AG:60:LEU:HA | 7:AG:60:LEU:HD13 | 1.67 | 0.42 |
| 8:AH:7:LEU:HA | 8:AH:7:LEU:HD12 | 1.89 | 0.42 |
| 31:C7:19:ARG:HG2 | 31:C7:19:ARG:HH11 | 1.83 | 0.42 |
| 26:C2:21:LEU:HA | 26:C2:21:LEU:HD23 | 1.81 | 0.42 |
| 35:DB:105:PHE:O | 35:DB:107:THR:N | 2.52 | 0.42 |
| 34:BA:690:G:C6 | 34:BA:691:G:C6 | 3.07 | 0.42 |
| 34:DA:1303:C:N4 | 34:DA:1304:G:C6 | 2.87 | 0.42 |
| 37:BD:52:SER:O | 37:BD:56:VAL:HG23 | 2.20 | 0.42 |
| 37:DD:64:LEU:HB2 | 37:DD:198:VAL:HG11 | 2.01 | 0.42 |
| 34:BA:1521:G:H2' | 34:BA:1522:U:C6 | 2.54 | 0.42 |
| 34:DA:229:U:H2' | 34:DA:230:G:O4' | 2.19 | 0.42 |
| 59:BZ:247:ARG:HG3 | 59:BZ:247:ARG:NH1 | 2.34 | 0.42 |
| 59:BZ:73:PHE:CZ | 59:BZ:78:ARG:NH1 | 2.79 | 0.42 |
| 34:BA:924:C:H2' | 34:BA:925:G:H8 | 1.85 | 0.42 |
| 34:DA:1074:G:O2' | 34:DA:1101:A:N1 | 2.44 | 0.42 |
| 1:CA:2126:A:N6 | 1:CA:2163:C:H5' | 2.34 | 0.42 |
| 42:DI:8:GLY:O | 42:DI:14:VAL:HA | 2.19 | 0.42 |
| 6:CF:31:HIS:O | 6:CF:34:TRP:HB3 | 2.20 | 0.42 |
| 30:C6:8:LYS:HD3 | 32:C8:34:TRP:CG | 2.54 | 0.42 |
| 43:BJ:61:GLU:OE1 | 47:BN:49:HIS:HE1 | 2.03 | 0.42 |
| 34:BA:342:C:O2' | 34:BA:343:U:H5' | 2.19 | 0.42 |
| 24:C0:72:ARG:HE | 24:C0:75:LEU:HD12 | 1.85 | 0.42 |
| 1:CA:1404:C:H2' | 1:CA:1405:U:H6 | 1.85 | 0.42 |
| 2:AB:66:A:N6 | 2:AB:108:U:H2' | 2.35 | 0.42 |
| 11:CN:34:LEU:HD12 | 11:CN:34:LEU:HA | 1.61 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:16:MET:CE | 4:CD:208:LYS:HD3 | 2.50 | 0.42 |
| 11:CN:43:THR:HA | 11:CN:44:PRO:HD3 | 1.82 | 0.42 |
| 1:CA:253:C:OP2 | 32:C8:5:LYS:NZ | 2.44 | 0.42 |
| 33:C9:14:CYS:HA | 33:C9:27:CYS:HB2 | 2.02 | 0.42 |
| 1:AA:485:U:H5'' | 31:A7:40:TRP:CD2 | 2.54 | 0.42 |
| 19:AV:28:GLU:HG3 | 19:AV:29:PRO:HD2 | 2.01 | 0.42 |
| 1:AA:579:G:H2' | 1:AA:580:U:C6 | 2.55 | 0.42 |
| 23:CZ:100:VAL:HA | 23:CZ:101:PRO:HD3 | 1.90 | 0.42 |
| 1:CA:924:C:H2' | 1:CA:925:C:C6 | 2.54 | 0.42 |
| 21:AX:24:GLY:O | 21:AX:83:VAL:HG22 | 2.19 | 0.42 |
| 34:BA:1055:A:C5 | 34:BA:1206:G:C2 | 3.07 | 0.42 |
| 26:C2:22:GLU:OE2 | 26:C2:68:ARG:NH2 | 2.52 | 0.42 |
| 1:AA:2267:G:H21 | 24:A0:9:SER:HB3 | 1.84 | 0.42 |
| 15:CR:18:LEU:HD23 | 15:CR:18:LEU:HA | 1.64 | 0.42 |
| 50:BQ:87:LYS:HA | 50:BQ:87:LYS:HD3 | 1.84 | 0.42 |
| 59:BZ:422:GLU:H | 59:BZ:422:GLU:HG3 | 1.61 | 0.42 |
| 2:CB:78:A:C2 | 2:CB:100:A:C4 | 3.07 | 0.42 |
| 1:AA:1271:G:O3' | 19:AV:84:LYS:HE2 | 2.19 | 0.42 |
| 58:BY:38:A:H2' | 58:BY:39:PSU:O4' | 2.20 | 0.42 |
| 11:AN:85:ILE:HA | 11:AN:86:PRO:HD3 | 1.81 | 0.42 |
| 1:AA:2595:G:N3 | 56:BW:76:F3N:C2 | 2.82 | 0.42 |
| 59:BZ:100:VAL:HG12 | 59:BZ:100:VAL:O | 2.19 | 0.42 |
| 59:DZ:285:ASP:N | 59:DZ:285:ASP:OD2 | 2.53 | 0.42 |
| 34:BA:155:C:N4 | 34:BA:167:G:O6 | 2.53 | 0.42 |
| 1:CA:330:A:H2 | 1:CA:1210:A:HO2' | 1.65 | 0.42 |
| 1:CA:814:C:H2' | 1:CA:815:C:H6 | 1.85 | 0.42 |
| 13:CP:85:LEU:HD23 | 13:CP:88:LEU:HD12 | 2.01 | 0.42 |
| 3:CC:195:ARG:NH1 | 3:CC:195:ARG:HG3 | 2.35 | 0.42 |
| 59:BZ:-34:ARG:O | 59:BZ:-32:LEU:N | 2.52 | 0.42 |
| 10:AL:101:TRP:O | 10:AL:105:LEU:HD12 | 2.19 | 0.42 |
| 1:CA:956:G:N2 | 1:CA:959:A:H3' | 2.34 | 0.42 |
| 13:CP:84:ASN:OD1 | 13:CP:117:GLU:HB2 | 2.19 | 0.42 |
| 1:CA:18:C:H2' | 1:CA:19:C:H6 | 1.83 | 0.42 |
| 1:AA:2150:C:H2' | 1:AA:2151:C:H6 | 1.84 | 0.42 |
| 40:DG:26:PHE:CD1 | 40:DG:62:PHE:CE1 | 3.07 | 0.42 |
| 34:DA:26:A:O2' | 37:DD:209:ARG:NH2 | 2.53 | 0.42 |
| 34:DA:165:C:H2' | 34:DA:166:G:H8 | 1.84 | 0.42 |
| 34:BA:836:G:OP2 | 51:BR:61:LYS:HE3 | 2.19 | 0.42 |
| 25:C1:80:LEU:HD23 | 25:C1:82:LEU:HD21 | 2.01 | 0.42 |
| 34:BA:1002:G:C2 | 34:BA:1003:G:H1' | 2.55 | 0.42 |
| 1:CA:862:G:O2' | 2:CB:78:A:N3 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:2595:G:N3 | 56:BW:76:F3N:H2 | 2.35 | 0.42 |
| 41:BH:49:GLU:HG2 | 41:BH:62:TYR:HE1 | 1.85 | 0.42 |
| 40:DG:28:ASN:HD21 | 40:DG:36:LYS:NZ | 2.16 | 0.42 |
| 59:DZ:443:HIS:HA | 59:DZ:444:PRO:HD2 | 1.79 | 0.42 |
| 51:BR:45:SER:OG | 51:BR:47:THR:HG22 | 2.20 | 0.42 |
| 12:CO:98:VAL:CG1 | 12:CO:117:LEU:HB3 | 2.48 | 0.42 |
| 1:CA:2756:U:H1' | 1:CA:2757:A:H5'' | 2.01 | 0.42 |
| 45:BL:27:LEU:HA | 45:BL:27:LEU:HD12 | 1.84 | 0.42 |
| 45:BL:24:VAL:HB | 45:BL:27:LEU:HD22 | 2.01 | 0.42 |
| 34:DA:923:A:N6 | 34:DA:1392:G:O6 | 2.52 | 0.42 |
| 7:CG:86:MET:HA | 7:CG:87:PRO:HD2 | 1.93 | 0.42 |
| 1:CA:1473:G:H2' | 1:CA:1474:C:O4' | 2.19 | 0.42 |
| 7:CG:136:ARG:HD2 | 7:CG:137:GLU:HG3 | 2.01 | 0.42 |
| 1:CA:1104:C:H2' | 1:CA:1105:U:C6 | 2.55 | 0.42 |
| 36:DC:22:TRP:HB2 | 36:DC:23:TYR:H | 1.69 | 0.42 |
| 47:BN:33:VAL:HA | 47:BN:40:CYS:HA | 2.02 | 0.42 |
| 40:DG:79:ARG:HB3 | 40:DG:80:VAL:H | 1.42 | 0.42 |
| 1:CA:686:G:N2 | 1:CA:788:A:H61 | 2.17 | 0.42 |
| 37:BD:158:ILE:H | 37:BD:158:ILE:HG12 | 1.61 | 0.42 |
| 59:DZ:31:ARG:HA | 59:DZ:31:ARG:HE | 1.83 | 0.42 |
| 1:CA:315:G:H2' | 1:CA:316:C:C6 | 2.55 | 0.42 |
| 1:CA:794:G:H2' | 1:CA:795:C:C6 | 2.55 | 0.42 |
| 56:DW:37:MIA:H2' | 56:DW:38:A:O4' | 2.19 | 0.42 |
| 1:AA:726:C:H2' | 1:AA:727:G:H8 | 1.85 | 0.42 |
| 34:BA:162:A:C8 | 34:BA:163:C:H1' | 2.55 | 0.42 |
| 3:CC:6:LYS:N | 3:CC:9:ARG:HH12 | 2.17 | 0.42 |
| 59:BZ:21:ILE:HD12 | 59:BZ:87:HIS:NE2 | 2.35 | 0.42 |
| 56:BW:19:G:H4' | 56:BW:20:U:OP1 | 2.19 | 0.42 |
| 38:DE:100:VAL:HG12 | 38:DE:107:ARG:HH21 | 1.85 | 0.42 |
| 1:CA:1070:A:H5' | 1:CA:1072:C:OP2 | 2.19 | 0.42 |
| 36:DC:32:LEU:O | 36:DC:36:ASP:HB2 | 2.19 | 0.42 |
| 35:DB:55:PHE:HD1 | 35:DB:58:ILE:HD12 | 1.83 | 0.42 |
| 17:AT:18:ASP:OD2 | 17:AT:18:ASP:N | 2.53 | 0.42 |
| 34:DA:1041:A:H5' | 34:DA:1042:G:OP2 | 2.20 | 0.42 |
| 34:BA:1092:A:N3 | 34:BA:1183:A:N6 | 2.67 | 0.42 |
| 3:AC:225:ILE:O | 3:AC:227:PRO:HD3 | 2.19 | 0.42 |
| 38:BE:152:ARG:HA | 41:BH:64:LYS:HZ2 | 1.84 | 0.42 |
| 59:DZ:630:GLN:CG | 59:DZ:646:PHE:HB2 | 2.50 | 0.42 |
| 1:CA:86:C:P | 22:CY:32:PRO:HG2 | 2.60 | 0.42 |
| 34:BA:134:A:N6 | 49:BP:25:ARG:NH1 | 2.68 | 0.42 |
| 1:CA:910:A:H2' | 1:CA:2264:C:O2' | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:AA:2289:G:OP2 | 24:A0:10:THR:HG21 | 2.20 | 0.42 |
| 1:CA:590:A:H2' | 1:CA:591:C:O4' | 2.19 | 0.42 |
| 34:BA:1456:G:H1' | 53:BT:39:LYS:HZ3 | 1.85 | 0.42 |
| 2:CB:11:C:OP2 | 2:CB:12:C:N4 | 2.33 | 0.42 |
| 14:AQ:31:ASP:OD2 | 14:AQ:107:ALA:HA | 2.20 | 0.42 |
| 1:CA:1889:A:N1 | 1:CA:2234:G:H1' | 2.34 | 0.42 |
| 7:CG:33:ARG:CZ | 7:CG:33:ARG:HB2 | 2.50 | 0.42 |
| 1:AA:1911:A:N1 | 1:AA:2246:G:H1' | 2.34 | 0.42 |
| 34:DA:1418:A:H5'' | 34:DA:1419:G:OP2 | 2.19 | 0.42 |
| 1:CA:1615:C:C5 | 1:CA:1617:C:C4 | 3.07 | 0.42 |
| 1:CA:610:G:N2 | 1:CA:619:G:H1' | 2.34 | 0.42 |
| 24:A0:56:ASP:O | 24:A0:57:PHE:HB2 | 2.19 | 0.42 |
| 34:BA:1486:G:H2' | 34:BA:1487:G:O4' | 2.20 | 0.42 |
| 51:BR:46:GLU:HG3 | 51:BR:46:GLU:H | 1.52 | 0.42 |
| 13:CP:2:LYS:HB2 | 13:CP:2:LYS:HE2 | 1.84 | 0.42 |
| 17:AT:53:ARG:HB3 | 17:AT:53:ARG:CZ | 2.49 | 0.42 |
| 5:AE:178:GLU:CD | 5:AE:178:GLU:H | 2.21 | 0.42 |
| 6:AF:181:LEU:HA | 6:AF:181:LEU:HD12 | 1.81 | 0.42 |
| 9:CK:56:ASN:HA | 9:CK:83:TYR:HA | 2.02 | 0.42 |
| 1:AA:1634:C:H2' | 1:AA:1635:C:C6 | 2.53 | 0.42 |
| 34:DA:784:C:H2' | 34:DA:785:G:C8 | 2.54 | 0.42 |
| 1:CA:2712:U:H2' | 1:CA:2714:G:H5'' | 2.01 | 0.42 |
| 1:AA:2200:C:H2' | 1:AA:2201:C:C6 | 2.55 | 0.42 |
| 3:AC:54:ARG:HE | 3:AC:57:GLN:HG2 | 1.83 | 0.42 |
| 3:CC:20:VAL:O | 3:CC:21:TYR:CB | 2.59 | 0.42 |
| 1:CA:1155:A:H5'' | 18:CU:55:ARG:NH1 | 2.26 | 0.42 |
| 59:BZ:111:SER:O | 59:BZ:148:LEU:HD21 | 2.20 | 0.42 |
| 34:BA:1054:C:C4 | 56:BW:34:G:H1' | 2.55 | 0.42 |
| 1:AA:1117:G:O2' | 1:AA:1135:G:OP2 | 2.30 | 0.42 |
| 18:CU:76:TYR:HH | 18:CU:92:ARG:NH1 | 2.18 | 0.42 |
| 34:BA:1250:A:H4' | 42:BI:68:GLY:N | 2.35 | 0.42 |
| 1:CA:2112:G:C5 | 1:CA:2113:U:H1' | 2.55 | 0.42 |
| 59:DZ:280:LEU:HA | 59:DZ:281:PRO:HD3 | 1.92 | 0.42 |
| 36:BC:8:ILE:HG22 | 47:BN:49:HIS:O | 2.19 | 0.42 |
| 3:CC:225:ILE:O | 3:CC:227:PRO:HD3 | 2.19 | 0.42 |
| 53:DT:57:ARG:HH12 | 53:DT:100:ILE:CD1 | 2.33 | 0.42 |
| 59:BZ:2:LYS:HA | 59:BZ:5:LEU:HB2 | 2.00 | 0.42 |
| 13:AP:65:ARG:HG3 | 13:AP:66:GLY:N | 2.34 | 0.42 |
| 22:CY:68:HIS:CE1 | 22:CY:70:SER:HB3 | 2.55 | 0.42 |
| 53:BT:99:LEU:HA | 53:BT:100:ILE:O | 2.19 | 0.42 |
| 23:AZ:98:MET:O | 23:AZ:125:LEU:HD12 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AN:4:TYR:CE2 | 18:AU:100:VAL:HG11 | 2.54 | 0.42 |
| 23:CZ:40:ASP:OD2 | 23:CZ:42:VAL:HG12 | 2.20 | 0.42 |
| 34:DA:685:G:C2 | 34:DA:686:U:C4 | 3.08 | 0.42 |
| 34:BA:1028:C:H2' | 34:BA:1029:C:H4' | 2.02 | 0.42 |
| 23:AZ:107:THR:HA | 23:AZ:108:PRO:HD3 | 1.71 | 0.42 |
| 34:DA:1144:G:N2 | 34:DA:1146:A:H62 | 2.18 | 0.42 |
| 44:DK:84:VAL:HG11 | 44:DK:91:ARG:HD2 | 2.00 | 0.42 |
| 37:BD:116:GLN:NE2 | 37:BD:157:LEU:HD11 | 2.35 | 0.42 |
| 16:AS:110:LEU:HA | 16:AS:110:LEU:HD12 | 1.75 | 0.42 |
| 1:CA:1810:A:H2' | 1:CA:1811:G:O4' | 2.18 | 0.42 |
| 17:CT:41:ARG:NH1 | 34:DA:346:G:OP1 | 2.49 | 0.42 |
| 8:AH:33:LEU:HD21 | 8:AH:136:ILE:HG13 | 2.01 | 0.42 |
| 49:DP:36:ILE:HD12 | 49:DP:56:ALA:HB2 | 2.02 | 0.42 |
| 1:CA:373:U:H1' | 1:CA:423:A:N3 | 2.34 | 0.42 |
| 40:BG:103:TRP:CH2 | 40:BG:141:VAL:HG21 | 2.55 | 0.42 |
| 1:AA:2703:C:O3' | 1:AA:2881:C:H4' | 2.20 | 0.42 |
| 1:CA:572:A:H5'' | 1:CA:573:G:OP2 | 2.19 | 0.42 |
| 15:CR:12:ARG:HG3 | 15:CR:12:ARG:HH11 | 1.84 | 0.42 |
| 1:AA:645:G:H2' | 1:AA:645:G:N3 | 2.33 | 0.42 |
| 59:DZ:286:ILE:O | 59:DZ:286:ILE:HG12 | 2.19 | 0.42 |
| 50:DQ:52:LYS:HE3 | 50:DQ:52:LYS:HB2 | 1.83 | 0.42 |
| 57:BX:39:C:O2' | 58:BY:35:A:O2' | 2.38 | 0.42 |
| 59:BZ:268:GLY:HA2 | 59:BZ:271:LEU:HD13 | 2.02 | 0.42 |
| 38:BE:31:LEU:HD23 | 38:BE:45:PHE:CD1 | 2.55 | 0.42 |
| 35:DB:184:VAL:N | 35:DB:198:ASP:OD2 | 2.50 | 0.42 |
| 3:CC:48:LEU:CD2 | 3:CC:59:VAL:HG21 | 2.50 | 0.42 |
| 34:DA:992:U:H3 | 34:DA:1044:A:N6 | 2.12 | 0.42 |
| 59:DZ:463:VAL:HA | 59:DZ:466:LEU:HB2 | 2.02 | 0.42 |
| 34:DA:1004:A:H62 | 34:DA:1037:C:C2' | 2.30 | 0.42 |
| 1:CA:814:C:O2' | 1:CA:815:C:H5' | 2.20 | 0.42 |
| 1:CA:2285:C:OP2 | 30:C6:6:ARG:NH1 | 2.52 | 0.42 |
| 1:AA:330:U:H2' | 1:AA:331:G:O4' | 2.20 | 0.42 |
| 1:CA:2628:C:H1' | 1:CA:2781:A:H2' | 2.01 | 0.42 |
| 34:BA:342:C:N3 | 34:BA:348:G:N2 | 2.68 | 0.42 |
| 1:CA:86:C:H4' | 1:CA:104:U:H1' | 2.02 | 0.42 |
| 34:DA:688:G:H2' | 34:DA:689:C:C6 | 2.55 | 0.42 |
| 57:DX:47:U:N3 | 57:DX:50:U:OP1 | 2.52 | 0.42 |
| 5:CE:36:ARG:HG2 | 5:CE:47:VAL:HG12 | 2.01 | 0.42 |
| 1:AA:1831:C:OP2 | 4:AD:183:ARG:NH2 | 2.53 | 0.42 |
| 1:AA:800:C:H2' | 1:AA:801:C:H6 | 1.85 | 0.42 |
| 1:AA:2340:A:H2' | 1:AA:2341:G:C8 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:2258:C:O2' | 1:CA:2427:C:OP2 | 2.34 | 0.42 |
| 40:BG:78:ARG:HG2 | 40:BG:79:ARG:N | 2.35 | 0.42 |
| 5:AE:49:LEU:HD22 | 5:AE:81:ILE:HG13 | 2.01 | 0.42 |
| 53:BT:81:LYS:O | 53:BT:85:MET:HG3 | 2.19 | 0.42 |
| 1:AA:2408:G:H5' | 25:A1:25:LYS:HE2 | 2.02 | 0.42 |
| 34:BA:158:G:N2 | 34:BA:163:C:O2 | 2.50 | 0.42 |
| 1:AA:2022:G:OP1 | 15:AR:5:LYS:NZ | 2.49 | 0.42 |
| 13:CP:47:ASP:HA | 13:CP:48:PRO:HD3 | 1.87 | 0.42 |
| 34:BA:1368:G:OP2 | 42:BI:112:LYS:HG3 | 2.20 | 0.42 |
| 11:CN:120:LEU:HD22 | 11:CN:122:VAL:HG23 | 2.01 | 0.42 |
| 8:CH:42:ARG:HH12 | 8:CH:53:GLU:HB2 | 1.84 | 0.42 |
| 57:DX:58:A:H4' | 57:DX:59:A:OP1 | 2.18 | 0.42 |
| 4:CD:132:PRO:HD3 | 4:CD:190:TYR:CZ | 2.55 | 0.42 |
| 1:AA:1764:G:C6 | 1:AA:1765:U:C4 | 3.08 | 0.42 |
| 34:DA:232:G:H1' | 34:DA:262:A:N1 | 2.35 | 0.42 |
| 34:BA:106:C:O2 | 34:BA:379:C:H4' | 2.20 | 0.42 |
| 1:AA:540:A:H2 | 1:AA:1306:G:N3 | 2.17 | 0.42 |
| 1:CA:2689:U:P | 1:CA:2719:G:H22 | 2.43 | 0.42 |
| 8:CH:88:LEU:HD22 | 8:CH:165:ALA:HA | 2.00 | 0.42 |
| 5:CE:24:THR:HG23 | 5:CE:184:VAL:HG13 | 2.00 | 0.42 |
| 33:A9:17:ILE:HA | 33:A9:17:ILE:HD12 | 1.72 | 0.42 |
| 15:CR:51:LEU:HA | 15:CR:51:LEU:HD23 | 1.74 | 0.42 |
| 17:CT:118:ARG:HG2 | 34:DA:1442(A):G:C8 | 2.55 | 0.42 |
| 26:C2:2:LYS:HE3 | 26:C2:2:LYS:HB3 | 1.92 | 0.42 |
| 40:BG:45:ASP:O | 40:BG:49:ILE:HG13 | 2.20 | 0.42 |
| 1:AA:233:A:C2 | 1:AA:244:A:C4 | 3.07 | 0.42 |
| 59:BZ:94:VAL:HB | 59:BZ:98:MET:HB2 | 2.02 | 0.42 |
| 22:AY:55:TYR:H | 22:AY:55:TYR:HD1 | 1.68 | 0.42 |
| 22:AY:90:LEU:HA | 22:AY:90:LEU:HD12 | 1.75 | 0.42 |
| 1:AA:2554:A:H4' | 1:AA:2555:G:C8 | 2.55 | 0.42 |
| 1:CA:2583:G:N3 | 56:DW:76:F3N:H2 | 2.35 | 0.42 |
| 45:DL:32:PHE:CB | 45:DL:84:LEU:HD11 | 2.46 | 0.42 |
| 45:DL:84:LEU:HD13 | 45:DL:85:ILE:N | 2.35 | 0.42 |
| 23:CZ:150:LEU:HB3 | 23:CZ:171:ILE:HD11 | 2.02 | 0.42 |
| 3:CC:42:VAL:O | 3:CC:216:THR:C | 2.59 | 0.42 |
| 57:DX:72:A:H2' | 57:DX:73:A:C8 | 2.55 | 0.42 |
| 34:DA:1263:C:H2' | 34:DA:1264:C:C6 | 2.55 | 0.42 |
| 1:AA:1091:A:C8 | 1:AA:1093:G:C2 | 3.08 | 0.42 |
| 1:AA:1500:A:O2' | 1:AA:1501:U:H2' | 2.20 | 0.42 |
| 34:DA:834:C:C4 | 34:DA:835:U:C4 | 3.08 | 0.42 |
| 41:BH:64:LYS:HB3 | 41:BH:79:VAL:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:DE:139:LEU:C | 38:DE:141:GLN:N | 2.72 | 0.42 |
| 46:DM:82:MET:HE3 | 46:DM:92:HIS:HB3 | 2.01 | 0.42 |
| 23:CZ:145:GLU:HG2 | 23:CZ:146:ILE:HD12 | 2.01 | 0.42 |
| 5:AE:51:PHE:CE2 | 5:AE:52:LEU:HG | 2.55 | 0.42 |
| 1:CA:857:C:OP2 | 24:C0:77:ARG:NH2 | 2.52 | 0.42 |
| 36:DC:18:TRP:HE3 | 36:DC:18:TRP:H | 1.68 | 0.42 |
| 1:CA:1651:G:H2' | 1:CA:1652:A:O4' | 2.20 | 0.42 |
| 17:AT:45:PHE:CE1 | 17:AT:65:LYS:HD3 | 2.55 | 0.42 |
| 53:DT:55:ILE:HD13 | 53:DT:55:ILE:HA | 1.82 | 0.42 |
| 1:CA:503:A:H4' | 1:CA:504:U:H5'' | 2.02 | 0.42 |
| 1:CA:1713:U:H2' | 1:CA:1714:G:C8 | 2.55 | 0.42 |
| 34:BA:864:A:H2' | 34:BA:865:A:C8 | 2.55 | 0.42 |
| 7:CG:136:ARG:HD2 | 7:CG:136:ARG:C | 2.40 | 0.42 |
| 23:AZ:104:PHE:HB3 | 23:AZ:141:VAL:HG21 | 2.01 | 0.42 |
| 53:BT:14:LYS:O | 53:BT:18:GLN:HG3 | 2.20 | 0.42 |
| 25:A1:23:LYS:HE3 | 25:A1:23:LYS:HB2 | 1.90 | 0.42 |
| 1:CA:2335:A:C8 | 1:CA:2337:G:C5 | 3.07 | 0.42 |
| 32:A8:52:LYS:N | 32:A8:53:PRO:HD2 | 2.35 | 0.42 |
| 1:CA:1268:A:H2' | 1:CA:1269:A:O4' | 2.20 | 0.42 |
| 1:AA:1938:A:H2' | 1:AA:1939:U:O4' | 2.20 | 0.42 |
| 1:AA:1944:G:H2' | 1:AA:1945:U:C6 | 2.54 | 0.42 |
| 38:DE:24:ARG:NH1 | 55:DV:24:A:OP2 | 2.52 | 0.42 |
| 1:CA:748:G:O6 | 20:CW:90:ARG:NH1 | 2.52 | 0.42 |
| 16:CS:63:THR:HG23 | 16:CS:64:GLU:N | 2.35 | 0.42 |
| 9:CK:4:LYS:HA | 9:CK:5:ARG:HA | 1.86 | 0.42 |
| 21:CX:5:TYR:CE2 | 26:C2:30:ARG:HB3 | 2.54 | 0.42 |
| 21:CX:5:TYR:HB3 | 26:C2:33:MET:HB2 | 2.02 | 0.42 |
| 25:A1:85:LEU:HA | 25:A1:85:LEU:HD23 | 1.75 | 0.42 |
| 1:CA:1312:U:OP2 | 21:CX:63:LYS:NZ | 2.36 | 0.42 |
| 39:BF:4:TYR:HD1 | 39:BF:92:LYS:HA | 1.85 | 0.42 |
| 44:DK:72:ALA:HB1 | 44:DK:77:MET:HB2 | 2.01 | 0.42 |
| 12:CO:15:GLY:O | 12:CO:47:ILE:HG13 | 2.20 | 0.42 |
| 13:CP:3:LEU:HD12 | 13:CP:3:LEU:HA | 1.88 | 0.41 |
| 1:AA:1715:A:H4' | 1:AA:1716:A:O5' | 2.20 | 0.41 |
| 34:DA:114:U:O2' | 34:DA:115:G:H5' | 2.20 | 0.41 |
| 1:AA:1185:C:O3' | 11:AN:25:ARG:NH1 | 2.53 | 0.41 |
| 3:AC:48:LEU:CD2 | 3:AC:59:VAL:HG21 | 2.50 | 0.41 |
| 35:DB:214:ILE:H | 35:DB:214:ILE:HG12 | 1.64 | 0.41 |
| 1:AA:2348:A:N6 | 24:A0:43:THR:HG21 | 2.33 | 0.41 |
| 1:CA:1816:G:C8 | 4:CD:62:TYR:CE2 | 3.09 | 0.41 |
| 1:AA:2132:G:C6 | 1:AA:2142:G:C8 | 3.08 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BA:109:A:H2' | 34:BA:326:G:H21 | 1.83 | 0.41 |
| 37:BD:202:LEU:HD23 | 37:BD:202:LEU:HA | 1.74 | 0.41 |
| 34:BA:955:U:O2' | 52:BS:83:HIS:CD2 | 2.73 | 0.41 |
| 1:AA:2429:C:OP1 | 13:AP:65:ARG:NH2 | 2.53 | 0.41 |
| 57:DX:49:G:N2 | 57:DX:66:C:O2 | 2.53 | 0.41 |
| 34:DA:519:C:H2' | 34:DA:520:A:O4' | 2.20 | 0.41 |
| 34:DA:519:C:H2' | 34:DA:520:A:C8 | 2.55 | 0.41 |
| 5:CE:51:PHE:CE2 | 5:CE:52:LEU:HD13 | 2.55 | 0.41 |
| 38:BE:83:GLU:HG2 | 38:BE:88:LYS:HB2 | 2.02 | 0.41 |
| 11:CN:58:ASP:OD2 | 11:CN:59:LYS:HE3 | 2.20 | 0.41 |
| 41:DH:97:VAL:HG21 | 41:DH:128:GLY:HA2 | 2.02 | 0.41 |
| 34:DA:1328:C:H2' | 34:DA:1329:A:O4' | 2.20 | 0.41 |
| 18:CU:104:GLN:CD | 18:CU:104:GLN:H | 2.21 | 0.41 |
| 3:CC:60:ARG:NH2 | 3:CC:165:ARG:HH21 | 2.18 | 0.41 |
| 16:AS:74:ALA:HA | 16:AS:110:LEU:HD22 | 2.02 | 0.41 |
| 22:AY:76:CYS:HA | 22:AY:77:PRO:HD3 | 1.89 | 0.41 |
| 1:CA:2378:A:H4' | 16:CS:23:ARG:NH1 | 2.35 | 0.41 |
| 17:AT:32:TYR:HD2 | 17:AT:34:VAL:HG23 | 1.85 | 0.41 |
| 34:DA:1429:C:H2' | 34:DA:1430:C:C6 | 2.55 | 0.41 |
| 1:CA:623:G:H2' | 1:CA:624:C:C6 | 2.55 | 0.41 |
| 34:DA:1018:C:H2' | 34:DA:1019:C:O4' | 2.20 | 0.41 |
| 37:DD:28:SER:HB2 | 37:DD:29:PRO:HD2 | 2.01 | 0.41 |
| 52:BS:31:ILE:HD12 | 52:BS:49:ILE:HG12 | 2.01 | 0.41 |
| 34:BA:99:U:H2' | 34:BA:100:C:C6 | 2.55 | 0.41 |
| 34:BA:567:G:H2' | 34:BA:568:G:O4' | 2.19 | 0.41 |
| 34:BA:107:G:H2' | 34:BA:108:G:O4' | 2.20 | 0.41 |
| 1:CA:687:C:H1' | 31:C7:4:THR:HG22 | 2.02 | 0.41 |
| 34:BA:392:G:H2' | 34:BA:393:A:C8 | 2.55 | 0.41 |
| 1:AA:1961:U:OP1 | 1:AA:2616:U:O2' | 2.34 | 0.41 |
| 34:DA:918:A:H2' | 34:DA:919:A:O4' | 2.20 | 0.41 |
| 53:BT:63:ILE:HG22 | 53:BT:77:ALA:HB1 | 2.02 | 0.41 |
| 2:AB:88:C:H2' | 2:AB:89:G:O4' | 2.19 | 0.41 |
| 19:AV:97:LYS:HA | 19:AV:97:LYS:HD2 | 1.46 | 0.41 |
| 13:CP:46:LYS:HE3 | 13:CP:46:LYS:HB3 | 1.87 | 0.41 |
| 40:DG:104:LEU:HD13 | 40:DG:104:LEU:HA | 1.73 | 0.41 |
| 11:AN:115:ARG:HA | 11:AN:118:LYS:HE3 | 2.02 | 0.41 |
| 1:CA:403:U:H4' | 1:CA:404:C:H5' | 2.01 | 0.41 |
| 31:A7:31:LEU:HD22 | 31:A7:42:LEU:HD13 | 2.00 | 0.41 |
| 39:BF:2:ARG:CZ | 39:BF:69:GLU:HG2 | 2.50 | 0.41 |
| 1:CA:2206:G:H3' | 1:CA:2207:G:H8 | 1.75 | 0.41 |
| 35:BB:145:LEU:HD12 | 35:BB:149:LEU:HD12 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:AR:100:LEU:HD11 | 15:AR:113:LEU:HD23 | 2.02 | 0.41 |
| 1:CA:2137:C:H2' | 1:CA:2138:C:C6 | 2.55 | 0.41 |
| 56:DW:9:A:H8 | 56:DW:11:C:H41 | 1.67 | 0.41 |
| 1:CA:815:C:H2' | 1:CA:816:C:H6 | 1.84 | 0.41 |
| 3:AC:42:VAL:O | 3:AC:216:THR:C | 2.59 | 0.41 |
| 43:DJ:38:ILE:HG12 | 43:DJ:71:LEU:O | 2.20 | 0.41 |
| 34:DA:1119:C:H2' | 34:DA:1120:G:C8 | 2.54 | 0.41 |
| 18:CU:79:PHE:O | 18:CU:83:LEU:HD22 | 2.20 | 0.41 |
| 36:DC:184:TYR:HD1 | 36:DC:201:TYR:CE2 | 2.38 | 0.41 |
| 5:AE:144:ARG:HB3 | 5:AE:145:LYS:H | 1.45 | 0.41 |
| 5:CE:48:GLN:OE1 | 5:CE:78:LEU:HG | 2.21 | 0.41 |
| 18:CU:86:ALA:O | 19:CV:49:THR:HG23 | 2.20 | 0.41 |
| 1:CA:2183:C:H2' | 1:CA:2184:G:C8 | 2.52 | 0.41 |
| 59:BZ:264:LEU:HB2 | 64:BZ:702:GDP:C6 | 2.55 | 0.41 |
| 34:BA:143:A:H2 | 34:BA:220:G:H1 | 1.66 | 0.41 |
| 51:BR:40:LEU:O | 51:BR:43:PHE:N | 2.38 | 0.41 |
| 34:BA:382:A:H2' | 34:BA:383:A:C8 | 2.55 | 0.41 |
| 59:BZ:6:GLU:O | 59:BZ:10:LYS:N | 2.53 | 0.41 |
| 1:CA:590:A:OP1 | 6:CF:95:ARG:NH1 | 2.49 | 0.41 |
| 34:BA:1352:C:OP1 | 54:BU:3:LYS:NZ | 2.46 | 0.41 |
| 12:AO:1:MET:HE3 | 12:AO:32:TYR:CE1 | 2.55 | 0.41 |
| 1:CA:1469:A:H2' | 1:CA:1470:G:O4' | 2.20 | 0.41 |
| 1:CA:443:A:H1' | 1:CA:1201:C:O4' | 2.19 | 0.41 |
| 59:BZ:414:GLU:C | 59:BZ:416:LYS:H | 2.22 | 0.41 |
| 34:DA:1049:U:C6 | 34:DA:1201:A:H5' | 2.55 | 0.41 |
| 1:AA:2431:U:H2' | 1:AA:2432:C:C6 | 2.56 | 0.41 |
| 1:CA:888:C:P | 46:DM:93:ARG:HD3 | 2.59 | 0.41 |
| 34:DA:730:G:O2' | 34:DA:766:A:H5' | 2.20 | 0.41 |
| 34:BA:1152:A:H5' | 43:BJ:13:HIS:ND1 | 2.35 | 0.41 |
| 1:AA:696:C:P | 1:AA:696:C:H6 | 2.43 | 0.41 |
| 30:A6:19:ARG:N | 30:A6:19:ARG:HD2 | 2.35 | 0.41 |
| 34:BA:62:U:H5'' | 34:BA:385:C:H1' | 2.02 | 0.41 |
| 38:BE:127:ASN:HA | 38:BE:128:PRO:HD3 | 1.79 | 0.41 |
| 19:CV:82:ARG:O | 19:CV:83:ARG:HD3 | 2.20 | 0.41 |
| 6:CF:64:ILE:HD12 | 6:CF:65:TRP:CZ3 | 2.55 | 0.41 |
| 30:C6:40:CYS:SG | 30:C6:42:TRP:HB2 | 2.59 | 0.41 |
| 23:CZ:8:TYR:HB2 | 23:CZ:38:TYR:CZ | 2.55 | 0.41 |
| 46:DM:88:ARG:HG2 | 46:DM:98:VAL:HG12 | 2.03 | 0.41 |
| 34:DA:1090:U:H2' | 34:DA:1091:U:H6 | 1.86 | 0.41 |
| 45:BL:39:VAL:HG11 | 45:BL:41:ARG:NH1 | 2.35 | 0.41 |
| 1:AA:1403:U:H2' | 1:AA:1404:G:O4' | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:CZ:102:LEU:HD11 | 23:CZ:121:HIS:O | 2.20 | 0.41 |
| 16:CS:87:PHE:CE1 | 16:CS:102:ALA:HB2 | 2.55 | 0.41 |
| 12:AO:19:ILE:HB | 12:AO:41:ALA:HB1 | 2.01 | 0.41 |
| 21:AX:41:ASN:O | 21:AX:45:THR:HG23 | 2.20 | 0.41 |
| 13:AP:3:LEU:HA | 13:AP:3:LEU:HD12 | 1.75 | 0.41 |
| 1:CA:2127:G:H4' | 1:CA:2127:G:OP1 | 2.20 | 0.41 |
| 1:AA:1042:A:H4' | 18:AU:91:ASP:OD2 | 2.20 | 0.41 |
| 34:BA:1516:G:H2' | 34:BA:1518:A:OP2 | 2.20 | 0.41 |
| 23:CZ:157:LEU:HB3 | 23:CZ:161:VAL:HG13 | 2.02 | 0.41 |
| 1:AA:2481:A:H5' | 1:AA:2482:G:OP2 | 2.20 | 0.41 |
| 1:CA:1107:G:C2 | 1:CA:1108:U:C4 | 3.08 | 0.41 |
| 1:AA:1067:A:C3' | 1:AA:1067:A:C8 | 3.03 | 0.41 |
| 22:CY:98:VAL:HG23 | 22:CY:99:CYS:O | 2.20 | 0.41 |
| 13:CP:36:LYS:O | 13:CP:40:SER:HB3 | 2.20 | 0.41 |
| 1:AA:1098:C:H2' | 1:AA:1099:C:H6 | 1.84 | 0.41 |
| 59:BZ:358:MET:HE1 | 59:BZ:363:ARG:NH1 | 2.36 | 0.41 |
| 34:DA:137:C:H2' | 34:DA:138:G:H8 | 1.84 | 0.41 |
| 59:BZ:257:PRO:HB2 | 59:BZ:259:PHE:CE1 | 2.55 | 0.41 |
| 34:BA:1250:A:H2' | 34:BA:1251:A:C8 | 2.56 | 0.41 |
| 1:CA:1082:U:H5'' | 10:CL:122:ALA:HB1 | 2.02 | 0.41 |
| 34:DA:1130:A:H5' | 42:DI:18:PHE:CE2 | 2.55 | 0.41 |
| 34:BA:1118:C:H1' | 34:BA:1179:A:C4 | 2.56 | 0.41 |
| 34:BA:78:G:H22 | 34:BA:92:C:H42 | 1.67 | 0.41 |
| 34:DA:64:G:H4' | 34:DA:65:U:C3' | 2.49 | 0.41 |
| 1:AA:469:A:C6 | 6:AF:45:ARG:HD2 | 2.55 | 0.41 |
| 34:DA:1106:G:H4' | 36:DC:171:GLY:O | 2.20 | 0.41 |
| 34:DA:391:G:C6 | 34:DA:392:G:C5 | 3.08 | 0.41 |
| 1:CA:863:A:H2' | 1:CA:864:G:H8 | 1.84 | 0.41 |
| 1:CA:271(F):C:H2' | 1:CA:271(G):C:O4' | 2.20 | 0.41 |
| 23:CZ:67:LEU:HA | 23:CZ:68:PRO:HD3 | 1.73 | 0.41 |
| 34:BA:715:A:H2' | 34:BA:716:A:C8 | 2.55 | 0.41 |
| 40:DG:26:PHE:HB2 | 40:DG:101:LEU:HD22 | 2.01 | 0.41 |
| 9:CK:118:THR:O | 9:CK:120:LYS:N | 2.51 | 0.41 |
| 1:AA:733:G:OP1 | 31:A7:11:LYS:NZ | 2.50 | 0.41 |
| 50:DQ:15:MET:HE1 | 50:DQ:43:LEU:HD13 | 2.01 | 0.41 |
| 37:DD:60:GLU:OE1 | 37:DD:199:ASN:N | 2.52 | 0.41 |
| 1:CA:583:G:OP2 | 18:CU:10:ARG:HD2 | 2.20 | 0.41 |
| 1:AA:2124:U:H2' | 1:AA:2125:C:C6 | 2.54 | 0.41 |
| 1:AA:50:G:H4' | 1:AA:51:A:H5' | 2.01 | 0.41 |
| 4:AD:260:ARG:NH2 | 4:AD:264:LYS:HD3 | 2.35 | 0.41 |
| 23:AZ:129:SER:HA | 23:AZ:130:PRO:HD3 | 1.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:CP:87:ASP:HB3 | 13:CP:105:LEU:HD22 | 2.02 | 0.41 |
| 5:AE:108:SER:O | 5:AE:162:ALA:HA | 2.20 | 0.41 |
| 52:BS:48:THR:HA | 52:BS:60:VAL:O | 2.19 | 0.41 |
| 44:BK:33:THR:HA | 44:BK:39:PRO:HA | 2.02 | 0.41 |
| 8:AH:84:SER:HA | 8:AH:133:VAL:O | 2.20 | 0.41 |
| 1:CA:1656:C:H2' | 1:CA:1657:C:C6 | 2.56 | 0.41 |
| 7:AG:11:TYR:HA | 7:AG:15:VAL:HB | 2.01 | 0.41 |
| 1:AA:2164:C:H2' | 1:AA:2165:C:C6 | 2.55 | 0.41 |
| 16:AS:97:ARG:O | 16:AS:100:ALA:HB3 | 2.20 | 0.41 |
| 26:C2:49:LYS:HE2 | 26:C2:49:LYS:HB3 | 1.89 | 0.41 |
| 1:CA:1647:G:H3' | 1:CA:1647:G:OP2 | 2.20 | 0.41 |
| 15:AR:21:TYR:OH | 15:AR:43:GLU:HG2 | 2.20 | 0.41 |
| 1:CA:1401:G:H2' | 1:CA:1402:C:O4' | 2.21 | 0.41 |
| 34:BA:243:A:C2 | 34:BA:246:A:C8 | 3.09 | 0.41 |
| 1:CA:1638:C:H5'' | 1:CA:2710:C:O2' | 2.20 | 0.41 |
| 1:CA:2536:G:C6 | 1:CA:2537:U:C4 | 3.09 | 0.41 |
| 20:CW:53:SER:O | 20:CW:56:ALA:HB3 | 2.20 | 0.41 |
| 34:DA:1314:C:OP2 | 52:DS:4:SER:OG | 2.12 | 0.41 |
| 38:BE:74:GLY:HA3 | 38:BE:116:THR:HG22 | 2.01 | 0.41 |
| 1:CA:1860:G:H4' | 3:CC:206:LYS:HG3 | 1.76 | 0.41 |
| 59:DZ:165:GLN:O | 59:DZ:166:LEU:HD12 | 2.20 | 0.41 |
| 34:BA:565:U:H3' | 34:BA:566:G:H2' | 2.01 | 0.41 |
| 15:AR:36:THR:HG22 | 15:AR:37:THR:H | 1.84 | 0.41 |
| 7:AG:43:LEU:HA | 7:AG:43:LEU:HD12 | 1.81 | 0.41 |
| 52:BS:65:ASN:H | 52:BS:65:ASN:HD22 | 1.67 | 0.41 |
| 39:DF:61:LEU:HD23 | 39:DF:63:TYR:OH | 2.20 | 0.41 |
| 34:BA:1261:A:H3' | 34:BA:1262:C:H6 | 1.84 | 0.41 |
| 35:DB:212:GLN:O | 35:DB:216:SER:OG | 2.35 | 0.41 |
| 23:AZ:150:LEU:O | 23:AZ:171:ILE:HG13 | 2.20 | 0.41 |
| 1:AA:2147:G:OP1 | 3:AC:71:LYS:NZ | 2.52 | 0.41 |
| 1:CA:1652:A:O2' | 1:CA:1653:G:H5' | 2.20 | 0.41 |
| 1:AA:2173:G:H2' | 1:AA:2174:G:C8 | 2.56 | 0.41 |
| 23:AZ:152:ALA:HA | 23:AZ:155:LEU:HD22 | 2.02 | 0.41 |
| 34:DA:520:A:N1 | 34:DA:536:C:H1' | 2.35 | 0.41 |
| 53:BT:53:LEU:O | 53:BT:57:ARG:HG3 | 2.20 | 0.41 |
| 1:CA:888:C:H5'' | 1:CA:889:C:OP2 | 2.20 | 0.41 |
| 34:DA:1343:G:H2' | 34:DA:1344:C:C6 | 2.55 | 0.41 |
| 7:AG:97:ASP:O | 7:AG:101:ILE:HG13 | 2.20 | 0.41 |
| 8:AH:56:SER:OG | 8:AH:61:HIS:ND1 | 2.40 | 0.41 |
| 56:DW:4:C:N4 | 56:DW:5:G:O6 | 2.53 | 0.41 |
| 1:AA:659:C:H2' | 1:AA:660:C:C6 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:BA:28:G:O2' | 34:BA:296:U:OP1 | 2.30 | 0.41 |
| 17:AT:109:GLU:HG2 | 17:AT:112:ARG:HH21 | 1.85 | 0.41 |
| 34:BA:1220:G:N2 | 52:BS:54:GLY:O | 2.50 | 0.41 |
| 47:BN:8:GLU:OE2 | 47:BN:11:LYS:HD2 | 2.21 | 0.41 |
| 34:DA:546:G:P | 37:DD:72:GLU:HB3 | 2.60 | 0.41 |
| 34:DA:719:C:O2' | 51:DR:49:LYS:HB3 | 2.21 | 0.41 |
| 59:DZ:201:ILE:HG22 | 59:DZ:202:PRO:O | 2.20 | 0.41 |
| 59:BZ:427:ALA:O | 59:BZ:431:LEU:HD22 | 2.20 | 0.41 |
| 37:DD:100:ARG:HH11 | 37:DD:100:ARG:HG2 | 1.84 | 0.41 |
| 48:DO:32:LEU:HA | 48:DO:32:LEU:HD23 | 1.75 | 0.41 |
| 59:BZ:471:LYS:HB3 | 59:BZ:471:LYS:HE2 | 1.97 | 0.41 |
| 1:CA:1804:C:H6 | 1:CA:1804:C:O5' | 2.02 | 0.41 |
| 36:BC:131:ARG:HH11 | 38:BE:50:GLU:HG3 | 1.86 | 0.41 |
| 1:AA:170:A:H2' | 1:AA:171:A:C8 | 2.55 | 0.41 |
| 59:BZ:78:ARG:HH11 | 59:BZ:78:ARG:CB | 2.32 | 0.41 |
| 3:AC:31:LYS:H | 3:AC:31:LYS:HG2 | 1.57 | 0.41 |
| 13:CP:3:LEU:HD12 | 13:CP:6:LEU:HD12 | 2.02 | 0.41 |
| 34:DA:344:A:H4' | 34:DA:345:C:OP2 | 2.21 | 0.41 |
| 23:AZ:111:VAL:HG12 | 23:AZ:112:ARG:N | 2.35 | 0.41 |
| 1:CA:297:C:H2' | 1:CA:298:G:O4' | 2.20 | 0.41 |
| 34:BA:368:U:P | 59:BZ:351:ARG:HH11 | 2.43 | 0.41 |
| 34:BA:1318:A:H2' | 34:BA:1319:A:H5'' | 2.03 | 0.41 |
| 34:BA:1183:A:H3' | 34:BA:1184:G:C5' | 2.51 | 0.41 |
| 34:DA:1063:C:OP2 | 34:DA:1064:G:O2' | 2.23 | 0.41 |
| 46:BM:4:ILE:HA | 46:BM:5:ALA:HA | 1.90 | 0.41 |
| 34:DA:869:G:O5' | 34:DA:869:G:H8 | 2.03 | 0.41 |
| 59:DZ:38:ARG:HE | 59:DZ:38:ARG:HB2 | 1.60 | 0.41 |
| 4:CD:68:LYS:O | 4:CD:69:ARG:HB2 | 2.21 | 0.41 |
| 40:DG:26:PHE:CZ | 40:DG:30:ILE:HD11 | 2.56 | 0.41 |
| 34:BA:1053:G:O2' | 34:BA:1199:U:OP2 | 2.21 | 0.41 |
| 14:AQ:31:ASP:HB2 | 14:AQ:32:TYR:HD2 | 1.85 | 0.41 |
| 57:BX:19:G:H4' | 57:BX:20:U:OP2 | 2.21 | 0.41 |
| 34:BA:1130:A:C4 | 34:BA:1146:A:C2 | 3.08 | 0.41 |
| 59:BZ:414:GLU:O | 59:BZ:416:LYS:N | 2.54 | 0.41 |
| 1:CA:620:G:N3 | 1:CA:620:G:H2' | 2.35 | 0.41 |
| 38:DE:129:ILE:O | 38:DE:132:ALA:HB3 | 2.20 | 0.41 |
| 28:A4:69:LYS:HE2 | 52:BS:20:LEU:HD13 | 2.02 | 0.41 |
| 25:A1:23:LYS:HB3 | 25:A1:29:GLY:HA3 | 2.02 | 0.41 |
| 36:DC:112:SER:O | 36:DC:115:LEU:HB2 | 2.21 | 0.41 |
| 36:DC:33:LEU:O | 36:DC:37:GLN:N | 2.52 | 0.41 |
| 2:AB:41:U:C5 | 7:AG:70:VAL:HB | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:BB:167:PRO:HG3 | 35:BB:186:ALA:HB1 | 2.02 | 0.41 |
| 45:DL:124:LYS:HA | 45:DL:125:PRO:HD3 | 1.79 | 0.41 |
| 34:DA:511:C:C2 | 34:DA:512:U:C5 | 3.08 | 0.41 |
| 37:DD:78:LEU:HB3 | 37:DD:93:PHE:HE1 | 1.86 | 0.41 |
| 1:AA:1841:A:H2' | 1:AA:1842:G:O4' | 2.20 | 0.41 |
| 30:C6:34:LEU:HB2 | 30:C6:51:GLU:HB2 | 2.03 | 0.41 |
| 16:AS:67:ARG:HD2 | 16:AS:71:ARG:NH2 | 2.35 | 0.41 |
| 1:AA:1400:A:C8 | 1:AA:1401:G:C8 | 3.09 | 0.41 |
| 34:BA:7:G:H5' | 34:BA:298:A:O4' | 2.20 | 0.41 |
| 1:CA:859:G:O2' | 1:CA:916:G:O6 | 2.31 | 0.41 |
| 41:DH:9:MET:SD | 41:DH:26:VAL:HG21 | 2.61 | 0.41 |
| 1:AA:1704:C:H2' | 1:AA:1705:C:C6 | 2.55 | 0.41 |
| 39:DF:5:GLU:N | 39:DF:91:VAL:O | 2.47 | 0.41 |
| 40:DG:155:ARG:HB3 | 40:DG:155:ARG:CZ | 2.49 | 0.41 |
| 11:AN:138:LEU:HD22 | 11:AN:138:LEU:HA | 1.74 | 0.41 |
| 59:BZ:-20:LEU:HA | 59:BZ:-20:LEU:HD22 | 1.70 | 0.41 |
| 31:A7:33:ARG:NH2 | 65:A7:201:HOH:O | 2.54 | 0.41 |
| 1:AA:2202:U:C4 | 1:AA:2203:G:N7 | 2.88 | 0.41 |
| 59:BZ:88:VAL:HG23 | 59:BZ:117:GLN:HA | 2.02 | 0.41 |
| 42:BI:23:ASN:HB2 | 42:BI:25:LYS:NZ | 2.35 | 0.41 |
| 34:DA:1319:A:N6 | 34:DA:1361:G:H21 | 2.18 | 0.41 |
| 35:DB:155:LEU:HD11 | 35:DB:159:PRO:HD3 | 2.02 | 0.41 |
| 41:BH:113:SER:O | 41:BH:131:GLY:HA3 | 2.21 | 0.41 |
| 59:BZ:520:GLY:H | 59:BZ:562:ASP:CG | 2.23 | 0.41 |
| 7:AG:140:ILE:HG22 | 7:AG:141:PHE:CD1 | 2.56 | 0.41 |
| 1:CA:1081:U:O5' | 10:CL:125:ARG:HD3 | 2.20 | 0.41 |
| 59:DZ:346:LYS:HG3 | 59:DZ:346:LYS:HZ2 | 1.68 | 0.41 |
| 1:AA:277:G:H2' | 1:AA:278:G:C8 | 2.55 | 0.41 |
| 34:BA:149:A:H2' | 34:BA:150:C:H6 | 1.84 | 0.41 |
| 16:CS:39:ILE:HD13 | 16:CS:85:VAL:HG21 | 2.01 | 0.41 |
| 22:CY:49:VAL:HG11 | 22:CY:55:TYR:HD2 | 1.85 | 0.41 |
| 1:CA:184:C:H2' | 1:CA:185:U:H6 | 1.86 | 0.41 |
| 2:CB:19:G:H2' | 2:CB:20:C:O4' | 2.21 | 0.41 |
| 34:DA:67:C:H2' | 34:DA:68:G:C8 | 2.55 | 0.41 |
| 40:DG:26:PHE:CD1 | 40:DG:62:PHE:HE1 | 2.39 | 0.41 |
| 7:AG:126:ASP:CG | 7:AG:130:ASN:HD22 | 2.23 | 0.41 |
| 16:CS:65:VAL:O | 16:CS:68:GLN:HB2 | 2.21 | 0.41 |
| 37:BD:110:PHE:CE2 | 37:BD:148:VAL:HG23 | 2.55 | 0.41 |
| 1:AA:2595:G:H2' | 1:AA:2596:U:O4' | 2.21 | 0.41 |
| 26:C2:2:LYS:HG2 | 26:C2:5:GLU:OE1 | 2.20 | 0.41 |
| 5:CE:60:ASN:CG | 5:CE:62:PRO:HD2 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:2557:G:H2' | 1:CA:2558:C:C6 | 2.55 | 0.41 |
| 1:AA:52:A:H2' | 1:AA:53:G:O4' | 2.20 | 0.41 |
| 34:BA:911:U:OP2 | 45:BL:97:ARG:NH1 | 2.54 | 0.41 |
| 38:DE:60:TYR:CE1 | 38:DE:64:ARG:HD3 | 2.54 | 0.41 |
| 1:AA:2133:C:N3 | 1:AA:2167:C:O2' | 2.48 | 0.41 |
| 1:AA:2140:U:OP1 | 1:AA:2170:G:H4' | 2.20 | 0.41 |
| 4:AD:34:VAL:HA | 4:AD:62:TYR:O | 2.21 | 0.41 |
| 34:BA:5:U:H5'' | 34:BA:6:G:C5 | 2.55 | 0.41 |
| 59:BZ:309:LEU:HD21 | 59:BZ:335:LEU:HD13 | 2.03 | 0.41 |
| 1:CA:1645:G:H5'' | 1:CA:1646:C:O4' | 2.21 | 0.41 |
| 24:A0:70:GLN:HG2 | 24:A0:72:ARG:HG3 | 2.02 | 0.41 |
| 34:BA:303:A:H2' | 34:BA:304:U:O4' | 2.20 | 0.41 |
| 16:AS:89:ARG:HD2 | 16:AS:92:TYR:O | 2.21 | 0.41 |
| 1:CA:777:A:O2' | 1:CA:778:G:H5' | 2.20 | 0.41 |
| 34:DA:841:U:H6 | 34:DA:841:U:P | 2.43 | 0.41 |
| 46:BM:19:LEU:HA | 46:BM:19:LEU:HD12 | 1.85 | 0.41 |
| 41:DH:132:GLU:O | 41:DH:134:ILE:N | 2.54 | 0.41 |
| 59:BZ:443:HIS:HA | 59:BZ:444:PRO:HD2 | 1.91 | 0.41 |
| 34:BA:321:A:C2 | 34:BA:333:G:C2 | 3.08 | 0.41 |
| 34:BA:982:U:H4' | 34:BA:983:A:O5' | 2.21 | 0.41 |
| 23:CZ:153:SER:HB3 | 23:CZ:167:PRO:HB3 | 2.03 | 0.41 |
| 59:DZ:88:VAL:HG23 | 59:DZ:117:GLN:HE21 | 1.86 | 0.41 |
| 18:AU:112:ARG:HH11 | 18:AU:112:ARG:HG2 | 1.84 | 0.41 |
| 34:BA:741:G:H2' | 34:BA:742:G:O4' | 2.21 | 0.41 |
| 49:BP:5:ARG:O | 49:BP:20:VAL:N | 2.46 | 0.41 |
| 4:CD:148:GLU:OE1 | 4:CD:151:LYS:NZ | 2.34 | 0.41 |
| 1:CA:2732:G:H3' | 1:CA:2733:A:O4' | 2.21 | 0.41 |
| 1:AA:667:G:H21 | 1:AA:671:A:H2 | 1.69 | 0.41 |
| 34:DA:561:U:HO2' | 34:DA:562:C:P | 2.44 | 0.41 |
| 42:DI:17:VAL:HG23 | 42:DI:63:ILE:HG12 | 2.03 | 0.41 |
| 18:CU:76:TYR:O | 18:CU:79:PHE:HB3 | 2.20 | 0.41 |
| 43:BJ:38:ILE:HG13 | 43:BJ:71:LEU:HB3 | 2.02 | 0.41 |
| 1:CA:1668:A:O2' | 1:CA:1674:G:N7 | 2.49 | 0.41 |
| 34:BA:452:A:OP1 | 49:BP:43:LYS:NZ | 2.30 | 0.41 |
| 34:DA:255:G:H1' | 50:DQ:16:GLN:NE2 | 2.36 | 0.41 |
| 1:CA:335:C:H4' | 22:CY:73:ARG:NE | 2.35 | 0.41 |
| 34:BA:1165:C:HO2' | 34:BA:1166:G:P | 2.44 | 0.41 |
| 34:DA:1151:A:O2' | 34:DA:1152:A:O5' | 2.36 | 0.41 |
| 34:DA:1373:G:H8 | 34:DA:1373:G:O5' | 2.02 | 0.41 |
| 37:DD:15:GLU:HB3 | 37:DD:63:LYS:HD2 | 2.03 | 0.41 |
| 1:AA:2693:C:OP2 | 5:AE:109:LYS:NZ | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:BA:786:G:C2 | 34:BA:797:C:C2 | 3.09 | 0.41 |
| 1:CA:1890:A:H8 | 1:CA:1890:A:O5' | 2.04 | 0.41 |
| 13:AP:63:PRO:HD3 | 32:A8:27:THR:HG22 | 2.02 | 0.41 |
| 47:DN:14:PRO:HB2 | 47:DN:16:PHE:O | 2.21 | 0.41 |
| 34:DA:1410:G:H2' | 34:DA:1411:C:C6 | 2.56 | 0.41 |
| 46:BM:121:LYS:NZ | 56:BW:40:C:H4' | 2.36 | 0.41 |
| 23:AZ:104:PHE:O | 23:AZ:106:GLY:N | 2.54 | 0.41 |
| 34:DA:1429:C:H2' | 34:DA:1430:C:H6 | 1.85 | 0.41 |
| 1:CA:623:G:C6 | 1:CA:624:C:C4 | 3.09 | 0.41 |
| 1:AA:2170:G:H2' | 1:AA:2171:G:H8 | 1.86 | 0.41 |
| 1:AA:381:A:H2' | 1:AA:382:U:O4' | 2.21 | 0.41 |
| 38:BE:96:PRO:HA | 38:BE:117:ASP:OD2 | 2.21 | 0.41 |
| 53:BT:29:LYS:O | 53:BT:33:ILE:HG13 | 2.21 | 0.41 |
| 34:DA:662:G:H2' | 34:DA:663:A:C8 | 2.56 | 0.41 |
| 1:AA:1020:C:OP1 | 65:AA:4082:HOH:O | 2.22 | 0.41 |
| 1:CA:652:C:C2' | 1:CA:652(A):A:H5' | 2.50 | 0.41 |
| 1:CA:1291:C:H2' | 1:CA:1292:U:C6 | 2.56 | 0.41 |
| 6:CF:20:LEU:HA | 6:CF:20:LEU:HD23 | 1.75 | 0.41 |
| 45:DL:52:LEU:HD12 | 45:DL:52:LEU:HA | 1.78 | 0.41 |
| 41:BH:36:LEU:HD23 | 41:BH:36:LEU:HA | 1.80 | 0.41 |
| 7:AG:111:LEU:HA | 7:AG:111:LEU:HD23 | 1.89 | 0.41 |
| 1:CA:2380:C:O5' | 1:CA:2380:C:H6 | 2.02 | 0.41 |
| 8:CH:106:THR:OG1 | 8:CH:106:THR:O | 2.35 | 0.41 |
| 57:DX:14:A:C5 | 57:DX:22:G:C6 | 3.08 | 0.41 |
| 16:CS:93:LYS:HG2 | 16:CS:95:HIS:HB3 | 2.02 | 0.41 |
| 19:AV:25:LEU:HD12 | 19:AV:92:THR:HG21 | 2.02 | 0.41 |
| 23:CZ:14:LYS:HA | 23:CZ:15:PRO:HD3 | 1.79 | 0.41 |
| 34:DA:407:G:H5'' | 37:DD:115:ARG:HB3 | 2.02 | 0.41 |
| 25:C1:83:GLU:HA | 25:C1:84:GLY:HA2 | 1.60 | 0.41 |
| 59:BZ:171:GLU:C | 59:BZ:173:THR:H | 2.23 | 0.41 |
| 1:AA:2227:G:H3' | 1:AA:2228:G:N7 | 2.36 | 0.41 |
| 17:CT:109:GLU:O | 17:CT:113:LYS:HB2 | 2.21 | 0.41 |
| 3:CC:44:VAL:HG23 | 3:CC:176:VAL:CG2 | 2.51 | 0.41 |
| 34:DA:1319:A:H61 | 34:DA:1361:G:H21 | 1.68 | 0.41 |
| 35:DB:91:PRO:HB3 | 35:DB:154:LEU:HB3 | 2.03 | 0.41 |
| 34:DA:1273:G:H5' | 34:DA:1274:G:OP2 | 2.21 | 0.41 |
| 59:DZ:655:TYR:CZ | 59:DZ:659:LEU:HG | 2.56 | 0.41 |
| 38:BE:40:ARG:HB3 | 38:BE:66:MET:CE | 2.51 | 0.41 |
| 58:DY:36:A:H2' | 58:DY:37:MIA:O4' | 2.20 | 0.41 |
| 7:CG:15:VAL:HG22 | 7:CG:175:LEU:HB3 | 2.02 | 0.41 |
| 1:AA:2287:C:O2 | 14:AQ:85:LYS:HE2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:552:C:C4 | 1:AA:2792:U:H2' | 2.55 | 0.41 |
| 34:BA:1072:G:C5 | 34:BA:1073:U:C4 | 3.09 | 0.41 |
| 30:C6:9:LEU:HD11 | 30:C6:23:THR:HG23 | 2.02 | 0.41 |
| 36:BC:85:ARG:O | 36:BC:89:GLU:HG2 | 2.21 | 0.41 |
| 51:BR:39:VAL:O | 51:BR:42:ARG:HB2 | 2.20 | 0.41 |
| 1:CA:1823:G:OP1 | 4:CD:54:ARG:NH1 | 2.54 | 0.41 |
| 1:CA:1125:G:H5' | 33:C9:37:GLY:HA2 | 2.03 | 0.41 |
| 34:BA:418:C:H2' | 34:BA:419:C:C6 | 2.56 | 0.41 |
| 53:DT:63:ILE:HG21 | 53:DT:81:LYS:HG3 | 2.02 | 0.41 |
| 1:AA:2325:C:H4' | 7:AG:91:ARG:HG3 | 2.02 | 0.41 |
| 6:AF:64:ILE:H | 6:AF:64:ILE:HG13 | 1.59 | 0.41 |
| 23:CZ:30:ASN:ND2 | 23:CZ:90:VAL:HB | 2.35 | 0.41 |
| 1:CA:443:A:C6 | 6:CF:45:ARG:HD2 | 2.56 | 0.41 |
| 1:CA:479:A:H4' | 1:CA:480:A:OP1 | 2.20 | 0.41 |
| 34:DA:1057:G:H2' | 34:DA:1058:G:O4' | 2.21 | 0.41 |
| 3:AC:60:ARG:NH2 | 3:AC:165:ARG:HH21 | 2.18 | 0.41 |
| 1:CA:1657:C:H2' | 1:CA:1658:C:H6 | 1.85 | 0.41 |
| 25:C1:95:LEU:O | 25:C1:98:LEU:HB2 | 2.20 | 0.41 |
| 34:BA:1187:G:H2' | 34:BA:1188:A:C8 | 2.56 | 0.41 |
| 25:C1:53:VAL:O | 25:C1:56:GLN:HB2 | 2.21 | 0.41 |
| 12:CO:68:GLU:OE2 | 12:CO:78:ARG:NH1 | 2.51 | 0.41 |
| 34:DA:336:C:O2' | 34:DA:337:C:H5' | 2.21 | 0.41 |
| 1:CA:1445(A):C:H2' | 1:CA:1446:C:H6 | 1.86 | 0.41 |
| 59:BZ:538:TYR:OH | 59:BZ:577:SER:O | 2.30 | 0.41 |
| 32:C8:23:VAL:HA | 32:C8:48:PHE:O | 2.20 | 0.41 |
| 38:DE:41:VAL:HG22 | 38:DE:113:ALA:HA | 2.02 | 0.41 |
| 8:AH:83:TYR:CE2 | 8:AH:138:LYS:HB2 | 2.55 | 0.41 |
| 49:DP:58:TYR:O | 49:DP:61:SER:N | 2.52 | 0.41 |
| 1:AA:599:U:H2' | 1:AA:600:G:C8 | 2.56 | 0.41 |
| 17:AT:117:ASP:O | 17:AT:121:ILE:HG13 | 2.21 | 0.41 |
| 17:AT:61:PHE:CE1 | 17:AT:76:PHE:HB2 | 2.56 | 0.41 |
| 46:BM:49:THR:O | 46:BM:53:VAL:HG23 | 2.20 | 0.41 |
| 59:DZ:590:ILE:HD13 | 59:DZ:590:ILE:HA | 1.83 | 0.41 |
| 48:BO:66:LEU:HD12 | 48:BO:66:LEU:HA | 1.76 | 0.41 |
| 59:DZ:641:GLN:HB2 | 59:DZ:641:GLN:HE21 | 1.63 | 0.41 |
| 32:A8:31:HIS:O | 32:A8:32:LEU:HB2 | 2.20 | 0.41 |
| 34:DA:694:A:H2' | 34:DA:695:A:O4' | 2.21 | 0.41 |
| 3:AC:206:LYS:HB3 | 3:AC:206:LYS:HZ3 | 1.85 | 0.41 |
| 3:CC:11:LEU:HD22 | 3:CC:11:LEU:H | 1.86 | 0.41 |
| 35:BB:204:ASN:OD1 | 35:BB:205:ASP:N | 2.54 | 0.41 |
| 1:AA:2356:U:O2' | 30:A6:36:LEU:HD22 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:139:A:C8 | 1:AA:1454:C:O2' | 2.67 | 0.41 |
| 1:CA:2544:G:H1' | 1:CA:2646:C:H4' | 2.03 | 0.41 |
| 34:BA:1304:G:C6 | 34:BA:1305:G:N1 | 2.89 | 0.41 |
| 3:CC:16:ASP:HA | 3:CC:17:PRO:HD2 | 1.90 | 0.41 |
| 46:DM:20:THR:C | 46:DM:22:ILE:H | 2.24 | 0.41 |
| 46:DM:60:VAL:HG23 | 46:DM:64:TRP:CE3 | 2.56 | 0.41 |
| 6:CF:103:LYS:HA | 6:CF:106:ARG:HG3 | 2.01 | 0.41 |
| 18:CU:76:TYR:CZ | 18:CU:80:ILE:HG13 | 2.55 | 0.41 |
| 37:DD:135:LEU:C | 37:DD:137:SER:H | 2.23 | 0.41 |
| 3:AC:11:LEU:HD22 | 3:AC:11:LEU:H | 1.86 | 0.41 |
| 1:AA:354:A:O2' | 1:AA:355:A:C8 | 2.72 | 0.41 |
| 1:CA:2876:G:OP1 | 17:CT:3:ARG:HB2 | 2.21 | 0.41 |
| 34:DA:1122:U:H2' | 34:DA:1123:A:O4' | 2.20 | 0.41 |
| 34:BA:973:G:OP1 | 43:BJ:57:LYS:HE3 | 2.20 | 0.41 |
| 34:DA:1281:U:H5'' | 34:DA:1282:C:C5 | 2.56 | 0.41 |
| 6:CF:197:ASP:O | 6:CF:200:GLU:HB2 | 2.21 | 0.41 |
| 34:DA:1277:C:O2' | 34:DA:1279:A:H1' | 2.20 | 0.41 |
| 37:BD:167:GLY:H | 37:BD:168:ARG:NH2 | 2.19 | 0.41 |
| 59:BZ:125:ALA:CB | 59:BZ:132:ARG:NH1 | 2.84 | 0.41 |
| 35:BB:21:ARG:HB3 | 35:BB:39:ILE:HA | 2.02 | 0.41 |
| 41:DH:39:LEU:HD13 | 41:DH:39:LEU:HA | 1.96 | 0.41 |
| 59:DZ:168:ILE:HG12 | 59:DZ:205:TYR:CD2 | 2.55 | 0.41 |
| 53:DT:36:LEU:HD13 | 53:DT:36:LEU:HA | 1.57 | 0.41 |
| 1:AA:841:G:H2' | 1:AA:842:C:H6 | 1.85 | 0.41 |
| 1:CA:2404:C:O3' | 13:CP:77:ARG:NH2 | 2.54 | 0.41 |
| 34:BA:443:C:H2' | 34:BA:444:C:H6 | 1.86 | 0.41 |
| 1:CA:1485:G:H2' | 1:CA:1486:A:O4' | 2.20 | 0.41 |
| 12:AO:17:ARG:N | 12:AO:45:GLU:O | 2.40 | 0.41 |
| 1:CA:1002:G:H2' | 1:CA:1003:G:O4' | 2.21 | 0.41 |
| 34:DA:401:C:H1' | 34:DA:622:A:H1' | 2.02 | 0.41 |
| 19:CV:1:MET:HG2 | 19:CV:41:GLY:O | 2.20 | 0.41 |
| 1:CA:2630:G:H2' | 1:CA:2631:G:H8 | 1.86 | 0.41 |
| 59:DZ:164:MET:HG3 | 59:DZ:257:PRO:HB3 | 2.01 | 0.41 |
| 1:AA:1815:A:H4' | 1:AA:1816:A:C5' | 2.51 | 0.41 |
| 13:CP:93:GLY:H | 13:CP:123:LEU:HD21 | 1.86 | 0.41 |
| 34:BA:981:U:OP1 | 47:BN:6:LEU:HD11 | 2.21 | 0.41 |
| 34:BA:501:C:H1' | 34:BA:549:C:H1' | 2.03 | 0.41 |
| 33:A9:3:VAL:C | 33:A9:4:ARG:HG3 | 2.40 | 0.41 |
| 49:BP:7:ALA:O | 49:BP:9:PHE:CD1 | 2.73 | 0.41 |
| 11:CN:91:LEU:O | 11:CN:95:PRO:HB3 | 2.20 | 0.41 |
| 53:BT:18:GLN:O | 53:BT:22:ARG:HG3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:AA:1401:G:P | 4:AD:38:LYS:HE2 | 2.61 | 0.41 |
| 41:DH:134:ILE:HG22 | 41:DH:135:CYS:SG | 2.61 | 0.41 |
| 32:C8:26:LYS:HG2 | 32:C8:48:PHE:CD1 | 2.56 | 0.41 |
| 21:CX:4:ALA:HB1 | 21:CX:42:ALA:HA | 2.01 | 0.41 |
| 1:AA:1572:G:C6 | 1:AA:1573:G:C2 | 3.08 | 0.41 |
| 59:BZ:603:GLU:HG2 | 59:BZ:679:VAL:HG12 | 2.03 | 0.41 |
| 18:AU:47:TYR:HA | 18:AU:50:ARG:NH2 | 2.35 | 0.41 |
| 59:BZ:291:GLY:HA3 | 59:BZ:301:ILE:HD11 | 2.01 | 0.41 |
| 37:DD:26:CYS:HA | 63:DD:501:SF4:S3 | 2.61 | 0.41 |
| 56:DW:13:C:O2' | 56:DW:14:A:P | 2.79 | 0.41 |
| 40:DG:120:ILE:HG22 | 40:DG:124:LEU:CD1 | 2.50 | 0.41 |
| 1:AA:505:A:N3 | 1:AA:507:G:H5' | 2.35 | 0.41 |
| 36:BC:108:ASN:HA | 36:BC:109:PRO:HD2 | 1.91 | 0.41 |
| 34:BA:1142:G:H2' | 34:BA:1143:G:O4' | 2.21 | 0.41 |
| 50:DQ:89:LEU:HD23 | 50:DQ:89:LEU:HA | 1.64 | 0.41 |
| 34:DA:796:C:O5' | 34:DA:796:C:H6 | 2.04 | 0.41 |
| 1:AA:926:G:H8 | 1:AA:926:G:O5' | 2.02 | 0.41 |
| 40:DG:110:GLN:HE21 | 40:DG:110:GLN:HB3 | 1.71 | 0.41 |
| 34:BA:1169:A:N6 | 34:BA:1170:A:N1 | 2.69 | 0.41 |
| 38:BE:85:GLY:O | 38:BE:86:ALA:HB3 | 2.21 | 0.41 |
| 1:AA:1756:U:H2' | 1:AA:1757:C:C6 | 2.56 | 0.41 |
| 1:AA:1957:G:H1' | 1:AA:1986:G:N2 | 2.36 | 0.41 |
| 44:BK:56:GLY:O | 44:BK:89:ALA:HB3 | 2.21 | 0.41 |
| 19:AV:71:LEU:HD23 | 19:AV:71:LEU:HA | 1.94 | 0.41 |
| 34:BA:509:A:H3' | 34:BA:509:A:C8 | 2.55 | 0.41 |
| 4:AD:33:LEU:HD23 | 4:AD:33:LEU:HA | 1.94 | 0.41 |
| 1:CA:2801(A):A:H1' | 1:CA:2895:U:H1' | 2.03 | 0.41 |
| 46:BM:78:ILE:O | 46:BM:82:MET:HG3 | 2.21 | 0.41 |
| 20:CW:10:VAL:HG21 | 20:CW:103:ILE:HD12 | 2.01 | 0.41 |
| 1:CA:1019:U:OP1 | 1:CA:1035:U:O2' | 2.26 | 0.41 |
| 22:CY:99:CYS:SG | 22:CY:102:CYS:N | 2.93 | 0.41 |
| 3:CC:54:ARG:CZ | 3:CC:55:SER:O | 2.69 | 0.41 |
| 3:AC:224:ARG:HE | 3:AC:224:ARG:HB3 | 1.73 | 0.41 |
| 1:AA:2555:G:H2' | 1:AA:2556:G:C8 | 2.56 | 0.41 |
| 1:CA:2733:A:H2 | 5:CE:204:ALA:H | 1.68 | 0.41 |
| 34:DA:1030(A):G:N2 | 34:DA:1030(C):G:H3' | 2.36 | 0.41 |
| 34:DA:253:U:H2' | 34:DA:254:G:H8 | 1.85 | 0.41 |
| 34:BA:1254:C:H2' | 34:BA:1255:G:O4' | 2.21 | 0.41 |
| 37:BD:188:LEU:H | 37:BD:188:LEU:HD23 | 1.86 | 0.41 |
| 34:BA:1118:C:OP1 | 42:BI:9:ARG:NH1 | 2.54 | 0.41 |
| 14:CQ:85:LYS:HD3 | 24:C0:7:LEU:HG | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:CY:5:MET:HG2 | 22:CY:30:VAL:HG11 | 2.03 | 0.41 |
| 59:DZ:628:ARG:HD2 | 59:DZ:680:PRO:HG2 | 2.03 | 0.41 |
| 1:AA:1712:A:H2' | 1:AA:1713:G:O4' | 2.20 | 0.41 |
| 1:CA:1405:U:H2' | 1:CA:1406:U:C6 | 2.55 | 0.41 |
| 1:AA:1002:A:H5' | 14:AQ:76:LYS:HG2 | 2.03 | 0.41 |
| 7:CG:53:LEU:HD23 | 7:CG:53:LEU:HA | 1.83 | 0.41 |
| 35:BB:215:LEU:O | 35:BB:219:VAL:HG23 | 2.21 | 0.41 |
| 12:CO:113:LYS:O | 12:CO:117:LEU:HD12 | 2.21 | 0.41 |
| 1:CA:2330:G:H2' | 1:CA:2331:G:O4' | 2.20 | 0.41 |
| 13:AP:85:LEU:HD12 | 13:AP:116:GLY:O | 2.20 | 0.41 |
| 20:CW:70:TYR:O | 20:CW:107:LEU:HD12 | 2.21 | 0.41 |
| 1:CA:2745:C:H4' | 8:CH:142:GLY:O | 2.20 | 0.41 |
| 34:DA:1310:G:H5' | 46:DM:77:ASN:OD1 | 2.21 | 0.41 |
| 23:AZ:138:GLU:H | 23:AZ:156:LYS:HD3 | 1.86 | 0.41 |
| 59:DZ:327:PHE:CE1 | 59:DZ:376:ALA:HB2 | 2.56 | 0.41 |
| 1:AA:789:G:H4' | 1:AA:1723:A:H5' | 2.03 | 0.41 |
| 59:BZ:499:ARG:HB2 | 59:BZ:506:GLN:HB2 | 2.04 | 0.41 |
| 6:AF:62:ARG:NH1 | 6:AF:62:ARG:HB3 | 2.36 | 0.41 |
| 1:AA:1772:C:H6 | 1:AA:1772:C:O5' | 2.04 | 0.41 |
| 59:DZ:382:GLU:H | 59:DZ:382:GLU:HG2 | 1.76 | 0.41 |
| 1:CA:224:G:N7 | 1:CA:420:C:H4' | 2.36 | 0.41 |
| 59:BZ:350:GLU:OE1 | 59:BZ:382:GLU:N | 2.53 | 0.41 |
| 12:AO:66:LYS:HA | 12:AO:79:PHE:O | 2.21 | 0.41 |
| 59:BZ:-27:THR:O | 59:BZ:-23:LEU:HB2 | 2.21 | 0.41 |
| 37:DD:173:TRP:CD1 | 37:DD:174:LEU:HG | 2.56 | 0.40 |
| 59:DZ:221:ALA:HB1 | 59:DZ:228:MET:HB2 | 2.02 | 0.40 |
| 1:AA:1117:G:N2 | 1:AA:1135:G:HO2' | 2.18 | 0.40 |
| 38:BE:100:VAL:O | 38:BE:101:ILE:HD13 | 2.21 | 0.40 |
| 1:AA:325:G:C4 | 1:AA:326:C:C5 | 3.09 | 0.40 |
| 1:AA:2146:G:H5'' | 3:AC:175:PRO:HG3 | 2.03 | 0.40 |
| 46:DM:20:THR:HG22 | 46:DM:26:GLY:O | 2.21 | 0.40 |
| 1:CA:2164:C:H3' | 1:CA:2165:G:O4' | 2.21 | 0.40 |
| 34:DA:1207:G:H2' | 34:DA:1208:C:C6 | 2.55 | 0.40 |
| 5:CE:67:PHE:CE2 | 5:CE:74:PRO:HA | 2.56 | 0.40 |
| 3:AC:194:ILE:CD1 | 3:AC:227:PRO:CB | 2.99 | 0.40 |
| 1:AA:1855:G:OP1 | 4:AD:52:ARG:NH1 | 2.46 | 0.40 |
| 1:CA:1654:A:OP1 | 15:CR:1:MET:HA | 2.20 | 0.40 |
| 1:CA:811:U:P | 13:CP:29:LYS:H | 2.45 | 0.40 |
| 16:CS:111:GLU:O | 16:CS:112:PHE:HB3 | 2.22 | 0.40 |
| 34:BA:435:C:H2' | 34:BA:436:C:H6 | 1.85 | 0.40 |
| 1:CA:856:C:H3' | 1:CA:856:C:C6 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1652:A:OP1 | 15:CR:8:ARG:HD3 | 2.21 | 0.40 |
| 12:AO:47:ILE:HB | 12:AO:48:PRO:HD2 | 2.03 | 0.40 |
| 43:DJ:47:PHE:CZ | 47:DN:37:PHE:HE1 | 2.40 | 0.40 |
| 11:CN:128:HIS:HA | 11:CN:129:PRO:HD3 | 1.75 | 0.40 |
| 1:CA:1297:C:H2' | 1:CA:1298:C:H6 | 1.86 | 0.40 |
| 1:CA:2494:G:O2' | 14:CQ:80:GLU:HA | 2.22 | 0.40 |
| 34:DA:939:G:C6 | 34:DA:940:C:N4 | 2.90 | 0.40 |
| 42:BI:26:VAL:HG13 | 42:BI:61:ALA:HB3 | 2.03 | 0.40 |
| 34:BA:1015:A:N3 | 34:BA:1218:C:O2' | 2.45 | 0.40 |
| 8:AH:98:LEU:HD13 | 8:AH:125:VAL:CG2 | 2.51 | 0.40 |
| 35:BB:84:GLU:O | 35:BB:219:VAL:HG21 | 2.20 | 0.40 |
| 33:C9:9:ARG:HG2 | 33:C9:14:CYS:HB2 | 2.03 | 0.40 |
| 1:CA:2689:U:H2' | 1:CA:2689:U:O2 | 2.21 | 0.40 |
| 32:C8:26:LYS:HG2 | 32:C8:48:PHE:HD1 | 1.86 | 0.40 |
| 1:AA:1985:U:H4' | 1:AA:1986:G:OP1 | 2.20 | 0.40 |
| 49:DP:21:VAL:CG1 | 49:DP:34:GLU:HB3 | 2.51 | 0.40 |
| 1:AA:895:G:H2' | 1:AA:896:A:C8 | 2.56 | 0.40 |
| 1:AA:100:G:H5'' | 26:A2:3:LEU:CD1 | 2.51 | 0.40 |
| 11:AN:10:GLU:OE1 | 11:AN:11:PRO:HD2 | 2.21 | 0.40 |
| 14:AQ:81:VAL:HB | 24:A0:7:LEU:HD11 | 2.01 | 0.40 |
| 7:AG:132:ASN:HA | 7:AG:157:ILE:O | 2.22 | 0.40 |
| 1:CA:1283:G:N2 | 1:CA:1285:G:H3' | 2.36 | 0.40 |
| 47:BN:13:THR:HA | 47:BN:14:PRO:HD3 | 1.78 | 0.40 |
| 1:AA:347:G:C8 | 6:AF:171:PRO:HG3 | 2.56 | 0.40 |
| 5:CE:179:GLU:O | 5:CE:180:ASN:HB2 | 2.22 | 0.40 |
| 7:AG:125:PHE:HB3 | 7:AG:166:ASP:CG | 2.41 | 0.40 |
| 1:CA:2309:A:C6 | 1:CA:2310:A:C6 | 3.09 | 0.40 |
| 1:CA:190:A:OP2 | 25:C1:39:LYS:HE3 | 2.22 | 0.40 |
| 48:BO:27:VAL:O | 48:BO:31:LEU:HG | 2.21 | 0.40 |
| 1:AA:2819:A:C6 | 1:AA:2901:A:C8 | 3.09 | 0.40 |
| 51:DR:76:LEU:HA | 51:DR:76:LEU:HD12 | 1.56 | 0.40 |
| 17:AT:118:ARG:HH11 | 17:AT:118:ARG:HG3 | 1.86 | 0.40 |
| 35:BB:87:ARG:NH2 | 35:BB:220:ASP:OD1 | 2.42 | 0.40 |
| 1:AA:253:C:O2' | 1:AA:254:A:H2' | 2.22 | 0.40 |
| 1:AA:254:A:N6 | 1:AA:454:U:O2' | 2.46 | 0.40 |
| 50:BQ:29:HIS:HA | 50:BQ:30:PRO:HD2 | 1.79 | 0.40 |
| 50:BQ:27:PHE:CE2 | 50:BQ:36:ILE:HD11 | 2.55 | 0.40 |
| 34:BA:622:A:C8 | 34:BA:623:C:C5 | 3.09 | 0.40 |
| 34:BA:375:U:C2 | 34:BA:376:G:C8 | 3.10 | 0.40 |
| 22:AY:92:ASN:ND2 | 22:AY:92:ASN:N | 2.67 | 0.40 |
| 1:CA:2203:U:H2' | 1:CA:2205:C:C6 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:AT:23:ARG:HG3 | 17:AT:120:ARG:NH1 | 2.35 | 0.40 |
| 56:BW:52:G:H2' | 56:BW:53:G:O4' | 2.21 | 0.40 |
| 5:CE:75:VAL:HG13 | 5:CE:77:ILE:H | 1.86 | 0.40 |
| 47:BN:27:CYS:SG | 47:BN:29:ARG:HB2 | 2.61 | 0.40 |
| 1:CA:1721:G:H5' | 1:CA:1722:A:OP2 | 2.22 | 0.40 |
| 22:CY:30:VAL:O | 22:CY:32:PRO:HD3 | 2.22 | 0.40 |
| 35:DB:149:LEU:O | 35:DB:153:ARG:N | 2.47 | 0.40 |
| 23:AZ:150:LEU:C | 23:AZ:151:HIS:HD1 | 2.25 | 0.40 |
| 1:AA:1686:U:H4' | 1:AA:2711:C:H4' | 2.03 | 0.40 |
| 46:BM:60:VAL:HG13 | 46:BM:64:TRP:CZ3 | 2.55 | 0.40 |
| 59:BZ:188:TYR:CE1 | 59:BZ:196:ILE:HD12 | 2.56 | 0.40 |
| 5:AE:120:TRP:CE3 | 5:AE:155:LYS:HE2 | 2.56 | 0.40 |
| 34:DA:1014:A:H2' | 34:DA:1015:A:N9 | 2.36 | 0.40 |
| 34:DA:555:C:H2' | 34:DA:556:C:C6 | 2.56 | 0.40 |
| 1:AA:2650:G:P | 5:AE:82:ARG:HH22 | 2.44 | 0.40 |
| 38:BE:143:ARG:NH1 | 41:BH:77:GLU:OE1 | 2.54 | 0.40 |
| 6:AF:200:GLU:O | 6:AF:203:GLN:HB2 | 2.22 | 0.40 |
| 16:AS:74:ALA:HB2 | 16:AS:105:ALA:HA | 2.03 | 0.40 |
| 1:CA:248:G:H2' | 65:CA:3866:HOH:O | 2.20 | 0.40 |
| 4:CD:218:ARG:HB3 | 4:CD:219:PRO:HD2 | 2.03 | 0.40 |
| 12:AO:98:VAL:HG22 | 12:AO:118:ALA:HA | 2.04 | 0.40 |
| 34:DA:338:A:H2' | 34:DA:339:C:O4' | 2.21 | 0.40 |
| 1:CA:1627:G:OP2 | 65:CA:4545:HOH:O | 2.22 | 0.40 |
| 13:AP:144:GLU:HA | 13:AP:145:PRO:HD3 | 1.84 | 0.40 |
| 14:CQ:65:PHE:HB2 | 14:CQ:105:GLU:HB2 | 2.03 | 0.40 |
| 1:CA:947:G:H2' | 1:CA:948:G:C8 | 2.57 | 0.40 |
| 13:AP:106:LEU:HD23 | 13:AP:106:LEU:HA | 1.80 | 0.40 |
| 23:AZ:102:LEU:HA | 23:AZ:102:LEU:HD12 | 1.79 | 0.40 |
| 40:DG:139:GLU:O | 40:DG:143:ARG:N | 2.53 | 0.40 |
| 1:AA:1445:C:N4 | 65:AA:4432:HOH:O | 2.53 | 0.40 |
| 1:CA:2626:C:H2' | 1:CA:2627:G:O4' | 2.21 | 0.40 |
| 1:AA:2108:U:H2' | 1:AA:2109:G:C8 | 2.56 | 0.40 |
| 57:DX:8:4SU:O2 | 57:DX:21:A:H2 | 2.05 | 0.40 |
| 1:CA:2178:C:HO2' | 3:CC:169:THR:HB | 1.80 | 0.40 |
| 3:AC:54:ARG:CZ | 3:AC:55:SER:O | 2.69 | 0.40 |
| 34:DA:1073:U:O2' | 35:DB:104:ASN:OD1 | 2.35 | 0.40 |
| 34:DA:1237:C:OP1 | 34:DA:1238:A:H1' | 2.21 | 0.40 |
| 41:BH:6:ILE:HG12 | 41:BH:6:ILE:H | 1.53 | 0.40 |
| 34:BA:1316:G:O2' | 47:BN:18:VAL:HG11 | 2.20 | 0.40 |
| 6:CF:155:LEU:CD2 | 6:CF:186:ILE:HG13 | 2.50 | 0.40 |
| 2:CB:79:C:H2' | 2:CB:80:U:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:CD:26:LYS:HE2 | 4:CD:28:GLU:O | 2.21 | 0.40 |
| 1:AA:174:U:H4' | 1:AA:207:A:H4' | 2.03 | 0.40 |
| 14:AQ:109:VAL:HG13 | 14:AQ:113:GLN:HB2 | 2.03 | 0.40 |
| 1:AA:1824:C:H2' | 1:AA:1825:U:C6 | 2.57 | 0.40 |
| 1:CA:2667:C:N3 | 8:CH:110:SER:OG | 2.54 | 0.40 |
| 1:AA:2221:A:H3' | 1:AA:2222:C:H6 | 1.86 | 0.40 |
| 34:DA:1104:G:O5' | 35:DB:111:ARG:HD2 | 2.21 | 0.40 |
| 22:CY:49:VAL:HG21 | 22:CY:61:ILE:HG23 | 2.03 | 0.40 |
| 1:CA:2306:C:C4 | 1:CA:2307:G:C6 | 3.10 | 0.40 |
| 25:A1:20:ARG:HD3 | 25:A1:20:ARG:HH11 | 1.71 | 0.40 |
| 33:C9:17:ILE:HD12 | 33:C9:18:ARG:H | 1.86 | 0.40 |
| 46:BM:56:LEU:O | 46:BM:60:VAL:HG23 | 2.22 | 0.40 |
| 34:BA:1510:U:H2' | 34:BA:1511:G:C8 | 2.57 | 0.40 |
| 1:CA:1093:G:H1' | 1:CA:1099:G:N2 | 2.37 | 0.40 |
| 1:CA:1301:A:C8 | 1:CA:1303:G:C8 | 3.09 | 0.40 |
| 1:CA:2787:C:O2' | 1:CA:2810:A:O2' | 2.29 | 0.40 |
| 34:BA:708:C:H2' | 34:BA:709:G:C8 | 2.56 | 0.40 |
| 34:DA:790:A:OP1 | 57:DX:38:A:O2' | 2.37 | 0.40 |
| 14:CQ:18:LYS:HB2 | 14:CQ:18:LYS:HE3 | 1.75 | 0.40 |
| 58:BY:20:U:H4' | 58:BY:21:A:OP1 | 2.20 | 0.40 |
| 8:AH:41:MET:HE1 | 8:AH:65:HIS:HA | 2.03 | 0.40 |
| 1:AA:438:G:OP2 | 1:AA:2418:U:O2' | 2.36 | 0.40 |
| 37:DD:196:LEU:O | 37:DD:198:VAL:N | 2.48 | 0.40 |
| 40:DG:36:LYS:O | 40:DG:39:ALA:HB3 | 2.22 | 0.40 |
| 34:DA:1090:U:H2' | 34:DA:1091:U:C6 | 2.56 | 0.40 |
| 34:DA:1229:A:H2' | 34:DA:1230:C:H6 | 1.85 | 0.40 |
| 1:CA:527:C:C5 | 1:CA:2779:U:H2' | 2.57 | 0.40 |
| 39:DF:100:ASN:HD21 | 51:DR:23:LYS:HG2 | 1.86 | 0.40 |
| 1:CA:1826:G:H4' | 4:CD:242:ARG:CZ | 2.51 | 0.40 |
| 56:BW:24:G:C5 | 56:BW:25:C:C4 | 3.10 | 0.40 |
| 1:AA:96:C:OP1 | 26:A2:2:LYS:HE2 | 2.22 | 0.40 |
| 38:BE:8:GLU:HG3 | 38:BE:34:VAL:HG23 | 2.03 | 0.40 |
| 14:AQ:37:LEU:HA | 14:AQ:37:LEU:HD23 | 1.65 | 0.40 |
| 22:AY:5:MET:HB2 | 22:AY:5:MET:HE2 | 1.90 | 0.40 |
| 36:BC:18:TRP:HE3 | 36:BC:18:TRP:H | 1.68 | 0.40 |
| 51:DR:21:LYS:HB2 | 51:DR:21:LYS:HE2 | 1.85 | 0.40 |
| 10:AL:84:LEU:HD21 | 10:AL:96:VAL:HB | 2.03 | 0.40 |
| 26:C2:53:LEU:O | 26:C2:57:ILE:HG13 | 2.21 | 0.40 |
| 4:AD:223:GLY:HA3 | 4:AD:231:HIS:CE1 | 2.56 | 0.40 |
| 35:DB:193:ASP:HA | 35:DB:194:PRO:HD2 | 1.84 | 0.40 |
| 34:BA:986:A:H2' | 34:BA:987:G:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:DA:684:A:H1' | 44:DK:38:ASN:HB3 | 2.04 | 0.40 |
| 56:DW:32:PSU:C2 | 56:DW:33:U:C4 | 3.09 | 0.40 |
| 1:AA:2603:C:P | 4:AD:239:ARG:HG3 | 2.62 | 0.40 |
| 21:AX:65:ARG:HB2 | 21:AX:70:LEU:HD22 | 2.04 | 0.40 |
| 15:CR:84:ALA:HB3 | 15:CR:85:PRO:HD3 | 2.03 | 0.40 |
| 1:AA:1249:A:H61 | 1:AA:1286:U:H2' | 1.86 | 0.40 |
| 59:DZ:116:PRO:O | 59:DZ:117:GLN:HG3 | 2.22 | 0.40 |
| 59:BZ:404:VAL:HA | 59:BZ:405:PRO:HD3 | 1.80 | 0.40 |
| 13:CP:39:LYS:CB | 13:CP:45:LEU:HG | 2.41 | 0.40 |
| 1:AA:2203:G:HO2' | 1:AA:2204:G:P | 2.44 | 0.40 |
| 41:DH:51:VAL:HG12 | 41:DH:52:ASP:H | 1.86 | 0.40 |
| 43:DJ:29:ARG:HD3 | 43:DJ:29:ARG:HA | 1.83 | 0.40 |
| 34:BA:1330:U:C2' | 34:BA:1331:G:H5' | 2.51 | 0.40 |
| 41:BH:112:LEU:HB3 | 41:BH:133:LEU:HA | 2.03 | 0.40 |
| 23:CZ:120:ILE:HD11 | 23:CZ:171:ILE:C | 2.42 | 0.40 |
| 41:DH:84:ARG:HD2 | 41:DH:86:ILE:HD13 | 2.03 | 0.40 |
| 35:DB:16:HIS:CD2 | 35:DB:17:PHE:N | 2.90 | 0.40 |
| 7:AG:161:THR:HG22 | 7:AG:163:ALA:N | 2.33 | 0.40 |
| 59:DZ:105:ILE:HG22 | 59:DZ:280:LEU:HD11 | 2.03 | 0.40 |
| 5:AE:52:LEU:O | 5:AE:76:ARG:N | 2.54 | 0.40 |
| 11:AN:121:LYS:HG2 | 11:AN:130:HIS:CE1 | 2.57 | 0.40 |
| 34:BA:1350:A:N7 | 42:BI:118:LYS:NZ | 2.70 | 0.40 |
| 1:AA:704:U:H2' | 1:AA:705:C:H6 | 1.86 | 0.40 |
| 14:CQ:32:TYR:CZ | 14:CQ:133:ARG:HD3 | 2.56 | 0.40 |
| 42:DI:4:TYR:CG | 42:DI:88:TYR:HB2 | 2.57 | 0.40 |
| 34:BA:954:G:H2' | 34:BA:955:U:O4' | 2.21 | 0.40 |
| 38:BE:51:VAL:HB | 38:BE:52:PRO:HD3 | 2.04 | 0.40 |
| 34:BA:619:U:N3 | 37:BD:134:ASP:OD2 | 2.42 | 0.40 |
| 36:DC:181:ASN:OD1 | 36:DC:204:LEU:HD12 | 2.21 | 0.40 |
| 37:DD:97:LEU:HD23 | 37:DD:97:LEU:HA | 1.93 | 0.40 |
| 34:DA:186:C:H2' | 34:DA:187:C:C6 | 2.56 | 0.40 |
| 46:BM:80:ARG:NH2 | 52:BS:69:HIS:CE1 | 2.90 | 0.40 |
| 1:AA:2367:C:O3' | 24:A0:24:LYS:HE3 | 2.21 | 0.40 |
| 50:BQ:9:VAL:HG23 | 50:BQ:9:VAL:H | 1.57 | 0.40 |
| 16:CS:110:LEU:HA | 16:CS:110:LEU:HD12 | 1.74 | 0.40 |
| 35:BB:71:VAL:HG22 | 35:BB:93:VAL:CG2 | 2.52 | 0.40 |
| 35:DB:105:PHE:C | 35:DB:107:THR:H | 2.25 | 0.40 |
| 39:DF:100:ASN:ND2 | 51:DR:23:LYS:HE3 | 2.37 | 0.40 |
| 59:BZ:462:ILE:O | 59:BZ:466:LEU:HB2 | 2.21 | 0.40 |
| 1:AA:2225:U:O4' | 4:AD:151:LYS:HE2 | 2.21 | 0.40 |
| 38:BE:48:ALA:HB3 | 38:BE:54:ALA:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:461:U:H1' | 1:AA:462:C:H5 | 1.86 | 0.40 |
| 1:CA:2280:G:N3 | 1:CA:2388:A:H2 | 2.19 | 0.40 |
| 2:AB:43:C:O2' | 7:AG:95:ARG:HD2 | 2.22 | 0.40 |
| 5:AE:21:VAL:HG23 | 5:AE:185:LYS:HD2 | 2.04 | 0.40 |
| 6:AF:139:PHE:HB2 | 6:AF:166:ALA:HB1 | 2.03 | 0.40 |
| 1:AA:2247:G:H2' | 1:AA:2248:C:C6 | 2.56 | 0.40 |
| 40:DG:59:LEU:O | 40:DG:63:LYS:HE2 | 2.21 | 0.40 |
| 22:CY:79:CYS:O | 22:CY:81:LYS:HG3 | 2.21 | 0.40 |
| 36:BC:56:ASP:HB2 | 36:BC:67:THR:HB | 2.03 | 0.40 |
| 48:BO:43:LEU:HD23 | 48:BO:43:LEU:HA | 1.78 | 0.40 |
| 35:DB:223:ILE:H | 35:DB:223:ILE:HG13 | 1.74 | 0.40 |
| 6:AF:140:LEU:HD12 | 6:AF:140:LEU:HA | 1.75 | 0.40 |
| 59:DZ:355:LEU:HD12 | 59:DZ:355:LEU:HA | 1.93 | 0.40 |
| 19:CV:35:LEU:HA | 19:CV:36:PRO:HD3 | 1.94 | 0.40 |
| 50:BQ:81:ARG:HA | 50:BQ:81:ARG:HD2 | 1.90 | 0.40 |
| 1:CA:1913:A:H4' | 1:CA:1914:C:O5' | 2.20 | 0.40 |
| 1:CA:1913:A:C8 | 34:DA:1494:G:H4' | 2.57 | 0.40 |
| 34:DA:499:A:H4' | 34:DA:500:G:OP1 | 2.20 | 0.40 |
| 38:DE:36:ASP:C | 38:DE:38:GLN:H | 2.24 | 0.40 |
| 1:AA:632:A:H2' | 1:AA:633:G:O4' | 2.22 | 0.40 |
| 9:AK:23:SER:HA | 9:AK:117:LEU:O | 2.21 | 0.40 |
| 34:DA:976:G:N2 | 34:DA:1362:C:H2' | 2.37 | 0.40 |
| 22:AY:54:LYS:HA | 22:AY:55:TYR:HA | 1.95 | 0.40 |
| 59:DZ:160:ARG:HB3 | 59:DZ:256:THR:H | 1.87 | 0.40 |
| 34:DA:1222:G:C2 | 34:DA:1223:C:C2 | 3.09 | 0.40 |
| 1:CA:307:G:H2' | 1:CA:309:G:OP2 | 2.21 | 0.40 |
| 1:CA:1341:U:O2 | 21:CX:80:ILE:HD12 | 2.22 | 0.40 |
| 59:DZ:659:LEU:HA | 59:DZ:659:LEU:HD23 | 1.87 | 0.40 |
| 34:BA:1250:A:C2 | 34:BA:1370:G:H1' | 2.56 | 0.40 |
| 37:DD:203:VAL:O | 37:DD:206:PHE:HB3 | 2.22 | 0.40 |
| 36:BC:113:ALA:HB3 | 36:BC:114:PRO:HD3 | 2.04 | 0.40 |
| 34:DA:1132:C:H2' | 34:DA:1133:G:H8 | 1.86 | 0.40 |
| 35:DB:97:TRP:CH2 | 35:DB:102:LEU:HD13 | 2.57 | 0.40 |
| 37:DD:38:TYR:CE1 | 37:DD:45:GLN:HG3 | 2.57 | 0.40 |
| 36:DC:8:ILE:HG13 | 36:DC:16:ARG:HG2 | 2.02 | 0.40 |
| 34:DA:1125:U:O2' | 34:DA:1126:U:H2' | 2.21 | 0.40 |
| 34:DA:188:C:H2' | 34:DA:189:G:C8 | 2.53 | 0.40 |
| 1:CA:1740:G:H2' | 1:CA:1741:A:C8 | 2.57 | 0.40 |
| 6:AF:129:PHE:HB3 | 6:AF:132:VAL:CG1 | 2.52 | 0.40 |
| 34:BA:1106:G:H5'' | 36:BC:172:ARG:HG2 | 2.04 | 0.40 |
| 22:CY:13:VAL:O | 22:CY:24:VAL:HA | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 36:DC:140:ARG:NH1 | 36:DC:141:VAL:HG23 | 2.36 | 0.40 |
| 41:DH:40:ALA:O | 41:DH:43:GLY:N | 2.46 | 0.40 |
| 36:BC:20:SER:HB3 | 36:BC:22:TRP:NE1 | 2.37 | 0.40 |
| 34:BA:45:U:O5' | 34:BA:45:U:H6 | 2.04 | 0.40 |
| 1:AA:2371:C:H2' | 1:AA:2372:A:O4' | 2.22 | 0.40 |
| 1:AA:955:A:H2' | 1:AA:958:C:H5 | 1.86 | 0.40 |
| 6:AF:150:GLY:HA2 | 6:AF:172:TRP:CE3 | 2.56 | 0.40 |
| 18:AU:104:GLN:H | 18:AU:104:GLN:NE2 | 2.20 | 0.40 |
| 34:BA:1417:G:H22 | 34:BA:1482:G:H2' | 1.86 | 0.40 |
| 37:BD:110:PHE:H | 37:BD:110:PHE:HD1 | 1.70 | 0.40 |
| 1:AA:863:C:H2' | 1:AA:864:C:H6 | 1.86 | 0.40 |
| 6:CF:36:VAL:HG12 | 6:CF:40:GLN:OE1 | 2.21 | 0.40 |
| 34:DA:1409:C:H2' | 34:DA:1410:G:H8 | 1.86 | 0.40 |
| 42:DI:111:ARG:O | 42:DI:113:LYS:HD2 | 2.20 | 0.40 |
| 34:BA:185:A:H1' | 53:BT:81:LYS:HZ1 | 1.86 | 0.40 |
| 34:DA:719:C:N4 | 51:DR:71:LYS:HE2 | 2.37 | 0.40 |
| 49:DP:55:ARG:O | 49:DP:58:TYR:HB3 | 2.21 | 0.40 |
| 4:CD:242:ARG:HD3 | 4:CD:242:ARG:N | 2.36 | 0.40 |
| 5:AE:21:VAL:HA | 5:AE:22:PRO:HD3 | 1.89 | 0.40 |
| 34:BA:1082:G:H2' | 34:BA:1083:U:O4' | 2.22 | 0.40 |
| 59:DZ:682:GLN:O | 59:DZ:686:LYS:HB3 | 2.21 | 0.40 |
| 1:CA:1171:G:N2 | 1:CA:1179:C:C2 | 2.89 | 0.40 |
| 1:CA:2576:G:H1' | 65:CA:3997:HOH:O | 2.21 | 0.40 |
| 1:CA:277:C:H1' | 1:CA:278:A:P | 2.62 | 0.40 |
| 34:BA:456:C:H42 | 34:BA:475:G:H1 | 1.68 | 0.40 |
| 58:DY:8:4SU:H1' | 58:DY:48:C:O2 | 2.21 | 0.40 |
| 6:CF:148:LEU:HD11 | 6:CF:193:VAL:HG21 | 2.03 | 0.40 |
| 34:DA:643:C:H5' | 41:DH:31:PHE:CD1 | 2.57 | 0.40 |
| 59:DZ:71:THR:HG22 | 59:DZ:80:ASN:OD1 | 2.22 | 0.40 |
| 2:CB:101:G:H2' | 2:CB:102:A:O4' | 2.21 | 0.40 |
| 14:CQ:118:LEU:HA | 14:CQ:118:LEU:HD23 | 1.93 | 0.40 |
| 39:DF:50:TYR:CE2 | 51:DR:77:GLY:HA2 | 2.56 | 0.40 |
| 37:BD:61:LYS:HA | 37:BD:203:VAL:HG22 | 2.03 | 0.40 |
| 36:BC:33:LEU:HD11 | 47:BN:53:LEU:HD23 | 2.03 | 0.40 |
| 53:DT:56:MET:HE2 | 53:DT:88:VAL:HG21 | 2.03 | 0.40 |
| 18:CU:61:TRP:CD2 | 18:CU:93:LYS:HA | 2.56 | 0.40 |
| 34:DA:865:A:H5' | 34:DA:1078:U:O4 | 2.21 | 0.40 |

All (17) 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) |
|-------------------|--------------------------|--------------------------|-------------------|
| 3:AC:9:ARG:NH2 | 59:DZ:504:ARG:NH1[3_654] | 0.73 | 1.47 |
| 59:BZ:504:ARG:NH2 | 3:CC:9:ARG:NE[2_655] | 1.08 | 1.12 |
| 59:BZ:504:ARG:NH1 | 3:CC:9:ARG:NH1[2_655] | 1.09 | 1.11 |
| 3:AC:6:LYS:O | 59:DZ:501:THR:O[3_654] | 1.74 | 0.46 |
| 59:BZ:504:ARG:NH1 | 3:CC:9:ARG:NE[2_655] | 1.80 | 0.40 |
| 59:BZ:504:ARG:CZ | 3:CC:9:ARG:CZ[2_655] | 1.83 | 0.37 |
| 59:BZ:502:GLY:CA | 3:CC:9:ARG:CB[2_655] | 1.85 | 0.35 |
| 59:BZ:504:ARG:CZ | 3:CC:9:ARG:CD[2_655] | 1.85 | 0.35 |
| 3:AC:9:ARG:CZ | 59:DZ:504:ARG:NH1[3_654] | 1.85 | 0.35 |
| 3:AC:9:ARG:NH2 | 59:DZ:504:ARG:CZ[3_654] | 1.86 | 0.34 |
| 59:BZ:504:ARG:NH2 | 3:CC:9:ARG:CZ[2_655] | 1.91 | 0.29 |
| 59:BZ:504:ARG:NH1 | 3:CC:9:ARG:CD[2_655] | 2.04 | 0.16 |
| 59:BZ:504:ARG:NH2 | 3:CC:9:ARG:CD[2_655] | 2.07 | 0.13 |
| 1:AA:2154:U:O4 | 59:DZ:501:THR:OG1[3_654] | 2.08 | 0.12 |
| 1:AA:2158:C:O2' | 34:DA:1000:U:O2'[3_654] | 2.08 | 0.12 |
| 3:AC:9:ARG:CB | 59:DZ:502:GLY:CA[3_654] | 2.10 | 0.10 |
| 59:BZ:502:GLY:N | 3:CC:9:ARG:CB[2_655] | 2.17 | 0.03 |

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | AC | 133/228 (58%) | 90 (68%) | 25 (19%) | 18 (14%) | 0 | 1 |
| 3 | CC | 133/228 (58%) | 90 (68%) | 25 (19%) | 18 (14%) | 0 | 1 |
| 4 | AD | 273/276 (99%) | 248 (91%) | 22 (8%) | 3 (1%) | 17 | 50 |
| 4 | CD | 273/276 (99%) | 245 (90%) | 25 (9%) | 3 (1%) | 17 | 50 |
| 5 | AE | 202/206 (98%) | 189 (94%) | 12 (6%) | 1 (0%) | 34 | 69 |
| 5 | CE | 202/206 (98%) | 189 (94%) | 10 (5%) | 3 (2%) | 13 | 40 |
| 6 | AF | 201/210 (96%) | 185 (92%) | 16 (8%) | 0 | 100 | 100 |
| 6 | CF | 201/210 (96%) | 189 (94%) | 8 (4%) | 4 (2%) | 9 | 30 |
| 7 | AG | 179/182 (98%) | 159 (89%) | 14 (8%) | 6 (3%) | 5 | 16 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7 | CG | 179/182 (98%) | 154 (86%) | 19 (11%) | 6 (3%) | 5 | 16 |
| 8 | AH | 172/180 (96%) | 160 (93%) | 11 (6%) | 1 (1%) | 30 | 65 |
| 8 | CH | 172/180 (96%) | 153 (89%) | 13 (8%) | 6 (4%) | 4 | 15 |
| 9 | AK | 128/173 (74%) | 74 (58%) | 26 (20%) | 28 (22%) | 0 | 0 |
| 9 | CK | 128/173 (74%) | 80 (62%) | 28 (22%) | 20 (16%) | 0 | 0 |
| 10 | AL | 64/147 (44%) | 47 (73%) | 13 (20%) | 4 (6%) | 2 | 4 |
| 10 | CL | 64/147 (44%) | 44 (69%) | 17 (27%) | 3 (5%) | 3 | 9 |
| 11 | AN | 138/140 (99%) | 130 (94%) | 8 (6%) | 0 | 100 | 100 |
| 11 | CN | 138/140 (99%) | 126 (91%) | 10 (7%) | 2 (1%) | 14 | 42 |
| 12 | AO | 120/122 (98%) | 110 (92%) | 9 (8%) | 1 (1%) | 24 | 58 |
| 12 | CO | 120/122 (98%) | 110 (92%) | 9 (8%) | 1 (1%) | 24 | 58 |
| 13 | AP | 147/150 (98%) | 133 (90%) | 12 (8%) | 2 (1%) | 14 | 42 |
| 13 | CP | 147/150 (98%) | 129 (88%) | 15 (10%) | 3 (2%) | 9 | 30 |
| 14 | AQ | 139/141 (99%) | 128 (92%) | 11 (8%) | 0 | 100 | 100 |
| 14 | CQ | 139/141 (99%) | 123 (88%) | 13 (9%) | 3 (2%) | 8 | 28 |
| 15 | AR | 116/118 (98%) | 109 (94%) | 6 (5%) | 1 (1%) | 21 | 55 |
| 15 | CR | 116/118 (98%) | 104 (90%) | 11 (10%) | 1 (1%) | 21 | 55 |
| 16 | AS | 108/112 (96%) | 99 (92%) | 8 (7%) | 1 (1%) | 21 | 55 |
| 16 | CS | 108/112 (96%) | 89 (82%) | 17 (16%) | 2 (2%) | 10 | 32 |
| 17 | AT | 129/146 (88%) | 119 (92%) | 10 (8%) | 0 | 100 | 100 |
| 17 | CT | 129/146 (88%) | 120 (93%) | 9 (7%) | 0 | 100 | 100 |
| 18 | AU | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | CU | 114/118 (97%) | 108 (95%) | 6 (5%) | 0 | 100 | 100 |
| 19 | AV | 99/101 (98%) | 93 (94%) | 5 (5%) | 1 (1%) | 19 | 52 |
| 19 | CV | 99/101 (98%) | 90 (91%) | 7 (7%) | 2 (2%) | 9 | 30 |
| 20 | AW | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | CW | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 21 | AX | 93/96 (97%) | 89 (96%) | 3 (3%) | 1 (1%) | 17 | 50 |
| 21 | CX | 93/96 (97%) | 88 (95%) | 4 (4%) | 1 (1%) | 17 | 50 |
| 22 | AY | 105/110 (96%) | 95 (90%) | 9 (9%) | 1 (1%) | 19 | 52 |
| 22 | CY | 105/110 (96%) | 90 (86%) | 11 (10%) | 4 (4%) | 4 | 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 23 | AZ | 169/206 (82%) | 136 (80%) | 28 (17%) | 5 (3%) | 5 | 18 |
| 23 | CZ | 172/206 (84%) | 144 (84%) | 25 (14%) | 3 (2%) | 11 | 36 |
| 24 | A0 | 81/85 (95%) | 74 (91%) | 6 (7%) | 1 (1%) | 16 | 47 |
| 24 | C0 | 81/85 (95%) | 76 (94%) | 5 (6%) | 0 | 100 | 100 |
| 25 | A1 | 95/98 (97%) | 86 (90%) | 9 (10%) | 0 | 100 | 100 |
| 25 | C1 | 95/98 (97%) | 91 (96%) | 3 (3%) | 1 (1%) | 17 | 50 |
| 26 | A2 | 68/72 (94%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 26 | C2 | 68/72 (94%) | 64 (94%) | 4 (6%) | 0 | 100 | 100 |
| 27 | A3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 27 | C3 | 57/60 (95%) | 52 (91%) | 4 (7%) | 1 (2%) | 11 | 34 |
| 28 | A4 | 67/71 (94%) | 44 (66%) | 16 (24%) | 7 (10%) | 1 | 1 |
| 28 | C4 | 67/71 (94%) | 49 (73%) | 13 (19%) | 5 (8%) | 1 | 3 |
| 29 | A5 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 29 | C5 | 57/60 (95%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 30 | A6 | 51/54 (94%) | 48 (94%) | 3 (6%) | 0 | 100 | 100 |
| 30 | C6 | 51/54 (94%) | 45 (88%) | 6 (12%) | 0 | 100 | 100 |
| 31 | A7 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 31 | C7 | 46/49 (94%) | 44 (96%) | 0 | 2 (4%) | 3 | 10 |
| 32 | A8 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 32 | C8 | 62/65 (95%) | 58 (94%) | 2 (3%) | 2 (3%) | 5 | 17 |
| 33 | A9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 33 | C9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 35 | BB | 229/256 (90%) | 187 (82%) | 29 (13%) | 13 (6%) | 2 | 6 |
| 35 | DB | 229/256 (90%) | 177 (77%) | 37 (16%) | 15 (7%) | 1 | 4 |
| 36 | BC | 204/239 (85%) | 171 (84%) | 25 (12%) | 8 (4%) | 4 | 12 |
| 36 | DC | 204/239 (85%) | 171 (84%) | 30 (15%) | 3 (2%) | 13 | 40 |
| 37 | BD | 206/209 (99%) | 186 (90%) | 16 (8%) | 4 (2%) | 10 | 32 |
| 37 | DD | 206/209 (99%) | 180 (87%) | 20 (10%) | 6 (3%) | 6 | 19 |
| 38 | BE | 146/162 (90%) | 128 (88%) | 13 (9%) | 5 (3%) | 5 | 16 |
| 38 | DE | 146/162 (90%) | 128 (88%) | 12 (8%) | 6 (4%) | 3 | 11 |
| 39 | BF | 98/101 (97%) | 89 (91%) | 7 (7%) | 2 (2%) | 9 | 30 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 39 | DF | 98/101 (97%) | 91 (93%) | 6 (6%) | 1 (1%) | 19 | 52 |
| 40 | BG | 153/156 (98%) | 142 (93%) | 9 (6%) | 2 (1%) | 15 | 44 |
| 40 | DG | 153/156 (98%) | 132 (86%) | 19 (12%) | 2 (1%) | 15 | 44 |
| 41 | BH | 135/138 (98%) | 120 (89%) | 12 (9%) | 3 (2%) | 8 | 28 |
| 41 | DH | 135/138 (98%) | 121 (90%) | 12 (9%) | 2 (2%) | 13 | 40 |
| 42 | BI | 125/128 (98%) | 111 (89%) | 10 (8%) | 4 (3%) | 5 | 17 |
| 42 | DI | 125/128 (98%) | 111 (89%) | 12 (10%) | 2 (2%) | 12 | 38 |
| 43 | BJ | 95/105 (90%) | 81 (85%) | 9 (10%) | 5 (5%) | 2 | 7 |
| 43 | DJ | 94/105 (90%) | 77 (82%) | 10 (11%) | 7 (7%) | 1 | 3 |
| 44 | BK | 112/129 (87%) | 102 (91%) | 8 (7%) | 2 (2%) | 11 | 34 |
| 44 | DK | 112/129 (87%) | 98 (88%) | 10 (9%) | 4 (4%) | 4 | 14 |
| 45 | BL | 120/132 (91%) | 106 (88%) | 13 (11%) | 1 (1%) | 24 | 58 |
| 45 | DL | 120/132 (91%) | 109 (91%) | 11 (9%) | 0 | 100 | 100 |
| 46 | BM | 121/126 (96%) | 101 (84%) | 17 (14%) | 3 (2%) | 7 | 24 |
| 46 | DM | 120/126 (95%) | 98 (82%) | 13 (11%) | 9 (8%) | 1 | 3 |
| 47 | BN | 58/61 (95%) | 49 (84%) | 8 (14%) | 1 (2%) | 11 | 36 |
| 47 | DN | 58/61 (95%) | 53 (91%) | 4 (7%) | 1 (2%) | 11 | 36 |
| 48 | BO | 86/89 (97%) | 77 (90%) | 7 (8%) | 2 (2%) | 8 | 26 |
| 48 | DO | 86/89 (97%) | 72 (84%) | 12 (14%) | 2 (2%) | 8 | 26 |
| 49 | BP | 80/88 (91%) | 66 (82%) | 12 (15%) | 2 (2%) | 7 | 24 |
| 49 | DP | 80/88 (91%) | 66 (82%) | 13 (16%) | 1 (1%) | 15 | 44 |
| 50 | BQ | 97/105 (92%) | 87 (90%) | 9 (9%) | 1 (1%) | 19 | 52 |
| 50 | DQ | 97/105 (92%) | 85 (88%) | 12 (12%) | 0 | 100 | 100 |
| 51 | BR | 66/88 (75%) | 61 (92%) | 4 (6%) | 1 (2%) | 13 | 40 |
| 51 | DR | 66/88 (75%) | 61 (92%) | 5 (8%) | 0 | 100 | 100 |
| 52 | BS | 82/93 (88%) | 73 (89%) | 9 (11%) | 0 | 100 | 100 |
| 52 | DS | 81/93 (87%) | 67 (83%) | 12 (15%) | 2 (2%) | 7 | 24 |
| 53 | BT | 94/106 (89%) | 78 (83%) | 10 (11%) | 6 (6%) | 2 | 4 |
| 53 | DT | 94/106 (89%) | 78 (83%) | 12 (13%) | 4 (4%) | 3 | 10 |
| 54 | BU | 21/27 (78%) | 18 (86%) | 3 (14%) | 0 | 100 | 100 |
| 54 | DU | 21/27 (78%) | 19 (90%) | 1 (5%) | 1 (5%) | 3 | 9 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 59 | BZ | 722/758 (95%) | 598 (83%) | 92 (13%) | 32 (4%) | 3 | 10 |
| 59 | DZ | 726/758 (96%) | 594 (82%) | 97 (13%) | 35 (5%) | 3 | 9 |
| All | All | 13220/14444 (92%) | 11544 (87%) | 1298 (10%) | 378 (3%) | 6 | 19 |

All (378) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 42 | VAL |
| 3 | AC | 47 | LYS |
| 3 | AC | 68 | GLY |
| 3 | AC | 180 | SER |
| 3 | AC | 181 | PHE |
| 4 | AD | 275 | LYS |
| 7 | AG | 43 | LEU |
| 7 | AG | 47 | LYS |
| 7 | AG | 50 | ALA |
| 7 | AG | 126 | ASP |
| 9 | AK | 56 | ASN |
| 9 | AK | 71 | LEU |
| 9 | AK | 74 | LEU |
| 9 | AK | 75 | GLN |
| 9 | AK | 77 | PRO |
| 9 | AK | 80 | VAL |
| 9 | AK | 85 | ASP |
| 9 | AK | 104 | ILE |
| 9 | AK | 105 | PRO |
| 9 | AK | 107 | VAL |
| 9 | AK | 128 | LEU |
| 10 | AL | 115 | LEU |
| 16 | AS | 59 | LYS |
| 28 | A4 | 45 | GLY |
| 28 | A4 | 49 | PHE |
| 28 | A4 | 59 | PHE |
| 28 | A4 | 62 | ARG |
| 35 | BB | 17 | PHE |
| 35 | BB | 125 | PRO |
| 35 | BB | 231 | GLU |
| 36 | BC | 65 | ALA |
| 36 | BC | 66 | VAL |
| 37 | BD | 42 | GLN |
| 38 | BE | 98 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BG | 79 | ARG |
| 40 | BG | 80 | VAL |
| 41 | BH | 133 | LEU |
| 42 | BI | 41 | VAL |
| 42 | BI | 44 | VAL |
| 42 | BI | 54 | ASP |
| 43 | BJ | 79 | ARG |
| 53 | BT | 10 | LEU |
| 53 | BT | 100 | ILE |
| 59 | BZ | -57 | GLU |
| 59 | BZ | -33 | GLY |
| 59 | BZ | 88 | VAL |
| 59 | BZ | 97 | SER |
| 59 | BZ | 98 | MET |
| 59 | BZ | 171 | GLU |
| 59 | BZ | 183 | MET |
| 59 | BZ | 404 | VAL |
| 59 | BZ | 405 | PRO |
| 59 | BZ | 472 | VAL |
| 59 | BZ | 481 | VAL |
| 3 | CC | 42 | VAL |
| 3 | CC | 47 | LYS |
| 3 | CC | 68 | GLY |
| 3 | CC | 180 | SER |
| 3 | CC | 181 | PHE |
| 6 | CF | 130 | ALA |
| 7 | CG | 14 | GLU |
| 7 | CG | 51 | ARG |
| 7 | CG | 81 | LYS |
| 8 | CH | 92 | ILE |
| 8 | CH | 126 | PRO |
| 8 | CH | 143 | GLN |
| 8 | CH | 144 | VAL |
| 9 | CK | 69 | PRO |
| 9 | CK | 70 | GLU |
| 9 | CK | 71 | LEU |
| 9 | CK | 74 | LEU |
| 9 | CK | 75 | GLN |
| 9 | CK | 77 | PRO |
| 9 | CK | 80 | VAL |
| 9 | CK | 85 | ASP |
| 9 | CK | 105 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | CK | 107 | VAL |
| 10 | CL | 87 | GLY |
| 13 | CP | 38 | GLN |
| 21 | CX | 94 | GLY |
| 28 | C4 | 62 | ARG |
| 28 | C4 | 63 | TYR |
| 31 | C7 | 46 | VAL |
| 35 | DB | 10 | LEU |
| 35 | DB | 17 | PHE |
| 36 | DC | 98 | ASN |
| 40 | DG | 55 | GLY |
| 42 | DI | 54 | ASP |
| 43 | DJ | 56 | HIS |
| 43 | DJ | 79 | ARG |
| 46 | DM | 4 | ILE |
| 48 | DO | 19 | PRO |
| 53 | DT | 10 | LEU |
| 53 | DT | 100 | ILE |
| 59 | DZ | -65 | LYS |
| 59 | DZ | -57 | GLU |
| 59 | DZ | 85 | PRO |
| 59 | DZ | 117 | GLN |
| 59 | DZ | 160 | ARG |
| 59 | DZ | 183 | MET |
| 59 | DZ | 290 | LYS |
| 59 | DZ | 472 | VAL |
| 3 | AC | 53 | ARG |
| 3 | AC | 161 | ARG |
| 3 | AC | 179 | ALA |
| 4 | AD | 3 | VAL |
| 9 | AK | 91 | LYS |
| 9 | AK | 93 | LEU |
| 9 | AK | 125 | LEU |
| 9 | AK | 132 | ASP |
| 10 | AL | 82 | ALA |
| 15 | AR | 2 | ARG |
| 19 | AV | 79 | VAL |
| 21 | AX | 94 | GLY |
| 23 | AZ | 105 | VAL |
| 28 | A4 | 63 | TYR |
| 35 | BB | 10 | LEU |
| 35 | BB | 19 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | BC | 101 | LEU |
| 37 | BD | 179 | GLU |
| 39 | BF | 70 | ASP |
| 43 | BJ | 31 | GLY |
| 43 | BJ | 56 | HIS |
| 50 | BQ | 49 | GLU |
| 53 | BT | 47 | GLY |
| 59 | BZ | 85 | PRO |
| 59 | BZ | 92 | ILE |
| 59 | BZ | 114 | VAL |
| 59 | BZ | 400 | GLU |
| 59 | BZ | 402 | ILE |
| 59 | BZ | 418 | LYS |
| 59 | BZ | 688 | ILE |
| 3 | CC | 53 | ARG |
| 3 | CC | 161 | ARG |
| 3 | CC | 179 | ALA |
| 4 | CD | 3 | VAL |
| 6 | CF | 195 | ASP |
| 7 | CG | 96 | ARG |
| 9 | CK | 84 | GLU |
| 9 | CK | 93 | LEU |
| 23 | CZ | 105 | VAL |
| 28 | C4 | 11 | PRO |
| 28 | C4 | 45 | GLY |
| 35 | DB | 106 | LYS |
| 35 | DB | 123 | ALA |
| 36 | DC | 95 | THR |
| 37 | DD | 10 | ARG |
| 38 | DE | 140 | ARG |
| 40 | DG | 80 | VAL |
| 41 | DH | 133 | LEU |
| 43 | DJ | 75 | ILE |
| 44 | DK | 49 | GLY |
| 44 | DK | 117 | ASN |
| 46 | DM | 67 | GLU |
| 46 | DM | 106 | ASN |
| 52 | DS | 12 | ASP |
| 53 | DT | 46 | GLU |
| 54 | DU | 3 | LYS |
| 59 | DZ | 39 | ILE |
| 59 | DZ | 92 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | DZ | 402 | ILE |
| 59 | DZ | 403 | GLU |
| 59 | DZ | 404 | VAL |
| 59 | DZ | 479 | PRO |
| 59 | DZ | 481 | VAL |
| 59 | DZ | 600 | VAL |
| 3 | AC | 30 | VAL |
| 3 | AC | 43 | GLU |
| 3 | AC | 52 | PRO |
| 3 | AC | 69 | LEU |
| 3 | AC | 184 | GLU |
| 3 | AC | 202 | PRO |
| 3 | AC | 209 | PHE |
| 4 | AD | 125 | ILE |
| 7 | AG | 51 | ARG |
| 9 | AK | 20 | ALA |
| 9 | AK | 22 | GLY |
| 9 | AK | 39 | ALA |
| 9 | AK | 69 | PRO |
| 9 | AK | 101 | PRO |
| 10 | AL | 89 | HIS |
| 12 | AO | 5 | GLN |
| 13 | AP | 36 | LYS |
| 22 | AY | 54 | LYS |
| 23 | AZ | 65 | GLN |
| 36 | BC | 51 | GLY |
| 43 | BJ | 77 | PRO |
| 44 | BK | 105 | VAL |
| 46 | BM | 67 | GLU |
| 46 | BM | 113 | PRO |
| 48 | BO | 19 | PRO |
| 48 | BO | 86 | GLY |
| 51 | BR | 41 | LYS |
| 53 | BT | 71 | THR |
| 53 | BT | 102 | GLY |
| 59 | BZ | 115 | GLU |
| 59 | BZ | 170 | ARG |
| 59 | BZ | 315 | LYS |
| 59 | BZ | 320 | PRO |
| 3 | CC | 30 | VAL |
| 3 | CC | 43 | GLU |
| 3 | CC | 52 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | CC | 69 | LEU |
| 3 | CC | 184 | GLU |
| 3 | CC | 202 | PRO |
| 3 | CC | 209 | PHE |
| 4 | CD | 239 | ARG |
| 5 | CE | 52 | LEU |
| 6 | CF | 21 | ALA |
| 7 | CG | 52 | ILE |
| 9 | CK | 86 | PRO |
| 9 | CK | 128 | LEU |
| 9 | CK | 132 | ASP |
| 10 | CL | 89 | HIS |
| 11 | CN | 23 | LEU |
| 13 | CP | 122 | PRO |
| 16 | CS | 89 | ARG |
| 19 | CV | 24 | LYS |
| 23 | CZ | 31 | ARG |
| 23 | CZ | 114 | GLY |
| 25 | C1 | 3 | LYS |
| 28 | C4 | 46 | GLN |
| 31 | C7 | 45 | ALA |
| 35 | DB | 8 | LYS |
| 35 | DB | 16 | HIS |
| 35 | DB | 121 | LEU |
| 35 | DB | 125 | PRO |
| 35 | DB | 213 | LEU |
| 37 | DD | 47 | ARG |
| 43 | DJ | 36 | GLY |
| 43 | DJ | 55 | LYS |
| 43 | DJ | 77 | PRO |
| 44 | DK | 105 | VAL |
| 46 | DM | 5 | ALA |
| 46 | DM | 6 | GLY |
| 46 | DM | 101 | GLN |
| 46 | DM | 108 | ARG |
| 48 | DO | 88 | ARG |
| 52 | DS | 24 | ALA |
| 53 | DT | 102 | GLY |
| 59 | DZ | -25 | SER |
| 59 | DZ | 20 | HIS |
| 59 | DZ | 170 | ARG |
| 59 | DZ | 400 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | DZ | 418 | LYS |
| 59 | DZ | 598 | ASP |
| 59 | DZ | 599 | PRO |
| 59 | DZ | 651 | GLU |
| 3 | AC | 16 | ASP |
| 5 | AE | 52 | LEU |
| 9 | AK | 33 | PRO |
| 9 | AK | 86 | PRO |
| 9 | AK | 114 | GLY |
| 10 | AL | 81 | ALA |
| 24 | A0 | 57 | PHE |
| 35 | BB | 9 | GLU |
| 35 | BB | 16 | HIS |
| 35 | BB | 131 | PRO |
| 36 | BC | 50 | ALA |
| 38 | BE | 86 | ALA |
| 41 | BH | 51 | VAL |
| 42 | BI | 96 | LEU |
| 44 | BK | 49 | GLY |
| 59 | BZ | 172 | ASP |
| 59 | BZ | 469 | GLU |
| 59 | BZ | 596 | LYS |
| 59 | BZ | 641 | GLN |
| 59 | BZ | 671 | MET |
| 3 | CC | 16 | ASP |
| 4 | CD | 125 | ILE |
| 5 | CE | 74 | PRO |
| 8 | CH | 119 | GLU |
| 9 | CK | 91 | LYS |
| 9 | CK | 104 | ILE |
| 11 | CN | 2 | LYS |
| 15 | CR | 45 | ARG |
| 16 | CS | 84 | GLN |
| 19 | CV | 79 | VAL |
| 22 | CY | 78 | ALA |
| 27 | C3 | 59 | VAL |
| 32 | C8 | 57 | ARG |
| 35 | DB | 20 | GLU |
| 35 | DB | 131 | PRO |
| 37 | DD | 22 | LYS |
| 37 | DD | 171 | GLY |
| 38 | DE | 96 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | DE | 104 | ALA |
| 38 | DE | 107 | ARG |
| 42 | DI | 34 | ASN |
| 43 | DJ | 78 | ASN |
| 46 | DM | 35 | GLU |
| 47 | DN | 27 | CYS |
| 49 | DP | 53 | VAL |
| 59 | DZ | -33 | GLY |
| 59 | DZ | 416 | LYS |
| 59 | DZ | 471 | LYS |
| 59 | DZ | 559 | PRO |
| 3 | AC | 21 | TYR |
| 9 | AK | 120 | LYS |
| 9 | AK | 123 | GLU |
| 23 | AZ | 152 | ALA |
| 35 | BB | 56 | ARG |
| 35 | BB | 195 | ASP |
| 36 | BC | 129 | ALA |
| 36 | BC | 156 | ARG |
| 37 | BD | 178 | VAL |
| 46 | BM | 19 | LEU |
| 47 | BN | 58 | LYS |
| 49 | BP | 49 | LEU |
| 59 | BZ | 322 | VAL |
| 59 | BZ | 324 | ARG |
| 59 | BZ | 416 | LYS |
| 59 | BZ | 479 | PRO |
| 3 | CC | 21 | TYR |
| 6 | CF | 60 | SER |
| 7 | CG | 47 | LYS |
| 9 | CK | 119 | ALA |
| 10 | CL | 112 | MET |
| 22 | CY | 43 | ASN |
| 22 | CY | 102 | CYS |
| 35 | DB | 83 | MET |
| 37 | DD | 136 | PRO |
| 44 | DK | 106 | LYS |
| 59 | DZ | 180 | VAL |
| 59 | DZ | 473 | ASP |
| 59 | DZ | 477 | GLY |
| 3 | AC | 221 | PRO |
| 8 | AH | 148 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | AK | 31 | GLY |
| 9 | AK | 119 | ALA |
| 28 | A4 | 47 | GLN |
| 37 | BD | 109 | GLY |
| 38 | BE | 68 | GLU |
| 39 | BF | 39 | LYS |
| 49 | BP | 41 | PRO |
| 59 | BZ | 415 | PRO |
| 3 | CC | 221 | PRO |
| 8 | CH | 80 | SER |
| 9 | CK | 101 | PRO |
| 13 | CP | 29 | LYS |
| 14 | CQ | 115 | MET |
| 22 | CY | 51 | VAL |
| 35 | DB | 21 | ARG |
| 35 | DB | 202 | PRO |
| 36 | DC | 108 | ASN |
| 37 | DD | 5 | ILE |
| 59 | DZ | 199 | ILE |
| 7 | AG | 32 | PRO |
| 13 | AP | 122 | PRO |
| 23 | AZ | 158 | PRO |
| 35 | BB | 183 | PRO |
| 35 | BB | 234 | PRO |
| 38 | BE | 69 | VAL |
| 43 | BJ | 75 | ILE |
| 53 | BT | 96 | GLY |
| 59 | DZ | 116 | PRO |
| 35 | BB | 202 | PRO |
| 32 | C8 | 58 | ILE |
| 46 | DM | 85 | GLY |
| 9 | AK | 68 | LEU |
| 23 | AZ | 167 | PRO |
| 28 | A4 | 41 | PRO |
| 45 | BL | 125 | PRO |
| 14 | CQ | 27 | VAL |
| 35 | DB | 232 | PRO |
| 59 | DZ | 88 | VAL |
| 59 | DZ | 688 | ILE |
| 9 | CK | 68 | LEU |
| 14 | CQ | 88 | GLY |
| 38 | DE | 69 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DH | 83 | ILE |
| 36 | BC | 81 | GLY |
| 38 | BE | 85 | GLY |
| 41 | BH | 90 | GLY |
| 12 | CO | 110 | GLY |
| 38 | DE | 105 | VAL |
| 39 | DF | 40 | VAL |
| 5 | CE | 30 | PRO |

5.3.2 Protein sidechains [i](#)

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | AC | 111/180 (62%) | 103 (93%) | 8 (7%) | 18 | 45 |
| 3 | CC | 111/180 (62%) | 103 (93%) | 8 (7%) | 18 | 45 |
| 4 | AD | 215/218 (99%) | 189 (88%) | 26 (12%) | 6 | 18 |
| 4 | CD | 216/218 (99%) | 181 (84%) | 35 (16%) | 3 | 8 |
| 5 | AE | 164/166 (99%) | 140 (85%) | 24 (15%) | 4 | 11 |
| 5 | CE | 164/166 (99%) | 139 (85%) | 25 (15%) | 3 | 10 |
| 6 | AF | 160/166 (96%) | 134 (84%) | 26 (16%) | 3 | 8 |
| 6 | CF | 159/166 (96%) | 135 (85%) | 24 (15%) | 3 | 10 |
| 7 | AG | 143/156 (92%) | 119 (83%) | 24 (17%) | 2 | 8 |
| 7 | CG | 142/156 (91%) | 108 (76%) | 34 (24%) | 1 | 2 |
| 8 | AH | 144/148 (97%) | 128 (89%) | 16 (11%) | 8 | 23 |
| 8 | CH | 144/148 (97%) | 125 (87%) | 19 (13%) | 5 | 14 |
| 10 | AL | 50/111 (45%) | 45 (90%) | 5 (10%) | 9 | 27 |
| 10 | CL | 50/111 (45%) | 45 (90%) | 5 (10%) | 9 | 27 |
| 11 | AN | 118/119 (99%) | 94 (80%) | 24 (20%) | 1 | 4 |
| 11 | CN | 118/119 (99%) | 98 (83%) | 20 (17%) | 2 | 7 |
| 12 | AO | 100/100 (100%) | 83 (83%) | 17 (17%) | 2 | 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12 | CO | 100/100 (100%) | 83 (83%) | 17 (17%) | 2 | 7 |
| 13 | AP | 116/116 (100%) | 97 (84%) | 19 (16%) | 3 | 8 |
| 13 | CP | 115/116 (99%) | 99 (86%) | 16 (14%) | 4 | 13 |
| 14 | AQ | 111/111 (100%) | 90 (81%) | 21 (19%) | 2 | 5 |
| 14 | CQ | 111/111 (100%) | 95 (86%) | 16 (14%) | 4 | 12 |
| 15 | AR | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 | 3 |
| 15 | CR | 101/101 (100%) | 84 (83%) | 17 (17%) | 2 | 8 |
| 16 | AS | 87/88 (99%) | 71 (82%) | 16 (18%) | 2 | 6 |
| 16 | CS | 85/88 (97%) | 67 (79%) | 18 (21%) | 1 | 4 |
| 17 | AT | 115/127 (91%) | 97 (84%) | 18 (16%) | 3 | 9 |
| 17 | CT | 113/127 (89%) | 93 (82%) | 20 (18%) | 2 | 7 |
| 18 | AU | 93/94 (99%) | 77 (83%) | 16 (17%) | 2 | 7 |
| 18 | CU | 93/94 (99%) | 82 (88%) | 11 (12%) | 6 | 19 |
| 19 | AV | 80/82 (98%) | 65 (81%) | 15 (19%) | 2 | 6 |
| 19 | CV | 80/82 (98%) | 67 (84%) | 13 (16%) | 3 | 8 |
| 20 | AW | 90/92 (98%) | 80 (89%) | 10 (11%) | 8 | 23 |
| 20 | CW | 90/92 (98%) | 79 (88%) | 11 (12%) | 6 | 18 |
| 21 | AX | 77/78 (99%) | 73 (95%) | 4 (5%) | 29 | 62 |
| 21 | CX | 77/78 (99%) | 70 (91%) | 7 (9%) | 12 | 33 |
| 22 | AY | 85/91 (93%) | 73 (86%) | 12 (14%) | 4 | 12 |
| 22 | CY | 85/91 (93%) | 70 (82%) | 15 (18%) | 2 | 7 |
| 23 | AZ | 145/179 (81%) | 117 (81%) | 28 (19%) | 2 | 5 |
| 23 | CZ | 145/179 (81%) | 125 (86%) | 20 (14%) | 4 | 13 |
| 24 | A0 | 65/67 (97%) | 63 (97%) | 2 (3%) | 47 | 81 |
| 24 | C0 | 65/67 (97%) | 60 (92%) | 5 (8%) | 16 | 41 |
| 25 | A1 | 80/83 (96%) | 72 (90%) | 8 (10%) | 9 | 27 |
| 25 | C1 | 80/83 (96%) | 69 (86%) | 11 (14%) | 4 | 13 |
| 26 | A2 | 65/67 (97%) | 54 (83%) | 11 (17%) | 2 | 7 |
| 26 | C2 | 65/67 (97%) | 55 (85%) | 10 (15%) | 3 | 10 |
| 27 | A3 | 51/52 (98%) | 44 (86%) | 7 (14%) | 4 | 13 |
| 27 | C3 | 50/52 (96%) | 38 (76%) | 12 (24%) | 1 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 28 | A4 | 60/63 (95%) | 49 (82%) | 11 (18%) | 2 | 6 |
| 28 | C4 | 53/63 (84%) | 39 (74%) | 14 (26%) | 0 | 1 |
| 29 | A5 | 50/52 (96%) | 43 (86%) | 7 (14%) | 4 | 13 |
| 29 | C5 | 50/52 (96%) | 44 (88%) | 6 (12%) | 6 | 19 |
| 30 | A6 | 51/52 (98%) | 40 (78%) | 11 (22%) | 1 | 3 |
| 30 | C6 | 50/52 (96%) | 43 (86%) | 7 (14%) | 4 | 13 |
| 31 | A7 | 41/42 (98%) | 35 (85%) | 6 (15%) | 4 | 11 |
| 31 | C7 | 41/42 (98%) | 36 (88%) | 5 (12%) | 6 | 18 |
| 32 | A8 | 54/55 (98%) | 47 (87%) | 7 (13%) | 5 | 15 |
| 32 | C8 | 54/55 (98%) | 49 (91%) | 5 (9%) | 11 | 32 |
| 33 | A9 | 34/34 (100%) | 31 (91%) | 3 (9%) | 12 | 35 |
| 33 | C9 | 34/34 (100%) | 29 (85%) | 5 (15%) | 4 | 11 |
| 35 | BB | 192/220 (87%) | 144 (75%) | 48 (25%) | 1 | 2 |
| 35 | DB | 187/220 (85%) | 157 (84%) | 30 (16%) | 3 | 9 |
| 36 | BC | 143/188 (76%) | 124 (87%) | 19 (13%) | 5 | 14 |
| 36 | DC | 141/188 (75%) | 115 (82%) | 26 (18%) | 2 | 6 |
| 37 | BD | 170/181 (94%) | 146 (86%) | 24 (14%) | 4 | 12 |
| 37 | DD | 174/181 (96%) | 148 (85%) | 26 (15%) | 4 | 11 |
| 38 | BE | 113/123 (92%) | 104 (92%) | 9 (8%) | 15 | 40 |
| 38 | DE | 114/123 (93%) | 96 (84%) | 18 (16%) | 3 | 9 |
| 39 | BF | 84/90 (93%) | 71 (84%) | 13 (16%) | 3 | 10 |
| 39 | DF | 86/90 (96%) | 75 (87%) | 11 (13%) | 5 | 16 |
| 40 | BG | 119/127 (94%) | 98 (82%) | 21 (18%) | 2 | 7 |
| 40 | DG | 120/127 (94%) | 112 (93%) | 8 (7%) | 20 | 50 |
| 41 | BH | 114/119 (96%) | 98 (86%) | 16 (14%) | 4 | 13 |
| 41 | DH | 114/119 (96%) | 92 (81%) | 22 (19%) | 2 | 5 |
| 42 | BI | 91/99 (92%) | 72 (79%) | 19 (21%) | 1 | 4 |
| 42 | DI | 89/99 (90%) | 71 (80%) | 18 (20%) | 1 | 4 |
| 43 | BJ | 66/92 (72%) | 58 (88%) | 8 (12%) | 6 | 18 |
| 43 | DJ | 69/92 (75%) | 58 (84%) | 11 (16%) | 3 | 9 |
| 44 | BK | 83/99 (84%) | 71 (86%) | 12 (14%) | 4 | 11 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|-------------|----|
| 44 | DK | 83/99 (84%) | 74 (89%) | 9 (11%) | 8 | 23 |
| 45 | BL | 97/109 (89%) | 90 (93%) | 7 (7%) | 18 | 45 |
| 45 | DL | 97/109 (89%) | 86 (89%) | 11 (11%) | 7 | 22 |
| 46 | BM | 95/101 (94%) | 82 (86%) | 13 (14%) | 4 | 13 |
| 46 | DM | 92/101 (91%) | 76 (83%) | 16 (17%) | 2 | 7 |
| 47 | BN | 49/50 (98%) | 39 (80%) | 10 (20%) | 1 | 4 |
| 47 | DN | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 6 |
| 48 | BO | 78/80 (98%) | 64 (82%) | 14 (18%) | 2 | 6 |
| 48 | DO | 78/80 (98%) | 68 (87%) | 10 (13%) | 5 | 16 |
| 49 | BP | 69/74 (93%) | 56 (81%) | 13 (19%) | 2 | 6 |
| 49 | DP | 68/74 (92%) | 61 (90%) | 7 (10%) | 9 | 26 |
| 50 | BQ | 94/97 (97%) | 81 (86%) | 13 (14%) | 4 | 13 |
| 50 | DQ | 94/97 (97%) | 82 (87%) | 12 (13%) | 5 | 16 |
| 51 | BR | 59/77 (77%) | 47 (80%) | 12 (20%) | 1 | 4 |
| 51 | DR | 59/77 (77%) | 51 (86%) | 8 (14%) | 5 | 14 |
| 52 | BS | 70/80 (88%) | 61 (87%) | 9 (13%) | 5 | 16 |
| 52 | DS | 67/80 (84%) | 60 (90%) | 7 (10%) | 9 | 25 |
| 53 | BT | 70/82 (85%) | 59 (84%) | 11 (16%) | 3 | 9 |
| 53 | DT | 71/82 (87%) | 58 (82%) | 13 (18%) | 2 | 6 |
| 54 | BU | 18/22 (82%) | 16 (89%) | 2 (11%) | 8 | 23 |
| 54 | DU | 18/22 (82%) | 16 (89%) | 2 (11%) | 8 | 23 |
| 59 | BZ | 604/636 (95%) | 489 (81%) | 115 (19%) | 2 | 5 |
| 59 | DZ | 607/636 (95%) | 505 (83%) | 102 (17%) | 2 | 8 |
| All | All | 10652/11672 (91%) | 9013 (85%) | 1639 (15%) | 3 | 10 |

All (1639) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 28 | ARG |
| 3 | AC | 32 | GLU |
| 3 | AC | 48 | LEU |
| 3 | AC | 50 | ILE |
| 3 | AC | 53 | ARG |
| 3 | AC | 54 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 203 | GLU |
| 3 | AC | 208 | THR |
| 4 | AD | 12 | SER |
| 4 | AD | 13 | ARG |
| 4 | AD | 38 | LYS |
| 4 | AD | 61 | LEU |
| 4 | AD | 88 | ARG |
| 4 | AD | 94 | LEU |
| 4 | AD | 99 | ASP |
| 4 | AD | 103 | ARG |
| 4 | AD | 106 | ILE |
| 4 | AD | 113 | VAL |
| 4 | AD | 122 | ASP |
| 4 | AD | 126 | GLN |
| 4 | AD | 138 | VAL |
| 4 | AD | 142 | VAL |
| 4 | AD | 155 | LEU |
| 4 | AD | 175 | LEU |
| 4 | AD | 183 | ARG |
| 4 | AD | 193 | VAL |
| 4 | AD | 211 | ARG |
| 4 | AD | 229 | VAL |
| 4 | AD | 242 | ARG |
| 4 | AD | 253 | GLN |
| 4 | AD | 257 | LEU |
| 4 | AD | 259 | THR |
| 4 | AD | 260 | ARG |
| 4 | AD | 274 | ARG |
| 5 | AE | 1 | MET |
| 5 | AE | 9 | VAL |
| 5 | AE | 21 | VAL |
| 5 | AE | 34 | VAL |
| 5 | AE | 47 | VAL |
| 5 | AE | 48 | GLN |
| 5 | AE | 49 | LEU |
| 5 | AE | 75 | VAL |
| 5 | AE | 78 | LEU |
| 5 | AE | 82 | ARG |
| 5 | AE | 93 | VAL |
| 5 | AE | 97 | LYS |
| 5 | AE | 111 | ARG |
| 5 | AE | 116 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | AE | 119 | ARG |
| 5 | AE | 136 | ARG |
| 5 | AE | 144 | ARG |
| 5 | AE | 154 | LYS |
| 5 | AE | 163 | GLU |
| 5 | AE | 170 | LEU |
| 5 | AE | 175 | VAL |
| 5 | AE | 179 | GLU |
| 5 | AE | 181 | LEU |
| 5 | AE | 183 | LEU |
| 6 | AF | 12 | LEU |
| 6 | AF | 17 | ARG |
| 6 | AF | 19 | GLU |
| 6 | AF | 24 | LEU |
| 6 | AF | 33 | LEU |
| 6 | AF | 53 | THR |
| 6 | AF | 57 | VAL |
| 6 | AF | 64 | ILE |
| 6 | AF | 74 | ARG |
| 6 | AF | 82 | ILE |
| 6 | AF | 88 | VAL |
| 6 | AF | 95 | ARG |
| 6 | AF | 106 | ARG |
| 6 | AF | 110 | LEU |
| 6 | AF | 125 | LEU |
| 6 | AF | 132 | VAL |
| 6 | AF | 137 | LYS |
| 6 | AF | 140 | LEU |
| 6 | AF | 158 | THR |
| 6 | AF | 161 | GLU |
| 6 | AF | 162 | LEU |
| 6 | AF | 170 | LEU |
| 6 | AF | 183 | VAL |
| 6 | AF | 192 | LEU |
| 6 | AF | 195 | ASP |
| 6 | AF | 197 | ASP |
| 7 | AG | 5 | VAL |
| 7 | AG | 7 | LEU |
| 7 | AG | 21 | ARG |
| 7 | AG | 28 | VAL |
| 7 | AG | 31 | VAL |
| 7 | AG | 41 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 43 | LEU |
| 7 | AG | 45 | GLU |
| 7 | AG | 58 | GLN |
| 7 | AG | 60 | LEU |
| 7 | AG | 79 | ASN |
| 7 | AG | 82 | LEU |
| 7 | AG | 84 | LYS |
| 7 | AG | 86 | MET |
| 7 | AG | 91 | ARG |
| 7 | AG | 128 | ARG |
| 7 | AG | 140 | ILE |
| 7 | AG | 146 | TYR |
| 7 | AG | 153 | ARG |
| 7 | AG | 159 | VAL |
| 7 | AG | 170 | ARG |
| 7 | AG | 174 | GLU |
| 7 | AG | 175 | LEU |
| 7 | AG | 181 | ARG |
| 8 | AH | 3 | ARG |
| 8 | AH | 6 | ARG |
| 8 | AH | 13 | LYS |
| 8 | AH | 24 | VAL |
| 8 | AH | 25 | LYS |
| 8 | AH | 49 | VAL |
| 8 | AH | 57 | ASP |
| 8 | AH | 62 | LYS |
| 8 | AH | 69 | ARG |
| 8 | AH | 71 | LEU |
| 8 | AH | 97 | ARG |
| 8 | AH | 116 | GLU |
| 8 | AH | 122 | THR |
| 8 | AH | 125 | VAL |
| 8 | AH | 134 | SER |
| 8 | AH | 139 | GLN |
| 10 | AL | 77 | LEU |
| 10 | AL | 86 | LYS |
| 10 | AL | 100 | THR |
| 10 | AL | 105 | LEU |
| 10 | AL | 106 | GLU |
| 11 | AN | 5 | VAL |
| 11 | AN | 9 | VAL |
| 11 | AN | 15 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | AN | 21 | LYS |
| 11 | AN | 28 | THR |
| 11 | AN | 33 | LEU |
| 11 | AN | 34 | LEU |
| 11 | AN | 39 | ARG |
| 11 | AN | 48 | MET |
| 11 | AN | 61 | ARG |
| 11 | AN | 62 | VAL |
| 11 | AN | 67 | LEU |
| 11 | AN | 73 | THR |
| 11 | AN | 84 | LYS |
| 11 | AN | 87 | LEU |
| 11 | AN | 88 | GLU |
| 11 | AN | 97 | ARG |
| 11 | AN | 99 | LEU |
| 11 | AN | 120 | LEU |
| 11 | AN | 133 | GLN |
| 11 | AN | 136 | GLU |
| 11 | AN | 137 | LYS |
| 11 | AN | 138 | LEU |
| 11 | AN | 140 | VAL |
| 12 | AO | 8 | LEU |
| 12 | AO | 10 | VAL |
| 12 | AO | 17 | ARG |
| 12 | AO | 20 | MET |
| 12 | AO | 24 | VAL |
| 12 | AO | 28 | SER |
| 12 | AO | 35 | VAL |
| 12 | AO | 47 | ILE |
| 12 | AO | 52 | VAL |
| 12 | AO | 53 | LYS |
| 12 | AO | 80 | ASP |
| 12 | AO | 82 | ASN |
| 12 | AO | 91 | LEU |
| 12 | AO | 92 | GLU |
| 12 | AO | 94 | ARG |
| 12 | AO | 98 | VAL |
| 12 | AO | 113 | LYS |
| 13 | AP | 21 | ARG |
| 13 | AP | 42 | SER |
| 13 | AP | 55 | ARG |
| 13 | AP | 59 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | AP | 70 | GLN |
| 13 | AP | 74 | GLU |
| 13 | AP | 77 | ARG |
| 13 | AP | 83 | VAL |
| 13 | AP | 98 | GLU |
| 13 | AP | 99 | LEU |
| 13 | AP | 106 | LEU |
| 13 | AP | 112 | LEU |
| 13 | AP | 126 | VAL |
| 13 | AP | 135 | LEU |
| 13 | AP | 138 | LEU |
| 13 | AP | 139 | LYS |
| 13 | AP | 147 | LEU |
| 13 | AP | 148 | LEU |
| 13 | AP | 149 | GLU |
| 14 | AQ | 2 | LEU |
| 14 | AQ | 7 | MET |
| 14 | AQ | 8 | LYS |
| 14 | AQ | 16 | ARG |
| 14 | AQ | 21 | THR |
| 14 | AQ | 22 | LYS |
| 14 | AQ | 35 | VAL |
| 14 | AQ | 42 | ILE |
| 14 | AQ | 45 | GLN |
| 14 | AQ | 54 | MET |
| 14 | AQ | 59 | ARG |
| 14 | AQ | 60 | ARG |
| 14 | AQ | 75 | THR |
| 14 | AQ | 76 | LYS |
| 14 | AQ | 85 | LYS |
| 14 | AQ | 98 | LYS |
| 14 | AQ | 109 | VAL |
| 14 | AQ | 110 | THR |
| 14 | AQ | 115 | MET |
| 14 | AQ | 133 | ARG |
| 14 | AQ | 134 | ARG |
| 15 | AR | 6 | SER |
| 15 | AR | 9 | LYS |
| 15 | AR | 18 | LEU |
| 15 | AR | 27 | SER |
| 15 | AR | 28 | LEU |
| 15 | AR | 29 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AR | 33 | ARG |
| 15 | AR | 36 | THR |
| 15 | AR | 44 | LEU |
| 15 | AR | 45 | ARG |
| 15 | AR | 54 | LEU |
| 15 | AR | 57 | ARG |
| 15 | AR | 59 | ASP |
| 15 | AR | 60 | LEU |
| 15 | AR | 63 | ARG |
| 15 | AR | 65 | LEU |
| 15 | AR | 67 | LEU |
| 15 | AR | 79 | LEU |
| 15 | AR | 91 | GLN |
| 15 | AR | 96 | ARG |
| 15 | AR | 102 | GLU |
| 15 | AR | 111 | LEU |
| 16 | AS | 3 | ARG |
| 16 | AS | 14 | VAL |
| 16 | AS | 19 | LYS |
| 16 | AS | 20 | ARG |
| 16 | AS | 25 | ARG |
| 16 | AS | 36 | TYR |
| 16 | AS | 46 | VAL |
| 16 | AS | 48 | LEU |
| 16 | AS | 49 | VAL |
| 16 | AS | 50 | SER |
| 16 | AS | 57 | LYS |
| 16 | AS | 69 | VAL |
| 16 | AS | 83 | LYS |
| 16 | AS | 85 | VAL |
| 16 | AS | 93 | LYS |
| 16 | AS | 110 | LEU |
| 17 | AT | 6 | LEU |
| 17 | AT | 13 | ARG |
| 17 | AT | 17 | THR |
| 17 | AT | 23 | ARG |
| 17 | AT | 28 | VAL |
| 17 | AT | 40 | THR |
| 17 | AT | 49 | VAL |
| 17 | AT | 59 | THR |
| 17 | AT | 65 | LYS |
| 17 | AT | 67 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | AT | 74 | ARG |
| 17 | AT | 78 | LEU |
| 17 | AT | 85 | LYS |
| 17 | AT | 96 | ARG |
| 17 | AT | 108 | ARG |
| 17 | AT | 118 | ARG |
| 17 | AT | 125 | ARG |
| 17 | AT | 128 | GLU |
| 18 | AU | 5 | LYS |
| 18 | AU | 8 | VAL |
| 18 | AU | 13 | LYS |
| 18 | AU | 16 | LYS |
| 18 | AU | 19 | LYS |
| 18 | AU | 36 | ARG |
| 18 | AU | 52 | ARG |
| 18 | AU | 60 | LEU |
| 18 | AU | 74 | LEU |
| 18 | AU | 77 | SER |
| 18 | AU | 83 | LEU |
| 18 | AU | 92 | ARG |
| 18 | AU | 95 | LEU |
| 18 | AU | 103 | PRO |
| 18 | AU | 104 | GLN |
| 18 | AU | 112 | ARG |
| 19 | AV | 18 | LEU |
| 19 | AV | 20 | LEU |
| 19 | AV | 21 | ARG |
| 19 | AV | 28 | GLU |
| 19 | AV | 35 | LEU |
| 19 | AV | 43 | GLU |
| 19 | AV | 46 | VAL |
| 19 | AV | 51 | VAL |
| 19 | AV | 62 | LEU |
| 19 | AV | 72 | VAL |
| 19 | AV | 79 | VAL |
| 19 | AV | 85 | LYS |
| 19 | AV | 92 | THR |
| 19 | AV | 95 | LEU |
| 19 | AV | 100 | ARG |
| 20 | AW | 4 | LYS |
| 20 | AW | 11 | ARG |
| 20 | AW | 12 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | AW | 15 | ARG |
| 20 | AW | 19 | LEU |
| 20 | AW | 24 | ILE |
| 20 | AW | 51 | LEU |
| 20 | AW | 63 | ASP |
| 20 | AW | 98 | LYS |
| 20 | AW | 107 | LEU |
| 21 | AX | 2 | LYS |
| 21 | AX | 57 | LEU |
| 21 | AX | 65 | ARG |
| 21 | AX | 70 | LEU |
| 22 | AY | 7 | VAL |
| 22 | AY | 23 | ARG |
| 22 | AY | 31 | LEU |
| 22 | AY | 47 | LYS |
| 22 | AY | 55 | TYR |
| 22 | AY | 73 | ARG |
| 22 | AY | 85 | VAL |
| 22 | AY | 90 | LEU |
| 22 | AY | 91 | GLU |
| 22 | AY | 92 | ASN |
| 22 | AY | 106 | LEU |
| 22 | AY | 107 | ASP |
| 23 | AZ | 5 | LEU |
| 23 | AZ | 6 | LYS |
| 23 | AZ | 18 | LEU |
| 23 | AZ | 31 | ARG |
| 23 | AZ | 33 | LEU |
| 23 | AZ | 41 | LEU |
| 23 | AZ | 50 | GLN |
| 23 | AZ | 58 | VAL |
| 23 | AZ | 72 | ARG |
| 23 | AZ | 76 | LEU |
| 23 | AZ | 84 | GLU |
| 23 | AZ | 86 | VAL |
| 23 | AZ | 91 | LEU |
| 23 | AZ | 98 | MET |
| 23 | AZ | 102 | LEU |
| 23 | AZ | 117 | LEU |
| 23 | AZ | 120 | ILE |
| 23 | AZ | 126 | VAL |
| 23 | AZ | 128 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | AZ | 129 | SER |
| 23 | AZ | 141 | VAL |
| 23 | AZ | 146 | ILE |
| 23 | AZ | 148 | ASP |
| 23 | AZ | 149 | SER |
| 23 | AZ | 154 | ASP |
| 23 | AZ | 155 | LEU |
| 23 | AZ | 161 | VAL |
| 23 | AZ | 170 | THR |
| 24 | A0 | 20 | ARG |
| 24 | A0 | 55 | ARG |
| 25 | A1 | 21 | ARG |
| 25 | A1 | 30 | VAL |
| 25 | A1 | 40 | ARG |
| 25 | A1 | 46 | LEU |
| 25 | A1 | 52 | ARG |
| 25 | A1 | 59 | THR |
| 25 | A1 | 83 | GLU |
| 25 | A1 | 95 | LEU |
| 26 | A2 | 3 | LEU |
| 26 | A2 | 28 | LYS |
| 26 | A2 | 30 | ARG |
| 26 | A2 | 32 | LEU |
| 26 | A2 | 45 | SER |
| 26 | A2 | 53 | LEU |
| 26 | A2 | 59 | ARG |
| 26 | A2 | 62 | THR |
| 26 | A2 | 65 | ASN |
| 26 | A2 | 68 | ARG |
| 26 | A2 | 70 | GLN |
| 27 | A3 | 3 | ARG |
| 27 | A3 | 8 | LEU |
| 27 | A3 | 23 | LEU |
| 27 | A3 | 29 | ARG |
| 27 | A3 | 54 | VAL |
| 27 | A3 | 58 | VAL |
| 27 | A3 | 60 | GLU |
| 28 | A4 | 1 | MET |
| 28 | A4 | 3 | GLU |
| 28 | A4 | 5 | ILE |
| 28 | A4 | 34 | GLU |
| 28 | A4 | 46 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | A4 | 49 | PHE |
| 28 | A4 | 50 | VAL |
| 28 | A4 | 55 | ARG |
| 28 | A4 | 56 | VAL |
| 28 | A4 | 59 | PHE |
| 28 | A4 | 63 | TYR |
| 29 | A5 | 6 | VAL |
| 29 | A5 | 16 | ARG |
| 29 | A5 | 26 | THR |
| 29 | A5 | 29 | THR |
| 29 | A5 | 40 | LYS |
| 29 | A5 | 55 | ARG |
| 29 | A5 | 56 | LYS |
| 30 | A6 | 3 | SER |
| 30 | A6 | 4 | GLU |
| 30 | A6 | 6 | ARG |
| 30 | A6 | 7 | ILE |
| 30 | A6 | 9 | LEU |
| 30 | A6 | 14 | THR |
| 30 | A6 | 33 | LYS |
| 30 | A6 | 35 | GLU |
| 30 | A6 | 44 | ARG |
| 30 | A6 | 48 | VAL |
| 30 | A6 | 50 | ARG |
| 31 | A7 | 1 | MET |
| 31 | A7 | 9 | ARG |
| 31 | A7 | 10 | ARG |
| 31 | A7 | 41 | ARG |
| 31 | A7 | 43 | THR |
| 31 | A7 | 46 | VAL |
| 32 | A8 | 6 | THR |
| 32 | A8 | 30 | ARG |
| 32 | A8 | 31 | HIS |
| 32 | A8 | 32 | LEU |
| 32 | A8 | 37 | SER |
| 32 | A8 | 41 | ILE |
| 32 | A8 | 46 | ARG |
| 33 | A9 | 4 | ARG |
| 33 | A9 | 17 | ILE |
| 33 | A9 | 19 | ARG |
| 35 | BB | 8 | LYS |
| 35 | BB | 11 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 35 | BB | 15 | VAL |
| 35 | BB | 17 | PHE |
| 35 | BB | 19 | HIS |
| 35 | BB | 20 | GLU |
| 35 | BB | 21 | ARG |
| 35 | BB | 23 | ARG |
| 35 | BB | 24 | TRP |
| 35 | BB | 35 | GLU |
| 35 | BB | 37 | ASN |
| 35 | BB | 45 | GLN |
| 35 | BB | 48 | MET |
| 35 | BB | 58 | ILE |
| 35 | BB | 60 | ASP |
| 35 | BB | 67 | THR |
| 35 | BB | 75 | LYS |
| 35 | BB | 76 | GLN |
| 35 | BB | 78 | GLN |
| 35 | BB | 80 | ILE |
| 35 | BB | 84 | GLU |
| 35 | BB | 87 | ARG |
| 35 | BB | 93 | VAL |
| 35 | BB | 96 | ARG |
| 35 | BB | 97 | TRP |
| 35 | BB | 111 | ARG |
| 35 | BB | 112 | VAL |
| 35 | BB | 113 | HIS |
| 35 | BB | 126 | GLU |
| 35 | BB | 137 | ARG |
| 35 | BB | 145 | LEU |
| 35 | BB | 147 | LYS |
| 35 | BB | 150 | SER |
| 35 | BB | 153 | ARG |
| 35 | BB | 156 | LYS |
| 35 | BB | 160 | ASP |
| 35 | BB | 167 | PRO |
| 35 | BB | 168 | THR |
| 35 | BB | 169 | LYS |
| 35 | BB | 170 | GLU |
| 35 | BB | 178 | ARG |
| 35 | BB | 187 | LEU |
| 35 | BB | 195 | ASP |
| 35 | BB | 196 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | BB | 200 | ILE |
| 35 | BB | 208 | ILE |
| 35 | BB | 221 | LEU |
| 35 | BB | 230 | VAL |
| 36 | BC | 3 | ASN |
| 36 | BC | 28 | GLN |
| 36 | BC | 29 | TYR |
| 36 | BC | 37 | GLN |
| 36 | BC | 38 | ARG |
| 36 | BC | 44 | GLU |
| 36 | BC | 45 | LYS |
| 36 | BC | 49 | SER |
| 36 | BC | 52 | LEU |
| 36 | BC | 70 | VAL |
| 36 | BC | 77 | ILE |
| 36 | BC | 82 | GLU |
| 36 | BC | 118 | GLN |
| 36 | BC | 131 | ARG |
| 36 | BC | 188 | LEU |
| 36 | BC | 196 | LEU |
| 36 | BC | 202 | ILE |
| 36 | BC | 206 | GLU |
| 36 | BC | 207 | VAL |
| 37 | BD | 5 | ILE |
| 37 | BD | 15 | GLU |
| 37 | BD | 19 | LEU |
| 37 | BD | 28 | SER |
| 37 | BD | 31 | CYS |
| 37 | BD | 49 | ARG |
| 37 | BD | 57 | ARG |
| 37 | BD | 58 | LEU |
| 37 | BD | 65 | ARG |
| 37 | BD | 85 | LYS |
| 37 | BD | 86 | LYS |
| 37 | BD | 100 | ARG |
| 37 | BD | 108 | LEU |
| 37 | BD | 115 | ARG |
| 37 | BD | 118 | ARG |
| 37 | BD | 127 | THR |
| 37 | BD | 134 | ASP |
| 37 | BD | 135 | LEU |
| 37 | BD | 141 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | BD | 157 | LEU |
| 37 | BD | 158 | ILE |
| 37 | BD | 168 | ARG |
| 37 | BD | 188 | LEU |
| 37 | BD | 190 | ASP |
| 38 | BE | 10 | MET |
| 38 | BE | 13 | ILE |
| 38 | BE | 41 | VAL |
| 38 | BE | 47 | LYS |
| 38 | BE | 78 | HIS |
| 38 | BE | 79 | GLU |
| 38 | BE | 87 | SER |
| 38 | BE | 120 | THR |
| 38 | BE | 150 | ARG |
| 39 | BF | 28 | ARG |
| 39 | BF | 40 | VAL |
| 39 | BF | 45 | LEU |
| 39 | BF | 55 | ASP |
| 39 | BF | 69 | GLU |
| 39 | BF | 70 | ASP |
| 39 | BF | 71 | ARG |
| 39 | BF | 72 | VAL |
| 39 | BF | 73 | ASN |
| 39 | BF | 75 | LEU |
| 39 | BF | 82 | ARG |
| 39 | BF | 89 | MET |
| 39 | BF | 91 | VAL |
| 40 | BG | 8 | GLU |
| 40 | BG | 12 | LEU |
| 40 | BG | 21 | VAL |
| 40 | BG | 31 | MET |
| 40 | BG | 38 | LEU |
| 40 | BG | 50 | ILE |
| 40 | BG | 51 | GLN |
| 40 | BG | 56 | GLN |
| 40 | BG | 73 | MET |
| 40 | BG | 76 | ARG |
| 40 | BG | 78 | ARG |
| 40 | BG | 79 | ARG |
| 40 | BG | 91 | VAL |
| 40 | BG | 104 | LEU |
| 40 | BG | 113 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 40 | BG | 114 | ARG |
| 40 | BG | 131 | LYS |
| 40 | BG | 138 | LYS |
| 40 | BG | 139 | GLU |
| 40 | BG | 140 | ASP |
| 40 | BG | 155 | ARG |
| 41 | BH | 2 | LEU |
| 41 | BH | 6 | ILE |
| 41 | BH | 18 | ARG |
| 41 | BH | 21 | LYS |
| 41 | BH | 23 | SER |
| 41 | BH | 37 | ARG |
| 41 | BH | 51 | VAL |
| 41 | BH | 60 | ARG |
| 41 | BH | 63 | LEU |
| 41 | BH | 68 | ARG |
| 41 | BH | 78 | GLN |
| 41 | BH | 83 | ILE |
| 41 | BH | 99 | GLU |
| 41 | BH | 115 | SER |
| 41 | BH | 121 | ASP |
| 41 | BH | 122 | ARG |
| 42 | BI | 3 | GLN |
| 42 | BI | 7 | THR |
| 42 | BI | 17 | VAL |
| 42 | BI | 23 | ASN |
| 42 | BI | 27 | THR |
| 42 | BI | 56 | LEU |
| 42 | BI | 64 | THR |
| 42 | BI | 65 | VAL |
| 42 | BI | 75 | ASP |
| 42 | BI | 78 | LYS |
| 42 | BI | 81 | ILE |
| 42 | BI | 87 | GLN |
| 42 | BI | 97 | LYS |
| 42 | BI | 102 | LEU |
| 42 | BI | 104 | ARG |
| 42 | BI | 109 | VAL |
| 42 | BI | 111 | ARG |
| 42 | BI | 121 | ARG |
| 42 | BI | 128 | ARG |
| 43 | BJ | 5 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | BJ | 7 | LYS |
| 43 | BJ | 16 | LEU |
| 43 | BJ | 23 | ILE |
| 43 | BJ | 44 | VAL |
| 43 | BJ | 49 | VAL |
| 43 | BJ | 67 | THR |
| 43 | BJ | 92 | THR |
| 44 | BK | 25 | TYR |
| 44 | BK | 41 | THR |
| 44 | BK | 48 | ILE |
| 44 | BK | 63 | LEU |
| 44 | BK | 83 | ILE |
| 44 | BK | 84 | VAL |
| 44 | BK | 96 | ARG |
| 44 | BK | 98 | LEU |
| 44 | BK | 104 | GLN |
| 44 | BK | 105 | VAL |
| 44 | BK | 109 | VAL |
| 44 | BK | 114 | VAL |
| 45 | BL | 23 | LYS |
| 45 | BL | 27 | LEU |
| 45 | BL | 42 | THR |
| 45 | BL | 60 | LEU |
| 45 | BL | 86 | ARG |
| 45 | BL | 89 | ARG |
| 45 | BL | 97 | ARG |
| 46 | BM | 4 | ILE |
| 46 | BM | 17 | VAL |
| 46 | BM | 19 | LEU |
| 46 | BM | 20 | THR |
| 46 | BM | 43 | THR |
| 46 | BM | 56 | LEU |
| 46 | BM | 63 | THR |
| 46 | BM | 64 | TRP |
| 46 | BM | 70 | LEU |
| 46 | BM | 102 | ARG |
| 46 | BM | 109 | THR |
| 46 | BM | 110 | ARG |
| 46 | BM | 121 | LYS |
| 47 | BN | 3 | ARG |
| 47 | BN | 6 | LEU |
| 47 | BN | 7 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | BN | 9 | LYS |
| 47 | BN | 18 | VAL |
| 47 | BN | 32 | SER |
| 47 | BN | 33 | VAL |
| 47 | BN | 41 | ARG |
| 47 | BN | 44 | LEU |
| 47 | BN | 60 | SER |
| 48 | BO | 3 | ILE |
| 48 | BO | 5 | LYS |
| 48 | BO | 6 | GLU |
| 48 | BO | 22 | THR |
| 48 | BO | 26 | GLU |
| 48 | BO | 34 | LEU |
| 48 | BO | 35 | ARG |
| 48 | BO | 38 | ARG |
| 48 | BO | 39 | LEU |
| 48 | BO | 41 | GLU |
| 48 | BO | 66 | LEU |
| 48 | BO | 83 | GLU |
| 48 | BO | 87 | ILE |
| 48 | BO | 88 | ARG |
| 49 | BP | 1 | MET |
| 49 | BP | 6 | LEU |
| 49 | BP | 11 | SER |
| 49 | BP | 19 | ILE |
| 49 | BP | 20 | VAL |
| 49 | BP | 27 | LYS |
| 49 | BP | 36 | ILE |
| 49 | BP | 50 | LYS |
| 49 | BP | 60 | LEU |
| 49 | BP | 62 | VAL |
| 49 | BP | 67 | THR |
| 49 | BP | 69 | THR |
| 49 | BP | 71 | ARG |
| 50 | BQ | 6 | LEU |
| 50 | BQ | 36 | ILE |
| 50 | BQ | 45 | HIS |
| 50 | BQ | 60 | ILE |
| 50 | BQ | 63 | ARG |
| 50 | BQ | 68 | ARG |
| 50 | BQ | 72 | ARG |
| 50 | BQ | 78 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | BQ | 86 | GLU |
| 50 | BQ | 90 | ILE |
| 50 | BQ | 91 | ARG |
| 50 | BQ | 92 | ARG |
| 50 | BQ | 97 | SER |
| 51 | BR | 31 | LEU |
| 51 | BR | 32 | ARG |
| 51 | BR | 35 | ARG |
| 51 | BR | 37 | VAL |
| 51 | BR | 38 | GLU |
| 51 | BR | 45 | SER |
| 51 | BR | 46 | GLU |
| 51 | BR | 47 | THR |
| 51 | BR | 55 | ARG |
| 51 | BR | 65 | ILE |
| 51 | BR | 68 | LYS |
| 51 | BR | 76 | LEU |
| 52 | BS | 12 | ASP |
| 52 | BS | 28 | LYS |
| 52 | BS | 37 | ARG |
| 52 | BS | 38 | SER |
| 52 | BS | 62 | ILE |
| 52 | BS | 65 | ASN |
| 52 | BS | 78 | ARG |
| 52 | BS | 81 | ARG |
| 52 | BS | 85 | LYS |
| 53 | BT | 8 | ARG |
| 53 | BT | 13 | LEU |
| 53 | BT | 24 | LEU |
| 53 | BT | 43 | LEU |
| 53 | BT | 45 | GLN |
| 53 | BT | 56 | MET |
| 53 | BT | 58 | LYS |
| 53 | BT | 60 | GLU |
| 53 | BT | 62 | LEU |
| 53 | BT | 84 | LEU |
| 53 | BT | 100 | ILE |
| 54 | BU | 9 | ARG |
| 54 | BU | 10 | ARG |
| 59 | BZ | -64 | VAL |
| 59 | BZ | -42 | TYR |
| 59 | BZ | -29 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | BZ | -23 | LEU |
| 59 | BZ | -20 | LEU |
| 59 | BZ | -19 | GLU |
| 59 | BZ | -10 | ARG |
| 59 | BZ | -6 | ARG |
| 59 | BZ | -1 | GLU |
| 59 | BZ | 0 | ARG |
| 59 | BZ | 4 | ILE |
| 59 | BZ | 7 | ASN |
| 59 | BZ | 12 | LEU |
| 59 | BZ | 13 | ARG |
| 59 | BZ | 15 | ILE |
| 59 | BZ | 21 | ILE |
| 59 | BZ | 30 | GLU |
| 59 | BZ | 33 | LEU |
| 59 | BZ | 69 | VAL |
| 59 | BZ | 71 | THR |
| 59 | BZ | 75 | LYS |
| 59 | BZ | 76 | ASP |
| 59 | BZ | 78 | ARG |
| 59 | BZ | 87 | HIS |
| 59 | BZ | 89 | ASP |
| 59 | BZ | 92 | ILE |
| 59 | BZ | 99 | ARG |
| 59 | BZ | 102 | ASP |
| 59 | BZ | 105 | ILE |
| 59 | BZ | 112 | GLN |
| 59 | BZ | 130 | VAL |
| 59 | BZ | 132 | ARG |
| 59 | BZ | 139 | MET |
| 59 | BZ | 146 | LEU |
| 59 | BZ | 148 | LEU |
| 59 | BZ | 152 | THR |
| 59 | BZ | 156 | ARG |
| 59 | BZ | 160 | ARG |
| 59 | BZ | 166 | LEU |
| 59 | BZ | 170 | ARG |
| 59 | BZ | 172 | ASP |
| 59 | BZ | 196 | ILE |
| 59 | BZ | 198 | GLU |
| 59 | BZ | 203 | GLU |
| 59 | BZ | 207 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | BZ | 208 | GLN |
| 59 | BZ | 222 | ASP |
| 59 | BZ | 238 | THR |
| 59 | BZ | 239 | GLU |
| 59 | BZ | 240 | GLU |
| 59 | BZ | 247 | ARG |
| 59 | BZ | 255 | ILE |
| 59 | BZ | 267 | LYS |
| 59 | BZ | 269 | VAL |
| 59 | BZ | 282 | SER |
| 59 | BZ | 284 | LEU |
| 59 | BZ | 286 | ILE |
| 59 | BZ | 289 | ILE |
| 59 | BZ | 298 | VAL |
| 59 | BZ | 312 | LEU |
| 59 | BZ | 328 | ILE |
| 59 | BZ | 329 | ARG |
| 59 | BZ | 331 | TYR |
| 59 | BZ | 336 | THR |
| 59 | BZ | 349 | LYS |
| 59 | BZ | 352 | VAL |
| 59 | BZ | 354 | ARG |
| 59 | BZ | 356 | LEU |
| 59 | BZ | 362 | HIS |
| 59 | BZ | 363 | ARG |
| 59 | BZ | 368 | GLU |
| 59 | BZ | 369 | LEU |
| 59 | BZ | 374 | LEU |
| 59 | BZ | 381 | LYS |
| 59 | BZ | 382 | GLU |
| 59 | BZ | 389 | LEU |
| 59 | BZ | 397 | VAL |
| 59 | BZ | 399 | LEU |
| 59 | BZ | 402 | ILE |
| 59 | BZ | 406 | GLU |
| 59 | BZ | 420 | ASP |
| 59 | BZ | 421 | GLN |
| 59 | BZ | 422 | GLU |
| 59 | BZ | 431 | LEU |
| 59 | BZ | 433 | GLU |
| 59 | BZ | 437 | THR |
| 59 | BZ | 442 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | BZ | 446 | THR |
| 59 | BZ | 457 | LEU |
| 59 | BZ | 464 | ASP |
| 59 | BZ | 468 | ARG |
| 59 | BZ | 473 | ASP |
| 59 | BZ | 484 | ARG |
| 59 | BZ | 485 | GLU |
| 59 | BZ | 486 | THR |
| 59 | BZ | 504 | ARG |
| 59 | BZ | 506 | GLN |
| 59 | BZ | 512 | ILE |
| 59 | BZ | 572 | TYR |
| 59 | BZ | 600 | VAL |
| 59 | BZ | 614 | GLU |
| 59 | BZ | 630 | GLN |
| 59 | BZ | 634 | MET |
| 59 | BZ | 644 | ARG |
| 59 | BZ | 647 | VAL |
| 59 | BZ | 651 | GLU |
| 59 | BZ | 659 | LEU |
| 59 | BZ | 660 | ARG |
| 59 | BZ | 669 | PHE |
| 59 | BZ | 670 | VAL |
| 59 | BZ | 679 | VAL |
| 59 | BZ | 681 | LYS |
| 59 | BZ | 683 | VAL |
| 59 | BZ | 684 | GLN |
| 59 | BZ | 686 | LYS |
| 3 | CC | 28 | ARG |
| 3 | CC | 32 | GLU |
| 3 | CC | 48 | LEU |
| 3 | CC | 50 | ILE |
| 3 | CC | 53 | ARG |
| 3 | CC | 54 | ARG |
| 3 | CC | 203 | GLU |
| 3 | CC | 208 | THR |
| 4 | CD | 3 | VAL |
| 4 | CD | 5 | LYS |
| 4 | CD | 12 | SER |
| 4 | CD | 13 | ARG |
| 4 | CD | 14 | ARG |
| 4 | CD | 26 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | CD | 32 | SER |
| 4 | CD | 54 | ARG |
| 4 | CD | 61 | LEU |
| 4 | CD | 71 | ASP |
| 4 | CD | 89 | SER |
| 4 | CD | 94 | LEU |
| 4 | CD | 99 | ASP |
| 4 | CD | 101 | GLU |
| 4 | CD | 103 | ARG |
| 4 | CD | 106 | ILE |
| 4 | CD | 111 | LEU |
| 4 | CD | 113 | VAL |
| 4 | CD | 134 | ARG |
| 4 | CD | 138 | VAL |
| 4 | CD | 141 | VAL |
| 4 | CD | 142 | VAL |
| 4 | CD | 165 | ILE |
| 4 | CD | 211 | ARG |
| 4 | CD | 212 | SER |
| 4 | CD | 217 | ARG |
| 4 | CD | 221 | VAL |
| 4 | CD | 229 | VAL |
| 4 | CD | 242 | ARG |
| 4 | CD | 257 | LEU |
| 4 | CD | 259 | THR |
| 4 | CD | 260 | ARG |
| 4 | CD | 262 | ARG |
| 4 | CD | 270 | ILE |
| 4 | CD | 276 | LYS |
| 5 | CE | 12 | THR |
| 5 | CE | 21 | VAL |
| 5 | CE | 34 | VAL |
| 5 | CE | 40 | GLU |
| 5 | CE | 45 | THR |
| 5 | CE | 49 | LEU |
| 5 | CE | 58 | ARG |
| 5 | CE | 61 | ARG |
| 5 | CE | 75 | VAL |
| 5 | CE | 77 | ILE |
| 5 | CE | 78 | LEU |
| 5 | CE | 79 | ARG |
| 5 | CE | 82 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | CE | 89 | ASP |
| 5 | CE | 111 | ARG |
| 5 | CE | 116 | VAL |
| 5 | CE | 119 | ARG |
| 5 | CE | 144 | ARG |
| 5 | CE | 154 | LYS |
| 5 | CE | 170 | LEU |
| 5 | CE | 175 | VAL |
| 5 | CE | 181 | LEU |
| 5 | CE | 184 | VAL |
| 5 | CE | 195 | LEU |
| 5 | CE | 202 | LYS |
| 6 | CF | 17 | ARG |
| 6 | CF | 19 | GLU |
| 6 | CF | 24 | LEU |
| 6 | CF | 32 | LEU |
| 6 | CF | 40 | GLN |
| 6 | CF | 50 | SER |
| 6 | CF | 53 | THR |
| 6 | CF | 57 | VAL |
| 6 | CF | 70 | THR |
| 6 | CF | 74 | ARG |
| 6 | CF | 77 | ASP |
| 6 | CF | 88 | VAL |
| 6 | CF | 95 | ARG |
| 6 | CF | 106 | ARG |
| 6 | CF | 107 | LYS |
| 6 | CF | 110 | LEU |
| 6 | CF | 135 | LYS |
| 6 | CF | 140 | LEU |
| 6 | CF | 158 | THR |
| 6 | CF | 169 | ASN |
| 6 | CF | 175 | THR |
| 6 | CF | 186 | ILE |
| 6 | CF | 192 | LEU |
| 6 | CF | 200 | GLU |
| 7 | CG | 3 | LEU |
| 7 | CG | 4 | ASP |
| 7 | CG | 5 | VAL |
| 7 | CG | 16 | ARG |
| 7 | CG | 18 | GLU |
| 7 | CG | 28 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CG | 31 | VAL |
| 7 | CG | 33 | ARG |
| 7 | CG | 35 | GLU |
| 7 | CG | 43 | LEU |
| 7 | CG | 49 | ASP |
| 7 | CG | 60 | LEU |
| 7 | CG | 70 | VAL |
| 7 | CG | 71 | THR |
| 7 | CG | 79 | ASN |
| 7 | CG | 80 | PHE |
| 7 | CG | 91 | ARG |
| 7 | CG | 111 | LEU |
| 7 | CG | 115 | ARG |
| 7 | CG | 116 | ASP |
| 7 | CG | 128 | ARG |
| 7 | CG | 130 | ASN |
| 7 | CG | 133 | LEU |
| 7 | CG | 136 | ARG |
| 7 | CG | 139 | LEU |
| 7 | CG | 143 | GLU |
| 7 | CG | 145 | THR |
| 7 | CG | 148 | MET |
| 7 | CG | 152 | LEU |
| 7 | CG | 153 | ARG |
| 7 | CG | 159 | VAL |
| 7 | CG | 162 | THR |
| 7 | CG | 165 | THR |
| 7 | CG | 170 | ARG |
| 8 | CH | 3 | ARG |
| 8 | CH | 27 | LYS |
| 8 | CH | 33 | LEU |
| 8 | CH | 41 | MET |
| 8 | CH | 44 | VAL |
| 8 | CH | 69 | ARG |
| 8 | CH | 84 | SER |
| 8 | CH | 88 | LEU |
| 8 | CH | 98 | LEU |
| 8 | CH | 106 | THR |
| 8 | CH | 110 | SER |
| 8 | CH | 111 | HIS |
| 8 | CH | 122 | THR |
| 8 | CH | 124 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | CH | 129 | THR |
| 8 | CH | 136 | ILE |
| 8 | CH | 139 | GLN |
| 8 | CH | 147 | ASN |
| 8 | CH | 171 | LEU |
| 10 | CL | 86 | LYS |
| 10 | CL | 93 | ARG |
| 10 | CL | 96 | VAL |
| 10 | CL | 112 | MET |
| 10 | CL | 117 | THR |
| 11 | CN | 2 | LYS |
| 11 | CN | 3 | THR |
| 11 | CN | 5 | VAL |
| 11 | CN | 12 | ARG |
| 11 | CN | 33 | LEU |
| 11 | CN | 34 | LEU |
| 11 | CN | 43 | THR |
| 11 | CN | 46 | VAL |
| 11 | CN | 48 | MET |
| 11 | CN | 82 | LEU |
| 11 | CN | 87 | LEU |
| 11 | CN | 97 | ARG |
| 11 | CN | 99 | LEU |
| 11 | CN | 104 | LYS |
| 11 | CN | 119 | ARG |
| 11 | CN | 120 | LEU |
| 11 | CN | 127 | ASP |
| 11 | CN | 133 | GLN |
| 11 | CN | 138 | LEU |
| 11 | CN | 140 | VAL |
| 12 | CO | 1 | MET |
| 12 | CO | 5 | GLN |
| 12 | CO | 10 | VAL |
| 12 | CO | 14 | THR |
| 12 | CO | 24 | VAL |
| 12 | CO | 28 | SER |
| 12 | CO | 66 | LYS |
| 12 | CO | 69 | ILE |
| 12 | CO | 77 | ILE |
| 12 | CO | 78 | ARG |
| 12 | CO | 85 | VAL |
| 12 | CO | 86 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | CO | 92 | GLU |
| 12 | CO | 98 | VAL |
| 12 | CO | 108 | GLU |
| 12 | CO | 113 | LYS |
| 12 | CO | 117 | LEU |
| 13 | CP | 2 | LYS |
| 13 | CP | 3 | LEU |
| 13 | CP | 38 | GLN |
| 13 | CP | 40 | SER |
| 13 | CP | 42 | SER |
| 13 | CP | 45 | LEU |
| 13 | CP | 55 | ARG |
| 13 | CP | 56 | SER |
| 13 | CP | 64 | LYS |
| 13 | CP | 65 | ARG |
| 13 | CP | 75 | ILE |
| 13 | CP | 83 | VAL |
| 13 | CP | 95 | VAL |
| 13 | CP | 106 | LEU |
| 13 | CP | 131 | SER |
| 13 | CP | 148 | LEU |
| 14 | CQ | 1 | MET |
| 14 | CQ | 3 | MET |
| 14 | CQ | 7 | MET |
| 14 | CQ | 8 | LYS |
| 14 | CQ | 12 | GLN |
| 14 | CQ | 16 | ARG |
| 14 | CQ | 21 | THR |
| 14 | CQ | 35 | VAL |
| 14 | CQ | 45 | GLN |
| 14 | CQ | 60 | ARG |
| 14 | CQ | 75 | THR |
| 14 | CQ | 109 | VAL |
| 14 | CQ | 110 | THR |
| 14 | CQ | 115 | MET |
| 14 | CQ | 128 | LYS |
| 14 | CQ | 131 | ILE |
| 15 | CR | 1 | MET |
| 15 | CR | 18 | LEU |
| 15 | CR | 27 | SER |
| 15 | CR | 28 | LEU |
| 15 | CR | 29 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | CR | 36 | THR |
| 15 | CR | 44 | LEU |
| 15 | CR | 60 | LEU |
| 15 | CR | 65 | LEU |
| 15 | CR | 67 | LEU |
| 15 | CR | 75 | LEU |
| 15 | CR | 79 | LEU |
| 15 | CR | 86 | ARG |
| 15 | CR | 96 | ARG |
| 15 | CR | 100 | LEU |
| 15 | CR | 111 | LEU |
| 15 | CR | 114 | VAL |
| 16 | CS | 3 | ARG |
| 16 | CS | 13 | ARG |
| 16 | CS | 14 | VAL |
| 16 | CS | 19 | LYS |
| 16 | CS | 20 | ARG |
| 16 | CS | 25 | ARG |
| 16 | CS | 35 | ILE |
| 16 | CS | 36 | TYR |
| 16 | CS | 49 | VAL |
| 16 | CS | 58 | LEU |
| 16 | CS | 64 | GLU |
| 16 | CS | 67 | ARG |
| 16 | CS | 68 | GLN |
| 16 | CS | 69 | VAL |
| 16 | CS | 78 | LEU |
| 16 | CS | 80 | LEU |
| 16 | CS | 103 | GLU |
| 16 | CS | 110 | LEU |
| 17 | CT | 6 | LEU |
| 17 | CT | 8 | LYS |
| 17 | CT | 28 | VAL |
| 17 | CT | 34 | VAL |
| 17 | CT | 49 | VAL |
| 17 | CT | 51 | ARG |
| 17 | CT | 53 | ARG |
| 17 | CT | 59 | THR |
| 17 | CT | 64 | ARG |
| 17 | CT | 74 | ARG |
| 17 | CT | 78 | LEU |
| 17 | CT | 85 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | CT | 89 | VAL |
| 17 | CT | 93 | ARG |
| 17 | CT | 96 | ARG |
| 17 | CT | 113 | LYS |
| 17 | CT | 115 | ARG |
| 17 | CT | 118 | ARG |
| 17 | CT | 123 | GLN |
| 17 | CT | 124 | ASP |
| 18 | CU | 6 | THR |
| 18 | CU | 8 | VAL |
| 18 | CU | 13 | LYS |
| 18 | CU | 31 | SER |
| 18 | CU | 60 | LEU |
| 18 | CU | 74 | LEU |
| 18 | CU | 83 | LEU |
| 18 | CU | 92 | ARG |
| 18 | CU | 101 | ARG |
| 18 | CU | 104 | GLN |
| 18 | CU | 108 | GLU |
| 19 | CV | 1 | MET |
| 19 | CV | 6 | LYS |
| 19 | CV | 15 | GLU |
| 19 | CV | 18 | LEU |
| 19 | CV | 19 | LYS |
| 19 | CV | 51 | VAL |
| 19 | CV | 52 | VAL |
| 19 | CV | 61 | VAL |
| 19 | CV | 62 | LEU |
| 19 | CV | 66 | ARG |
| 19 | CV | 73 | SER |
| 19 | CV | 79 | VAL |
| 19 | CV | 95 | LEU |
| 20 | CW | 11 | ARG |
| 20 | CW | 15 | ARG |
| 20 | CW | 17 | VAL |
| 20 | CW | 19 | LEU |
| 20 | CW | 23 | LEU |
| 20 | CW | 37 | ARG |
| 20 | CW | 51 | LEU |
| 20 | CW | 63 | ASP |
| 20 | CW | 100 | THR |
| 20 | CW | 101 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | CW | 107 | LEU |
| 21 | CX | 35 | THR |
| 21 | CX | 45 | THR |
| 21 | CX | 57 | LEU |
| 21 | CX | 60 | ARG |
| 21 | CX | 76 | ARG |
| 21 | CX | 87 | GLN |
| 21 | CX | 92 | LEU |
| 22 | CY | 2 | ARG |
| 22 | CY | 6 | HIS |
| 22 | CY | 7 | VAL |
| 22 | CY | 9 | LYS |
| 22 | CY | 21 | LYS |
| 22 | CY | 23 | ARG |
| 22 | CY | 37 | VAL |
| 22 | CY | 43 | ASN |
| 22 | CY | 47 | LYS |
| 22 | CY | 49 | VAL |
| 22 | CY | 50 | ARG |
| 22 | CY | 70 | SER |
| 22 | CY | 73 | ARG |
| 22 | CY | 91 | GLU |
| 22 | CY | 102 | CYS |
| 23 | CZ | 5 | LEU |
| 23 | CZ | 18 | LEU |
| 23 | CZ | 33 | LEU |
| 23 | CZ | 41 | LEU |
| 23 | CZ | 56 | VAL |
| 23 | CZ | 61 | LEU |
| 23 | CZ | 66 | SER |
| 23 | CZ | 71 | VAL |
| 23 | CZ | 86 | VAL |
| 23 | CZ | 91 | LEU |
| 23 | CZ | 102 | LEU |
| 23 | CZ | 107 | THR |
| 23 | CZ | 120 | ILE |
| 23 | CZ | 128 | VAL |
| 23 | CZ | 129 | SER |
| 23 | CZ | 136 | PHE |
| 23 | CZ | 144 | LEU |
| 23 | CZ | 146 | ILE |
| 23 | CZ | 154 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | CZ | 170 | THR |
| 24 | C0 | 3 | HIS |
| 24 | C0 | 19 | LYS |
| 24 | C0 | 20 | ARG |
| 24 | C0 | 36 | ILE |
| 24 | C0 | 44 | ARG |
| 25 | C1 | 21 | ARG |
| 25 | C1 | 35 | THR |
| 25 | C1 | 40 | ARG |
| 25 | C1 | 51 | VAL |
| 25 | C1 | 52 | ARG |
| 25 | C1 | 59 | THR |
| 25 | C1 | 80 | LEU |
| 25 | C1 | 86 | SER |
| 25 | C1 | 89 | GLU |
| 25 | C1 | 95 | LEU |
| 25 | C1 | 97 | LEU |
| 26 | C2 | 2 | LYS |
| 26 | C2 | 19 | VAL |
| 26 | C2 | 32 | LEU |
| 26 | C2 | 40 | SER |
| 26 | C2 | 41 | ILE |
| 26 | C2 | 44 | LEU |
| 26 | C2 | 53 | LEU |
| 26 | C2 | 66 | GLU |
| 26 | C2 | 67 | LYS |
| 26 | C2 | 70 | GLN |
| 27 | C3 | 3 | ARG |
| 27 | C3 | 5 | LYS |
| 27 | C3 | 6 | VAL |
| 27 | C3 | 8 | LEU |
| 27 | C3 | 18 | ASP |
| 27 | C3 | 23 | LEU |
| 27 | C3 | 24 | LYS |
| 27 | C3 | 30 | ARG |
| 27 | C3 | 31 | LEU |
| 27 | C3 | 34 | GLU |
| 27 | C3 | 54 | VAL |
| 27 | C3 | 56 | VAL |
| 28 | C4 | 1 | MET |
| 28 | C4 | 3 | GLU |
| 28 | C4 | 5 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | C4 | 10 | VAL |
| 28 | C4 | 34 | GLU |
| 28 | C4 | 36 | CYS |
| 28 | C4 | 41 | PRO |
| 28 | C4 | 50 | VAL |
| 28 | C4 | 56 | VAL |
| 28 | C4 | 58 | ARG |
| 28 | C4 | 61 | ARG |
| 28 | C4 | 63 | TYR |
| 28 | C4 | 68 | ARG |
| 28 | C4 | 69 | LYS |
| 29 | C5 | 6 | VAL |
| 29 | C5 | 16 | ARG |
| 29 | C5 | 29 | THR |
| 29 | C5 | 35 | GLU |
| 29 | C5 | 40 | LYS |
| 29 | C5 | 48 | GLU |
| 30 | C6 | 5 | VAL |
| 30 | C6 | 6 | ARG |
| 30 | C6 | 23 | THR |
| 30 | C6 | 27 | LYS |
| 30 | C6 | 28 | ARG |
| 30 | C6 | 44 | ARG |
| 30 | C6 | 48 | VAL |
| 31 | C7 | 1 | MET |
| 31 | C7 | 9 | ARG |
| 31 | C7 | 14 | LYS |
| 31 | C7 | 39 | ARG |
| 31 | C7 | 43 | THR |
| 32 | C8 | 14 | VAL |
| 32 | C8 | 26 | LYS |
| 32 | C8 | 30 | ARG |
| 32 | C8 | 31 | HIS |
| 32 | C8 | 34 | TRP |
| 33 | C9 | 4 | ARG |
| 33 | C9 | 17 | ILE |
| 33 | C9 | 19 | ARG |
| 33 | C9 | 26 | ILE |
| 33 | C9 | 35 | ARG |
| 35 | DB | 7 | VAL |
| 35 | DB | 10 | LEU |
| 35 | DB | 15 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | DB | 23 | ARG |
| 35 | DB | 24 | TRP |
| 35 | DB | 51 | LEU |
| 35 | DB | 60 | ASP |
| 35 | DB | 67 | THR |
| 35 | DB | 80 | ILE |
| 35 | DB | 95 | GLN |
| 35 | DB | 97 | TRP |
| 35 | DB | 108 | ILE |
| 35 | DB | 115 | LEU |
| 35 | DB | 117 | GLU |
| 35 | DB | 128 | GLU |
| 35 | DB | 135 | GLN |
| 35 | DB | 154 | LEU |
| 35 | DB | 155 | LEU |
| 35 | DB | 157 | ARG |
| 35 | DB | 158 | LEU |
| 35 | DB | 162 | ILE |
| 35 | DB | 163 | PHE |
| 35 | DB | 179 | LYS |
| 35 | DB | 185 | ILE |
| 35 | DB | 187 | LEU |
| 35 | DB | 189 | ASP |
| 35 | DB | 212 | GLN |
| 35 | DB | 215 | LEU |
| 35 | DB | 217 | ARG |
| 35 | DB | 224 | GLN |
| 36 | DC | 3 | ASN |
| 36 | DC | 15 | THR |
| 36 | DC | 16 | ARG |
| 36 | DC | 21 | ARG |
| 36 | DC | 22 | TRP |
| 36 | DC | 29 | TYR |
| 36 | DC | 30 | ARG |
| 36 | DC | 47 | LEU |
| 36 | DC | 48 | TYR |
| 36 | DC | 52 | LEU |
| 36 | DC | 72 | LYS |
| 36 | DC | 91 | LEU |
| 36 | DC | 104 | GLN |
| 36 | DC | 105 | GLU |
| 36 | DC | 108 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 36 | DC | 115 | LEU |
| 36 | DC | 116 | VAL |
| 36 | DC | 127 | ARG |
| 36 | DC | 128 | PHE |
| 36 | DC | 140 | ARG |
| 36 | DC | 152 | ILE |
| 36 | DC | 153 | VAL |
| 36 | DC | 154 | SER |
| 36 | DC | 190 | ARG |
| 36 | DC | 191 | THR |
| 36 | DC | 195 | VAL |
| 37 | DD | 3 | ARG |
| 37 | DD | 10 | ARG |
| 37 | DD | 25 | ARG |
| 37 | DD | 31 | CYS |
| 37 | DD | 34 | GLU |
| 37 | DD | 47 | ARG |
| 37 | DD | 53 | ASP |
| 37 | DD | 57 | ARG |
| 37 | DD | 58 | LEU |
| 37 | DD | 61 | LYS |
| 37 | DD | 63 | LYS |
| 37 | DD | 65 | ARG |
| 37 | DD | 73 | ARG |
| 37 | DD | 96 | LEU |
| 37 | DD | 102 | ASP |
| 37 | DD | 107 | ARG |
| 37 | DD | 108 | LEU |
| 37 | DD | 127 | THR |
| 37 | DD | 135 | LEU |
| 37 | DD | 137 | SER |
| 37 | DD | 150 | GLU |
| 37 | DD | 155 | LEU |
| 37 | DD | 187 | ARG |
| 37 | DD | 188 | LEU |
| 37 | DD | 194 | LEU |
| 37 | DD | 208 | SER |
| 38 | DE | 10 | MET |
| 38 | DE | 16 | THR |
| 38 | DE | 18 | ARG |
| 38 | DE | 31 | LEU |
| 38 | DE | 41 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38 | DE | 47 | LYS |
| 38 | DE | 53 | LEU |
| 38 | DE | 71 | LEU |
| 38 | DE | 75 | THR |
| 38 | DE | 78 | HIS |
| 38 | DE | 82 | VAL |
| 38 | DE | 87 | SER |
| 38 | DE | 89 | ILE |
| 38 | DE | 91 | LEU |
| 38 | DE | 107 | ARG |
| 38 | DE | 117 | ASP |
| 38 | DE | 120 | THR |
| 38 | DE | 150 | ARG |
| 39 | DF | 7 | ASN |
| 39 | DF | 10 | LEU |
| 39 | DF | 21 | LEU |
| 39 | DF | 27 | GLN |
| 39 | DF | 28 | ARG |
| 39 | DF | 69 | GLU |
| 39 | DF | 72 | VAL |
| 39 | DF | 75 | LEU |
| 39 | DF | 82 | ARG |
| 39 | DF | 87 | ARG |
| 39 | DF | 93 | SER |
| 40 | DG | 32 | ARG |
| 40 | DG | 57 | GLU |
| 40 | DG | 75 | VAL |
| 40 | DG | 98 | SER |
| 40 | DG | 104 | LEU |
| 40 | DG | 114 | ARG |
| 40 | DG | 115 | ARG |
| 40 | DG | 155 | ARG |
| 41 | DH | 2 | LEU |
| 41 | DH | 3 | THR |
| 41 | DH | 24 | THR |
| 41 | DH | 26 | VAL |
| 41 | DH | 37 | ARG |
| 41 | DH | 39 | LEU |
| 41 | DH | 51 | VAL |
| 41 | DH | 52 | ASP |
| 41 | DH | 60 | ARG |
| 41 | DH | 63 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41 | DH | 65 | TYR |
| 41 | DH | 78 | GLN |
| 41 | DH | 84 | ARG |
| 41 | DH | 85 | ARG |
| 41 | DH | 98 | LYS |
| 41 | DH | 111 | ILE |
| 41 | DH | 112 | LEU |
| 41 | DH | 119 | LEU |
| 41 | DH | 120 | THR |
| 41 | DH | 125 | ARG |
| 41 | DH | 127 | LEU |
| 41 | DH | 133 | LEU |
| 42 | DI | 23 | ASN |
| 42 | DI | 27 | THR |
| 42 | DI | 31 | GLN |
| 42 | DI | 41 | VAL |
| 42 | DI | 53 | VAL |
| 42 | DI | 64 | THR |
| 42 | DI | 65 | VAL |
| 42 | DI | 85 | LEU |
| 42 | DI | 89 | ASN |
| 42 | DI | 92 | TYR |
| 42 | DI | 102 | LEU |
| 42 | DI | 104 | ARG |
| 42 | DI | 108 | VAL |
| 42 | DI | 109 | VAL |
| 42 | DI | 113 | LYS |
| 42 | DI | 124 | GLN |
| 42 | DI | 125 | TYR |
| 42 | DI | 128 | ARG |
| 43 | DJ | 6 | ILE |
| 43 | DJ | 21 | GLN |
| 43 | DJ | 30 | SER |
| 43 | DJ | 34 | VAL |
| 43 | DJ | 43 | ARG |
| 43 | DJ | 46 | ARG |
| 43 | DJ | 59 | SER |
| 43 | DJ | 67 | THR |
| 43 | DJ | 72 | VAL |
| 43 | DJ | 85 | LEU |
| 43 | DJ | 96 | ILE |
| 44 | DK | 14 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44 | DK | 18 | ARG |
| 44 | DK | 30 | VAL |
| 44 | DK | 33 | THR |
| 44 | DK | 54 | ARG |
| 44 | DK | 92 | GLU |
| 44 | DK | 109 | VAL |
| 44 | DK | 120 | ARG |
| 44 | DK | 126 | ARG |
| 45 | DL | 33 | ARG |
| 45 | DL | 42 | THR |
| 45 | DL | 47 | LYS |
| 45 | DL | 52 | LEU |
| 45 | DL | 53 | ARG |
| 45 | DL | 75 | HIS |
| 45 | DL | 89 | ARG |
| 45 | DL | 92 | ASP |
| 45 | DL | 102 | ARG |
| 45 | DL | 104 | VAL |
| 45 | DL | 114 | LYS |
| 46 | DM | 3 | ARG |
| 46 | DM | 8 | GLU |
| 46 | DM | 11 | ARG |
| 46 | DM | 15 | VAL |
| 46 | DM | 27 | LYS |
| 46 | DM | 29 | ARG |
| 46 | DM | 52 | GLU |
| 46 | DM | 66 | LEU |
| 46 | DM | 70 | LEU |
| 46 | DM | 73 | GLU |
| 46 | DM | 77 | ASN |
| 46 | DM | 90 | LEU |
| 46 | DM | 92 | HIS |
| 46 | DM | 106 | ASN |
| 46 | DM | 110 | ARG |
| 46 | DM | 121 | LYS |
| 47 | DN | 3 | ARG |
| 47 | DN | 13 | THR |
| 47 | DN | 15 | LYS |
| 47 | DN | 18 | VAL |
| 47 | DN | 22 | THR |
| 47 | DN | 29 | ARG |
| 47 | DN | 33 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | DN | 44 | LEU |
| 47 | DN | 46 | GLU |
| 48 | DO | 3 | ILE |
| 48 | DO | 4 | THR |
| 48 | DO | 5 | LYS |
| 48 | DO | 7 | GLU |
| 48 | DO | 22 | THR |
| 48 | DO | 38 | ARG |
| 48 | DO | 39 | LEU |
| 48 | DO | 48 | LYS |
| 48 | DO | 66 | LEU |
| 48 | DO | 68 | ARG |
| 49 | DP | 1 | MET |
| 49 | DP | 2 | VAL |
| 49 | DP | 4 | ILE |
| 49 | DP | 5 | ARG |
| 49 | DP | 45 | THR |
| 49 | DP | 60 | LEU |
| 49 | DP | 62 | VAL |
| 50 | DQ | 6 | LEU |
| 50 | DQ | 50 | LYS |
| 50 | DQ | 52 | LYS |
| 50 | DQ | 63 | ARG |
| 50 | DQ | 69 | LYS |
| 50 | DQ | 72 | ARG |
| 50 | DQ | 74 | LEU |
| 50 | DQ | 79 | SER |
| 50 | DQ | 86 | GLU |
| 50 | DQ | 91 | ARG |
| 50 | DQ | 96 | GLU |
| 50 | DQ | 98 | LEU |
| 51 | DR | 32 | ARG |
| 51 | DR | 37 | VAL |
| 51 | DR | 41 | LYS |
| 51 | DR | 42 | ARG |
| 51 | DR | 53 | ARG |
| 51 | DR | 65 | ILE |
| 51 | DR | 76 | LEU |
| 51 | DR | 85 | LEU |
| 52 | DS | 6 | LYS |
| 52 | DS | 12 | ASP |
| 52 | DS | 22 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | DS | 33 | THR |
| 52 | DS | 65 | ASN |
| 52 | DS | 78 | ARG |
| 52 | DS | 83 | HIS |
| 53 | DT | 10 | LEU |
| 53 | DT | 24 | LEU |
| 53 | DT | 36 | LEU |
| 53 | DT | 46 | GLU |
| 53 | DT | 56 | MET |
| 53 | DT | 61 | SER |
| 53 | DT | 62 | LEU |
| 53 | DT | 71 | THR |
| 53 | DT | 79 | ARG |
| 53 | DT | 80 | ARG |
| 53 | DT | 84 | LEU |
| 53 | DT | 89 | ARG |
| 53 | DT | 93 | GLU |
| 54 | DU | 10 | ARG |
| 54 | DU | 15 | ARG |
| 59 | DZ | -55 | LEU |
| 59 | DZ | -53 | ASP |
| 59 | DZ | -47 | ASP |
| 59 | DZ | -29 | LEU |
| 59 | DZ | -20 | LEU |
| 59 | DZ | -13 | GLN |
| 59 | DZ | -10 | ARG |
| 59 | DZ | -6 | ARG |
| 59 | DZ | -5 | LYS |
| 59 | DZ | 7 | ASN |
| 59 | DZ | 8 | ASP |
| 59 | DZ | 9 | LEU |
| 59 | DZ | 12 | LEU |
| 59 | DZ | 15 | ILE |
| 59 | DZ | 21 | ILE |
| 59 | DZ | 25 | LYS |
| 59 | DZ | 26 | THR |
| 59 | DZ | 30 | GLU |
| 59 | DZ | 31 | ARG |
| 59 | DZ | 33 | LEU |
| 59 | DZ | 70 | THR |
| 59 | DZ | 75 | LYS |
| 59 | DZ | 92 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | DZ | 100 | VAL |
| 59 | DZ | 105 | ILE |
| 59 | DZ | 112 | GLN |
| 59 | DZ | 117 | GLN |
| 59 | DZ | 121 | VAL |
| 59 | DZ | 132 | ARG |
| 59 | DZ | 146 | LEU |
| 59 | DZ | 163 | VAL |
| 59 | DZ | 170 | ARG |
| 59 | DZ | 196 | ILE |
| 59 | DZ | 204 | GLU |
| 59 | DZ | 207 | ASP |
| 59 | DZ | 215 | LYS |
| 59 | DZ | 228 | MET |
| 59 | DZ | 232 | LEU |
| 59 | DZ | 236 | GLU |
| 59 | DZ | 240 | GLU |
| 59 | DZ | 255 | ILE |
| 59 | DZ | 264 | LEU |
| 59 | DZ | 277 | VAL |
| 59 | DZ | 285 | ASP |
| 59 | DZ | 286 | ILE |
| 59 | DZ | 292 | THR |
| 59 | DZ | 297 | GLU |
| 59 | DZ | 299 | VAL |
| 59 | DZ | 302 | HIS |
| 59 | DZ | 312 | LEU |
| 59 | DZ | 322 | VAL |
| 59 | DZ | 326 | THR |
| 59 | DZ | 328 | ILE |
| 59 | DZ | 341 | VAL |
| 59 | DZ | 355 | LEU |
| 59 | DZ | 363 | ARG |
| 59 | DZ | 369 | LEU |
| 59 | DZ | 377 | VAL |
| 59 | DZ | 382 | GLU |
| 59 | DZ | 385 | THR |
| 59 | DZ | 396 | ARG |
| 59 | DZ | 399 | LEU |
| 59 | DZ | 403 | GLU |
| 59 | DZ | 421 | GLN |
| 59 | DZ | 422 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59 | DZ | 426 | GLN |
| 59 | DZ | 437 | THR |
| 59 | DZ | 442 | THR |
| 59 | DZ | 443 | HIS |
| 59 | DZ | 446 | THR |
| 59 | DZ | 471 | LYS |
| 59 | DZ | 473 | ASP |
| 59 | DZ | 475 | ASN |
| 59 | DZ | 488 | THR |
| 59 | DZ | 504 | ARG |
| 59 | DZ | 512 | ILE |
| 59 | DZ | 536 | LYS |
| 59 | DZ | 537 | GLU |
| 59 | DZ | 547 | GLU |
| 59 | DZ | 572 | TYR |
| 59 | DZ | 578 | SER |
| 59 | DZ | 598 | ASP |
| 59 | DZ | 600 | VAL |
| 59 | DZ | 601 | ILE |
| 59 | DZ | 602 | LEU |
| 59 | DZ | 612 | THR |
| 59 | DZ | 614 | GLU |
| 59 | DZ | 623 | ASP |
| 59 | DZ | 624 | LEU |
| 59 | DZ | 625 | ASN |
| 59 | DZ | 630 | GLN |
| 59 | DZ | 631 | ILE |
| 59 | DZ | 649 | LEU |
| 59 | DZ | 651 | GLU |
| 59 | DZ | 659 | LEU |
| 59 | DZ | 660 | ARG |
| 59 | DZ | 668 | SER |
| 59 | DZ | 675 | HIS |
| 59 | DZ | 679 | VAL |
| 59 | DZ | 681 | LYS |
| 59 | DZ | 686 | LYS |
| 59 | DZ | 689 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 67 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 189 | ASN |
| 3 | AC | 200 | HIS |
| 4 | AD | 126 | GLN |
| 4 | AD | 253 | GLN |
| 5 | AE | 85 | ASN |
| 6 | AF | 169 | ASN |
| 6 | AF | 203 | GLN |
| 7 | AG | 40 | ASN |
| 7 | AG | 41 | GLN |
| 7 | AG | 132 | ASN |
| 11 | AN | 131 | GLN |
| 13 | AP | 38 | GLN |
| 15 | AR | 71 | GLN |
| 16 | AS | 95 | HIS |
| 18 | AU | 94 | ASN |
| 21 | AX | 31 | HIS |
| 21 | AX | 82 | GLN |
| 22 | AY | 92 | ASN |
| 23 | AZ | 34 | ASN |
| 26 | A2 | 9 | GLN |
| 27 | A3 | 32 | GLN |
| 33 | A9 | 36 | GLN |
| 35 | BB | 40 | HIS |
| 35 | BB | 45 | GLN |
| 36 | BC | 6 | HIS |
| 36 | BC | 118 | GLN |
| 36 | BC | 136 | GLN |
| 36 | BC | 162 | GLN |
| 36 | BC | 176 | HIS |
| 36 | BC | 181 | ASN |
| 37 | BD | 45 | GLN |
| 37 | BD | 119 | GLN |
| 37 | BD | 123 | HIS |
| 37 | BD | 125 | HIS |
| 37 | BD | 160 | GLN |
| 37 | BD | 161 | ASN |
| 38 | BE | 56 | GLN |
| 38 | BE | 141 | GLN |
| 39 | BF | 73 | ASN |
| 40 | BG | 28 | ASN |
| 40 | BG | 51 | GLN |
| 40 | BG | 64 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | BG | 97 | GLN |
| 42 | BI | 23 | ASN |
| 42 | BI | 89 | ASN |
| 42 | BI | 124 | GLN |
| 43 | BJ | 56 | HIS |
| 44 | BK | 104 | GLN |
| 45 | BL | 78 | GLN |
| 47 | BN | 49 | HIS |
| 48 | BO | 9 | GLN |
| 48 | BO | 28 | GLN |
| 49 | BP | 13 | HIS |
| 50 | BQ | 16 | GLN |
| 52 | BS | 65 | ASN |
| 52 | BS | 69 | HIS |
| 53 | BT | 26 | ASN |
| 53 | BT | 45 | GLN |
| 53 | BT | 75 | ASN |
| 59 | BZ | -50 | GLN |
| 59 | BZ | -13 | GLN |
| 59 | BZ | 77 | HIS |
| 59 | BZ | 112 | GLN |
| 59 | BZ | 154 | GLN |
| 59 | BZ | 208 | GLN |
| 59 | BZ | 362 | HIS |
| 59 | BZ | 475 | ASN |
| 59 | BZ | 500 | GLN |
| 59 | BZ | 573 | HIS |
| 59 | BZ | 641 | GLN |
| 59 | BZ | 675 | HIS |
| 59 | BZ | 677 | GLN |
| 59 | BZ | 682 | GLN |
| 3 | CC | 67 | HIS |
| 3 | CC | 189 | ASN |
| 3 | CC | 200 | HIS |
| 4 | CD | 87 | ASN |
| 4 | CD | 96 | HIS |
| 4 | CD | 164 | GLN |
| 4 | CD | 253 | GLN |
| 6 | CF | 69 | HIS |
| 6 | CF | 75 | HIS |
| 6 | CF | 169 | ASN |
| 6 | CF | 203 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | CG | 40 | ASN |
| 10 | CL | 116 | ASN |
| 11 | CN | 133 | GLN |
| 13 | CP | 38 | GLN |
| 14 | CQ | 45 | GLN |
| 15 | CR | 13 | HIS |
| 15 | CR | 31 | HIS |
| 16 | CS | 95 | HIS |
| 18 | CU | 104 | GLN |
| 18 | CU | 117 | GLN |
| 20 | CW | 60 | ASN |
| 21 | CX | 31 | HIS |
| 23 | CZ | 132 | ASN |
| 33 | C9 | 36 | GLN |
| 35 | DB | 16 | HIS |
| 35 | DB | 45 | GLN |
| 35 | DB | 76 | GLN |
| 35 | DB | 94 | ASN |
| 36 | DC | 3 | ASN |
| 36 | DC | 28 | GLN |
| 36 | DC | 37 | GLN |
| 36 | DC | 104 | GLN |
| 36 | DC | 123 | GLN |
| 37 | DD | 123 | HIS |
| 37 | DD | 125 | HIS |
| 37 | DD | 160 | GLN |
| 39 | DF | 7 | ASN |
| 39 | DF | 27 | GLN |
| 39 | DF | 94 | GLN |
| 39 | DF | 100 | ASN |
| 40 | DG | 28 | ASN |
| 40 | DG | 51 | GLN |
| 40 | DG | 96 | GLN |
| 40 | DG | 97 | GLN |
| 40 | DG | 110 | GLN |
| 41 | DH | 15 | ASN |
| 42 | DI | 31 | GLN |
| 42 | DI | 58 | HIS |
| 42 | DI | 73 | GLN |
| 42 | DI | 89 | ASN |
| 42 | DI | 124 | GLN |
| 43 | DJ | 13 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | DJ | 21 | GLN |
| 43 | DJ | 62 | HIS |
| 43 | DJ | 68 | HIS |
| 44 | DK | 93 | GLN |
| 45 | DL | 49 | ASN |
| 45 | DL | 78 | GLN |
| 45 | DL | 99 | HIS |
| 46 | DM | 40 | ASN |
| 46 | DM | 92 | HIS |
| 48 | DO | 28 | GLN |
| 50 | DQ | 16 | GLN |
| 52 | DS | 23 | ASN |
| 52 | DS | 69 | HIS |
| 52 | DS | 83 | HIS |
| 53 | DT | 75 | ASN |
| 59 | DZ | -50 | GLN |
| 59 | DZ | 7 | ASN |
| 59 | DZ | 117 | GLN |
| 59 | DZ | 165 | GLN |
| 59 | DZ | 270 | GLN |
| 59 | DZ | 302 | HIS |
| 59 | DZ | 421 | GLN |
| 59 | DZ | 509 | HIS |
| 59 | DZ | 630 | GLN |
| 59 | DZ | 641 | GLN |
| 59 | DZ | 664 | GLN |
| 59 | DZ | 677 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 2866/2915 (98%) | 477 (16%) | 41 (1%) |
| 1 | CA | 2860/2915 (98%) | 517 (18%) | 37 (1%) |
| 2 | AB | 119/121 (98%) | 11 (9%) | 0 |
| 2 | CB | 119/121 (98%) | 19 (15%) | 0 |
| 34 | BA | 1494/1521 (98%) | 265 (17%) | 21 (1%) |
| 34 | DA | 1501/1521 (98%) | 284 (18%) | 23 (1%) |
| 55 | BV | 12/24 (50%) | 3 (25%) | 0 |
| 55 | DV | 11/24 (45%) | 1 (9%) | 0 |
| 56 | BW | 70/76 (92%) | 18 (25%) | 1 (1%) |
| 56 | DW | 67/76 (88%) | 22 (32%) | 2 (2%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 57 | BX | 74/77 (96%) | 10 (13%) | 0 |
| 57 | DX | 74/77 (96%) | 13 (17%) | 0 |
| 58 | BY | 71/76 (93%) | 20 (28%) | 2 (2%) |
| 58 | DY | 69/76 (90%) | 19 (27%) | 0 |
| All | All | 9407/9620 (97%) | 1679 (17%) | 127 (1%) |

All (1679) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 12 | U |
| 1 | AA | 13 | A |
| 1 | AA | 34 | C |
| 1 | AA | 45 | C |
| 1 | AA | 62 | U |
| 1 | AA | 70 | A |
| 1 | AA | 71 | U |
| 1 | AA | 73 | A |
| 1 | AA | 74 | G |
| 1 | AA | 83 | A |
| 1 | AA | 91 | G |
| 1 | AA | 94 | G |
| 1 | AA | 99 | G |
| 1 | AA | 116 | A |
| 1 | AA | 117 | A |
| 1 | AA | 118 | U |
| 1 | AA | 120 | G |
| 1 | AA | 137 | G |
| 1 | AA | 149 | A |
| 1 | AA | 185 | A |
| 1 | AA | 186 | A |
| 1 | AA | 188 | A |
| 1 | AA | 189 | U |
| 1 | AA | 190 | C |
| 1 | AA | 194 | G |
| 1 | AA | 203 | G |
| 1 | AA | 204 | G |
| 1 | AA | 205 | A |
| 1 | AA | 210 | A |
| 1 | AA | 211 | A |
| 1 | AA | 217 | A |
| 1 | AA | 218 | A |
| 1 | AA | 222 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 237 | G |
| 1 | AA | 239 | G |
| 1 | AA | 262 | C |
| 1 | AA | 269 | G |
| 1 | AA | 271 | U |
| 1 | AA | 272 | U |
| 1 | AA | 273 | G |
| 1 | AA | 274 | U |
| 1 | AA | 276 | C |
| 1 | AA | 279 | G |
| 1 | AA | 289 | G |
| 1 | AA | 299 | G |
| 1 | AA | 303 | C |
| 1 | AA | 311 | C |
| 1 | AA | 335 | A |
| 1 | AA | 348 | A |
| 1 | AA | 353 | G |
| 1 | AA | 354 | A |
| 1 | AA | 376 | G |
| 1 | AA | 387 | G |
| 1 | AA | 407 | U |
| 1 | AA | 413 | G |
| 1 | AA | 423 | G |
| 1 | AA | 434 | G |
| 1 | AA | 438 | G |
| 1 | AA | 439 | A |
| 1 | AA | 455 | A |
| 1 | AA | 469 | A |
| 1 | AA | 470 | C |
| 1 | AA | 474 | U |
| 1 | AA | 477 | C |
| 1 | AA | 482 | C |
| 1 | AA | 483 | A |
| 1 | AA | 496 | A |
| 1 | AA | 501 | U |
| 1 | AA | 505 | A |
| 1 | AA | 507 | G |
| 1 | AA | 519 | G |
| 1 | AA | 529 | U |
| 1 | AA | 530 | A |
| 1 | AA | 534 | C |
| 1 | AA | 551 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 553 | A |
| 1 | AA | 555 | G |
| 1 | AA | 556 | C |
| 1 | AA | 557 | A |
| 1 | AA | 558 | G |
| 1 | AA | 569 | G |
| 1 | AA | 573 | G |
| 1 | AA | 574 | G |
| 1 | AA | 586 | G |
| 1 | AA | 596 | G |
| 1 | AA | 598 | A |
| 1 | AA | 609 | A |
| 1 | AA | 616 | G |
| 1 | AA | 626 | A |
| 1 | AA | 627 | G |
| 1 | AA | 630 | U |
| 1 | AA | 633 | G |
| 1 | AA | 639 | G |
| 1 | AA | 641 | G |
| 1 | AA | 644 | G |
| 1 | AA | 659 | C |
| 1 | AA | 662 | A |
| 1 | AA | 670 | C |
| 1 | AA | 671 | A |
| 1 | AA | 692 | C |
| 1 | AA | 693 | G |
| 1 | AA | 697 | C |
| 1 | AA | 716 | G |
| 1 | AA | 717 | A |
| 1 | AA | 733 | G |
| 1 | AA | 762 | G |
| 1 | AA | 777 | C |
| 1 | AA | 785 | G |
| 1 | AA | 787 | U |
| 1 | AA | 793 | A |
| 1 | AA | 794 | U |
| 1 | AA | 811 | A |
| 1 | AA | 812 | G |
| 1 | AA | 822 | G |
| 1 | AA | 823 | G |
| 1 | AA | 829 | A |
| 1 | AA | 831 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 832 | G |
| 1 | AA | 837 | C |
| 1 | AA | 839 | G |
| 1 | AA | 852 | G |
| 1 | AA | 859 | C |
| 1 | AA | 866 | A |
| 1 | AA | 867 | A |
| 1 | AA | 874 | U |
| 1 | AA | 875 | U |
| 1 | AA | 877 | G |
| 1 | AA | 888 | A |
| 1 | AA | 906 | G |
| 1 | AA | 924 | U |
| 1 | AA | 927 | G |
| 1 | AA | 931 | C |
| 1 | AA | 932 | C |
| 1 | AA | 933 | C |
| 1 | AA | 934 | A |
| 1 | AA | 935 | C |
| 1 | AA | 936 | C |
| 1 | AA | 937 | A |
| 1 | AA | 938 | G |
| 1 | AA | 939 | C |
| 1 | AA | 940 | C |
| 1 | AA | 942 | A |
| 1 | AA | 943 | C |
| 1 | AA | 945 | A |
| 1 | AA | 946 | A |
| 1 | AA | 953 | U |
| 1 | AA | 956 | A |
| 1 | AA | 957 | A |
| 1 | AA | 960 | C |
| 1 | AA | 972 | A |
| 1 | AA | 977 | G |
| 1 | AA | 986 | A |
| 1 | AA | 990 | A |
| 1 | AA | 991 | G |
| 1 | AA | 1003 | U |
| 1 | AA | 1004 | A |
| 1 | AA | 1006 | C |
| 1 | AA | 1019 | G |
| 1 | AA | 1020 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 1029 | A |
| 1 | AA | 1036 | A |
| 1 | AA | 1042 | A |
| 1 | AA | 1051 | C |
| 1 | AA | 1054 | C |
| 1 | AA | 1058 | U |
| 1 | AA | 1059 | C |
| 1 | AA | 1068 | G |
| 1 | AA | 1072 | U |
| 1 | AA | 1077 | G |
| 1 | AA | 1079 | U |
| 1 | AA | 1084 | C |
| 1 | AA | 1092 | A |
| 1 | AA | 1093 | G |
| 1 | AA | 1096 | A |
| 1 | AA | 1099 | C |
| 1 | AA | 1100 | A |
| 1 | AA | 1101 | G |
| 1 | AA | 1105 | G |
| 1 | AA | 1106 | U |
| 1 | AA | 1107 | U |
| 1 | AA | 1108 | G |
| 1 | AA | 1111 | U |
| 1 | AA | 1112 | U |
| 1 | AA | 1116 | A |
| 1 | AA | 1121 | C |
| 1 | AA | 1122 | C |
| 1 | AA | 1125 | C |
| 1 | AA | 1126 | C |
| 1 | AA | 1129 | U |
| 1 | AA | 1134 | A |
| 1 | AA | 1136 | U |
| 1 | AA | 1139 | G |
| 1 | AA | 1154 | U |
| 1 | AA | 1155 | C |
| 1 | AA | 1156 | G |
| 1 | AA | 1174 | A |
| 1 | AA | 1180 | C |
| 1 | AA | 1181 | G |
| 1 | AA | 1184 | G |
| 1 | AA | 1196 | C |
| 1 | AA | 1197 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1210 | G |
| 1 | AA | 1217 | G |
| 1 | AA | 1218 | G |
| 1 | AA | 1219 | A |
| 1 | AA | 1220 | U |
| 1 | AA | 1221 | G |
| 1 | AA | 1222 | A |
| 1 | AA | 1223 | C |
| 1 | AA | 1255 | A |
| 1 | AA | 1256 | U |
| 1 | AA | 1265 | A |
| 1 | AA | 1287 | A |
| 1 | AA | 1290 | G |
| 1 | AA | 1294 | G |
| 1 | AA | 1299 | A |
| 1 | AA | 1302 | G |
| 1 | AA | 1317 | G |
| 1 | AA | 1318 | A |
| 1 | AA | 1322 | A |
| 1 | AA | 1346 | U |
| 1 | AA | 1347 | A |
| 1 | AA | 1349 | G |
| 1 | AA | 1367 | A |
| 1 | AA | 1391 | C |
| 1 | AA | 1405 | A |
| 1 | AA | 1406 | A |
| 1 | AA | 1411 | A |
| 1 | AA | 1425 | A |
| 1 | AA | 1430 | A |
| 1 | AA | 1431 | G |
| 1 | AA | 1462 | G |
| 1 | AA | 1463 | C |
| 1 | AA | 1466 | U |
| 1 | AA | 1467 | G |
| 1 | AA | 1468 | G |
| 1 | AA | 1473 | A |
| 1 | AA | 1474 | C |
| 1 | AA | 1491 | A |
| 1 | AA | 1496 | A |
| 1 | AA | 1497 | G |
| 1 | AA | 1500 | A |
| 1 | AA | 1502 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1508 | G |
| 1 | AA | 1514 | C |
| 1 | AA | 1518 | A |
| 1 | AA | 1525 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1539 | C |
| 1 | AA | 1554 | A |
| 1 | AA | 1555 | C |
| 1 | AA | 1556 | A |
| 1 | AA | 1578 | C |
| 1 | AA | 1587 | U |
| 1 | AA | 1589 | A |
| 1 | AA | 1590 | C |
| 1 | AA | 1605 | A |
| 1 | AA | 1607 | G |
| 1 | AA | 1613 | A |
| 1 | AA | 1616 | A |
| 1 | AA | 1625 | U |
| 1 | AA | 1627 | A |
| 1 | AA | 1628 | G |
| 1 | AA | 1630 | A |
| 1 | AA | 1631 | C |
| 1 | AA | 1632 | A |
| 1 | AA | 1654 | A |
| 1 | AA | 1655 | A |
| 1 | AA | 1656 | A |
| 1 | AA | 1695 | C |
| 1 | AA | 1721 | G |
| 1 | AA | 1743 | G |
| 1 | AA | 1747 | A |
| 1 | AA | 1764 | G |
| 1 | AA | 1767 | A |
| 1 | AA | 1776 | G |
| 1 | AA | 1787 | G |
| 1 | AA | 1788 | U |
| 1 | AA | 1793 | A |
| 1 | AA | 1794 | G |
| 1 | AA | 1795 | G |
| 1 | AA | 1804 | A |
| 1 | AA | 1811 | A |
| 1 | AA | 1813 | C |
| 1 | AA | 1822 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | AA | 1831 | C |
| 1 | AA | 1833 | A |
| 1 | AA | 1847 | G |
| 1 | AA | 1850 | A |
| 1 | AA | 1870 | G |
| 1 | AA | 1878 | A |
| 1 | AA | 1889 | G |
| 1 | AA | 1890 | A |
| 1 | AA | 1892 | G |
| 1 | AA | 1898 | A |
| 1 | AA | 1900 | G |
| 1 | AA | 1911 | A |
| 1 | AA | 1922 | A |
| 1 | AA | 1928 | G |
| 1 | AA | 1935 | A |
| 1 | AA | 1941 | A |
| 1 | AA | 1951 | G |
| 1 | AA | 1952 | G |
| 1 | AA | 1953 | U |
| 1 | AA | 1956 | C |
| 1 | AA | 1960 | A |
| 1 | AA | 1977 | U |
| 1 | AA | 1985 | U |
| 1 | AA | 1987 | C |
| 1 | AA | 1989 | C |
| 1 | AA | 1992 | A |
| 1 | AA | 1993 | A |
| 1 | AA | 1994 | A |
| 1 | AA | 2003 | A |
| 1 | AA | 2014 | G |
| 1 | AA | 2015 | U |
| 1 | AA | 2019 | G |
| 1 | AA | 2028 | C |
| 1 | AA | 2042 | A |
| 1 | AA | 2045 | G |
| 1 | AA | 2053 | A |
| 1 | AA | 2055 | A |
| 1 | AA | 2065 | C |
| 1 | AA | 2073 | A |
| 1 | AA | 2077 | C |
| 1 | AA | 2078 | G |
| 1 | AA | 2082 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 2083 | G |
| 1 | AA | 2084 | A |
| 1 | AA | 2091 | G |
| 1 | AA | 2123 | G |
| 1 | AA | 2132 | G |
| 1 | AA | 2133 | C |
| 1 | AA | 2141 | A |
| 1 | AA | 2143 | G |
| 1 | AA | 2144 | U |
| 1 | AA | 2149 | G |
| 1 | AA | 2152 | U |
| 1 | AA | 2153 | G |
| 1 | AA | 2154 | U |
| 1 | AA | 2155 | G |
| 1 | AA | 2156 | A |
| 1 | AA | 2157 | A |
| 1 | AA | 2158 | C |
| 1 | AA | 2159 | C |
| 1 | AA | 2160 | C |
| 1 | AA | 2162 | C |
| 1 | AA | 2163 | G |
| 1 | AA | 2164 | C |
| 1 | AA | 2165 | C |
| 1 | AA | 2169 | G |
| 1 | AA | 2173 | G |
| 1 | AA | 2175 | G |
| 1 | AA | 2179 | G |
| 1 | AA | 2180 | A |
| 1 | AA | 2181 | G |
| 1 | AA | 2182 | G |
| 1 | AA | 2188 | G |
| 1 | AA | 2190 | G |
| 1 | AA | 2191 | A |
| 1 | AA | 2194 | U |
| 1 | AA | 2195 | A |
| 1 | AA | 2196 | C |
| 1 | AA | 2198 | A |
| 1 | AA | 2199 | C |
| 1 | AA | 2200 | C |
| 1 | AA | 2203 | G |
| 1 | AA | 2204 | G |
| 1 | AA | 2205 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 2206 | G |
| 1 | AA | 2210 | C |
| 1 | AA | 2211 | U |
| 1 | AA | 2213 | G |
| 1 | AA | 2214 | G |
| 1 | AA | 2220 | A |
| 1 | AA | 2221 | A |
| 1 | AA | 2227 | G |
| 1 | AA | 2228 | G |
| 1 | AA | 2229 | A |
| 1 | AA | 2237 | A |
| 1 | AA | 2251 | G |
| 1 | AA | 2252 | C |
| 1 | AA | 2280 | A |
| 1 | AA | 2285 | A |
| 1 | AA | 2287 | C |
| 1 | AA | 2295 | C |
| 1 | AA | 2298 | A |
| 1 | AA | 2299 | A |
| 1 | AA | 2317 | A |
| 1 | AA | 2319 | G |
| 1 | AA | 2320 | G |
| 1 | AA | 2324 | U |
| 1 | AA | 2332 | A |
| 1 | AA | 2337 | G |
| 1 | AA | 2346 | G |
| 1 | AA | 2348 | A |
| 1 | AA | 2352 | G |
| 1 | AA | 2359 | C |
| 1 | AA | 2362 | C |
| 1 | AA | 2366 | G |
| 1 | AA | 2373 | A |
| 1 | AA | 2391 | G |
| 1 | AA | 2395 | G |
| 1 | AA | 2397 | C |
| 1 | AA | 2418 | U |
| 1 | AA | 2426 | G |
| 1 | AA | 2436 | C |
| 1 | AA | 2437 | A |
| 1 | AA | 2441 | G |
| 1 | AA | 2442 | A |
| 1 | AA | 2443 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 2446 | A |
| 1 | AA | 2447 | A |
| 1 | AA | 2451 | A |
| 1 | AA | 2452 | C |
| 1 | AA | 2453 | C |
| 1 | AA | 2459 | G |
| 1 | AA | 2460 | A |
| 1 | AA | 2461 | U |
| 1 | AA | 2471 | A |
| 1 | AA | 2488 | A |
| 1 | AA | 2490 | A |
| 1 | AA | 2506 | G |
| 1 | AA | 2514 | G |
| 1 | AA | 2517 | G |
| 1 | AA | 2530 | A |
| 1 | AA | 2541 | G |
| 1 | AA | 2566 | U |
| 1 | AA | 2567 | U |
| 1 | AA | 2578 | A |
| 1 | AA | 2579 | G |
| 1 | AA | 2585 | C |
| 1 | AA | 2594 | G |
| 1 | AA | 2614 | A |
| 1 | AA | 2621 | U |
| 1 | AA | 2623 | U |
| 1 | AA | 2624 | C |
| 1 | AA | 2640 | C |
| 1 | AA | 2641 | A |
| 1 | AA | 2642 | G |
| 1 | AA | 2644 | A |
| 1 | AA | 2653 | G |
| 1 | AA | 2658 | C |
| 1 | AA | 2666 | A |
| 1 | AA | 2675 | G |
| 1 | AA | 2701 | U |
| 1 | AA | 2702 | C |
| 1 | AA | 2714 | U |
| 1 | AA | 2715 | C |
| 1 | AA | 2725 | A |
| 1 | AA | 2726 | A |
| 1 | AA | 2727 | G |
| 1 | AA | 2739 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 2740 | G |
| 1 | AA | 2746 | A |
| 1 | AA | 2752 | U |
| 1 | AA | 2768 | C |
| 1 | AA | 2771 | A |
| 1 | AA | 2774 | G |
| 1 | AA | 2778 | A |
| 1 | AA | 2779 | G |
| 1 | AA | 2791 | A |
| 1 | AA | 2803 | A |
| 1 | AA | 2804 | C |
| 1 | AA | 2813 | G |
| 1 | AA | 2828 | G |
| 1 | AA | 2830 | A |
| 1 | AA | 2831 | A |
| 1 | AA | 2843 | G |
| 1 | AA | 2845 | A |
| 1 | AA | 2847 | G |
| 1 | AA | 2871 | G |
| 1 | AA | 2882 | G |
| 1 | AA | 2883 | A |
| 1 | AA | 2890 | C |
| 1 | AA | 2902 | G |
| 1 | AA | 2903 | G |
| 2 | AB | 2 | C |
| 2 | AB | 9 | G |
| 2 | AB | 12 | C |
| 2 | AB | 21 | G |
| 2 | AB | 45 | A |
| 2 | AB | 47 | C |
| 2 | AB | 56 | G |
| 2 | AB | 67 | G |
| 2 | AB | 73 | A |
| 2 | AB | 110 | G |
| 2 | AB | 116 | G |
| 34 | BA | 5 | U |
| 34 | BA | 7 | G |
| 34 | BA | 9 | G |
| 34 | BA | 29 | G |
| 34 | BA | 30 | U |
| 34 | BA | 32 | A |
| 34 | BA | 39 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 34 | BA | 47 | C |
| 34 | BA | 48 | C |
| 34 | BA | 50 | A |
| 34 | BA | 51 | A |
| 34 | BA | 58 | C |
| 34 | BA | 61 | G |
| 34 | BA | 69 | G |
| 34 | BA | 77 | G |
| 34 | BA | 79 | G |
| 34 | BA | 91 | C |
| 34 | BA | 97 | G |
| 34 | BA | 101 | A |
| 34 | BA | 115 | G |
| 34 | BA | 116 | A |
| 34 | BA | 121 | C |
| 34 | BA | 129(A) | G |
| 34 | BA | 131 | C |
| 34 | BA | 139 | G |
| 34 | BA | 161 | A |
| 34 | BA | 163 | C |
| 34 | BA | 174 | C |
| 34 | BA | 182 | U |
| 34 | BA | 189(D) | C |
| 34 | BA | 189(F) | U |
| 34 | BA | 195 | A |
| 34 | BA | 197 | A |
| 34 | BA | 199 | G |
| 34 | BA | 202 | U |
| 34 | BA | 204 | U |
| 34 | BA | 216 | G |
| 34 | BA | 222 | U |
| 34 | BA | 247 | G |
| 34 | BA | 251 | G |
| 34 | BA | 266 | G |
| 34 | BA | 267 | C |
| 34 | BA | 289 | G |
| 34 | BA | 301 | G |
| 34 | BA | 321 | A |
| 34 | BA | 328 | C |
| 34 | BA | 332 | G |
| 34 | BA | 342 | C |
| 34 | BA | 343 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | BA | 346 | G |
| 34 | BA | 347 | G |
| 34 | BA | 348 | G |
| 34 | BA | 351 | G |
| 34 | BA | 352 | C |
| 34 | BA | 353 | A |
| 34 | BA | 354 | G |
| 34 | BA | 355 | C |
| 34 | BA | 365 | U |
| 34 | BA | 367 | U |
| 34 | BA | 372 | C |
| 34 | BA | 373 | A |
| 34 | BA | 383 | A |
| 34 | BA | 384 | G |
| 34 | BA | 388 | G |
| 34 | BA | 397 | A |
| 34 | BA | 398 | C |
| 34 | BA | 406 | G |
| 34 | BA | 412 | A |
| 34 | BA | 413 | G |
| 34 | BA | 424 | G |
| 34 | BA | 429 | U |
| 34 | BA | 439 | A |
| 34 | BA | 442 | C |
| 34 | BA | 452 | A |
| 34 | BA | 470 | C |
| 34 | BA | 485 | G |
| 34 | BA | 496 | A |
| 34 | BA | 498 | U |
| 34 | BA | 505 | G |
| 34 | BA | 509 | A |
| 34 | BA | 510 | A |
| 34 | BA | 511 | C |
| 34 | BA | 513 | C |
| 34 | BA | 518 | C |
| 34 | BA | 524 | G |
| 34 | BA | 527 | G |
| 34 | BA | 531 | U |
| 34 | BA | 532 | A |
| 34 | BA | 533 | A |
| 34 | BA | 536 | C |
| 34 | BA | 547 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | BA | 559 | A |
| 34 | BA | 561 | U |
| 34 | BA | 572 | A |
| 34 | BA | 573 | A |
| 34 | BA | 576 | G |
| 34 | BA | 577 | G |
| 34 | BA | 596 | C |
| 34 | BA | 607 | A |
| 34 | BA | 616 | G |
| 34 | BA | 618 | C |
| 34 | BA | 630 | G |
| 34 | BA | 631 | G |
| 34 | BA | 632 | A |
| 34 | BA | 634 | C |
| 34 | BA | 653 | A |
| 34 | BA | 661 | G |
| 34 | BA | 665 | A |
| 34 | BA | 666 | G |
| 34 | BA | 667 | G |
| 34 | BA | 671 | G |
| 34 | BA | 673 | G |
| 34 | BA | 687 | A |
| 34 | BA | 688 | G |
| 34 | BA | 695 | A |
| 34 | BA | 723 | U |
| 34 | BA | 724 | G |
| 34 | BA | 728 | A |
| 34 | BA | 731 | G |
| 34 | BA | 749 | C |
| 34 | BA | 755 | G |
| 34 | BA | 765 | G |
| 34 | BA | 786 | G |
| 34 | BA | 788 | U |
| 34 | BA | 792 | A |
| 34 | BA | 793 | U |
| 34 | BA | 794 | A |
| 34 | BA | 815 | A |
| 34 | BA | 817 | C |
| 34 | BA | 828 | A |
| 34 | BA | 832 | C |
| 34 | BA | 840 | C |
| 34 | BA | 841 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | BA | 848 | C |
| 34 | BA | 851 | G |
| 34 | BA | 859 | A |
| 34 | BA | 860 | A |
| 34 | BA | 874 | G |
| 34 | BA | 875 | C |
| 34 | BA | 876 | G |
| 34 | BA | 902 | G |
| 34 | BA | 908 | A |
| 34 | BA | 914 | A |
| 34 | BA | 926 | G |
| 34 | BA | 927 | G |
| 34 | BA | 932 | C |
| 34 | BA | 934 | C |
| 34 | BA | 935 | A |
| 34 | BA | 942 | G |
| 34 | BA | 960 | U |
| 34 | BA | 961 | U |
| 34 | BA | 968 | A |
| 34 | BA | 969 | A |
| 34 | BA | 971 | G |
| 34 | BA | 972 | C |
| 34 | BA | 974 | A |
| 34 | BA | 975 | A |
| 34 | BA | 976 | G |
| 34 | BA | 977 | A |
| 34 | BA | 982 | U |
| 34 | BA | 992 | U |
| 34 | BA | 993 | G |
| 34 | BA | 1000 | U |
| 34 | BA | 1003 | G |
| 34 | BA | 1004 | A |
| 34 | BA | 1005 | A |
| 34 | BA | 1008 | C |
| 34 | BA | 1009 | G |
| 34 | BA | 1016 | A |
| 34 | BA | 1019 | C |
| 34 | BA | 1022 | G |
| 34 | BA | 1023 | G |
| 34 | BA | 1025 | U |
| 34 | BA | 1027 | C |
| 34 | BA | 1028 | C |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | BA | 1030 | C |
| 34 | BA | 1030(A) | G |
| 34 | BA | 1030(C) | G |
| 34 | BA | 1031 | G |
| 34 | BA | 1033 | G |
| 34 | BA | 1045 | C |
| 34 | BA | 1054 | C |
| 34 | BA | 1065 | U |
| 34 | BA | 1066 | C |
| 34 | BA | 1068 | G |
| 34 | BA | 1070 | U |
| 34 | BA | 1081 | G |
| 34 | BA | 1094 | G |
| 34 | BA | 1095 | U |
| 34 | BA | 1101 | A |
| 34 | BA | 1108 | G |
| 34 | BA | 1123 | A |
| 34 | BA | 1124 | G |
| 34 | BA | 1125 | U |
| 34 | BA | 1126 | U |
| 34 | BA | 1134 | G |
| 34 | BA | 1136 | U |
| 34 | BA | 1137 | C |
| 34 | BA | 1138 | G |
| 34 | BA | 1139 | G |
| 34 | BA | 1140 | C |
| 34 | BA | 1141 | C |
| 34 | BA | 1145 | C |
| 34 | BA | 1146 | A |
| 34 | BA | 1152 | A |
| 34 | BA | 1159 | U |
| 34 | BA | 1166 | G |
| 34 | BA | 1183 | A |
| 34 | BA | 1184 | G |
| 34 | BA | 1187 | G |
| 34 | BA | 1189 | C |
| 34 | BA | 1196 | U |
| 34 | BA | 1197 | G |
| 34 | BA | 1202 | G |
| 34 | BA | 1212 | U |
| 34 | BA | 1213 | A |
| 34 | BA | 1227 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 34 | BA | 1236 | A |
| 34 | BA | 1238 | A |
| 34 | BA | 1240 | U |
| 34 | BA | 1253 | G |
| 34 | BA | 1256 | A |
| 34 | BA | 1257 | U |
| 34 | BA | 1258 | G |
| 34 | BA | 1260 | C |
| 34 | BA | 1270 | C |
| 34 | BA | 1273 | G |
| 34 | BA | 1278 | U |
| 34 | BA | 1279 | A |
| 34 | BA | 1280 | A |
| 34 | BA | 1286 | A |
| 34 | BA | 1287 | A |
| 34 | BA | 1299 | A |
| 34 | BA | 1300 | G |
| 34 | BA | 1302 | U |
| 34 | BA | 1321 | C |
| 34 | BA | 1335 | C |
| 34 | BA | 1336 | C |
| 34 | BA | 1338 | G |
| 34 | BA | 1340 | A |
| 34 | BA | 1347 | G |
| 34 | BA | 1353 | G |
| 34 | BA | 1359 | C |
| 34 | BA | 1360 | A |
| 34 | BA | 1363 | C |
| 34 | BA | 1364 | U |
| 34 | BA | 1370 | G |
| 34 | BA | 1397 | C |
| 34 | BA | 1419 | G |
| 34 | BA | 1442 | G |
| 34 | BA | 1442(A) | G |
| 34 | BA | 1447 | A |
| 34 | BA | 1452 | C |
| 34 | BA | 1492 | A |
| 34 | BA | 1494 | G |
| 34 | BA | 1502 | A |
| 34 | BA | 1503 | A |
| 34 | BA | 1504 | G |
| 34 | BA | 1506 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | BA | 1516 | G |
| 34 | BA | 1517 | G |
| 34 | BA | 1519 | A |
| 34 | BA | 1529 | G |
| 34 | BA | 1530 | G |
| 34 | BA | 1531 | A |
| 55 | BV | 13 | A |
| 55 | BV | 23 | A |
| 55 | BV | 24 | A |
| 56 | BW | 3 | C |
| 56 | BW | 8 | 4SU |
| 56 | BW | 9 | A |
| 56 | BW | 13 | C |
| 56 | BW | 14 | A |
| 56 | BW | 19 | G |
| 56 | BW | 20 | U |
| 56 | BW | 21 | A |
| 56 | BW | 24 | G |
| 56 | BW | 45 | U |
| 56 | BW | 46 | 7MG |
| 56 | BW | 47 | U |
| 56 | BW | 48 | C |
| 56 | BW | 49 | C |
| 56 | BW | 64 | A |
| 56 | BW | 68 | C |
| 56 | BW | 73 | A |
| 56 | BW | 74 | C |
| 57 | BX | 13 | C |
| 57 | BX | 19 | G |
| 57 | BX | 21 | A |
| 57 | BX | 34 | C |
| 57 | BX | 42 | G |
| 57 | BX | 47 | U |
| 57 | BX | 49 | G |
| 57 | BX | 56 | C |
| 57 | BX | 58 | A |
| 57 | BX | 68 | C |
| 58 | BY | 5 | G |
| 58 | BY | 6 | G |
| 58 | BY | 9 | A |
| 58 | BY | 13 | C |
| 58 | BY | 14 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 58 | BY | 20 | U |
| 58 | BY | 21 | A |
| 58 | BY | 26 | A |
| 58 | BY | 36 | A |
| 58 | BY | 41 | C |
| 58 | BY | 42 | C |
| 58 | BY | 44 | G |
| 58 | BY | 45 | U |
| 58 | BY | 46 | 7MG |
| 58 | BY | 47 | U |
| 58 | BY | 48 | C |
| 58 | BY | 57 | G |
| 58 | BY | 59 | U |
| 58 | BY | 60 | U |
| 58 | BY | 68 | C |
| 1 | CA | 12 | U |
| 1 | CA | 13 | A |
| 1 | CA | 34 | C |
| 1 | CA | 36 | G |
| 1 | CA | 41 | C |
| 1 | CA | 45 | C |
| 1 | CA | 64 | A |
| 1 | CA | 71 | A |
| 1 | CA | 74 | A |
| 1 | CA | 75 | G |
| 1 | CA | 84 | A |
| 1 | CA | 90 | U |
| 1 | CA | 95 | G |
| 1 | CA | 100 | G |
| 1 | CA | 102 | G |
| 1 | CA | 118 | A |
| 1 | CA | 119 | A |
| 1 | CA | 120 | U |
| 1 | CA | 141 | A |
| 1 | CA | 154(A) | C |
| 1 | CA | 157 | U |
| 1 | CA | 173 | G |
| 1 | CA | 196 | A |
| 1 | CA | 205 | G |
| 1 | CA | 214 | G |
| 1 | CA | 215 | G |
| 1 | CA | 216 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 221 | A |
| 1 | CA | 222 | A |
| 1 | CA | 225 | A |
| 1 | CA | 228 | A |
| 1 | CA | 229 | A |
| 1 | CA | 248 | G |
| 1 | CA | 250 | G |
| 1 | CA | 271(I) | G |
| 1 | CA | 271(K) | U |
| 1 | CA | 271(L) | U |
| 1 | CA | 271(M) | G |
| 1 | CA | 271(N) | U |
| 1 | CA | 271(O) | C |
| 1 | CA | 272(A) | U |
| 1 | CA | 272(B) | G |
| 1 | CA | 277 | C |
| 1 | CA | 278 | A |
| 1 | CA | 283 | A |
| 1 | CA | 294 | A |
| 1 | CA | 299 | A |
| 1 | CA | 304 | G |
| 1 | CA | 311 | A |
| 1 | CA | 329 | G |
| 1 | CA | 330 | A |
| 1 | CA | 338 | G |
| 1 | CA | 342 | G |
| 1 | CA | 345 | A |
| 1 | CA | 352 | G |
| 1 | CA | 357 | A |
| 1 | CA | 362 | U |
| 1 | CA | 363 | G |
| 1 | CA | 363(B) | G |
| 1 | CA | 363(C) | G |
| 1 | CA | 363(F) | A |
| 1 | CA | 386 | G |
| 1 | CA | 395 | U |
| 1 | CA | 407 | G |
| 1 | CA | 411 | G |
| 1 | CA | 412 | A |
| 1 | CA | 422 | A |
| 1 | CA | 428 | A |
| 1 | CA | 443 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | CA | 444 | C |
| 1 | CA | 455 | C |
| 1 | CA | 456 | C |
| 1 | CA | 457 | A |
| 1 | CA | 470 | A |
| 1 | CA | 471 | A |
| 1 | CA | 481 | G |
| 1 | CA | 501 | A |
| 1 | CA | 504 | U |
| 1 | CA | 505 | A |
| 1 | CA | 509 | C |
| 1 | CA | 528 | A |
| 1 | CA | 529 | A |
| 1 | CA | 530 | G |
| 1 | CA | 531 | C |
| 1 | CA | 532 | A |
| 1 | CA | 533 | G |
| 1 | CA | 545 | G |
| 1 | CA | 563 | G |
| 1 | CA | 573 | G |
| 1 | CA | 575 | A |
| 1 | CA | 586 | A |
| 1 | CA | 587 | C |
| 1 | CA | 588 | U |
| 1 | CA | 599 | G |
| 1 | CA | 603 | A |
| 1 | CA | 604 | G |
| 1 | CA | 606 | U |
| 1 | CA | 607 | U |
| 1 | CA | 614(B) | G |
| 1 | CA | 614(C) | A |
| 1 | CA | 615 | G |
| 1 | CA | 616 | G |
| 1 | CA | 627 | A |
| 1 | CA | 631 | A |
| 1 | CA | 637 | A |
| 1 | CA | 645 | C |
| 1 | CA | 646 | A |
| 1 | CA | 652(A) | A |
| 1 | CA | 652(B) | A |
| 1 | CA | 652(C) | G |
| 1 | CA | 652(U) | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | CA | 668 | G |
| 1 | CA | 669 | G |
| 1 | CA | 686 | G |
| 1 | CA | 709 | U |
| 1 | CA | 730 | C |
| 1 | CA | 752 | A |
| 1 | CA | 753 | C |
| 1 | CA | 764 | A |
| 1 | CA | 765 | G |
| 1 | CA | 774 | A |
| 1 | CA | 775 | G |
| 1 | CA | 776 | G |
| 1 | CA | 782 | A |
| 1 | CA | 784 | A |
| 1 | CA | 785 | G |
| 1 | CA | 790 | C |
| 1 | CA | 792 | G |
| 1 | CA | 805 | G |
| 1 | CA | 812 | C |
| 1 | CA | 819 | A |
| 1 | CA | 827 | U |
| 1 | CA | 828 | U |
| 1 | CA | 857 | C |
| 1 | CA | 859 | G |
| 1 | CA | 866 | A |
| 1 | CA | 879 | G |
| 1 | CA | 880 | G |
| 1 | CA | 884 | C |
| 1 | CA | 886 | C |
| 1 | CA | 887 | A |
| 1 | CA | 888 | C |
| 1 | CA | 889 | C |
| 1 | CA | 890 | A |
| 1 | CA | 893 | C |
| 1 | CA | 896 | A |
| 1 | CA | 897 | C |
| 1 | CA | 898 | C |
| 1 | CA | 900 | A |
| 1 | CA | 901 | A |
| 1 | CA | 902 | C |
| 1 | CA | 910 | A |
| 1 | CA | 917 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 931 | G |
| 1 | CA | 932 | G |
| 1 | CA | 938 | G |
| 1 | CA | 941 | A |
| 1 | CA | 945 | A |
| 1 | CA | 946 | G |
| 1 | CA | 958 | U |
| 1 | CA | 959 | A |
| 1 | CA | 961 | C |
| 1 | CA | 968 | G |
| 1 | CA | 974 | G |
| 1 | CA | 975 | C |
| 1 | CA | 983 | A |
| 1 | CA | 996 | A |
| 1 | CA | 1002 | G |
| 1 | CA | 1005 | C |
| 1 | CA | 1012 | U |
| 1 | CA | 1013 | C |
| 1 | CA | 1016 | G |
| 1 | CA | 1022 | G |
| 1 | CA | 1033 | U |
| 1 | CA | 1036 | G |
| 1 | CA | 1038 | C |
| 1 | CA | 1039 | G |
| 1 | CA | 1042 | G |
| 1 | CA | 1046 | A |
| 1 | CA | 1047 | G |
| 1 | CA | 1048 | A |
| 1 | CA | 1053 | C |
| 1 | CA | 1054 | A |
| 1 | CA | 1055 | G |
| 1 | CA | 1058 | G |
| 1 | CA | 1059 | G |
| 1 | CA | 1060 | U |
| 1 | CA | 1061 | U |
| 1 | CA | 1062 | G |
| 1 | CA | 1063 | G |
| 1 | CA | 1064 | C |
| 1 | CA | 1069 | A |
| 1 | CA | 1070 | A |
| 1 | CA | 1073 | A |
| 1 | CA | 1076 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1081 | U |
| 1 | CA | 1083 | U |
| 1 | CA | 1088 | A |
| 1 | CA | 1090 | U |
| 1 | CA | 1100 | C |
| 1 | CA | 1101 | U |
| 1 | CA | 1107 | G |
| 1 | CA | 1109 | C |
| 1 | CA | 1110 | G |
| 1 | CA | 1111 | A |
| 1 | CA | 1112 | G |
| 1 | CA | 1113 | U |
| 1 | CA | 1116 | C |
| 1 | CA | 1119 | C |
| 1 | CA | 1128 | A |
| 1 | CA | 1135 | C |
| 1 | CA | 1136 | G |
| 1 | CA | 1139 | G |
| 1 | CA | 1151 | G |
| 1 | CA | 1155 | A |
| 1 | CA | 1204 | A |
| 1 | CA | 1210 | A |
| 1 | CA | 1211 | U |
| 1 | CA | 1220 | A |
| 1 | CA | 1241 | A |
| 1 | CA | 1252 | G |
| 1 | CA | 1253 | A |
| 1 | CA | 1256 | G |
| 1 | CA | 1271 | G |
| 1 | CA | 1272 | A |
| 1 | CA | 1273 | U |
| 1 | CA | 1287 | A |
| 1 | CA | 1300 | U |
| 1 | CA | 1301 | A |
| 1 | CA | 1308 | A |
| 1 | CA | 1314 | C |
| 1 | CA | 1327 | C |
| 1 | CA | 1342 | A |
| 1 | CA | 1359 | A |
| 1 | CA | 1360 | A |
| 1 | CA | 1365 | A |
| 1 | CA | 1368 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 1370 | C |
| 1 | CA | 1379 | A |
| 1 | CA | 1384 | A |
| 1 | CA | 1385 | G |
| 1 | CA | 1386 | C |
| 1 | CA | 1395 | A |
| 1 | CA | 1416 | G |
| 1 | CA | 1417 | C |
| 1 | CA | 1419 | A |
| 1 | CA | 1420 | U |
| 1 | CA | 1421 | G |
| 1 | CA | 1427 | A |
| 1 | CA | 1428 | C |
| 1 | CA | 1436 | G |
| 1 | CA | 1437 | C |
| 1 | CA | 1445 | A |
| 1 | CA | 1449 | A |
| 1 | CA | 1450 | G |
| 1 | CA | 1455 | G |
| 1 | CA | 1459 | G |
| 1 | CA | 1465 | G |
| 1 | CA | 1467 | C |
| 1 | CA | 1471 | A |
| 1 | CA | 1482 | G |
| 1 | CA | 1490 | A |
| 1 | CA | 1493 | C |
| 1 | CA | 1494 | A |
| 1 | CA | 1496 | A |
| 1 | CA | 1497 | U |
| 1 | CA | 1509 | C |
| 1 | CA | 1509(A) | A |
| 1 | CA | 1525 | G |
| 1 | CA | 1531 | C |
| 1 | CA | 1532 | C |
| 1 | CA | 1533 | G |
| 1 | CA | 1542 | A |
| 1 | CA | 1547 | C |
| 1 | CA | 1554 | A |
| 1 | CA | 1558 | A |
| 1 | CA | 1559 | G |
| 1 | CA | 1560 | G |
| 1 | CA | 1566 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1569 | A |
| 1 | CA | 1578 | U |
| 1 | CA | 1582 | C |
| 1 | CA | 1584 | C |
| 1 | CA | 1586 | A |
| 1 | CA | 1608 | A |
| 1 | CA | 1609 | A |
| 1 | CA | 1616 | A |
| 1 | CA | 1648 | C |
| 1 | CA | 1654 | A |
| 1 | CA | 1674 | G |
| 1 | CA | 1676 | A |
| 1 | CA | 1696 | G |
| 1 | CA | 1700 | A |
| 1 | CA | 1701 | A |
| 1 | CA | 1703 | G |
| 1 | CA | 1722 | A |
| 1 | CA | 1739 | U |
| 1 | CA | 1756 | G |
| 1 | CA | 1763 | G |
| 1 | CA | 1764 | G |
| 1 | CA | 1773 | A |
| 1 | CA | 1780 | A |
| 1 | CA | 1791 | A |
| 1 | CA | 1800 | C |
| 1 | CA | 1801 | G |
| 1 | CA | 1812 | A |
| 1 | CA | 1816 | G |
| 1 | CA | 1829 | A |
| 1 | CA | 1835 | G |
| 1 | CA | 1847 | A |
| 1 | CA | 1848 | A |
| 1 | CA | 1866 | C |
| 1 | CA | 1877 | A |
| 1 | CA | 1878 | G |
| 1 | CA | 1883 | G |
| 1 | CA | 1889 | A |
| 1 | CA | 1900 | A |
| 1 | CA | 1906 | G |
| 1 | CA | 1913 | A |
| 1 | CA | 1914 | C |
| 1 | CA | 1929 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 1930 | G |
| 1 | CA | 1934 | C |
| 1 | CA | 1952 | A |
| 1 | CA | 1955 | U |
| 1 | CA | 1963 | U |
| 1 | CA | 1967 | C |
| 1 | CA | 1970 | A |
| 1 | CA | 1971 | A |
| 1 | CA | 1972 | A |
| 1 | CA | 1983 | C |
| 1 | CA | 1992 | G |
| 1 | CA | 1993 | U |
| 1 | CA | 1997 | G |
| 1 | CA | 2005 | A |
| 1 | CA | 2020 | A |
| 1 | CA | 2023 | G |
| 1 | CA | 2031 | A |
| 1 | CA | 2032 | G |
| 1 | CA | 2033 | A |
| 1 | CA | 2038 | G |
| 1 | CA | 2043 | C |
| 1 | CA | 2046 | G |
| 1 | CA | 2055 | C |
| 1 | CA | 2056 | G |
| 1 | CA | 2060 | A |
| 1 | CA | 2061 | G |
| 1 | CA | 2062 | A |
| 1 | CA | 2063 | C |
| 1 | CA | 2069 | G |
| 1 | CA | 2082 | A |
| 1 | CA | 2096 | U |
| 1 | CA | 2102 | U |
| 1 | CA | 2106 | G |
| 1 | CA | 2110 | G |
| 1 | CA | 2111 | C |
| 1 | CA | 2112 | G |
| 1 | CA | 2113 | U |
| 1 | CA | 2115 | G |
| 1 | CA | 2116 | G |
| 1 | CA | 2117 | A |
| 1 | CA | 2119 | A |
| 1 | CA | 2122 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 2124 | G |
| 1 | CA | 2126 | A |
| 1 | CA | 2127 | G |
| 1 | CA | 2130 | U |
| 1 | CA | 2131 | G |
| 1 | CA | 2132 | U |
| 1 | CA | 2133 | G |
| 1 | CA | 2134 | A |
| 1 | CA | 2135 | A |
| 1 | CA | 2136 | C |
| 1 | CA | 2137 | C |
| 1 | CA | 2142 | C |
| 1 | CA | 2144 | U |
| 1 | CA | 2146 | C |
| 1 | CA | 2148 | G |
| 1 | CA | 2150 | U |
| 1 | CA | 2153 | G |
| 1 | CA | 2154 | G |
| 1 | CA | 2157 | G |
| 1 | CA | 2158 | A |
| 1 | CA | 2161 | C |
| 1 | CA | 2162 | G |
| 1 | CA | 2164 | C |
| 1 | CA | 2165 | G |
| 1 | CA | 2166 | G |
| 1 | CA | 2167 | U |
| 1 | CA | 2168 | G |
| 1 | CA | 2169 | A |
| 1 | CA | 2170 | A |
| 1 | CA | 2172 | U |
| 1 | CA | 2173 | A |
| 1 | CA | 2178 | C |
| 1 | CA | 2181 | G |
| 1 | CA | 2185 | C |
| 1 | CA | 2186 | G |
| 1 | CA | 2188 | C |
| 1 | CA | 2189 | U |
| 1 | CA | 2192 | G |
| 1 | CA | 2198 | A |
| 1 | CA | 2206 | G |
| 1 | CA | 2207 | G |
| 1 | CA | 2208 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 2218 | U |
| 1 | CA | 2225 | A |
| 1 | CA | 2238 | G |
| 1 | CA | 2239 | G |
| 1 | CA | 2240 | C |
| 1 | CA | 2248 | C |
| 1 | CA | 2268 | A |
| 1 | CA | 2269 | A |
| 1 | CA | 2275 | C |
| 1 | CA | 2278 | A |
| 1 | CA | 2279 | G |
| 1 | CA | 2283 | C |
| 1 | CA | 2287 | A |
| 1 | CA | 2289 | G |
| 1 | CA | 2294 | C |
| 1 | CA | 2305 | A |
| 1 | CA | 2308 | G |
| 1 | CA | 2312 | U |
| 1 | CA | 2319 | G |
| 1 | CA | 2320 | A |
| 1 | CA | 2321 | G |
| 1 | CA | 2325 | G |
| 1 | CA | 2334 | G |
| 1 | CA | 2336 | A |
| 1 | CA | 2343 | C |
| 1 | CA | 2347 | C |
| 1 | CA | 2350 | C |
| 1 | CA | 2354 | G |
| 1 | CA | 2376 | A |
| 1 | CA | 2383 | G |
| 1 | CA | 2385 | C |
| 1 | CA | 2406 | U |
| 1 | CA | 2410 | G |
| 1 | CA | 2423 | U |
| 1 | CA | 2424 | C |
| 1 | CA | 2425 | A |
| 1 | CA | 2428 | G |
| 1 | CA | 2429 | G |
| 1 | CA | 2430 | A |
| 1 | CA | 2435 | A |
| 1 | CA | 2439 | A |
| 1 | CA | 2440 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | CA | 2441 | C |
| 1 | CA | 2448 | A |
| 1 | CA | 2452 | C |
| 1 | CA | 2474 | C |
| 1 | CA | 2476 | A |
| 1 | CA | 2491 | U |
| 1 | CA | 2492 | U |
| 1 | CA | 2494 | G |
| 1 | CA | 2498 | C |
| 1 | CA | 2502 | G |
| 1 | CA | 2505 | G |
| 1 | CA | 2506 | U |
| 1 | CA | 2518 | A |
| 1 | CA | 2520 | C |
| 1 | CA | 2529 | G |
| 1 | CA | 2554 | U |
| 1 | CA | 2564 | A |
| 1 | CA | 2566 | A |
| 1 | CA | 2567 | G |
| 1 | CA | 2573 | C |
| 1 | CA | 2582 | G |
| 1 | CA | 2602 | A |
| 1 | CA | 2611 | U |
| 1 | CA | 2612 | C |
| 1 | CA | 2629 | A |
| 1 | CA | 2630 | G |
| 1 | CA | 2632 | A |
| 1 | CA | 2636 | U |
| 1 | CA | 2654 | A |
| 1 | CA | 2663 | G |
| 1 | CA | 2669 | G |
| 1 | CA | 2673 | G |
| 1 | CA | 2689 | U |
| 1 | CA | 2690 | C |
| 1 | CA | 2703 | C |
| 1 | CA | 2712(A) | A |
| 1 | CA | 2713 | A |
| 1 | CA | 2718 | G |
| 1 | CA | 2721 | A |
| 1 | CA | 2726 | U |
| 1 | CA | 2733 | A |
| 1 | CA | 2739 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | CA | 2744 | G |
| 1 | CA | 2748 | A |
| 1 | CA | 2751 | G |
| 1 | CA | 2757 | A |
| 1 | CA | 2758 | A |
| 1 | CA | 2761 | G |
| 1 | CA | 2764 | A |
| 1 | CA | 2765 | A |
| 1 | CA | 2766 | G |
| 1 | CA | 2778 | A |
| 1 | CA | 2793 | G |
| 1 | CA | 2794 | C |
| 1 | CA | 2802 | G |
| 1 | CA | 2808 | U |
| 1 | CA | 2818 | G |
| 1 | CA | 2820 | A |
| 1 | CA | 2821 | A |
| 1 | CA | 2833 | G |
| 1 | CA | 2835 | A |
| 1 | CA | 2839 | G |
| 1 | CA | 2872 | G |
| 1 | CA | 2876 | G |
| 1 | CA | 2880 | C |
| 1 | CA | 2892 | A |
| 1 | CA | 2893 | G |
| 1 | CA | 2894 | G |
| 1 | CA | 2896 | C |
| 1 | CA | 2897 | U |
| 2 | CB | 2 | C |
| 2 | CB | 7 | G |
| 2 | CB | 8 | U |
| 2 | CB | 12 | C |
| 2 | CB | 13 | A |
| 2 | CB | 15 | A |
| 2 | CB | 25 | A |
| 2 | CB | 28 | C |
| 2 | CB | 30 | C |
| 2 | CB | 32 | C |
| 2 | CB | 42 | C |
| 2 | CB | 52 | A |
| 2 | CB | 56 | G |
| 2 | CB | 58 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | CB | 73 | A |
| 2 | CB | 85 | G |
| 2 | CB | 95 | C |
| 2 | CB | 106 | G |
| 2 | CB | 110 | G |
| 34 | DA | 5 | U |
| 34 | DA | 9 | G |
| 34 | DA | 22 | G |
| 34 | DA | 26 | A |
| 34 | DA | 32 | A |
| 34 | DA | 39 | G |
| 34 | DA | 47 | C |
| 34 | DA | 48 | C |
| 34 | DA | 50 | A |
| 34 | DA | 51 | A |
| 34 | DA | 60 | A |
| 34 | DA | 61 | G |
| 34 | DA | 65 | U |
| 34 | DA | 66 | G |
| 34 | DA | 73 | G |
| 34 | DA | 80 | G |
| 34 | DA | 88 | A |
| 34 | DA | 89 | C |
| 34 | DA | 97 | G |
| 34 | DA | 98 | G |
| 34 | DA | 101 | A |
| 34 | DA | 116 | A |
| 34 | DA | 121 | C |
| 34 | DA | 122 | G |
| 34 | DA | 129(A) | G |
| 34 | DA | 131 | C |
| 34 | DA | 144 | G |
| 34 | DA | 151 | A |
| 34 | DA | 163 | C |
| 34 | DA | 180 | U |
| 34 | DA | 182 | U |
| 34 | DA | 189(E) | U |
| 34 | DA | 189(F) | U |
| 34 | DA | 189(K) | U |
| 34 | DA | 195 | A |
| 34 | DA | 197 | A |
| 34 | DA | 201 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DA | 203 | U |
| 34 | DA | 204 | U |
| 34 | DA | 216 | G |
| 34 | DA | 221 | C |
| 34 | DA | 231 | G |
| 34 | DA | 247 | G |
| 34 | DA | 251 | G |
| 34 | DA | 258 | G |
| 34 | DA | 266 | G |
| 34 | DA | 267 | C |
| 34 | DA | 269 | C |
| 34 | DA | 281 | G |
| 34 | DA | 289 | G |
| 34 | DA | 301 | G |
| 34 | DA | 317 | G |
| 34 | DA | 321 | A |
| 34 | DA | 328 | C |
| 34 | DA | 332 | G |
| 34 | DA | 344 | A |
| 34 | DA | 352 | C |
| 34 | DA | 353 | A |
| 34 | DA | 354 | G |
| 34 | DA | 355 | C |
| 34 | DA | 367 | U |
| 34 | DA | 372 | C |
| 34 | DA | 373 | A |
| 34 | DA | 384 | G |
| 34 | DA | 398 | C |
| 34 | DA | 406 | G |
| 34 | DA | 410 | G |
| 34 | DA | 412 | A |
| 34 | DA | 413 | G |
| 34 | DA | 423 | G |
| 34 | DA | 424 | G |
| 34 | DA | 429 | U |
| 34 | DA | 430 | A |
| 34 | DA | 439 | A |
| 34 | DA | 442 | C |
| 34 | DA | 452 | A |
| 34 | DA | 461 | A |
| 34 | DA | 485 | G |
| 34 | DA | 496 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | DA | 498 | U |
| 34 | DA | 505 | G |
| 34 | DA | 509 | A |
| 34 | DA | 510 | A |
| 34 | DA | 511 | C |
| 34 | DA | 513 | C |
| 34 | DA | 518 | C |
| 34 | DA | 527 | G |
| 34 | DA | 531 | U |
| 34 | DA | 532 | A |
| 34 | DA | 533 | A |
| 34 | DA | 547 | A |
| 34 | DA | 559 | A |
| 34 | DA | 561 | U |
| 34 | DA | 563 | A |
| 34 | DA | 564 | C |
| 34 | DA | 571 | U |
| 34 | DA | 572 | A |
| 34 | DA | 573 | A |
| 34 | DA | 576 | G |
| 34 | DA | 577 | G |
| 34 | DA | 581 | G |
| 34 | DA | 596 | C |
| 34 | DA | 601 | C |
| 34 | DA | 607 | A |
| 34 | DA | 620 | C |
| 34 | DA | 630 | G |
| 34 | DA | 632 | A |
| 34 | DA | 651 | C |
| 34 | DA | 653 | A |
| 34 | DA | 654 | G |
| 34 | DA | 665 | A |
| 34 | DA | 671 | G |
| 34 | DA | 687 | A |
| 34 | DA | 688 | G |
| 34 | DA | 695 | A |
| 34 | DA | 703 | G |
| 34 | DA | 720 | C |
| 34 | DA | 723 | U |
| 34 | DA | 724 | G |
| 34 | DA | 731 | G |
| 34 | DA | 749 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DA | 753 | A |
| 34 | DA | 755 | G |
| 34 | DA | 777 | A |
| 34 | DA | 792 | A |
| 34 | DA | 793 | U |
| 34 | DA | 794 | A |
| 34 | DA | 802 | A |
| 34 | DA | 817 | C |
| 34 | DA | 819 | A |
| 34 | DA | 821 | G |
| 34 | DA | 828 | A |
| 34 | DA | 829 | G |
| 34 | DA | 833 | U |
| 34 | DA | 836 | G |
| 34 | DA | 840 | C |
| 34 | DA | 841 | U |
| 34 | DA | 848 | C |
| 34 | DA | 851 | G |
| 34 | DA | 853 | G |
| 34 | DA | 859 | A |
| 34 | DA | 874 | G |
| 34 | DA | 902 | G |
| 34 | DA | 914 | A |
| 34 | DA | 916 | G |
| 34 | DA | 922 | G |
| 34 | DA | 926 | G |
| 34 | DA | 927 | G |
| 34 | DA | 934 | C |
| 34 | DA | 935 | A |
| 34 | DA | 960 | U |
| 34 | DA | 961 | U |
| 34 | DA | 968 | A |
| 34 | DA | 969 | A |
| 34 | DA | 971 | G |
| 34 | DA | 972 | C |
| 34 | DA | 974 | A |
| 34 | DA | 975 | A |
| 34 | DA | 976 | G |
| 34 | DA | 977 | A |
| 34 | DA | 984 | C |
| 34 | DA | 989 | C |
| 34 | DA | 991 | U |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | DA | 992 | U |
| 34 | DA | 993 | G |
| 34 | DA | 999 | C |
| 34 | DA | 1002 | G |
| 34 | DA | 1003 | G |
| 34 | DA | 1005 | A |
| 34 | DA | 1006 | C |
| 34 | DA | 1017 | G |
| 34 | DA | 1022 | G |
| 34 | DA | 1023 | G |
| 34 | DA | 1024 | G |
| 34 | DA | 1025 | U |
| 34 | DA | 1026 | G |
| 34 | DA | 1027 | C |
| 34 | DA | 1028 | C |
| 34 | DA | 1030 | C |
| 34 | DA | 1030(A) | G |
| 34 | DA | 1030(B) | C |
| 34 | DA | 1030(C) | G |
| 34 | DA | 1038 | C |
| 34 | DA | 1041 | A |
| 34 | DA | 1046 | A |
| 34 | DA | 1052 | U |
| 34 | DA | 1054 | C |
| 34 | DA | 1065 | U |
| 34 | DA | 1066 | C |
| 34 | DA | 1081 | G |
| 34 | DA | 1089 | G |
| 34 | DA | 1094 | G |
| 34 | DA | 1095 | U |
| 34 | DA | 1100 | C |
| 34 | DA | 1101 | A |
| 34 | DA | 1117 | G |
| 34 | DA | 1121 | U |
| 34 | DA | 1122 | U |
| 34 | DA | 1124 | G |
| 34 | DA | 1125 | U |
| 34 | DA | 1129 | C |
| 34 | DA | 1130 | A |
| 34 | DA | 1136 | U |
| 34 | DA | 1137 | C |
| 34 | DA | 1138 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 34 | DA | 1139 | G |
| 34 | DA | 1146 | A |
| 34 | DA | 1152 | A |
| 34 | DA | 1154 | G |
| 34 | DA | 1157 | A |
| 34 | DA | 1159 | U |
| 34 | DA | 1166 | G |
| 34 | DA | 1181 | G |
| 34 | DA | 1183 | A |
| 34 | DA | 1184 | G |
| 34 | DA | 1196 | U |
| 34 | DA | 1202 | G |
| 34 | DA | 1211 | U |
| 34 | DA | 1212 | U |
| 34 | DA | 1213 | A |
| 34 | DA | 1220 | G |
| 34 | DA | 1227 | A |
| 34 | DA | 1228 | C |
| 34 | DA | 1238 | A |
| 34 | DA | 1240 | U |
| 34 | DA | 1241 | G |
| 34 | DA | 1253 | G |
| 34 | DA | 1254 | C |
| 34 | DA | 1256 | A |
| 34 | DA | 1257 | U |
| 34 | DA | 1258 | G |
| 34 | DA | 1260 | C |
| 34 | DA | 1273 | G |
| 34 | DA | 1275 | A |
| 34 | DA | 1278 | U |
| 34 | DA | 1279 | A |
| 34 | DA | 1280 | A |
| 34 | DA | 1281 | U |
| 34 | DA | 1282 | C |
| 34 | DA | 1285 | A |
| 34 | DA | 1287 | A |
| 34 | DA | 1299 | A |
| 34 | DA | 1300 | G |
| 34 | DA | 1305 | G |
| 34 | DA | 1317 | C |
| 34 | DA | 1319 | A |
| 34 | DA | 1322 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 34 | DA | 1338 | G |
| 34 | DA | 1340 | A |
| 34 | DA | 1346 | A |
| 34 | DA | 1347 | G |
| 34 | DA | 1353 | G |
| 34 | DA | 1358 | U |
| 34 | DA | 1360 | A |
| 34 | DA | 1363 | C |
| 34 | DA | 1368 | G |
| 34 | DA | 1370 | G |
| 34 | DA | 1379 | G |
| 34 | DA | 1381 | U |
| 34 | DA | 1397 | C |
| 34 | DA | 1401 | G |
| 34 | DA | 1419 | G |
| 34 | DA | 1442 | G |
| 34 | DA | 1442(A) | G |
| 34 | DA | 1442(B) | A |
| 34 | DA | 1446 | U |
| 34 | DA | 1447 | A |
| 34 | DA | 1452 | C |
| 34 | DA | 1456 | G |
| 34 | DA | 1487 | G |
| 34 | DA | 1492 | A |
| 34 | DA | 1493 | A |
| 34 | DA | 1494 | G |
| 34 | DA | 1497 | G |
| 34 | DA | 1502 | A |
| 34 | DA | 1503 | A |
| 34 | DA | 1504 | G |
| 34 | DA | 1506 | U |
| 34 | DA | 1517 | G |
| 34 | DA | 1520 | G |
| 34 | DA | 1529 | G |
| 34 | DA | 1530 | G |
| 34 | DA | 1531 | A |
| 34 | DA | 1532 | U |
| 55 | DV | 24 | A |
| 56 | DW | 3 | C |
| 56 | DW | 7 | A |
| 56 | DW | 8 | 4SU |
| 56 | DW | 9 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56 | DW | 13 | C |
| 56 | DW | 14 | A |
| 56 | DW | 15 | G |
| 56 | DW | 19 | G |
| 56 | DW | 22 | G |
| 56 | DW | 23 | A |
| 56 | DW | 46 | 7MG |
| 56 | DW | 47 | U |
| 56 | DW | 48 | C |
| 56 | DW | 49 | C |
| 56 | DW | 50 | U |
| 56 | DW | 61 | C |
| 56 | DW | 62 | C |
| 56 | DW | 67 | C |
| 56 | DW | 68 | C |
| 56 | DW | 70 | G |
| 56 | DW | 73 | A |
| 56 | DW | 74 | C |
| 57 | DX | 13 | C |
| 57 | DX | 18 | G |
| 57 | DX | 19 | G |
| 57 | DX | 20 | U |
| 57 | DX | 21 | A |
| 57 | DX | 22 | G |
| 57 | DX | 30 | G |
| 57 | DX | 47 | U |
| 57 | DX | 48 | C |
| 57 | DX | 59 | A |
| 57 | DX | 61 | C |
| 57 | DX | 68 | C |
| 57 | DX | 75 | C |
| 58 | DY | 9 | A |
| 58 | DY | 13 | C |
| 58 | DY | 14 | A |
| 58 | DY | 19 | G |
| 58 | DY | 26 | A |
| 58 | DY | 34 | G |
| 58 | DY | 39 | PSU |
| 58 | DY | 45 | U |
| 58 | DY | 46 | 7MG |
| 58 | DY | 47 | U |
| 58 | DY | 48 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58 | DY | 49 | C |
| 58 | DY | 54 | 5MU |
| 58 | DY | 55 | PSU |
| 58 | DY | 57 | G |
| 58 | DY | 58 | A |
| 58 | DY | 59 | U |
| 58 | DY | 65 | G |
| 58 | DY | 70 | G |

All (127) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 185 | A |
| 1 | AA | 188 | A |
| 1 | AA | 271 | U |
| 1 | AA | 302 | A |
| 1 | AA | 334 | A |
| 1 | AA | 572 | A |
| 1 | AA | 641 | G |
| 1 | AA | 716 | G |
| 1 | AA | 793 | A |
| 1 | AA | 811 | A |
| 1 | AA | 821 | A |
| 1 | AA | 945 | A |
| 1 | AA | 1019 | G |
| 1 | AA | 1098 | C |
| 1 | AA | 1154 | U |
| 1 | AA | 1188 | A |
| 1 | AA | 1219 | A |
| 1 | AA | 1220 | U |
| 1 | AA | 1221 | G |
| 1 | AA | 1255 | A |
| 1 | AA | 1286 | U |
| 1 | AA | 1321 | A |
| 1 | AA | 1347 | A |
| 1 | AA | 1425 | A |
| 1 | AA | 1442 | U |
| 1 | AA | 1466 | U |
| 1 | AA | 1654 | A |
| 1 | AA | 1655 | A |
| 1 | AA | 1793 | A |
| 1 | AA | 2014 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | AA | 2148 | A |
| 1 | AA | 2203 | G |
| 1 | AA | 2209 | G |
| 1 | AA | 2320 | G |
| 1 | AA | 2345 | A |
| 1 | AA | 2418 | U |
| 1 | AA | 2442 | A |
| 1 | AA | 2451 | A |
| 1 | AA | 2623 | U |
| 1 | AA | 2701 | U |
| 1 | AA | 2902 | G |
| 34 | BA | 115 | G |
| 34 | BA | 243 | A |
| 34 | BA | 266 | G |
| 34 | BA | 347 | G |
| 34 | BA | 353 | A |
| 34 | BA | 509 | A |
| 34 | BA | 560 | U |
| 34 | BA | 687 | A |
| 34 | BA | 748 | C |
| 34 | BA | 793 | U |
| 34 | BA | 839 | U |
| 34 | BA | 913 | A |
| 34 | BA | 991 | U |
| 34 | BA | 1065 | U |
| 34 | BA | 1067 | A |
| 34 | BA | 1165 | C |
| 34 | BA | 1201 | A |
| 34 | BA | 1285 | A |
| 34 | BA | 1335 | C |
| 34 | BA | 1442 | G |
| 34 | BA | 1530 | G |
| 56 | BW | 13 | C |
| 58 | BY | 19 | G |
| 58 | BY | 58 | A |
| 1 | CA | 195 | A |
| 1 | CA | 196 | A |
| 1 | CA | 249 | C |
| 1 | CA | 271(K) | U |
| 1 | CA | 271(M) | G |
| 1 | CA | 277 | C |
| 1 | CA | 310 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | CA | 529 | A |
| 1 | CA | 685 | A |
| 1 | CA | 752 | A |
| 1 | CA | 764 | A |
| 1 | CA | 774 | A |
| 1 | CA | 776 | G |
| 1 | CA | 856 | C |
| 1 | CA | 900 | A |
| 1 | CA | 1057 | A |
| 1 | CA | 1063 | G |
| 1 | CA | 1210 | A |
| 1 | CA | 1301 | A |
| 1 | CA | 1420 | U |
| 1 | CA | 1427 | A |
| 1 | CA | 1558 | A |
| 1 | CA | 1608 | A |
| 1 | CA | 1653 | G |
| 1 | CA | 1913 | A |
| 1 | CA | 1992 | G |
| 1 | CA | 1997 | G |
| 1 | CA | 2110 | G |
| 1 | CA | 2126 | A |
| 1 | CA | 2318 | G |
| 1 | CA | 2406 | U |
| 1 | CA | 2439 | A |
| 1 | CA | 2581 | G |
| 1 | CA | 2611 | U |
| 1 | CA | 2689 | U |
| 1 | CA | 2726 | U |
| 1 | CA | 2756 | U |
| 34 | DA | 60 | A |
| 34 | DA | 65 | U |
| 34 | DA | 115 | G |
| 34 | DA | 243 | A |
| 34 | DA | 266 | G |
| 34 | DA | 353 | A |
| 34 | DA | 429 | U |
| 34 | DA | 509 | A |
| 34 | DA | 532 | A |
| 34 | DA | 560 | U |
| 34 | DA | 687 | A |
| 34 | DA | 748 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | DA | 793 | U |
| 34 | DA | 840 | C |
| 34 | DA | 913 | A |
| 34 | DA | 991 | U |
| 34 | DA | 992 | U |
| 34 | DA | 1064 | G |
| 34 | DA | 1065 | U |
| 34 | DA | 1183 | A |
| 34 | DA | 1201 | A |
| 34 | DA | 1442 | G |
| 34 | DA | 1492 | A |
| 56 | DW | 13 | C |
| 56 | DW | 14 | A |

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

40 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 56 | PSU | BW | 32 | 60,56 | 13,21,22 | 1.25 | 1 (7%) | 18,30,33 | 3.35 | 6 (33%) |
| 56 | MIA | BW | 37 | 56 | 21,31,32 | 1.88 | 2 (9%) | 26,44,47 | 1.92 | 7 (26%) |
| 56 | PSU | BW | 39 | 56 | 13,21,22 | 0.74 | 0 | 18,30,33 | 3.50 | 5 (27%) |
| 56 | 7MG | BW | 46 | 56 | 19,26,27 | 1.00 | 1 (5%) | 24,39,42 | 2.92 | 7 (29%) |
| 56 | 5MU | BW | 54 | 56 | 12,22,23 | 0.50 | 0 | 14,32,35 | 2.57 | 2 (14%) |
| 56 | PSU | BW | 55 | 56 | 13,21,22 | 0.66 | 0 | 18,30,33 | 3.46 | 6 (33%) |
| 56 | F3N | BW | 76 | 1,56 | 27,36,37 | 1.34 | 5 (18%) | 31,51,54 | 2.34 | 3 (9%) |
| 56 | 4SU | BW | 8 | 56 | 11,21,22 | 1.25 | 1 (9%) | 13,30,33 | 1.17 | 1 (7%) |
| 57 | 5MC | BX | 32 | 57 | 13,22,23 | 1.14 | 1 (7%) | 15,32,35 | 1.51 | 3 (20%) |
| 57 | 5MU | BX | 54 | 60,57 | 12,22,23 | 0.47 | 0 | 14,32,35 | 2.53 | 2 (14%) |
| 57 | PSU | BX | 55 | 57 | 13,21,22 | 1.46 | 1 (7%) | 18,30,33 | 3.41 | 6 (33%) |
| 57 | 31H | BX | 76 | 60,57 | 25,34,35 | 1.25 | 4 (16%) | 26,47,50 | 3.08 | 5 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 57 | 4SU | BX | 8 | 57 | 11,21,22 | 1.18 | 1 (9%) | 13,30,33 | 1.31 | 1 (7%) |
| 58 | PSU | BY | 32 | 58 | 13,21,22 | 0.77 | 0 | 18,30,33 | 3.46 | 5 (27%) |
| 58 | MIA | BY | 37 | 58 | 15,24,32 | 1.27 | 2 (13%) | 16,35,47 | 2.23 | 3 (18%) |
| 58 | PSU | BY | 39 | 58 | 13,21,22 | 1.23 | 1 (7%) | 18,30,33 | 3.33 | 6 (33%) |
| 58 | 7MG | BY | 46 | 58 | 19,26,27 | 1.02 | 1 (5%) | 24,39,42 | 3.07 | 6 (25%) |
| 58 | 5MU | BY | 54 | 58 | 12,22,23 | 0.36 | 0 | 14,32,35 | 2.43 | 2 (14%) |
| 58 | PSU | BY | 55 | 58 | 13,21,22 | 1.27 | 1 (7%) | 18,30,33 | 3.38 | 6 (33%) |
| 58 | 4SU | BY | 8 | 58 | 11,21,22 | 1.27 | 1 (9%) | 13,30,33 | 1.24 | 1 (7%) |
| 56 | PSU | DW | 32 | 56 | 13,21,22 | 0.84 | 1 (7%) | 18,30,33 | 3.35 | 6 (33%) |
| 56 | MIA | DW | 37 | 56 | 15,24,32 | 1.20 | 2 (13%) | 16,35,47 | 2.10 | 2 (12%) |
| 56 | PSU | DW | 39 | 56 | 13,21,22 | 1.32 | 1 (7%) | 18,30,33 | 3.55 | 6 (33%) |
| 56 | 7MG | DW | 46 | 56 | 19,26,27 | 0.96 | 1 (5%) | 24,39,42 | 2.89 | 6 (25%) |
| 56 | 5MU | DW | 54 | 56 | 12,22,23 | 0.34 | 0 | 14,32,35 | 2.42 | 2 (14%) |
| 56 | PSU | DW | 55 | 56 | 13,21,22 | 0.99 | 1 (7%) | 18,30,33 | 3.53 | 6 (33%) |
| 56 | F3N | DW | 76 | 1,56 | 27,36,37 | 1.46 | 5 (18%) | 31,51,54 | 2.46 | 5 (16%) |
| 56 | 4SU | DW | 8 | 56 | 11,21,22 | 1.24 | 1 (9%) | 13,30,33 | 1.30 | 1 (7%) |
| 57 | 5MC | DX | 32 | 57 | 13,22,23 | 1.51 | 1 (7%) | 15,32,35 | 1.01 | 2 (13%) |
| 57 | 5MU | DX | 54 | 57 | 12,22,23 | 0.42 | 0 | 14,32,35 | 2.12 | 2 (14%) |
| 57 | PSU | DX | 55 | 57 | 13,21,22 | 1.01 | 1 (7%) | 18,30,33 | 3.41 | 5 (27%) |
| 57 | 31H | DX | 76 | 60,57 | 25,34,35 | 1.24 | 4 (16%) | 26,47,50 | 3.07 | 5 (19%) |
| 57 | 4SU | DX | 8 | 57 | 11,21,22 | 1.30 | 1 (9%) | 13,30,33 | 1.00 | 1 (7%) |
| 58 | PSU | DY | 32 | 58 | 13,21,22 | 1.15 | 1 (7%) | 18,30,33 | 3.42 | 6 (33%) |
| 58 | MIA | DY | 37 | 58 | 15,24,32 | 1.17 | 2 (13%) | 16,35,47 | 2.12 | 2 (12%) |
| 58 | PSU | DY | 39 | 58 | 13,21,22 | 1.17 | 2 (15%) | 18,30,33 | 3.39 | 5 (27%) |
| 58 | 7MG | DY | 46 | 58 | 19,26,27 | 1.07 | 1 (5%) | 24,39,42 | 3.29 | 8 (33%) |
| 58 | 5MU | DY | 54 | 58 | 12,22,23 | 0.36 | 0 | 14,32,35 | 2.35 | 2 (14%) |
| 58 | PSU | DY | 55 | 58 | 13,21,22 | 1.20 | 1 (7%) | 18,30,33 | 3.34 | 6 (33%) |
| 58 | 4SU | DY | 8 | 58 | 11,21,22 | 1.28 | 1 (9%) | 13,30,33 | 1.25 | 1 (7%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 56 | PSU | BW | 32 | 60,56 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|------------|---------|
| 56 | MIA | BW | 37 | 56 | - | 0/11/33/34 | 0/3/3/3 |
| 56 | PSU | BW | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 7MG | BW | 46 | 56 | - | 0/7/37/38 | 0/3/3/3 |
| 56 | 5MU | BW | 54 | 56 | - | 0/3/25/26 | 0/2/2/2 |
| 56 | PSU | BW | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | F3N | BW | 76 | 1,56 | - | 0/15/37/38 | 0/4/4/4 |
| 56 | 4SU | BW | 8 | 56 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | 5MC | BX | 32 | 57 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | 5MU | BX | 54 | 60,57 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | PSU | BX | 55 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 31H | BX | 76 | 60,57 | - | 1/18/40/41 | 0/3/3/3 |
| 57 | 4SU | BX | 8 | 57 | - | 0/3/25/26 | 0/2/2/2 |
| 58 | PSU | BY | 32 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | MIA | BY | 37 | 58 | - | 0/3/25/34 | 0/3/3/3 |
| 58 | PSU | BY | 39 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | 7MG | BY | 46 | 58 | - | 0/7/37/38 | 0/3/3/3 |
| 58 | 5MU | BY | 54 | 58 | - | 0/3/25/26 | 0/2/2/2 |
| 58 | PSU | BY | 55 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | 4SU | BY | 8 | 58 | - | 0/3/25/26 | 0/2/2/2 |
| 56 | PSU | DW | 32 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | MIA | DW | 37 | 56 | - | 0/3/25/34 | 0/3/3/3 |
| 56 | PSU | DW | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 7MG | DW | 46 | 56 | - | 0/7/37/38 | 0/3/3/3 |
| 56 | 5MU | DW | 54 | 56 | - | 0/3/25/26 | 0/2/2/2 |
| 56 | PSU | DW | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | F3N | DW | 76 | 1,56 | - | 0/15/37/38 | 0/4/4/4 |
| 56 | 4SU | DW | 8 | 56 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | 5MC | DX | 32 | 57 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | 5MU | DX | 54 | 57 | - | 0/3/25/26 | 0/2/2/2 |
| 57 | PSU | DX | 55 | 57 | - | 0/7/25/26 | 0/2/2/2 |
| 57 | 31H | DX | 76 | 60,57 | - | 1/18/40/41 | 0/3/3/3 |
| 57 | 4SU | DX | 8 | 57 | - | 0/3/25/26 | 0/2/2/2 |
| 58 | PSU | DY | 32 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | MIA | DY | 37 | 58 | - | 0/3/25/34 | 0/3/3/3 |
| 58 | PSU | DY | 39 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | 7MG | DY | 46 | 58 | - | 0/7/37/38 | 0/3/3/3 |
| 58 | 5MU | DY | 54 | 58 | - | 0/3/25/26 | 0/2/2/2 |
| 58 | PSU | DY | 55 | 58 | - | 0/7/25/26 | 0/2/2/2 |
| 58 | 4SU | DY | 8 | 58 | - | 0/3/25/26 | 0/2/2/2 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 56 | BW | 37 | MIA | C2-S10 | -7.59 | 1.69 | 1.75 |
| 57 | BX | 55 | PSU | C5-C1' | -4.74 | 1.48 | 1.52 |
| 56 | DW | 39 | PSU | C5-C1' | -4.33 | 1.48 | 1.52 |
| 58 | BY | 55 | PSU | C5-C1' | -4.06 | 1.48 | 1.52 |
| 57 | DX | 8 | 4SU | C4-S4 | -4.04 | 1.59 | 1.67 |
| 56 | BW | 32 | PSU | C5-C1' | -4.04 | 1.48 | 1.52 |
| 58 | BY | 8 | 4SU | C4-S4 | -3.92 | 1.59 | 1.67 |
| 58 | BY | 39 | PSU | C5-C1' | -3.89 | 1.48 | 1.52 |
| 56 | DW | 76 | F3N | CB-CG | -3.86 | 1.41 | 1.51 |
| 58 | DY | 8 | 4SU | C4-S4 | -3.83 | 1.60 | 1.67 |
| 56 | BW | 8 | 4SU | C4-S4 | -3.81 | 1.60 | 1.67 |
| 56 | DW | 8 | 4SU | C4-S4 | -3.70 | 1.60 | 1.67 |
| 58 | DY | 55 | PSU | C5-C1' | -3.69 | 1.49 | 1.52 |
| 56 | BW | 76 | F3N | CB-CG | -3.55 | 1.42 | 1.51 |
| 58 | DY | 32 | PSU | C5-C1' | -3.54 | 1.49 | 1.52 |
| 57 | BX | 76 | 31H | C5-C4 | -3.52 | 1.32 | 1.40 |
| 57 | DX | 76 | 31H | C5-C4 | -3.49 | 1.32 | 1.40 |
| 58 | DY | 39 | PSU | C5-C1' | -3.24 | 1.49 | 1.52 |
| 57 | BX | 8 | 4SU | C4-S4 | -3.17 | 1.61 | 1.67 |
| 56 | DW | 55 | PSU | C5-C1' | -2.94 | 1.49 | 1.52 |
| 57 | DX | 55 | PSU | C5-C1' | -2.90 | 1.49 | 1.52 |
| 56 | DW | 76 | F3N | C5-C4 | -2.56 | 1.34 | 1.40 |
| 56 | BW | 76 | F3N | C5-C4 | -2.52 | 1.34 | 1.40 |
| 56 | BW | 76 | F3N | C2'-C3' | -2.32 | 1.49 | 1.53 |
| 56 | DW | 32 | PSU | C5-C1' | -2.32 | 1.50 | 1.52 |
| 56 | DW | 76 | F3N | C5-N7 | -2.20 | 1.31 | 1.39 |
| 57 | BX | 76 | 31H | C5-N7 | -2.17 | 1.32 | 1.39 |
| 57 | DX | 76 | 31H | C5-N7 | -2.17 | 1.32 | 1.39 |
| 56 | BW | 76 | F3N | C5-N7 | -2.12 | 1.32 | 1.39 |
| 58 | DY | 39 | PSU | O4'-C1' | -2.01 | 1.41 | 1.44 |
| 57 | DX | 76 | 31H | CA-N | 2.08 | 1.47 | 1.45 |
| 57 | BX | 76 | 31H | CA-N | 2.11 | 1.47 | 1.45 |
| 58 | DY | 37 | MIA | C2-N3 | 2.12 | 1.36 | 1.32 |
| 58 | BY | 37 | MIA | C2-N3 | 2.29 | 1.36 | 1.32 |
| 56 | DW | 37 | MIA | C2-N3 | 2.33 | 1.36 | 1.32 |
| 56 | DW | 76 | F3N | C3'-N3' | 2.45 | 1.49 | 1.45 |
| 56 | BW | 76 | F3N | O4'-C1' | 2.58 | 1.44 | 1.41 |
| 57 | BX | 76 | 31H | C3'-N3' | 2.85 | 1.50 | 1.45 |
| 57 | DX | 76 | 31H | C3'-N3' | 2.86 | 1.50 | 1.45 |
| 56 | DW | 46 | 7MG | C5-C4 | 2.93 | 1.47 | 1.39 |
| 56 | BW | 46 | 7MG | C5-C4 | 3.04 | 1.47 | 1.39 |
| 58 | BY | 46 | 7MG | C5-C4 | 3.07 | 1.47 | 1.39 |
| 56 | BW | 37 | MIA | C5-C4 | 3.09 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 58 | DY | 46 | 7MG | C5-C4 | 3.27 | 1.48 | 1.39 |
| 58 | DY | 37 | MIA | C5-C4 | 3.38 | 1.48 | 1.40 |
| 56 | DW | 37 | MIA | C5-C4 | 3.39 | 1.48 | 1.40 |
| 58 | BY | 37 | MIA | C5-C4 | 3.55 | 1.48 | 1.40 |
| 57 | BX | 32 | 5MC | C5-C4 | 3.61 | 1.46 | 1.41 |
| 56 | DW | 76 | F3N | O4'-C1' | 3.76 | 1.46 | 1.41 |
| 57 | DX | 32 | 5MC | C5-C4 | 5.29 | 1.49 | 1.41 |

All (162) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 56 | DW | 76 | F3N | N3-C2-N1 | -11.79 | 119.87 | 128.89 |
| 56 | BW | 76 | F3N | N3-C2-N1 | -11.78 | 119.87 | 128.89 |
| 57 | BX | 76 | 31H | N3-C2-N1 | -11.65 | 119.97 | 128.89 |
| 57 | DX | 76 | 31H | N3-C2-N1 | -11.61 | 120.00 | 128.89 |
| 56 | BW | 39 | PSU | N1-C2-N3 | -11.47 | 121.02 | 128.33 |
| 58 | BY | 32 | PSU | N1-C2-N3 | -11.26 | 121.15 | 128.33 |
| 56 | DW | 39 | PSU | N1-C2-N3 | -11.12 | 121.24 | 128.33 |
| 57 | DX | 55 | PSU | N1-C2-N3 | -10.95 | 121.34 | 128.33 |
| 56 | BW | 55 | PSU | N1-C2-N3 | -10.86 | 121.41 | 128.33 |
| 58 | DY | 32 | PSU | N1-C2-N3 | -10.84 | 121.42 | 128.33 |
| 58 | DY | 39 | PSU | N1-C2-N3 | -10.82 | 121.43 | 128.33 |
| 58 | BY | 55 | PSU | N1-C2-N3 | -10.67 | 121.53 | 128.33 |
| 56 | DW | 55 | PSU | N1-C2-N3 | -10.61 | 121.56 | 128.33 |
| 58 | DY | 55 | PSU | N1-C2-N3 | -10.45 | 121.67 | 128.33 |
| 56 | DW | 32 | PSU | N1-C2-N3 | -10.38 | 121.71 | 128.33 |
| 56 | BW | 32 | PSU | N1-C2-N3 | -10.35 | 121.73 | 128.33 |
| 57 | BX | 55 | PSU | N1-C2-N3 | -10.31 | 121.75 | 128.33 |
| 58 | BY | 39 | PSU | N1-C2-N3 | -10.23 | 121.81 | 128.33 |
| 58 | DY | 46 | 7MG | C5-C4-N3 | -10.11 | 116.96 | 126.82 |
| 58 | BY | 46 | 7MG | C5-C4-N3 | -9.55 | 117.52 | 126.82 |
| 56 | DW | 46 | 7MG | C5-C4-N3 | -8.56 | 118.48 | 126.82 |
| 56 | BW | 46 | 7MG | C5-C4-N3 | -8.27 | 118.76 | 126.82 |
| 58 | BY | 37 | MIA | N3-C2-N1 | -7.52 | 123.14 | 128.89 |
| 56 | DW | 37 | MIA | N3-C2-N1 | -7.47 | 123.17 | 128.89 |
| 57 | DX | 76 | 31H | C4'-O4'-C1' | -7.42 | 101.57 | 109.72 |
| 57 | BX | 76 | 31H | C4'-O4'-C1' | -7.40 | 101.59 | 109.72 |
| 58 | DY | 37 | MIA | N3-C2-N1 | -7.39 | 123.23 | 128.89 |
| 57 | BX | 54 | 5MU | C5-C4-N3 | -6.42 | 117.99 | 125.14 |
| 56 | BW | 54 | 5MU | C5-C4-N3 | -6.17 | 118.27 | 125.14 |
| 58 | BY | 54 | 5MU | C5-C4-N3 | -5.76 | 118.73 | 125.14 |
| 56 | BW | 37 | MIA | C11-S10-C2 | -5.67 | 98.62 | 102.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56 | DW | 54 | 5MU | C5-C4-N3 | -5.62 | 118.88 | 125.14 |
| 58 | DY | 54 | 5MU | C5-C4-N3 | -5.54 | 118.97 | 125.14 |
| 56 | BW | 46 | 7MG | C5-C6-N1 | -5.09 | 115.63 | 123.46 |
| 57 | DX | 54 | 5MU | C5-C4-N3 | -5.07 | 119.50 | 125.14 |
| 56 | DW | 55 | PSU | C5-C1'-C2' | -5.06 | 106.53 | 115.52 |
| 58 | DY | 46 | 7MG | C5-C6-N1 | -4.96 | 115.83 | 123.46 |
| 58 | BY | 46 | 7MG | C5-C6-N1 | -4.86 | 115.99 | 123.46 |
| 56 | DW | 46 | 7MG | C5-C6-N1 | -4.78 | 116.11 | 123.46 |
| 57 | BX | 55 | PSU | C5-C6-N1 | -4.37 | 118.23 | 124.39 |
| 57 | BX | 8 | 4SU | C5-C4-N3 | -4.29 | 119.42 | 123.63 |
| 56 | DW | 8 | 4SU | C5-C4-N3 | -4.16 | 119.56 | 123.63 |
| 57 | BX | 55 | PSU | C5-C1'-C2' | -4.02 | 108.39 | 115.52 |
| 58 | BY | 8 | 4SU | C5-C4-N3 | -3.98 | 119.73 | 123.63 |
| 56 | BW | 55 | PSU | C5-C1'-C2' | -3.97 | 108.47 | 115.52 |
| 56 | DW | 39 | PSU | C5-C1'-C2' | -3.91 | 108.58 | 115.52 |
| 56 | BW | 8 | 4SU | C5-C4-N3 | -3.86 | 119.85 | 123.63 |
| 58 | DY | 8 | 4SU | C5-C4-N3 | -3.83 | 119.88 | 123.63 |
| 57 | DX | 55 | PSU | C5-C6-N1 | -3.74 | 119.11 | 124.39 |
| 58 | DY | 55 | PSU | C5-C6-N1 | -3.70 | 119.17 | 124.39 |
| 56 | BW | 37 | MIA | C4-C5-N7 | -3.62 | 106.15 | 109.48 |
| 56 | BW | 37 | MIA | C5-C6-N1 | -3.54 | 116.83 | 120.48 |
| 56 | DW | 76 | F3N | C4'-C3'-N3' | -3.42 | 106.47 | 113.61 |
| 58 | BY | 37 | MIA | C4-C5-N7 | -3.37 | 106.38 | 109.48 |
| 58 | DY | 32 | PSU | C5-C6-N1 | -3.37 | 119.63 | 124.39 |
| 58 | BY | 39 | PSU | C5-C6-N1 | -3.36 | 119.65 | 124.39 |
| 56 | DW | 39 | PSU | C5-C6-N1 | -3.29 | 119.75 | 124.39 |
| 56 | DW | 32 | PSU | C5-C6-N1 | -3.25 | 119.80 | 124.39 |
| 58 | BY | 39 | PSU | C5-C1'-C2' | -3.23 | 109.78 | 115.52 |
| 58 | BY | 55 | PSU | C5-C6-N1 | -3.23 | 119.84 | 124.39 |
| 56 | BW | 32 | PSU | C5-C6-N1 | -3.18 | 119.90 | 124.39 |
| 58 | BY | 32 | PSU | C5-C6-N1 | -3.18 | 119.90 | 124.39 |
| 56 | DW | 55 | PSU | C5-C6-N1 | -3.10 | 120.02 | 124.39 |
| 56 | BW | 37 | MIA | C12-N6-C6 | -3.06 | 119.62 | 123.42 |
| 58 | DY | 37 | MIA | C4-C5-N7 | -2.99 | 106.73 | 109.48 |
| 57 | BX | 76 | 31H | CA-N-CN | -2.98 | 118.25 | 122.82 |
| 57 | DX | 8 | 4SU | C5-C4-N3 | -2.97 | 120.72 | 123.63 |
| 56 | BW | 55 | PSU | C5-C6-N1 | -2.94 | 120.24 | 124.39 |
| 57 | DX | 76 | 31H | CA-N-CN | -2.94 | 118.30 | 122.82 |
| 58 | DY | 46 | 7MG | CM7-N7-C8 | -2.89 | 112.32 | 120.52 |
| 56 | DW | 37 | MIA | C4-C5-N7 | -2.87 | 106.84 | 109.48 |
| 56 | DW | 46 | 7MG | CM7-N7-C8 | -2.84 | 112.47 | 120.52 |
| 57 | BX | 76 | 31H | OCN-CN-N | -2.83 | 120.69 | 124.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56 | DW | 32 | PSU | C5-C1'-C2' | -2.81 | 110.53 | 115.52 |
| 56 | BW | 76 | F3N | C4'-C3'-N3' | -2.77 | 107.82 | 113.61 |
| 57 | DX | 76 | 31H | OCN-CN-N | -2.77 | 120.76 | 124.76 |
| 58 | BY | 46 | 7MG | CM7-N7-C8 | -2.71 | 112.84 | 120.52 |
| 56 | BW | 46 | 7MG | CM7-N7-C8 | -2.71 | 112.85 | 120.52 |
| 56 | BW | 32 | PSU | C5-C1'-C2' | -2.56 | 110.98 | 115.52 |
| 56 | BW | 39 | PSU | C5-C6-N1 | -2.55 | 120.79 | 124.39 |
| 58 | DY | 32 | PSU | C5-C1'-C2' | -2.50 | 111.07 | 115.52 |
| 58 | BY | 55 | PSU | C5-C1'-C2' | -2.38 | 111.29 | 115.52 |
| 56 | BW | 76 | F3N | C4'-O4'-C1' | -2.32 | 107.17 | 109.72 |
| 58 | DY | 39 | PSU | C5-C6-N1 | -2.20 | 121.28 | 124.39 |
| 58 | DY | 55 | PSU | C5-C1'-C2' | -2.20 | 111.61 | 115.52 |
| 56 | BW | 46 | 7MG | C5-C4-N9 | -2.15 | 103.00 | 106.18 |
| 57 | DX | 32 | 5MC | C5-C4-N3 | -2.15 | 117.67 | 121.27 |
| 57 | BX | 32 | 5MC | C5-C4-N3 | -2.11 | 117.73 | 121.27 |
| 58 | DY | 46 | 7MG | C5-C4-N9 | -2.09 | 103.11 | 106.18 |
| 57 | BX | 32 | 5MC | C5-C4-N4 | -2.05 | 119.17 | 122.20 |
| 56 | BW | 37 | MIA | N3-C2-N1 | -2.02 | 122.93 | 126.79 |
| 57 | DX | 32 | 5MC | N4-C4-N3 | 2.06 | 119.93 | 116.95 |
| 58 | BY | 46 | 7MG | CM7-N7-C5 | 2.06 | 130.98 | 124.09 |
| 56 | DW | 76 | F3N | C2'-C3'-C4' | 2.13 | 104.92 | 102.27 |
| 56 | BW | 46 | 7MG | CM7-N7-C5 | 2.14 | 131.26 | 124.09 |
| 58 | BY | 37 | MIA | C2-N1-C6 | 2.17 | 122.65 | 118.77 |
| 58 | DY | 39 | PSU | O4'-C1'-C2' | 2.19 | 106.96 | 104.73 |
| 56 | BW | 55 | PSU | O4'-C1'-C2' | 2.23 | 107.00 | 104.73 |
| 56 | DW | 46 | 7MG | CM7-N7-C5 | 2.24 | 131.57 | 124.09 |
| 58 | DY | 46 | 7MG | CM7-N7-C5 | 2.28 | 131.72 | 124.09 |
| 56 | DW | 55 | PSU | O4'-C1'-C2' | 2.31 | 107.09 | 104.73 |
| 56 | BW | 39 | PSU | O4'-C1'-C2' | 2.33 | 107.10 | 104.73 |
| 58 | DY | 46 | 7MG | C4-N9-C1' | 2.33 | 132.31 | 126.70 |
| 56 | BW | 37 | MIA | C5-C6-N6 | 2.35 | 124.33 | 120.47 |
| 56 | DW | 76 | F3N | C2'-C3'-N3' | 2.49 | 119.59 | 113.18 |
| 56 | DW | 32 | PSU | O4'-C1'-C2' | 2.58 | 107.36 | 104.73 |
| 58 | BY | 39 | PSU | O4'-C1'-C2' | 2.58 | 107.36 | 104.73 |
| 56 | DW | 39 | PSU | O4'-C1'-C2' | 2.78 | 107.56 | 104.73 |
| 58 | DY | 55 | PSU | O4'-C1'-C2' | 2.78 | 107.56 | 104.73 |
| 57 | DX | 55 | PSU | O4'-C1'-C2' | 2.81 | 107.60 | 104.73 |
| 58 | BY | 55 | PSU | O4'-C1'-C2' | 2.82 | 107.60 | 104.73 |
| 58 | BY | 32 | PSU | O4'-C1'-C2' | 2.82 | 107.61 | 104.73 |
| 56 | DW | 76 | F3N | O4'-C4'-C3' | 2.86 | 108.01 | 103.93 |
| 58 | DY | 32 | PSU | O4'-C1'-C2' | 2.87 | 107.66 | 104.73 |
| 57 | BX | 55 | PSU | O4'-C1'-C2' | 2.94 | 107.72 | 104.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 56 | BW | 32 | PSU | O4'-C1'-C2' | 3.02 | 107.80 | 104.73 |
| 56 | BW | 37 | MIA | C2-N1-C6 | 3.32 | 123.09 | 113.35 |
| 58 | DY | 39 | PSU | C6-N1-C2 | 3.59 | 121.24 | 115.47 |
| 56 | BW | 32 | PSU | C6-N1-C2 | 3.73 | 121.47 | 115.47 |
| 56 | DW | 55 | PSU | C6-N1-C2 | 3.90 | 121.75 | 115.47 |
| 58 | BY | 55 | PSU | C6-N1-C2 | 3.96 | 121.84 | 115.47 |
| 58 | BY | 39 | PSU | C6-N1-C2 | 3.96 | 121.84 | 115.47 |
| 56 | DW | 32 | PSU | C6-N1-C2 | 4.15 | 122.15 | 115.47 |
| 58 | DY | 32 | PSU | C6-N1-C2 | 4.17 | 122.17 | 115.47 |
| 57 | BX | 32 | 5MC | N4-C4-N3 | 4.24 | 123.09 | 116.95 |
| 56 | BW | 55 | PSU | C6-N1-C2 | 4.27 | 122.33 | 115.47 |
| 56 | DW | 39 | PSU | C6-N1-C2 | 4.29 | 122.37 | 115.47 |
| 58 | BY | 32 | PSU | C6-N1-C2 | 4.33 | 122.43 | 115.47 |
| 56 | BW | 39 | PSU | C6-N1-C2 | 4.34 | 122.45 | 115.47 |
| 57 | BX | 55 | PSU | C6-N1-C2 | 4.40 | 122.54 | 115.47 |
| 57 | DX | 55 | PSU | C6-N1-C2 | 4.40 | 122.55 | 115.47 |
| 58 | DY | 55 | PSU | C6-N1-C2 | 4.44 | 122.61 | 115.47 |
| 58 | BY | 46 | 7MG | C6-N1-C2 | 4.75 | 122.53 | 115.94 |
| 58 | DY | 46 | 7MG | C6-N1-C2 | 4.77 | 122.55 | 115.94 |
| 56 | DW | 46 | 7MG | C6-N1-C2 | 4.95 | 122.81 | 115.94 |
| 56 | BW | 46 | 7MG | C6-N1-C2 | 5.22 | 123.19 | 115.94 |
| 57 | DX | 76 | 31H | O4'-C1'-N9 | 5.30 | 119.18 | 108.10 |
| 57 | BX | 76 | 31H | O4'-C1'-N9 | 5.30 | 119.20 | 108.10 |
| 57 | BX | 55 | PSU | C4-N3-C2 | 5.71 | 120.18 | 115.25 |
| 57 | DX | 54 | 5MU | C4-N3-C2 | 5.79 | 120.25 | 115.25 |
| 58 | DY | 55 | PSU | C4-N3-C2 | 6.30 | 120.69 | 115.25 |
| 57 | DX | 55 | PSU | C4-N3-C2 | 6.41 | 120.79 | 115.25 |
| 56 | BW | 55 | PSU | C4-N3-C2 | 6.43 | 120.80 | 115.25 |
| 58 | DY | 54 | 5MU | C4-N3-C2 | 6.51 | 120.88 | 115.25 |
| 57 | BX | 54 | 5MU | C4-N3-C2 | 6.61 | 120.96 | 115.25 |
| 58 | BY | 39 | PSU | C4-N3-C2 | 6.63 | 120.98 | 115.25 |
| 58 | BY | 54 | 5MU | C4-N3-C2 | 6.68 | 121.02 | 115.25 |
| 56 | DW | 32 | PSU | C4-N3-C2 | 6.70 | 121.04 | 115.25 |
| 58 | DY | 32 | PSU | C4-N3-C2 | 6.71 | 121.05 | 115.25 |
| 56 | DW | 54 | 5MU | C4-N3-C2 | 6.76 | 121.09 | 115.25 |
| 56 | DW | 39 | PSU | C4-N3-C2 | 6.76 | 121.09 | 115.25 |
| 58 | BY | 32 | PSU | C4-N3-C2 | 6.81 | 121.13 | 115.25 |
| 58 | BY | 55 | PSU | C4-N3-C2 | 6.87 | 121.18 | 115.25 |
| 56 | BW | 54 | 5MU | C4-N3-C2 | 6.91 | 121.22 | 115.25 |
| 56 | BW | 39 | PSU | C4-N3-C2 | 6.96 | 121.26 | 115.25 |
| 56 | DW | 55 | PSU | C4-N3-C2 | 6.99 | 121.28 | 115.25 |
| 56 | BW | 32 | PSU | C4-N3-C2 | 7.06 | 121.35 | 115.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 56 | DW | 46 | 7MG | N3-C4-N9 | 7.39 | 137.84 | 126.75 |
| 58 | DY | 39 | PSU | C4-N3-C2 | 7.56 | 121.78 | 115.25 |
| 56 | BW | 46 | 7MG | N3-C4-N9 | 7.65 | 138.23 | 126.75 |
| 58 | BY | 46 | 7MG | N3-C4-N9 | 8.11 | 138.92 | 126.75 |
| 58 | DY | 46 | 7MG | N3-C4-N9 | 8.78 | 139.93 | 126.75 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 57 | DX | 76 | 31H | OCN-CN-N-CA |
| 57 | BX | 76 | 31H | OCN-CN-N-CA |

There are no ring outliers.

21 monomers are involved in 31 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56 | BW | 39 | PSU | 1 | 0 |
| 56 | BW | 55 | PSU | 1 | 0 |
| 56 | BW | 76 | F3N | 2 | 0 |
| 56 | BW | 8 | 4SU | 1 | 0 |
| 57 | BX | 32 | 5MC | 2 | 0 |
| 57 | BX | 55 | PSU | 1 | 0 |
| 58 | BY | 39 | PSU | 1 | 0 |
| 58 | BY | 8 | 4SU | 1 | 0 |
| 56 | DW | 32 | PSU | 1 | 0 |
| 56 | DW | 37 | MIA | 1 | 0 |
| 56 | DW | 46 | 7MG | 2 | 0 |
| 56 | DW | 54 | 5MU | 1 | 0 |
| 56 | DW | 55 | PSU | 1 | 0 |
| 56 | DW | 76 | F3N | 4 | 0 |
| 57 | DX | 55 | PSU | 1 | 0 |
| 57 | DX | 76 | 31H | 3 | 0 |
| 57 | DX | 8 | 4SU | 1 | 0 |
| 58 | DY | 37 | MIA | 2 | 0 |
| 58 | DY | 39 | PSU | 1 | 0 |
| 58 | DY | 55 | PSU | 3 | 0 |
| 58 | DY | 8 | 4SU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2073 ligands modelled in this entry, 2069 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 63 | SF4 | BD | 501 | 37 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 64 | GDP | BZ | 702 | 60 | 23,30,30 | 1.15 | 2 (8%) | 30,47,47 | 2.01 | 7 (23%) |
| 63 | SF4 | DD | 501 | 37 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 64 | GDP | DZ | 702 | 60 | 23,30,30 | 1.08 | 2 (8%) | 30,47,47 | 1.85 | 8 (26%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 63 | SF4 | BD | 501 | 37 | - | 0/0/48/48 | 0/6/5/5 |
| 64 | GDP | BZ | 702 | 60 | - | 0/12/32/32 | 0/3/3/3 |
| 63 | SF4 | DD | 501 | 37 | - | 0/0/48/48 | 0/6/5/5 |
| 64 | GDP | DZ | 702 | 60 | - | 0/12/32/32 | 0/3/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 64 | BZ | 702 | GDP | C6-C5 | 2.67 | 1.46 | 1.41 |
| 64 | DZ | 702 | GDP | C5-C4 | 2.96 | 1.47 | 1.40 |
| 64 | DZ | 702 | GDP | C6-C5 | 3.10 | 1.47 | 1.41 |
| 64 | BZ | 702 | GDP | C5-C4 | 3.13 | 1.47 | 1.40 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 64 | BZ | 702 | GDP | C5-C6-N1 | -5.06 | 116.67 | 123.59 |
| 64 | BZ | 702 | GDP | C2'-C1'-N9 | -4.63 | 107.22 | 114.29 |
| 64 | DZ | 702 | GDP | C5-C6-N1 | -4.40 | 117.57 | 123.59 |
| 64 | DZ | 702 | GDP | PA-O3A-PB | -3.38 | 121.33 | 132.67 |
| 64 | DZ | 702 | GDP | C2'-C1'-N9 | -3.25 | 109.32 | 114.29 |
| 64 | BZ | 702 | GDP | PA-O3A-PB | -3.04 | 122.48 | 132.67 |
| 64 | DZ | 702 | GDP | C6-C5-C4 | -3.00 | 117.32 | 120.90 |
| 64 | BZ | 702 | GDP | N3-C2-N1 | -2.83 | 123.13 | 127.44 |
| 64 | DZ | 702 | GDP | C4-C5-N7 | -2.53 | 107.15 | 109.48 |
| 64 | DZ | 702 | GDP | N3-C2-N1 | -2.53 | 123.59 | 127.44 |
| 64 | DZ | 702 | GDP | O3'-C3'-C4' | -2.33 | 104.06 | 111.05 |
| 64 | BZ | 702 | GDP | C4-C5-N7 | -2.15 | 107.50 | 109.48 |
| 64 | BZ | 702 | GDP | O4'-C1'-N9 | 2.02 | 112.32 | 108.10 |
| 64 | BZ | 702 | GDP | C6-N1-C2 | 4.58 | 122.29 | 115.94 |
| 64 | DZ | 702 | GDP | C6-N1-C2 | 4.68 | 122.44 | 115.94 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 63 | BD | 501 | SF4 | 1 | 0 |
| 64 | BZ | 702 | GDP | 6 | 0 |
| 63 | DD | 501 | SF4 | 1 | 0 |
| 64 | DZ | 702 | GDP | 7 | 0 |

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 | 2872/2915 (98%) | -0.13 | 60 (2%) 67 56 | 16, 36, 153, 292 | 0 |
| 1 | CA | 2868/2915 (98%) | -0.01 | 112 (3%) 43 31 | 25, 54, 187, 320 | 0 |
| 2 | AB | 120/121 (99%) | -0.38 | 0 100 100 | 26, 52, 72, 110 | 0 |
| 2 | CB | 120/121 (99%) | -0.08 | 0 100 100 | 55, 87, 110, 177 | 0 |
| 3 | AC | 137/228 (60%) | 4.05 | 114 (83%) 0 0 | 95, 162, 210, 232 | 0 |
| 3 | CC | 137/228 (60%) | 5.81 | 126 (91%) 0 0 | 115, 183, 225, 239 | 0 |
| 4 | AD | 275/276 (99%) | -0.47 | 2 (0%) 89 84 | 16, 35, 59, 113 | 0 |
| 4 | CD | 275/276 (99%) | -0.33 | 1 (0%) 93 90 | 19, 46, 73, 142 | 0 |
| 5 | AE | 204/206 (99%) | -0.47 | 0 100 100 | 8, 36, 67, 101 | 0 |
| 5 | CE | 204/206 (99%) | -0.27 | 0 100 100 | 25, 53, 88, 136 | 0 |
| 6 | AF | 203/210 (96%) | -0.41 | 1 (0%) 91 88 | 12, 37, 91, 175 | 0 |
| 6 | CF | 203/210 (96%) | -0.29 | 0 100 100 | 23, 63, 114, 164 | 0 |
| 7 | AG | 181/182 (99%) | -0.22 | 3 (1%) 73 63 | 41, 71, 110, 179 | 0 |
| 7 | CG | 181/182 (99%) | 0.32 | 8 (4%) 38 26 | 74, 106, 143, 190 | 0 |
| 8 | AH | 174/180 (96%) | -0.35 | 2 (1%) 82 74 | 30, 51, 81, 174 | 0 |
| 8 | CH | 174/180 (96%) | 0.63 | 12 (6%) 20 11 | 45, 94, 139, 208 | 0 |
| 9 | AK | 130/173 (75%) | 1.30 | 27 (20%) 1 1 | 62, 125, 191, 235 | 0 |
| 9 | CK | 130/173 (75%) | 2.94 | 73 (56%) 0 0 | 104, 173, 211, 231 | 0 |
| 10 | AL | 66/147 (44%) | 4.22 | 51 (77%) 0 0 | 134, 182, 226, 242 | 0 |
| 10 | CL | 66/147 (44%) | 5.96 | 53 (80%) 0 0 | 115, 198, 249, 257 | 0 |
| 11 | AN | 140/140 (100%) | -0.52 | 0 100 100 | 17, 34, 76, 106 | 0 |
| 11 | CN | 140/140 (100%) | -0.09 | 1 (0%) 89 84 | 33, 59, 97, 139 | 0 |
| 12 | AO | 122/122 (100%) | -0.32 | 0 100 100 | 20, 40, 67, 95 | 0 |
| 12 | CO | 122/122 (100%) | -0.29 | 0 100 100 | 33, 52, 83, 102 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13 | AP | 149/150 (99%) | -0.29 | 0 100 100 | 14, 44, 83, 127 | 0 |
| 13 | CP | 149/150 (99%) | 0.23 | 4 (2%) 58 45 | 29, 66, 112, 154 | 0 |
| 14 | AQ | 141/141 (100%) | -0.37 | 0 100 100 | 17, 39, 66, 97 | 0 |
| 14 | CQ | 141/141 (100%) | -0.32 | 0 100 100 | 33, 62, 91, 156 | 0 |
| 15 | AR | 118/118 (100%) | -0.47 | 0 100 100 | 17, 32, 57, 96 | 0 |
| 15 | CR | 118/118 (100%) | -0.26 | 0 100 100 | 29, 52, 78, 97 | 0 |
| 16 | AS | 110/112 (98%) | -0.15 | 0 100 100 | 32, 54, 81, 102 | 0 |
| 16 | CS | 110/112 (98%) | 0.28 | 4 (3%) 46 34 | 53, 82, 112, 143 | 0 |
| 17 | AT | 131/146 (89%) | -0.29 | 2 (1%) 76 68 | 23, 44, 94, 160 | 0 |
| 17 | CT | 131/146 (89%) | -0.31 | 0 100 100 | 37, 58, 99, 155 | 0 |
| 18 | AU | 116/118 (98%) | -0.56 | 0 100 100 | 15, 28, 48, 110 | 0 |
| 18 | CU | 116/118 (98%) | -0.27 | 1 (0%) 85 79 | 36, 52, 82, 123 | 0 |
| 19 | AV | 101/101 (100%) | -0.56 | 1 (0%) 84 77 | 19, 34, 63, 119 | 0 |
| 19 | CV | 101/101 (100%) | -0.03 | 1 (0%) 84 77 | 33, 72, 108, 138 | 0 |
| 20 | AW | 112/113 (99%) | -0.44 | 0 100 100 | 15, 29, 56, 134 | 0 |
| 20 | CW | 112/113 (99%) | -0.23 | 1 (0%) 85 79 | 27, 48, 86, 149 | 0 |
| 21 | AX | 95/96 (98%) | -0.44 | 1 (1%) 82 74 | 22, 38, 69, 125 | 0 |
| 21 | CX | 95/96 (98%) | 0.04 | 4 (4%) 40 28 | 40, 61, 93, 134 | 0 |
| 22 | AY | 107/110 (97%) | -0.28 | 1 (0%) 85 79 | 25, 48, 92, 129 | 0 |
| 22 | CY | 107/110 (97%) | 0.69 | 7 (6%) 22 13 | 43, 78, 114, 172 | 0 |
| 23 | AZ | 171/206 (83%) | 0.08 | 11 (6%) 23 14 | 33, 73, 144, 235 | 0 |
| 23 | CZ | 174/206 (84%) | 0.85 | 22 (12%) 5 2 | 60, 107, 174, 243 | 0 |
| 24 | A0 | 83/85 (97%) | -0.30 | 2 (2%) 62 50 | 18, 38, 68, 147 | 0 |
| 24 | C0 | 83/85 (97%) | 0.32 | 6 (7%) 18 10 | 37, 62, 96, 135 | 0 |
| 25 | A1 | 97/98 (98%) | -0.21 | 2 (2%) 67 56 | 23, 44, 85, 108 | 0 |
| 25 | C1 | 97/98 (98%) | -0.09 | 1 (1%) 84 77 | 33, 54, 107, 119 | 0 |
| 26 | A2 | 70/72 (97%) | -0.27 | 2 (2%) 55 43 | 22, 47, 74, 149 | 0 |
| 26 | C2 | 70/72 (97%) | 0.04 | 1 (1%) 78 69 | 51, 78, 99, 121 | 0 |
| 27 | A3 | 59/60 (98%) | -0.28 | 1 (1%) 73 63 | 18, 34, 63, 112 | 0 |
| 27 | C3 | 59/60 (98%) | 0.61 | 5 (8%) 13 6 | 43, 62, 108, 167 | 0 |
| 28 | A4 | 69/71 (97%) | 0.49 | 9 (13%) 5 2 | 60, 100, 186, 194 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28 | C4 | 69/71 (97%) | 0.98 | 13 (18%) 2 1 | 89, 138, 197, 212 | 0 |
| 29 | A5 | 59/60 (98%) | -0.56 | 0 100 100 | 15, 30, 55, 84 | 0 |
| 29 | C5 | 59/60 (98%) | -0.22 | 1 (1%) 73 63 | 29, 46, 77, 112 | 0 |
| 30 | A6 | 53/54 (98%) | -0.38 | 0 100 100 | 24, 42, 67, 91 | 0 |
| 30 | C6 | 53/54 (98%) | -0.08 | 1 (1%) 70 59 | 43, 63, 88, 103 | 0 |
| 31 | A7 | 48/49 (97%) | -0.26 | 2 (4%) 40 28 | 14, 26, 63, 126 | 0 |
| 31 | C7 | 48/49 (97%) | -0.08 | 1 (2%) 67 56 | 26, 38, 83, 105 | 0 |
| 32 | A8 | 64/65 (98%) | -0.43 | 0 100 100 | 17, 32, 46, 72 | 0 |
| 32 | C8 | 64/65 (98%) | -0.23 | 0 100 100 | 36, 51, 70, 101 | 0 |
| 33 | A9 | 37/37 (100%) | -0.11 | 0 100 100 | 23, 39, 60, 80 | 0 |
| 33 | C9 | 37/37 (100%) | 0.25 | 1 (2%) 58 45 | 42, 66, 96, 108 | 0 |
| 34 | BA | 1497/1521 (98%) | 0.05 | 35 (2%) 64 52 | 32, 76, 169, 302 | 0 |
| 34 | DA | 1503/1521 (98%) | 0.13 | 37 (2%) 61 48 | 40, 83, 174, 317 | 0 |
| 35 | BB | 231/256 (90%) | 0.49 | 18 (7%) 16 8 | 61, 108, 167, 197 | 0 |
| 35 | DB | 231/256 (90%) | 0.84 | 33 (14%) 4 2 | 77, 129, 184, 232 | 0 |
| 36 | BC | 206/239 (86%) | 0.33 | 8 (3%) 43 31 | 60, 103, 138, 194 | 0 |
| 36 | DC | 206/239 (86%) | 0.91 | 25 (12%) 6 3 | 77, 127, 170, 196 | 0 |
| 37 | BD | 208/209 (99%) | 0.07 | 3 (1%) 78 69 | 51, 82, 121, 168 | 0 |
| 37 | DD | 208/209 (99%) | -0.01 | 2 (0%) 84 77 | 47, 80, 112, 165 | 0 |
| 38 | BE | 148/162 (91%) | -0.08 | 0 100 100 | 48, 73, 111, 140 | 0 |
| 38 | DE | 148/162 (91%) | 0.20 | 4 (2%) 58 45 | 46, 89, 128, 151 | 0 |
| 39 | BF | 100/101 (99%) | -0.21 | 0 100 100 | 45, 80, 116, 137 | 0 |
| 39 | DF | 100/101 (99%) | -0.17 | 1 (1%) 84 77 | 49, 80, 104, 121 | 0 |
| 40 | BG | 155/156 (99%) | 0.28 | 13 (8%) 14 6 | 59, 88, 132, 174 | 0 |
| 40 | DG | 155/156 (99%) | 0.68 | 17 (10%) 7 3 | 67, 103, 142, 192 | 0 |
| 41 | BH | 137/138 (99%) | 0.09 | 1 (0%) 89 84 | 45, 76, 106, 135 | 0 |
| 41 | DH | 137/138 (99%) | 0.38 | 6 (4%) 38 26 | 55, 88, 127, 170 | 0 |
| 42 | BI | 127/128 (99%) | 0.61 | 10 (7%) 15 8 | 50, 101, 140, 166 | 0 |
| 42 | DI | 127/128 (99%) | 1.32 | 28 (22%) 1 1 | 66, 118, 159, 201 | 0 |
| 43 | BJ | 97/105 (92%) | 0.82 | 14 (14%) 3 2 | 53, 113, 158, 199 | 0 |
| 43 | DJ | 96/105 (91%) | 1.47 | 25 (26%) 1 0 | 70, 134, 181, 195 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 44 | BK | 114/129 (88%) | -0.26 | 0 100 100 | 45, 72, 112, 129 | 0 |
| 44 | DK | 114/129 (88%) | -0.01 | 1 (0%) 85 79 | 44, 80, 118, 139 | 0 |
| 45 | BL | 122/132 (92%) | -0.22 | 0 100 100 | 38, 63, 88, 113 | 0 |
| 45 | DL | 122/132 (92%) | -0.01 | 2 (1%) 74 66 | 37, 72, 94, 141 | 0 |
| 46 | BM | 123/126 (97%) | 0.54 | 9 (7%) 18 10 | 55, 95, 129, 222 | 0 |
| 46 | DM | 122/126 (96%) | 0.90 | 16 (13%) 5 2 | 71, 125, 153, 188 | 0 |
| 47 | BN | 60/61 (98%) | 0.57 | 4 (6%) 21 12 | 65, 95, 123, 138 | 0 |
| 47 | DN | 60/61 (98%) | 1.71 | 20 (33%) 0 0 | 84, 123, 166, 208 | 0 |
| 48 | BO | 88/89 (98%) | -0.04 | 2 (2%) 64 52 | 39, 68, 110, 142 | 0 |
| 48 | DO | 88/89 (98%) | 0.26 | 0 100 100 | 43, 78, 112, 127 | 0 |
| 49 | BP | 82/88 (93%) | 0.35 | 2 (2%) 62 50 | 54, 76, 109, 134 | 0 |
| 49 | DP | 82/88 (93%) | 0.19 | 2 (2%) 62 50 | 53, 70, 96, 131 | 0 |
| 50 | BQ | 99/105 (94%) | -0.07 | 0 100 100 | 43, 69, 97, 110 | 0 |
| 50 | DQ | 99/105 (94%) | 0.10 | 0 100 100 | 51, 74, 103, 123 | 0 |
| 51 | BR | 68/88 (77%) | 0.48 | 4 (5%) 26 16 | 48, 73, 112, 135 | 0 |
| 51 | DR | 68/88 (77%) | 0.48 | 4 (5%) 26 16 | 46, 78, 116, 135 | 0 |
| 52 | BS | 84/93 (90%) | 1.07 | 16 (19%) 2 1 | 67, 110, 163, 180 | 0 |
| 52 | DS | 83/93 (89%) | 1.89 | 39 (46%) 0 0 | 92, 141, 187, 229 | 0 |
| 53 | BT | 96/106 (90%) | 0.25 | 1 (1%) 84 77 | 53, 77, 115, 169 | 0 |
| 53 | DT | 96/106 (90%) | 0.29 | 1 (1%) 84 77 | 52, 77, 117, 132 | 0 |
| 54 | BU | 23/27 (85%) | 0.78 | 3 (13%) 5 2 | 56, 89, 104, 114 | 0 |
| 54 | DU | 23/27 (85%) | 1.73 | 9 (39%) 0 0 | 79, 109, 130, 142 | 0 |
| 55 | BV | 13/24 (54%) | 1.63 | 5 (38%) 0 0 | 49, 87, 172, 178 | 0 |
| 55 | DV | 12/24 (50%) | 2.51 | 7 (58%) 0 0 | 63, 120, 171, 199 | 0 |
| 56 | BW | 66/76 (86%) | 2.49 | 32 (48%) 0 0 | 64, 169, 230, 256 | 0 |
| 56 | DW | 64/76 (84%) | 3.51 | 44 (68%) 0 0 | 92, 197, 239, 263 | 0 |
| 57 | BX | 71/77 (92%) | -0.02 | 0 100 100 | 34, 78, 124, 188 | 0 |
| 57 | DX | 71/77 (92%) | 0.21 | 2 (2%) 56 44 | 34, 100, 148, 162 | 0 |
| 58 | BY | 67/76 (88%) | 0.88 | 9 (13%) 4 2 | 39, 159, 224, 266 | 0 |
| 58 | DY | 66/76 (86%) | 1.30 | 15 (22%) 1 1 | 57, 178, 229, 251 | 0 |
| 59 | BZ | 728/758 (96%) | 1.11 | 156 (21%) 1 1 | 41, 107, 195, 257 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 59 | DZ | 730/758 (96%) | 1.56 | 230 (31%) 1 0 | 38, 116, 213, 248 | 0 |
| All | All | 22848/24064 (94%) | 0.26 | 1669 (7%) 18 10 | 8, 68, 177, 320 | 0 |

All (1669) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 59 | BZ | 503 | GLY | 25.7 |
| 10 | CL | 137 | GLU | 19.6 |
| 3 | CC | 174 | ALA | 18.4 |
| 10 | CL | 138 | VAL | 16.2 |
| 59 | BZ | 502 | GLY | 15.5 |
| 3 | CC | 172 | ILE | 14.5 |
| 3 | CC | 176 | VAL | 14.4 |
| 10 | AL | 135 | GLY | 14.3 |
| 3 | CC | 69 | LEU | 14.1 |
| 59 | DZ | 688 | ILE | 14.0 |
| 46 | DM | 123 | ALA | 13.3 |
| 59 | DZ | 419 | ALA | 13.3 |
| 10 | CL | 133 | SER | 13.2 |
| 59 | BZ | 472 | VAL | 13.1 |
| 59 | DZ | 426 | GLN | 13.0 |
| 34 | DA | 1030(B) | C | 12.9 |
| 56 | DW | 71 | G | 12.9 |
| 3 | CC | 177 | GLY | 12.9 |
| 3 | CC | 162 | ILE | 12.8 |
| 59 | DZ | 422 | GLU | 12.5 |
| 9 | CK | 50 | ARG | 12.5 |
| 59 | DZ | 417 | THR | 12.5 |
| 59 | DZ | 425 | SER | 12.3 |
| 9 | AK | 49 | ALA | 12.1 |
| 3 | CC | 41 | THR | 12.1 |
| 3 | CC | 59 | VAL | 11.9 |
| 10 | CL | 82 | ALA | 11.8 |
| 10 | CL | 114 | ASP | 11.7 |
| 40 | DG | 83 | ALA | 11.4 |
| 3 | CC | 163 | GLU | 11.4 |
| 3 | CC | 164 | PHE | 11.4 |
| 59 | BZ | 419 | ALA | 11.2 |
| 10 | CL | 126 | MET | 11.1 |
| 3 | CC | 180 | SER | 11.0 |
| 3 | AC | 159 | ALA | 10.8 |
| 59 | DZ | 404 | VAL | 10.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 59 | DZ | 684 | GLN | 10.7 |
| 3 | CC | 160 | GLY | 10.7 |
| 10 | AL | 86 | LYS | 10.6 |
| 9 | CK | 49 | ALA | 10.6 |
| 40 | DG | 82 | GLY | 10.5 |
| 10 | AL | 134 | MET | 10.4 |
| 3 | CC | 175 | PRO | 10.3 |
| 3 | CC | 28 | ARG | 10.3 |
| 56 | DW | 72 | C | 10.1 |
| 10 | AL | 92 | GLY | 10.0 |
| 10 | CL | 94 | GLU | 9.9 |
| 56 | DW | 70 | G | 9.9 |
| 59 | DZ | 421 | GLN | 9.9 |
| 10 | CL | 95 | LYS | 9.9 |
| 59 | DZ | 444 | PRO | 9.9 |
| 3 | AC | 174 | ALA | 9.8 |
| 59 | DZ | 487 | ILE | 9.7 |
| 10 | CL | 105 | LEU | 9.7 |
| 10 | CL | 125 | ARG | 9.7 |
| 3 | AC | 219 | MET | 9.7 |
| 3 | AC | 57 | GLN | 9.7 |
| 3 | CC | 35 | THR | 9.6 |
| 3 | CC | 67 | HIS | 9.6 |
| 9 | CK | 53 | VAL | 9.6 |
| 3 | CC | 68 | GLY | 9.5 |
| 3 | CC | 171 | ALA | 9.5 |
| 9 | CK | 96 | PHE | 9.5 |
| 3 | CC | 61 | GLY | 9.4 |
| 10 | AL | 131 | ALA | 9.4 |
| 59 | DZ | 420 | ASP | 9.4 |
| 59 | DZ | 521 | SER | 9.4 |
| 59 | BZ | 91 | THR | 9.4 |
| 9 | AK | 48 | GLY | 9.3 |
| 59 | DZ | 594 | VAL | 9.3 |
| 3 | AC | 44 | VAL | 9.3 |
| 9 | AK | 50 | ARG | 9.2 |
| 59 | DZ | 593 | ALA | 9.2 |
| 10 | CL | 84 | LEU | 9.1 |
| 59 | BZ | 684 | GLN | 9.1 |
| 3 | CC | 44 | VAL | 9.1 |
| 59 | DZ | 634 | MET | 9.0 |
| 10 | CL | 83 | GLY | 9.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 59 | DZ | 472 | VAL | 9.0 |
| 43 | DJ | 10 | GLY | 9.0 |
| 3 | AC | 203 | GLU | 9.0 |
| 59 | DZ | 488 | THR | 8.9 |
| 10 | CL | 115 | LEU | 8.7 |
| 3 | CC | 70 | GLY | 8.7 |
| 46 | DM | 124 | PRO | 8.7 |
| 1 | CA | 1087 | G | 8.5 |
| 3 | CC | 182 | PRO | 8.5 |
| 59 | DZ | 473 | ASP | 8.5 |
| 22 | CY | 1 | MET | 8.5 |
| 34 | BA | 1030(B) | C | 8.4 |
| 3 | CC | 219 | MET | 8.4 |
| 10 | CL | 127 | ILE | 8.4 |
| 59 | DZ | 418 | LYS | 8.4 |
| 10 | AL | 138 | VAL | 8.4 |
| 9 | AK | 51 | LEU | 8.3 |
| 9 | CK | 97 | ALA | 8.3 |
| 23 | CZ | 144 | LEU | 8.3 |
| 56 | BW | 72 | C | 8.3 |
| 10 | CL | 88 | ALA | 8.3 |
| 3 | CC | 10 | ALA | 8.2 |
| 59 | DZ | 432 | ALA | 8.2 |
| 3 | CC | 56 | ASP | 8.2 |
| 10 | CL | 131 | ALA | 8.1 |
| 59 | DZ | 428 | LEU | 8.1 |
| 59 | BZ | 531 | GLY | 8.0 |
| 3 | CC | 58 | ASN | 8.0 |
| 59 | BZ | 501 | THR | 8.0 |
| 3 | CC | 66 | PRO | 8.0 |
| 3 | CC | 159 | ALA | 8.0 |
| 3 | CC | 221 | PRO | 8.0 |
| 47 | DN | 17 | LYS | 7.9 |
| 59 | DZ | 462 | ILE | 7.9 |
| 3 | CC | 37 | LYS | 7.9 |
| 46 | BM | 124 | PRO | 7.8 |
| 3 | CC | 170 | GLY | 7.8 |
| 10 | CL | 135 | GLY | 7.8 |
| 3 | CC | 166 | ASN | 7.7 |
| 10 | CL | 130 | SER | 7.7 |
| 10 | AL | 89 | HIS | 7.7 |
| 9 | CK | 51 | LEU | 7.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 59 | DZ | 503 | GLY | 7.7 |
| 3 | CC | 57 | GLN | 7.7 |
| 56 | DW | 3 | C | 7.7 |
| 10 | AL | 136 | VAL | 7.6 |
| 9 | AK | 88 | ALA | 7.6 |
| 3 | AC | 176 | VAL | 7.6 |
| 3 | CC | 48 | LEU | 7.6 |
| 34 | BA | 1002 | G | 7.6 |
| 1 | CA | 2146 | C | 7.6 |
| 56 | BW | 71 | G | 7.6 |
| 10 | CL | 98 | ARG | 7.6 |
| 34 | DA | 1001(A) | G | 7.6 |
| 10 | CL | 107 | ILE | 7.5 |
| 59 | BZ | 685 | GLU | 7.5 |
| 9 | CK | 116 | ILE | 7.5 |
| 10 | CL | 129 | GLY | 7.5 |
| 9 | CK | 99 | SER | 7.5 |
| 59 | DZ | 681 | LYS | 7.5 |
| 3 | CC | 60 | ARG | 7.5 |
| 9 | CK | 89 | ALA | 7.4 |
| 59 | BZ | 481 | VAL | 7.4 |
| 9 | CK | 115 | GLN | 7.4 |
| 10 | AL | 87 | GLY | 7.4 |
| 59 | BZ | 471 | LYS | 7.4 |
| 3 | AC | 65 | LEU | 7.4 |
| 3 | CC | 183 | PRO | 7.4 |
| 56 | DW | 6 | G | 7.4 |
| 59 | DZ | 416 | LYS | 7.3 |
| 10 | CL | 113 | PRO | 7.3 |
| 3 | CC | 36 | ALA | 7.3 |
| 59 | BZ | 90 | PHE | 7.3 |
| 3 | AC | 32 | GLU | 7.3 |
| 3 | AC | 221 | PRO | 7.3 |
| 10 | CL | 99 | ILE | 7.3 |
| 3 | CC | 40 | GLU | 7.3 |
| 3 | CC | 63 | VAL | 7.3 |
| 34 | DA | 1036 | G | 7.2 |
| 59 | DZ | 639 | ASN | 7.2 |
| 3 | CC | 217 | THR | 7.2 |
| 35 | DB | 232 | PRO | 7.2 |
| 3 | CC | 178 | LYS | 7.2 |
| 10 | AL | 83 | GLY | 7.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 9 | CK | 25 | PHE | 7.1 |
| 3 | AC | 170 | GLY | 7.1 |
| 10 | CL | 122 | ALA | 7.1 |
| 3 | CC | 42 | VAL | 7.1 |
| 3 | CC | 173 | HIS | 7.1 |
| 3 | AC | 52 | PRO | 7.1 |
| 59 | DZ | 486 | THR | 7.1 |
| 9 | AK | 53 | VAL | 7.1 |
| 59 | DZ | 464 | ASP | 7.0 |
| 34 | DA | 1030(A) | G | 7.0 |
| 55 | DV | 24 | A | 7.0 |
| 46 | BM | 123 | ALA | 7.0 |
| 59 | DZ | 415 | PRO | 6.9 |
| 3 | CC | 190 | ILE | 6.9 |
| 59 | DZ | 430 | ARG | 6.9 |
| 3 | AC | 59 | VAL | 6.9 |
| 56 | DW | 73 | A | 6.8 |
| 3 | CC | 199 | ALA | 6.8 |
| 10 | CL | 123 | ALA | 6.8 |
| 10 | CL | 80 | LYS | 6.8 |
| 28 | A4 | 57 | GLU | 6.8 |
| 10 | AL | 91 | PRO | 6.8 |
| 3 | CC | 179 | ALA | 6.8 |
| 59 | DZ | 429 | ALA | 6.8 |
| 10 | CL | 108 | ALA | 6.8 |
| 3 | AC | 190 | ILE | 6.7 |
| 10 | AL | 94 | GLU | 6.7 |
| 3 | AC | 56 | ASP | 6.7 |
| 59 | DZ | 424 | LEU | 6.7 |
| 9 | CK | 90 | ALA | 6.7 |
| 40 | BG | 82 | GLY | 6.7 |
| 3 | CC | 210 | LEU | 6.7 |
| 46 | DM | 122 | LYS | 6.7 |
| 56 | DW | 5 | G | 6.7 |
| 3 | AC | 192 | ALA | 6.7 |
| 3 | CC | 200 | HIS | 6.7 |
| 3 | AC | 161 | ARG | 6.6 |
| 59 | DZ | 463 | VAL | 6.6 |
| 3 | CC | 46 | ALA | 6.6 |
| 3 | CC | 220 | GLY | 6.6 |
| 9 | CK | 101 | PRO | 6.6 |
| 59 | DZ | 465 | ARG | 6.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 59 | DZ | 499 | ARG | 6.6 |
| 59 | BZ | 504 | ARG | 6.5 |
| 34 | BA | 1036 | G | 6.5 |
| 10 | CL | 81 | ALA | 6.5 |
| 59 | DZ | 500 | GLN | 6.5 |
| 59 | BZ | 89 | ASP | 6.5 |
| 3 | AC | 49 | GLY | 6.5 |
| 59 | DZ | 626 | ALA | 6.5 |
| 59 | DZ | 504 | ARG | 6.5 |
| 3 | CC | 192 | ALA | 6.4 |
| 56 | DW | 69 | G | 6.4 |
| 59 | DZ | 89 | ASP | 6.4 |
| 3 | CC | 71 | LYS | 6.4 |
| 10 | CL | 110 | GLN | 6.4 |
| 59 | DZ | 427 | ALA | 6.4 |
| 3 | CC | 12 | LEU | 6.4 |
| 59 | DZ | 562 | ASP | 6.3 |
| 42 | BI | 19 | LEU | 6.3 |
| 3 | CC | 24 | ASP | 6.3 |
| 3 | CC | 184 | GLU | 6.3 |
| 9 | CK | 84 | GLU | 6.3 |
| 1 | CA | 2155 | G | 6.3 |
| 3 | AC | 48 | LEU | 6.3 |
| 3 | AC | 172 | ILE | 6.3 |
| 10 | AL | 78 | ILE | 6.3 |
| 28 | C4 | 57 | GLU | 6.2 |
| 59 | BZ | 422 | GLU | 6.2 |
| 1 | CA | 2173 | A | 6.2 |
| 3 | CC | 189 | ASN | 6.2 |
| 59 | DZ | 90 | PHE | 6.2 |
| 59 | DZ | 467 | LYS | 6.2 |
| 3 | AC | 166 | ASN | 6.2 |
| 59 | BZ | 477 | GLY | 6.2 |
| 3 | AC | 34 | ALA | 6.2 |
| 10 | AL | 96 | VAL | 6.2 |
| 10 | CL | 101 | TRP | 6.2 |
| 59 | BZ | 538 | TYR | 6.2 |
| 3 | CC | 208 | THR | 6.2 |
| 3 | CC | 52 | PRO | 6.2 |
| 3 | CC | 188 | ASP | 6.1 |
| 3 | AC | 33 | LEU | 6.1 |
| 25 | C1 | 2 | SER | 6.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 175 | PRO | 6.1 |
| 9 | CK | 85 | ASP | 6.1 |
| 10 | AL | 120 | LEU | 6.1 |
| 3 | AC | 197 | LEU | 6.0 |
| 1 | CA | 1088 | A | 6.0 |
| 56 | BW | 73 | A | 6.0 |
| 56 | BW | 3 | C | 6.0 |
| 9 | AK | 90 | ALA | 6.0 |
| 3 | AC | 14 | LYS | 6.0 |
| 1 | AA | 2168 | C | 6.0 |
| 3 | CC | 187 | ALA | 6.0 |
| 3 | CC | 216 | THR | 6.0 |
| 9 | CK | 43 | ALA | 6.0 |
| 59 | DZ | 585 | ALA | 6.0 |
| 9 | AK | 89 | ALA | 5.9 |
| 9 | CK | 98 | LYS | 5.9 |
| 56 | DW | 15 | G | 5.9 |
| 56 | DW | 7 | A | 5.9 |
| 56 | DW | 4 | C | 5.9 |
| 42 | DI | 30 | GLY | 5.9 |
| 56 | DW | 2 | C | 5.9 |
| 59 | DZ | 614 | GLU | 5.9 |
| 35 | DB | 132 | LYS | 5.8 |
| 59 | DZ | 538 | TYR | 5.8 |
| 9 | CK | 44 | LEU | 5.8 |
| 27 | C3 | 60 | GLU | 5.8 |
| 10 | CL | 109 | LYS | 5.8 |
| 59 | BZ | 424 | LEU | 5.8 |
| 3 | CC | 5 | GLY | 5.8 |
| 56 | BW | 70 | G | 5.8 |
| 59 | DZ | 435 | ASP | 5.8 |
| 3 | CC | 4 | HIS | 5.8 |
| 59 | DZ | 461 | ILE | 5.8 |
| 9 | AK | 105 | PRO | 5.8 |
| 10 | CL | 97 | GLY | 5.8 |
| 23 | AZ | 112 | ARG | 5.8 |
| 59 | BZ | 639 | ASN | 5.7 |
| 3 | AC | 64 | SER | 5.7 |
| 56 | DW | 18 | G | 5.7 |
| 59 | DZ | 640 | ALA | 5.7 |
| 22 | AY | 1 | MET | 5.7 |
| 3 | AC | 218 | THR | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | AA | 932 | C | 5.6 |
| 59 | BZ | 681 | LYS | 5.6 |
| 1 | CA | 1065 | U | 5.6 |
| 59 | BZ | 505 | GLY | 5.6 |
| 40 | DG | 156 | TRP | 5.6 |
| 3 | CC | 203 | GLU | 5.6 |
| 1 | CA | 1067 | A | 5.6 |
| 3 | AC | 164 | PHE | 5.6 |
| 34 | DA | 1030(C) | G | 5.6 |
| 1 | CA | 2111 | C | 5.6 |
| 34 | BA | 1001(A) | G | 5.6 |
| 9 | CK | 100 | ASN | 5.6 |
| 59 | BZ | 93 | GLU | 5.6 |
| 3 | CC | 65 | LEU | 5.6 |
| 3 | AC | 28 | ARG | 5.5 |
| 3 | AC | 69 | LEU | 5.5 |
| 1 | CA | 2139 | C | 5.5 |
| 59 | BZ | 421 | GLN | 5.5 |
| 59 | DZ | 470 | PHE | 5.5 |
| 59 | DZ | 685 | GLU | 5.5 |
| 1 | AA | 2167 | C | 5.5 |
| 59 | DZ | 501 | THR | 5.5 |
| 1 | CA | 2145 | C | 5.5 |
| 56 | BW | 15 | G | 5.5 |
| 10 | CL | 75 | SER | 5.5 |
| 59 | DZ | 506 | GLN | 5.5 |
| 9 | CK | 31 | GLY | 5.5 |
| 59 | DZ | 595 | GLN | 5.5 |
| 59 | DZ | 559 | PRO | 5.5 |
| 59 | BZ | 231 | TYR | 5.4 |
| 59 | DZ | 522 | GLY | 5.4 |
| 3 | AC | 200 | HIS | 5.4 |
| 3 | CC | 39 | ASP | 5.4 |
| 1 | AA | 1221 | G | 5.4 |
| 3 | CC | 161 | ARG | 5.4 |
| 10 | CL | 112 | MET | 5.4 |
| 3 | CC | 165 | ARG | 5.4 |
| 10 | CL | 93 | ARG | 5.4 |
| 10 | CL | 96 | VAL | 5.4 |
| 10 | AL | 95 | LYS | 5.4 |
| 1 | CA | 1078 | U | 5.4 |
| 59 | DZ | 569 | ASP | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | C4 | 68 | ARG | 5.4 |
| 59 | BZ | 415 | PRO | 5.4 |
| 3 | AC | 23 | ILE | 5.4 |
| 3 | CC | 211 | ARG | 5.3 |
| 10 | CL | 124 | ALA | 5.3 |
| 55 | BV | 24 | A | 5.3 |
| 3 | AC | 13 | GLU | 5.3 |
| 10 | CL | 85 | GLU | 5.3 |
| 3 | AC | 26 | ALA | 5.3 |
| 9 | CK | 105 | PRO | 5.3 |
| 1 | CA | 1091 | G | 5.3 |
| 59 | BZ | 426 | GLN | 5.3 |
| 1 | AA | 935 | C | 5.3 |
| 3 | CC | 197 | LEU | 5.3 |
| 23 | CZ | 106 | GLY | 5.3 |
| 3 | AC | 171 | ALA | 5.3 |
| 59 | BZ | 435 | ASP | 5.2 |
| 52 | DS | 30 | LEU | 5.2 |
| 3 | AC | 204 | GLY | 5.2 |
| 34 | BA | 1003 | G | 5.2 |
| 59 | DZ | 612 | THR | 5.2 |
| 36 | BC | 2 | GLY | 5.2 |
| 59 | BZ | 530 | VAL | 5.2 |
| 59 | DZ | 655 | TYR | 5.2 |
| 3 | AC | 162 | ILE | 5.2 |
| 1 | AA | 2160 | C | 5.2 |
| 3 | AC | 30 | VAL | 5.2 |
| 59 | BZ | 473 | ASP | 5.2 |
| 3 | AC | 160 | GLY | 5.2 |
| 40 | DG | 81 | GLY | 5.2 |
| 3 | AC | 60 | ARG | 5.2 |
| 59 | BZ | 444 | PRO | 5.2 |
| 10 | CL | 111 | LYS | 5.2 |
| 3 | CC | 31 | LYS | 5.2 |
| 10 | AL | 93 | ARG | 5.2 |
| 3 | CC | 204 | GLY | 5.2 |
| 3 | CC | 185 | LYS | 5.2 |
| 9 | CK | 125 | LEU | 5.2 |
| 10 | AL | 124 | ALA | 5.2 |
| 1 | AA | 2165 | C | 5.1 |
| 59 | DZ | 683 | VAL | 5.1 |
| 47 | DN | 38 | GLY | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 59 | DZ | 474 | ALA | 5.1 |
| 3 | CC | 34 | ALA | 5.1 |
| 59 | DZ | 670 | VAL | 5.1 |
| 59 | DZ | 468 | ARG | 5.1 |
| 10 | CL | 136 | VAL | 5.1 |
| 56 | DW | 22 | G | 5.1 |
| 3 | AC | 50 | ILE | 5.1 |
| 59 | DZ | 491 | VAL | 5.1 |
| 59 | DZ | 686 | LYS | 5.1 |
| 59 | DZ | 528 | ALA | 5.1 |
| 59 | DZ | 471 | LYS | 5.1 |
| 3 | CC | 50 | ILE | 5.0 |
| 59 | DZ | 405 | PRO | 5.0 |
| 9 | CK | 39 | ALA | 5.0 |
| 1 | CA | 229 | A | 5.0 |
| 3 | AC | 194 | ILE | 5.0 |
| 59 | DZ | 680 | PRO | 5.0 |
| 3 | CC | 62 | THR | 5.0 |
| 10 | AL | 100 | THR | 5.0 |
| 25 | A1 | 2 | SER | 5.0 |
| 59 | BZ | 432 | ALA | 5.0 |
| 1 | AA | 1555 | C | 5.0 |
| 10 | AL | 85 | GLU | 5.0 |
| 23 | CZ | 107 | THR | 5.0 |
| 3 | CC | 33 | LEU | 4.9 |
| 3 | CC | 32 | GLU | 4.9 |
| 59 | DZ | 664 | GLN | 4.9 |
| 52 | DS | 64 | GLU | 4.9 |
| 1 | CA | 2156 | G | 4.9 |
| 1 | AA | 942 | A | 4.9 |
| 59 | DZ | 520 | GLY | 4.9 |
| 52 | DS | 71 | LEU | 4.9 |
| 46 | DM | 121 | LYS | 4.9 |
| 42 | DI | 7 | THR | 4.9 |
| 3 | CC | 38 | PHE | 4.9 |
| 59 | DZ | 413 | ILE | 4.9 |
| 59 | BZ | 227 | ILE | 4.9 |
| 52 | DS | 35 | SER | 4.9 |
| 3 | CC | 181 | PHE | 4.9 |
| 9 | CK | 77 | PRO | 4.8 |
| 36 | DC | 64 | VAL | 4.8 |
| 34 | DA | 1033 | G | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 35 | BB | 136 | VAL | 4.8 |
| 1 | CA | 2140 | C | 4.8 |
| 3 | CC | 8 | TYR | 4.8 |
| 59 | BZ | 454 | MET | 4.8 |
| 34 | BA | 1030(A) | G | 4.8 |
| 59 | DZ | 616 | TYR | 4.8 |
| 23 | CZ | 156 | LYS | 4.8 |
| 1 | AA | 931 | C | 4.8 |
| 59 | BZ | 597 | GLY | 4.8 |
| 59 | DZ | 662 | LYS | 4.8 |
| 59 | BZ | 418 | LYS | 4.8 |
| 28 | C4 | 56 | VAL | 4.8 |
| 9 | CK | 57 | THR | 4.8 |
| 59 | BZ | 576 | ASP | 4.8 |
| 47 | DN | 25 | VAL | 4.8 |
| 3 | AC | 24 | ASP | 4.8 |
| 23 | AZ | 114 | GLY | 4.7 |
| 59 | DZ | 541 | ALA | 4.7 |
| 59 | DZ | 543 | GLN | 4.7 |
| 59 | BZ | 540 | PRO | 4.7 |
| 3 | CC | 14 | LYS | 4.7 |
| 46 | DM | 82 | MET | 4.7 |
| 3 | CC | 6 | LYS | 4.7 |
| 59 | DZ | 494 | GLU | 4.7 |
| 1 | CA | 1509 | C | 4.7 |
| 1 | CA | 2147 | G | 4.7 |
| 3 | CC | 167 | ASP | 4.7 |
| 55 | DV | 14 | A | 4.7 |
| 59 | DZ | 584 | ILE | 4.7 |
| 1 | CA | 1066 | U | 4.7 |
| 1 | CA | 2154 | G | 4.7 |
| 43 | DJ | 71 | LEU | 4.6 |
| 3 | AC | 40 | GLU | 4.6 |
| 3 | AC | 9 | ARG | 4.6 |
| 59 | BZ | 449 | THR | 4.6 |
| 10 | CL | 78 | ILE | 4.6 |
| 56 | BW | 2 | C | 4.6 |
| 1 | CA | 1089 | G | 4.6 |
| 3 | CC | 45 | HIS | 4.6 |
| 3 | AC | 71 | LYS | 4.6 |
| 10 | AL | 132 | ARG | 4.6 |
| 34 | DA | 1030(D) | A | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 59 | DZ | 615 | GLU | 4.6 |
| 40 | BG | 80 | VAL | 4.6 |
| 1 | CA | 2148 | G | 4.6 |
| 3 | AC | 198 | GLU | 4.6 |
| 3 | CC | 43 | GLU | 4.6 |
| 3 | AC | 27 | ALA | 4.5 |
| 1 | AA | 2138 | G | 4.5 |
| 46 | BM | 121 | LYS | 4.5 |
| 10 | AL | 102 | GLU | 4.5 |
| 59 | DZ | 682 | GLN | 4.5 |
| 1 | CA | 2159 | G | 4.5 |
| 59 | DZ | 87 | HIS | 4.5 |
| 10 | CL | 79 | ARG | 4.5 |
| 9 | CK | 86 | PRO | 4.5 |
| 34 | DA | 1002 | G | 4.5 |
| 35 | DB | 139 | LYS | 4.5 |
| 46 | BM | 122 | LYS | 4.5 |
| 35 | DB | 135 | GLN | 4.5 |
| 9 | CK | 103 | GLY | 4.5 |
| 56 | DW | 14 | A | 4.5 |
| 10 | AL | 127 | ILE | 4.5 |
| 1 | AA | 2147 | G | 4.5 |
| 9 | CK | 118 | THR | 4.5 |
| 23 | CZ | 114 | GLY | 4.5 |
| 1 | CA | 2112 | G | 4.5 |
| 36 | DC | 188 | LEU | 4.5 |
| 56 | DW | 13 | C | 4.5 |
| 56 | DW | 56 | C | 4.5 |
| 59 | DZ | 476 | VAL | 4.5 |
| 59 | DZ | 551 | GLN | 4.5 |
| 9 | CK | 65 | GLU | 4.5 |
| 10 | AL | 84 | LEU | 4.5 |
| 56 | BW | 44 | G | 4.5 |
| 59 | DZ | 635 | GLU | 4.5 |
| 1 | CA | 885 | C | 4.4 |
| 3 | AC | 58 | ASN | 4.4 |
| 23 | AZ | 107 | THR | 4.4 |
| 59 | DZ | 689 | LYS | 4.4 |
| 56 | BW | 69 | G | 4.4 |
| 3 | AC | 186 | LEU | 4.4 |
| 9 | AK | 131 | MET | 4.4 |
| 52 | DS | 12 | ASP | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 59 | BZ | 413 | ILE | 4.4 |
| 59 | DZ | 530 | VAL | 4.4 |
| 10 | AL | 111 | LYS | 4.4 |
| 34 | DA | 1001 | A | 4.4 |
| 59 | DZ | 663 | THR | 4.4 |
| 59 | DZ | 598 | ASP | 4.4 |
| 3 | AC | 195 | ARG | 4.4 |
| 59 | DZ | 489 | LYS | 4.4 |
| 59 | BZ | 594 | VAL | 4.4 |
| 34 | BA | 1031 | G | 4.4 |
| 56 | BW | 14 | A | 4.4 |
| 3 | AC | 211 | ARG | 4.4 |
| 23 | AZ | 144 | LEU | 4.4 |
| 59 | DZ | 407 | PRO | 4.4 |
| 9 | CK | 37 | THR | 4.4 |
| 59 | BZ | 428 | LEU | 4.4 |
| 9 | CK | 56 | ASN | 4.3 |
| 3 | CC | 202 | PRO | 4.3 |
| 10 | AL | 99 | ILE | 4.3 |
| 9 | AK | 54 | ALA | 4.3 |
| 47 | BN | 2 | ALA | 4.3 |
| 52 | BS | 71 | LEU | 4.3 |
| 56 | DW | 67 | C | 4.3 |
| 3 | AC | 43 | GLU | 4.3 |
| 3 | AC | 163 | GLU | 4.3 |
| 3 | AC | 213 | VAL | 4.3 |
| 28 | A4 | 56 | VAL | 4.3 |
| 9 | CK | 119 | ALA | 4.3 |
| 1 | CA | 1079 | C | 4.3 |
| 59 | DZ | 540 | PRO | 4.3 |
| 35 | DB | 228 | GLY | 4.3 |
| 34 | BA | 1030(C) | G | 4.3 |
| 43 | BJ | 98 | ILE | 4.3 |
| 56 | BW | 1 | G | 4.3 |
| 3 | AC | 167 | ASP | 4.3 |
| 3 | AC | 70 | GLY | 4.3 |
| 9 | CK | 24 | PHE | 4.3 |
| 3 | CC | 215 | VAL | 4.3 |
| 1 | CA | 888 | C | 4.3 |
| 43 | DJ | 74 | ILE | 4.3 |
| 36 | DC | 196 | LEU | 4.3 |
| 1 | AA | 2163 | G | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | CC | 9 | ARG | 4.2 |
| 1 | CA | 1086 | A | 4.2 |
| 10 | AL | 137 | GLU | 4.2 |
| 34 | DA | 1026 | G | 4.2 |
| 35 | DB | 187 | LEU | 4.2 |
| 55 | DV | 23 | A | 4.2 |
| 59 | BZ | 500 | GLN | 4.2 |
| 10 | AL | 79 | ARG | 4.2 |
| 10 | AL | 114 | ASP | 4.2 |
| 34 | DA | 1021 | G | 4.2 |
| 35 | BB | 135 | GLN | 4.2 |
| 59 | BZ | 433 | GLU | 4.2 |
| 59 | DZ | 433 | GLU | 4.2 |
| 59 | BZ | 457 | LEU | 4.2 |
| 59 | DZ | 597 | GLY | 4.2 |
| 59 | BZ | 641 | GLN | 4.2 |
| 59 | DZ | 529 | ILE | 4.2 |
| 36 | DC | 189 | ALA | 4.2 |
| 10 | CL | 92 | GLY | 4.2 |
| 43 | DJ | 9 | ARG | 4.2 |
| 1 | CA | 2141 | G | 4.2 |
| 34 | DA | 1035 | A | 4.2 |
| 46 | DM | 120 | LYS | 4.2 |
| 52 | DS | 6 | LYS | 4.2 |
| 52 | DS | 32 | LYS | 4.2 |
| 8 | CH | 49 | VAL | 4.2 |
| 59 | DZ | 454 | MET | 4.2 |
| 59 | DZ | 455 | GLY | 4.2 |
| 3 | CC | 198 | GLU | 4.2 |
| 43 | DJ | 47 | PHE | 4.1 |
| 59 | DZ | 436 | PRO | 4.1 |
| 46 | DM | 119 | GLY | 4.1 |
| 3 | AC | 31 | LYS | 4.1 |
| 3 | AC | 206 | LYS | 4.1 |
| 59 | DZ | 575 | VAL | 4.1 |
| 3 | CC | 13 | GLU | 4.1 |
| 58 | DY | 53 | G | 4.1 |
| 40 | BG | 79 | ARG | 4.1 |
| 40 | DG | 79 | ARG | 4.1 |
| 59 | BZ | 468 | ARG | 4.1 |
| 9 | AK | 99 | SER | 4.1 |
| 59 | DZ | 676 | TYR | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 59 | DZ | 617 | MET | 4.1 |
| 9 | CK | 46 | GLN | 4.1 |
| 9 | AK | 104 | ILE | 4.1 |
| 59 | DZ | 539 | ILE | 4.1 |
| 59 | DZ | 638 | GLY | 4.1 |
| 34 | DA | 1032 | G | 4.1 |
| 59 | DZ | 586 | GLY | 4.1 |
| 59 | BZ | 430 | ARG | 4.1 |
| 10 | AL | 82 | ALA | 4.1 |
| 47 | DN | 2 | ALA | 4.1 |
| 3 | CC | 226 | ASN | 4.1 |
| 56 | DW | 31 | A | 4.1 |
| 10 | CL | 104 | VAL | 4.1 |
| 3 | AC | 177 | GLY | 4.1 |
| 10 | CL | 128 | ALA | 4.1 |
| 3 | AC | 182 | PRO | 4.1 |
| 10 | AL | 98 | ARG | 4.1 |
| 3 | AC | 188 | ASP | 4.1 |
| 59 | DZ | 630 | GLN | 4.0 |
| 59 | DZ | 408 | VAL | 4.0 |
| 3 | AC | 180 | SER | 4.0 |
| 59 | BZ | 577 | SER | 4.0 |
| 59 | BZ | 411 | VAL | 4.0 |
| 59 | DZ | 581 | ALA | 4.0 |
| 56 | DW | 23 | A | 4.0 |
| 59 | DZ | 448 | GLN | 4.0 |
| 59 | DZ | 505 | GLY | 4.0 |
| 3 | CC | 186 | LEU | 4.0 |
| 3 | AC | 66 | PRO | 4.0 |
| 40 | BG | 85 | TYR | 4.0 |
| 42 | DI | 27 | THR | 4.0 |
| 59 | DZ | 460 | GLU | 4.0 |
| 59 | DZ | 469 | GLU | 4.0 |
| 9 | CK | 129 | PRO | 4.0 |
| 34 | BA | 1030(D) | A | 4.0 |
| 3 | AC | 29 | LEU | 4.0 |
| 56 | DW | 19 | G | 4.0 |
| 3 | AC | 4 | HIS | 4.0 |
| 3 | CC | 64 | SER | 4.0 |
| 59 | BZ | 423 | LYS | 4.0 |
| 34 | BA | 1035 | A | 4.0 |
| 55 | BV | 12 | A | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 56 | DW | 58 | A | 4.0 |
| 3 | AC | 220 | GLY | 4.0 |
| 47 | DN | 34 | TYR | 4.0 |
| 59 | DZ | 40 | HIS | 4.0 |
| 40 | BG | 83 | ALA | 4.0 |
| 59 | DZ | 502 | GLY | 4.0 |
| 10 | AL | 88 | ALA | 4.0 |
| 23 | CZ | 108 | PRO | 3.9 |
| 59 | BZ | 470 | PHE | 3.9 |
| 34 | DA | 1257 | U | 3.9 |
| 59 | DZ | 527 | ASN | 3.9 |
| 59 | DZ | 446 | THR | 3.9 |
| 36 | DC | 87 | LEU | 3.9 |
| 52 | BS | 40 | ILE | 3.9 |
| 59 | DZ | 458 | HIS | 3.9 |
| 52 | DS | 26 | GLY | 3.9 |
| 59 | DZ | 523 | PHE | 3.9 |
| 3 | CC | 53 | ARG | 3.9 |
| 36 | DC | 39 | ILE | 3.9 |
| 59 | DZ | 567 | LEU | 3.9 |
| 10 | CL | 132 | ARG | 3.9 |
| 34 | BA | 1030 | C | 3.9 |
| 3 | CC | 22 | THR | 3.9 |
| 1 | CA | 2131 | G | 3.9 |
| 1 | CA | 1104 | C | 3.9 |
| 10 | AL | 90 | LYS | 3.9 |
| 59 | DZ | 434 | GLU | 3.9 |
| 58 | DY | 34 | G | 3.9 |
| 56 | DW | 49 | C | 3.9 |
| 59 | DZ | 660 | ARG | 3.9 |
| 3 | CC | 196 | ALA | 3.9 |
| 16 | CS | 58 | LEU | 3.9 |
| 59 | DZ | 457 | LEU | 3.9 |
| 24 | C0 | 3 | HIS | 3.9 |
| 59 | DZ | 423 | LYS | 3.9 |
| 10 | AL | 107 | ILE | 3.8 |
| 43 | DJ | 40 | LEU | 3.8 |
| 59 | DZ | 601 | ILE | 3.8 |
| 59 | BZ | 194 | THR | 3.8 |
| 59 | BZ | 616 | TYR | 3.8 |
| 9 | CK | 23 | SER | 3.8 |
| 1 | CA | 2160 | G | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 189 | ASN | 3.8 |
| 34 | DA | 1531 | A | 3.8 |
| 10 | AL | 81 | ALA | 3.8 |
| 59 | DZ | 517 | LEU | 3.8 |
| 34 | BA | 1034 | G | 3.8 |
| 3 | AC | 41 | THR | 3.8 |
| 59 | DZ | 645 | ALA | 3.8 |
| 9 | CK | 52 | PHE | 3.8 |
| 3 | AC | 202 | PRO | 3.8 |
| 59 | DZ | 447 | GLY | 3.8 |
| 47 | DN | 39 | LEU | 3.8 |
| 59 | BZ | 602 | LEU | 3.8 |
| 51 | BR | 22 | VAL | 3.8 |
| 1 | AA | 934 | A | 3.8 |
| 59 | BZ | 634 | MET | 3.8 |
| 9 | CK | 76 | GLY | 3.8 |
| 56 | BW | 20 | U | 3.8 |
| 59 | DZ | 623 | ASP | 3.8 |
| 35 | DB | 136 | VAL | 3.8 |
| 59 | DZ | 631 | ILE | 3.8 |
| 3 | AC | 224 | ARG | 3.8 |
| 1 | CA | 2142 | C | 3.8 |
| 23 | AZ | 113 | ALA | 3.8 |
| 52 | BS | 80 | TYR | 3.8 |
| 56 | BW | 6 | G | 3.8 |
| 1 | AA | 2183 | C | 3.8 |
| 46 | DM | 98 | VAL | 3.8 |
| 59 | BZ | 436 | PRO | 3.8 |
| 3 | AC | 209 | PHE | 3.7 |
| 28 | A4 | 52 | THR | 3.7 |
| 1 | AA | 1114 | G | 3.7 |
| 59 | BZ | 578 | SER | 3.7 |
| 59 | DZ | 641 | GLN | 3.7 |
| 1 | CA | 1090 | U | 3.7 |
| 3 | CC | 213 | VAL | 3.7 |
| 23 | AZ | 115 | GLY | 3.7 |
| 35 | DB | 133 | LYS | 3.7 |
| 42 | DI | 42 | ARG | 3.7 |
| 1 | AA | 2134 | G | 3.7 |
| 10 | CL | 86 | LYS | 3.7 |
| 42 | DI | 9 | ARG | 3.7 |
| 3 | AC | 46 | ALA | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 59 | DZ | 512 | ILE | 3.7 |
| 35 | DB | 121 | LEU | 3.7 |
| 59 | DZ | 578 | SER | 3.7 |
| 40 | DG | 80 | VAL | 3.7 |
| 1 | CA | 2138 | C | 3.6 |
| 9 | AK | 97 | ALA | 3.6 |
| 56 | BW | 13 | C | 3.6 |
| 51 | DR | 23 | LYS | 3.6 |
| 59 | BZ | 434 | GLU | 3.6 |
| 3 | AC | 68 | GLY | 3.6 |
| 56 | BW | 19 | G | 3.6 |
| 56 | DW | 24 | G | 3.6 |
| 59 | DZ | 431 | LEU | 3.6 |
| 9 | CK | 42 | GLN | 3.6 |
| 59 | BZ | 642 | VAL | 3.6 |
| 59 | BZ | 670 | VAL | 3.6 |
| 9 | CK | 88 | ALA | 3.6 |
| 9 | CK | 106 | GLN | 3.6 |
| 3 | AC | 67 | HIS | 3.6 |
| 44 | DK | 25 | TYR | 3.6 |
| 28 | A4 | 55 | ARG | 3.6 |
| 58 | DY | 35 | A | 3.6 |
| 1 | CA | 2116 | G | 3.6 |
| 36 | BC | 190 | ARG | 3.6 |
| 56 | DW | 28 | G | 3.6 |
| 3 | AC | 193 | PHE | 3.6 |
| 59 | DZ | 438 | PHE | 3.6 |
| 3 | AC | 25 | GLU | 3.6 |
| 59 | DZ | 596 | LYS | 3.6 |
| 58 | DY | 57 | G | 3.6 |
| 59 | DZ | 600 | VAL | 3.6 |
| 4 | AD | 276 | LYS | 3.6 |
| 59 | DZ | 519 | ARG | 3.6 |
| 3 | AC | 187 | ALA | 3.6 |
| 23 | AZ | 147 | GLY | 3.6 |
| 3 | CC | 225 | ILE | 3.6 |
| 56 | DW | 29 | G | 3.6 |
| 59 | BZ | 420 | ASP | 3.6 |
| 7 | CG | 2 | PRO | 3.6 |
| 35 | DB | 131 | PRO | 3.6 |
| 59 | BZ | 489 | LYS | 3.6 |
| 1 | CA | 887 | A | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 55 | BV | 23 | A | 3.6 |
| 46 | BM | 2 | ALA | 3.5 |
| 3 | AC | 38 | PHE | 3.5 |
| 59 | DZ | 514 | VAL | 3.5 |
| 59 | DZ | 443 | HIS | 3.5 |
| 1 | CA | 652(B) | A | 3.5 |
| 59 | BZ | 671 | MET | 3.5 |
| 3 | AC | 10 | ALA | 3.5 |
| 3 | AC | 191 | ARG | 3.5 |
| 36 | DC | 190 | ARG | 3.5 |
| 10 | AL | 139 | VAL | 3.5 |
| 43 | DJ | 72 | VAL | 3.5 |
| 59 | BZ | 612 | THR | 3.5 |
| 9 | CK | 45 | LYS | 3.5 |
| 24 | C0 | 75 | LEU | 3.5 |
| 59 | DZ | 666 | ARG | 3.5 |
| 1 | CA | 1058 | G | 3.5 |
| 34 | DA | 1034 | G | 3.5 |
| 52 | BS | 48 | THR | 3.5 |
| 59 | BZ | 638 | GLY | 3.5 |
| 10 | CL | 134 | MET | 3.5 |
| 9 | AK | 101 | PRO | 3.5 |
| 40 | DG | 78 | ARG | 3.5 |
| 46 | DM | 78 | ILE | 3.5 |
| 59 | DZ | 629 | GLY | 3.5 |
| 36 | DC | 187 | ALA | 3.5 |
| 3 | CC | 209 | PHE | 3.5 |
| 59 | DZ | 437 | THR | 3.5 |
| 10 | AL | 115 | LEU | 3.5 |
| 55 | DV | 21 | C | 3.5 |
| 1 | CA | 1103 | A | 3.5 |
| 23 | CZ | 115 | GLY | 3.5 |
| 43 | DJ | 73 | ASP | 3.5 |
| 1 | AA | 2161 | C | 3.4 |
| 1 | CA | 1102 | C | 3.4 |
| 56 | BW | 5 | G | 3.4 |
| 56 | DW | 10 | G | 3.4 |
| 59 | DZ | 654 | GLY | 3.4 |
| 43 | BJ | 72 | VAL | 3.4 |
| 1 | CA | 1068 | G | 3.4 |
| 58 | DY | 19 | G | 3.4 |
| 59 | DZ | 160 | ARG | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | CY | 55 | TYR | 3.4 |
| 1 | CA | 652(U) | G | 3.4 |
| 1 | CA | 2114 | A | 3.4 |
| 56 | BW | 22 | G | 3.4 |
| 28 | C4 | 67 | TYR | 3.4 |
| 43 | DJ | 6 | ILE | 3.4 |
| 3 | AC | 173 | HIS | 3.4 |
| 59 | DZ | 637 | ARG | 3.4 |
| 56 | BW | 65 | G | 3.4 |
| 40 | DG | 8 | GLU | 3.4 |
| 34 | BA | 1029 | C | 3.4 |
| 52 | BS | 84 | GLY | 3.4 |
| 3 | AC | 15 | VAL | 3.4 |
| 40 | BG | 156 | TRP | 3.4 |
| 59 | BZ | 414 | GLU | 3.4 |
| 36 | DC | 197 | GLY | 3.3 |
| 56 | DW | 48 | C | 3.3 |
| 43 | DJ | 27 | ALA | 3.3 |
| 1 | CA | 883 | G | 3.3 |
| 1 | CA | 2125 | G | 3.3 |
| 10 | AL | 133 | SER | 3.3 |
| 58 | DY | 56 | C | 3.3 |
| 10 | CL | 118 | THR | 3.3 |
| 21 | CX | 68 | ARG | 3.3 |
| 1 | CA | 1095 | A | 3.3 |
| 59 | BZ | 689 | LYS | 3.3 |
| 59 | BZ | 425 | SER | 3.3 |
| 11 | CN | 8 | GLN | 3.3 |
| 1 | AA | 698 | G | 3.3 |
| 59 | BZ | 463 | VAL | 3.3 |
| 59 | BZ | 537 | GLU | 3.3 |
| 43 | BJ | 10 | GLY | 3.3 |
| 59 | DZ | 677 | GLN | 3.3 |
| 3 | AC | 208 | THR | 3.3 |
| 28 | A4 | 50 | VAL | 3.3 |
| 21 | CX | 1 | MET | 3.3 |
| 55 | DV | 13 | A | 3.3 |
| 9 | CK | 78 | SER | 3.3 |
| 35 | BB | 133 | LYS | 3.3 |
| 56 | BW | 4 | C | 3.3 |
| 59 | DZ | 513 | LYS | 3.3 |
| 36 | DC | 32 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 10 | AL | 101 | TRP | 3.3 |
| 41 | DH | 99 | GLU | 3.3 |
| 56 | BW | 21 | A | 3.3 |
| 10 | AL | 76 | TYR | 3.3 |
| 40 | BG | 81 | GLY | 3.3 |
| 3 | CC | 214 | TYR | 3.3 |
| 34 | BA | 1026 | G | 3.3 |
| 59 | DZ | 459 | LEU | 3.3 |
| 3 | CC | 201 | LYS | 3.3 |
| 59 | DZ | 561 | VAL | 3.3 |
| 59 | DZ | 642 | VAL | 3.3 |
| 1 | AA | 2166 | U | 3.3 |
| 59 | BZ | 546 | ILE | 3.3 |
| 59 | DZ | 587 | SER | 3.3 |
| 59 | DZ | 624 | LEU | 3.3 |
| 1 | CA | 652(C) | G | 3.2 |
| 34 | DA | 1031 | G | 3.2 |
| 42 | BI | 8 | GLY | 3.2 |
| 3 | CC | 25 | GLU | 3.2 |
| 36 | DC | 159 | GLY | 3.2 |
| 59 | BZ | 412 | ALA | 3.2 |
| 43 | DJ | 89 | ASP | 3.2 |
| 3 | CC | 222 | SER | 3.2 |
| 35 | DB | 164 | VAL | 3.2 |
| 1 | CA | 886 | C | 3.2 |
| 59 | DZ | 475 | ASN | 3.2 |
| 40 | BG | 154 | TYR | 3.2 |
| 40 | DG | 154 | TYR | 3.2 |
| 59 | DZ | 572 | TYR | 3.2 |
| 9 | CK | 54 | ALA | 3.2 |
| 34 | BA | 1028 | C | 3.2 |
| 59 | BZ | 459 | LEU | 3.2 |
| 40 | BG | 78 | ARG | 3.2 |
| 3 | AC | 178 | LYS | 3.2 |
| 23 | CZ | 149 | SER | 3.2 |
| 52 | DS | 80 | TYR | 3.2 |
| 35 | DB | 140 | HIS | 3.2 |
| 9 | CK | 122 | VAL | 3.2 |
| 52 | DS | 44 | MET | 3.2 |
| 9 | CK | 26 | LEU | 3.2 |
| 35 | DB | 229 | VAL | 3.2 |
| 59 | DZ | 560 | VAL | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 165 | ARG | 3.2 |
| 28 | C4 | 32 | TYR | 3.2 |
| 59 | DZ | 537 | GLU | 3.2 |
| 37 | DD | 23 | GLY | 3.2 |
| 56 | BW | 23 | A | 3.2 |
| 59 | BZ | 474 | ALA | 3.2 |
| 59 | BZ | 535 | PRO | 3.2 |
| 59 | DZ | 599 | PRO | 3.2 |
| 3 | AC | 21 | TYR | 3.2 |
| 42 | BI | 4 | TYR | 3.2 |
| 43 | DJ | 38 | ILE | 3.2 |
| 59 | DZ | 568 | TYR | 3.2 |
| 1 | CA | 884 | C | 3.2 |
| 1 | AA | 2131 | U | 3.2 |
| 59 | BZ | 493 | VAL | 3.1 |
| 59 | BZ | 615 | GLU | 3.1 |
| 1 | AA | 2162 | C | 3.1 |
| 27 | C3 | 59 | VAL | 3.1 |
| 35 | DB | 214 | ILE | 3.1 |
| 21 | CX | 69 | TYR | 3.1 |
| 24 | C0 | 8 | GLY | 3.1 |
| 34 | DA | 1042 | G | 3.1 |
| 58 | DY | 18 | G | 3.1 |
| 23 | CZ | 96 | VAL | 3.1 |
| 34 | DA | 1043 | C | 3.1 |
| 58 | BY | 35 | A | 3.1 |
| 35 | DB | 122 | PHE | 3.1 |
| 10 | AL | 122 | ALA | 3.1 |
| 23 | CZ | 50 | GLN | 3.1 |
| 9 | CK | 73 | GLY | 3.1 |
| 35 | BB | 233 | SER | 3.1 |
| 46 | DM | 92 | HIS | 3.1 |
| 3 | CC | 193 | PHE | 3.1 |
| 56 | BW | 49 | C | 3.1 |
| 56 | DW | 68 | C | 3.1 |
| 21 | CX | 92 | LEU | 3.1 |
| 36 | DC | 198 | VAL | 3.1 |
| 59 | BZ | 491 | VAL | 3.1 |
| 59 | DZ | 235 | GLU | 3.1 |
| 59 | DZ | 515 | GLU | 3.1 |
| 59 | DZ | 613 | PRO | 3.1 |
| 59 | BZ | 541 | ALA | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | CA | 2143 | C | 3.1 |
| 1 | AA | 2141 | A | 3.1 |
| 1 | AA | 2174 | G | 3.1 |
| 1 | AA | 2176 | G | 3.1 |
| 56 | DW | 30 | G | 3.1 |
| 59 | DZ | 576 | ASP | 3.1 |
| 59 | DZ | 580 | MET | 3.1 |
| 3 | CC | 206 | LYS | 3.1 |
| 9 | CK | 4 | LYS | 3.1 |
| 34 | BA | 1039 | C | 3.1 |
| 56 | BW | 7 | A | 3.1 |
| 59 | BZ | 438 | PHE | 3.0 |
| 1 | CA | 1093 | G | 3.0 |
| 56 | DW | 57 | G | 3.0 |
| 59 | BZ | 442 | THR | 3.0 |
| 59 | DZ | 91 | THR | 3.0 |
| 59 | BZ | 447 | GLY | 3.0 |
| 59 | BZ | 613 | PRO | 3.0 |
| 35 | DB | 48 | MET | 3.0 |
| 43 | BJ | 73 | ASP | 3.0 |
| 34 | BA | 202 | U | 3.0 |
| 9 | CK | 30 | GLN | 3.0 |
| 34 | DA | 1003 | G | 3.0 |
| 1 | AA | 2164 | C | 3.0 |
| 28 | C4 | 59 | PHE | 3.0 |
| 42 | DI | 18 | PHE | 3.0 |
| 28 | C4 | 50 | VAL | 3.0 |
| 52 | DS | 61 | TYR | 3.0 |
| 10 | AL | 110 | GLN | 3.0 |
| 1 | CA | 2168 | G | 3.0 |
| 24 | C0 | 7 | LEU | 3.0 |
| 59 | DZ | 687 | LEU | 3.0 |
| 34 | DA | 1532 | U | 3.0 |
| 59 | BZ | 680 | PRO | 3.0 |
| 1 | CA | 1080 | C | 3.0 |
| 56 | BW | 68 | C | 3.0 |
| 52 | DS | 4 | SER | 3.0 |
| 3 | AC | 210 | LEU | 3.0 |
| 58 | DY | 52 | G | 3.0 |
| 1 | CA | 2804 | C | 3.0 |
| 9 | CK | 132 | ASP | 3.0 |
| 3 | AC | 185 | LYS | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | AL | 97 | GLY | 3.0 |
| 58 | BY | 20 | U | 3.0 |
| 1 | AA | 2159 | C | 3.0 |
| 23 | CZ | 169 | GLU | 3.0 |
| 36 | DC | 91 | LEU | 3.0 |
| 38 | DE | 31 | LEU | 3.0 |
| 59 | BZ | 494 | GLU | 3.0 |
| 3 | AC | 181 | PHE | 3.0 |
| 9 | AK | 37 | THR | 3.0 |
| 59 | BZ | 417 | THR | 3.0 |
| 10 | CL | 119 | ASP | 3.0 |
| 1 | AA | 2153 | G | 3.0 |
| 1 | CA | 2149 | G | 3.0 |
| 1 | CA | 2157 | G | 3.0 |
| 34 | BA | 1033 | G | 3.0 |
| 43 | DJ | 98 | ILE | 3.0 |
| 58 | DY | 36 | A | 3.0 |
| 28 | C4 | 44 | THR | 3.0 |
| 52 | DS | 39 | THR | 3.0 |
| 59 | BZ | 658 | ASP | 3.0 |
| 9 | CK | 47 | ASN | 3.0 |
| 26 | A2 | 70 | GLN | 3.0 |
| 37 | BD | 179 | GLU | 3.0 |
| 43 | DJ | 85 | LEU | 3.0 |
| 3 | AC | 212 | SER | 3.0 |
| 59 | DZ | 618 | GLY | 2.9 |
| 43 | BJ | 38 | ILE | 2.9 |
| 1 | CA | 882 | G | 2.9 |
| 1 | CA | 2110 | G | 2.9 |
| 28 | C4 | 49 | PHE | 2.9 |
| 43 | DJ | 26 | ALA | 2.9 |
| 42 | DI | 54 | ASP | 2.9 |
| 59 | BZ | 688 | ILE | 2.9 |
| 1 | CA | 1098 | A | 2.9 |
| 34 | DA | 1004 | A | 2.9 |
| 46 | DM | 64 | TRP | 2.9 |
| 59 | DZ | 627 | ARG | 2.9 |
| 51 | DR | 21 | LYS | 2.9 |
| 42 | DI | 36 | TYR | 2.9 |
| 22 | CY | 46 | LYS | 2.9 |
| 49 | DP | 48 | TRP | 2.9 |
| 28 | A4 | 66 | SER | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 46 | BM | 24 | GLY | 2.9 |
| 59 | DZ | 481 | VAL | 2.9 |
| 1 | AA | 34 | C | 2.9 |
| 3 | CC | 49 | GLY | 2.9 |
| 56 | BW | 56 | C | 2.9 |
| 43 | BJ | 5 | ARG | 2.9 |
| 1 | CA | 1059 | G | 2.9 |
| 1 | CA | 2153 | G | 2.9 |
| 22 | CY | 63 | LYS | 2.9 |
| 35 | DB | 203 | GLY | 2.9 |
| 59 | BZ | 495 | GLY | 2.9 |
| 34 | DA | 1027 | C | 2.9 |
| 52 | DS | 48 | THR | 2.9 |
| 59 | BZ | 635 | GLU | 2.9 |
| 57 | DX | 70 | G | 2.9 |
| 23 | AZ | 143 | GLY | 2.9 |
| 1 | AA | 1141 | A | 2.9 |
| 35 | BB | 78 | GLN | 2.9 |
| 46 | DM | 102 | ARG | 2.9 |
| 52 | DS | 29 | ARG | 2.9 |
| 59 | DZ | 542 | VAL | 2.9 |
| 55 | DV | 22 | U | 2.9 |
| 9 | CK | 74 | LEU | 2.9 |
| 47 | DN | 36 | PHE | 2.9 |
| 3 | AC | 61 | GLY | 2.9 |
| 53 | BT | 9 | ASN | 2.9 |
| 1 | AA | 1113 | A | 2.9 |
| 1 | CA | 1077 | A | 2.9 |
| 56 | BW | 67 | C | 2.9 |
| 36 | BC | 91 | LEU | 2.9 |
| 52 | DS | 82 | GLY | 2.9 |
| 47 | DN | 4 | LYS | 2.9 |
| 52 | DS | 65 | ASN | 2.9 |
| 59 | BZ | 458 | HIS | 2.9 |
| 1 | CA | 652(T) | C | 2.8 |
| 1 | CA | 1536 | C | 2.8 |
| 23 | AZ | 146 | ILE | 2.8 |
| 47 | DN | 35 | ARG | 2.8 |
| 7 | CG | 182 | LYS | 2.8 |
| 8 | CH | 13 | LYS | 2.8 |
| 59 | BZ | 640 | ALA | 2.8 |
| 56 | DW | 59 | U | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 2177 | G | 2.8 |
| 34 | DA | 1030 | C | 2.8 |
| 3 | CC | 227 | PRO | 2.8 |
| 28 | C4 | 52 | THR | 2.8 |
| 59 | DZ | 411 | VAL | 2.8 |
| 25 | A1 | 98 | LEU | 2.8 |
| 56 | DW | 60 | U | 2.8 |
| 8 | CH | 29 | PRO | 2.8 |
| 4 | CD | 262 | ARG | 2.8 |
| 10 | CL | 102 | GLU | 2.8 |
| 3 | CC | 23 | ILE | 2.8 |
| 7 | AG | 49 | ASP | 2.8 |
| 34 | BA | 1001 | A | 2.8 |
| 59 | BZ | 232 | LEU | 2.8 |
| 59 | BZ | 431 | LEU | 2.8 |
| 59 | DZ | 555 | LEU | 2.8 |
| 59 | BZ | 665 | GLY | 2.8 |
| 1 | CA | 645 | C | 2.8 |
| 1 | CA | 2803 | C | 2.8 |
| 59 | BZ | 499 | ARG | 2.8 |
| 46 | DM | 42 | ALA | 2.8 |
| 59 | BZ | 429 | ALA | 2.8 |
| 59 | DZ | 678 | GLU | 2.8 |
| 9 | AK | 83 | TYR | 2.8 |
| 9 | CK | 58 | LEU | 2.8 |
| 36 | DC | 204 | LEU | 2.8 |
| 52 | DS | 31 | ILE | 2.8 |
| 16 | CS | 57 | LYS | 2.8 |
| 23 | CZ | 162 | GLU | 2.8 |
| 1 | CA | 1074 | G | 2.8 |
| 57 | DX | 4 | G | 2.8 |
| 47 | DN | 61 | TRP | 2.8 |
| 38 | DE | 144 | THR | 2.8 |
| 59 | BZ | 523 | PHE | 2.8 |
| 52 | BS | 27 | GLU | 2.8 |
| 3 | CC | 54 | ARG | 2.8 |
| 59 | DZ | 573 | HIS | 2.8 |
| 1 | AA | 2178 | G | 2.8 |
| 35 | DB | 138 | LEU | 2.8 |
| 59 | BZ | 596 | LYS | 2.8 |
| 59 | DZ | 492 | ASP | 2.8 |
| 59 | BZ | 507 | TYR | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 26 | C2 | 1 | MET | 2.8 |
| 1 | CA | 898 | C | 2.8 |
| 34 | BA | 163 | C | 2.8 |
| 59 | DZ | 532 | GLY | 2.8 |
| 43 | BJ | 71 | LEU | 2.8 |
| 1 | AA | 2169 | G | 2.8 |
| 36 | BC | 193 | TYR | 2.8 |
| 54 | DU | 6 | ARG | 2.8 |
| 23 | CZ | 139 | VAL | 2.8 |
| 47 | BN | 11 | LYS | 2.8 |
| 52 | DS | 42 | PRO | 2.8 |
| 3 | AC | 55 | SER | 2.7 |
| 35 | DB | 115 | LEU | 2.7 |
| 36 | BC | 204 | LEU | 2.7 |
| 3 | AC | 216 | THR | 2.7 |
| 23 | CZ | 152 | ALA | 2.7 |
| 34 | BA | 204 | U | 2.7 |
| 41 | DH | 61 | VAL | 2.7 |
| 42 | DI | 17 | VAL | 2.7 |
| 59 | DZ | 554 | PRO | 2.7 |
| 43 | BJ | 35 | SER | 2.7 |
| 51 | DR | 58 | LEU | 2.7 |
| 59 | DZ | 510 | VAL | 2.7 |
| 59 | DZ | 608 | VAL | 2.7 |
| 56 | DW | 44 | G | 2.7 |
| 1 | CA | 652(D) | C | 2.7 |
| 3 | CC | 29 | LEU | 2.7 |
| 24 | A0 | 3 | HIS | 2.7 |
| 34 | DA | 1038 | C | 2.7 |
| 59 | DZ | 619 | ASP | 2.7 |
| 40 | BG | 84 | ASN | 2.7 |
| 1 | AA | 218 | A | 2.7 |
| 47 | DN | 13 | THR | 2.7 |
| 52 | DS | 67 | VAL | 2.7 |
| 41 | DH | 128 | GLY | 2.7 |
| 42 | DI | 66 | ARG | 2.7 |
| 7 | CG | 19 | LEU | 2.7 |
| 52 | BS | 20 | LEU | 2.7 |
| 41 | DH | 54 | ASP | 2.7 |
| 52 | DS | 13 | ASP | 2.7 |
| 42 | BI | 12 | GLU | 2.7 |
| 59 | BZ | 579 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | CA | 1085 | A | 2.7 |
| 42 | DI | 26 | VAL | 2.7 |
| 54 | DU | 17 | THR | 2.7 |
| 3 | AC | 12 | LEU | 2.7 |
| 7 | AG | 51 | ARG | 2.7 |
| 9 | CK | 126 | ALA | 2.7 |
| 31 | A7 | 47 | ARG | 2.7 |
| 59 | DZ | 236 | GLU | 2.7 |
| 1 | CA | 896 | A | 2.7 |
| 3 | CC | 20 | VAL | 2.7 |
| 34 | BA | 1447 | A | 2.7 |
| 42 | DI | 4 | TYR | 2.7 |
| 59 | BZ | 408 | VAL | 2.7 |
| 59 | DZ | 493 | VAL | 2.7 |
| 52 | DS | 16 | LEU | 2.7 |
| 40 | BG | 4 | ARG | 2.7 |
| 23 | CZ | 138 | GLU | 2.7 |
| 1 | CA | 2115 | G | 2.7 |
| 34 | BA | 1024 | G | 2.7 |
| 1 | CA | 1082 | U | 2.7 |
| 59 | DZ | 611 | THR | 2.7 |
| 52 | DS | 34 | TRP | 2.7 |
| 59 | BZ | 677 | GLN | 2.7 |
| 10 | AL | 116 | ASN | 2.7 |
| 1 | CA | 2166 | G | 2.7 |
| 52 | DS | 81 | ARG | 2.7 |
| 56 | BW | 24 | G | 2.7 |
| 59 | BZ | 575 | VAL | 2.7 |
| 9 | CK | 19 | ARG | 2.7 |
| 3 | AC | 217 | THR | 2.7 |
| 37 | BD | 163 | GLU | 2.7 |
| 59 | BZ | 498 | ILE | 2.7 |
| 3 | AC | 39 | ASP | 2.7 |
| 59 | DZ | 477 | GLY | 2.7 |
| 59 | DZ | 531 | GLY | 2.7 |
| 1 | CA | 1092 | C | 2.7 |
| 3 | AC | 53 | ARG | 2.7 |
| 3 | AC | 47 | LYS | 2.6 |
| 3 | CC | 47 | LYS | 2.6 |
| 59 | BZ | 346 | LYS | 2.6 |
| 59 | DZ | 83 | ASP | 2.6 |
| 59 | BZ | 630 | GLN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 696 | C | 2.6 |
| 36 | DC | 206 | GLU | 2.6 |
| 59 | BZ | 653 | PHE | 2.6 |
| 1 | AA | 2180 | A | 2.6 |
| 1 | AA | 930 | G | 2.6 |
| 3 | CC | 26 | ALA | 2.6 |
| 59 | BZ | 393 | ASP | 2.6 |
| 42 | DI | 87 | GLN | 2.6 |
| 47 | DN | 49 | HIS | 2.6 |
| 47 | DN | 50 | LYS | 2.6 |
| 59 | BZ | 522 | GLY | 2.6 |
| 9 | CK | 36 | GLU | 2.6 |
| 13 | CP | 92 | GLU | 2.6 |
| 58 | BY | 56 | C | 2.6 |
| 42 | DI | 5 | TYR | 2.6 |
| 10 | CL | 91 | PRO | 2.6 |
| 28 | C4 | 69 | LYS | 2.6 |
| 59 | BZ | 437 | THR | 2.6 |
| 42 | BI | 17 | VAL | 2.6 |
| 59 | BZ | 514 | VAL | 2.6 |
| 1 | CA | 34 | C | 2.6 |
| 40 | DG | 16 | LEU | 2.6 |
| 56 | DW | 11 | C | 2.6 |
| 1 | CA | 2158 | A | 2.6 |
| 43 | DJ | 77 | PRO | 2.6 |
| 56 | DW | 21 | A | 2.6 |
| 59 | BZ | 598 | ASP | 2.6 |
| 59 | DZ | 412 | ALA | 2.6 |
| 3 | CC | 191 | ARG | 2.6 |
| 6 | AF | 17 | ARG | 2.6 |
| 9 | CK | 107 | VAL | 2.6 |
| 3 | AC | 201 | LYS | 2.6 |
| 54 | DU | 14 | TRP | 2.6 |
| 34 | DA | 1037 | C | 2.6 |
| 59 | BZ | 455 | GLY | 2.6 |
| 52 | BS | 83 | HIS | 2.6 |
| 35 | BB | 139 | LYS | 2.6 |
| 8 | AH | 2 | SER | 2.6 |
| 1 | CA | 1072 | C | 2.6 |
| 42 | DI | 8 | GLY | 2.6 |
| 54 | DU | 16 | GLY | 2.6 |
| 9 | AK | 72 | ASP | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | CK | 121 | ASP | 2.6 |
| 1 | AA | 1142 | A | 2.6 |
| 28 | A4 | 68 | ARG | 2.6 |
| 36 | BC | 126 | ARG | 2.6 |
| 59 | DZ | 414 | GLU | 2.6 |
| 1 | CA | 2144 | U | 2.6 |
| 3 | AC | 35 | THR | 2.6 |
| 8 | CH | 2 | SER | 2.6 |
| 23 | CZ | 150 | LEU | 2.6 |
| 35 | DB | 118 | LEU | 2.6 |
| 42 | DI | 19 | LEU | 2.6 |
| 13 | CP | 149 | GLU | 2.6 |
| 19 | CV | 101 | GLY | 2.6 |
| 28 | A4 | 53 | GLU | 2.6 |
| 40 | DG | 4 | ARG | 2.6 |
| 54 | DU | 24 | ARG | 2.6 |
| 23 | AZ | 108 | PRO | 2.6 |
| 43 | BJ | 7 | LYS | 2.6 |
| 56 | DW | 41 | C | 2.6 |
| 1 | CA | 1046 | A | 2.6 |
| 35 | DB | 19 | HIS | 2.6 |
| 41 | DH | 122 | ARG | 2.6 |
| 38 | DE | 81 | GLU | 2.6 |
| 46 | BM | 119 | GLY | 2.6 |
| 59 | DZ | 590 | ILE | 2.6 |
| 59 | BZ | 617 | MET | 2.6 |
| 59 | DZ | 588 | MET | 2.6 |
| 1 | CA | 879 | G | 2.6 |
| 8 | CH | 57 | ASP | 2.6 |
| 42 | DI | 75 | ASP | 2.6 |
| 9 | AK | 77 | PRO | 2.6 |
| 56 | BW | 57 | G | 2.6 |
| 3 | AC | 63 | VAL | 2.6 |
| 33 | C9 | 37 | GLY | 2.5 |
| 40 | BG | 8 | GLU | 2.5 |
| 59 | DZ | 508 | GLY | 2.5 |
| 1 | CA | 2113 | U | 2.5 |
| 59 | BZ | 475 | ASN | 2.5 |
| 59 | BZ | 619 | ASP | 2.5 |
| 1 | CA | 1075 | C | 2.5 |
| 27 | A3 | 60 | GLU | 2.5 |
| 35 | BB | 140 | HIS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 43 | BJ | 8 | LEU | 2.5 |
| 1 | CA | 1083 | U | 2.5 |
| 1 | CA | 1094 | U | 2.5 |
| 3 | AC | 36 | ALA | 2.5 |
| 42 | DI | 64 | THR | 2.5 |
| 51 | BR | 24 | ALA | 2.5 |
| 3 | CC | 7 | ARG | 2.5 |
| 43 | BJ | 29 | ARG | 2.5 |
| 9 | AK | 27 | VAL | 2.5 |
| 43 | DJ | 39 | PRO | 2.5 |
| 59 | DZ | 440 | VAL | 2.5 |
| 36 | DC | 89 | GLU | 2.5 |
| 19 | AV | 101 | GLY | 2.5 |
| 58 | BY | 34 | G | 2.5 |
| 10 | AL | 118 | THR | 2.5 |
| 59 | DZ | 552 | SER | 2.5 |
| 59 | DZ | 511 | LYS | 2.5 |
| 1 | CA | 1026 | U | 2.5 |
| 27 | C3 | 6 | VAL | 2.5 |
| 34 | BA | 1037 | C | 2.5 |
| 46 | BM | 34 | LEU | 2.5 |
| 40 | DG | 7 | ALA | 2.5 |
| 58 | BY | 6 | G | 2.5 |
| 52 | DS | 25 | LYS | 2.5 |
| 36 | DC | 19 | GLU | 2.5 |
| 36 | DC | 63 | ASN | 2.5 |
| 52 | BS | 19 | VAL | 2.5 |
| 59 | DZ | 490 | PRO | 2.5 |
| 59 | DZ | 636 | PRO | 2.5 |
| 3 | CC | 195 | ARG | 2.5 |
| 42 | DI | 105 | ASP | 2.5 |
| 59 | DZ | 393 | ASP | 2.5 |
| 1 | AA | 1143 | U | 2.5 |
| 9 | CK | 67 | GLY | 2.5 |
| 10 | AL | 105 | LEU | 2.5 |
| 1 | CA | 1081 | U | 2.5 |
| 1 | AA | 1109 | G | 2.5 |
| 34 | DA | 1022 | G | 2.5 |
| 21 | AX | 94 | GLY | 2.5 |
| 3 | AC | 11 | LEU | 2.5 |
| 9 | CK | 40 | LEU | 2.5 |
| 59 | BZ | 595 | GLN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | CC | 223 | VAL | 2.5 |
| 23 | CZ | 46 | LYS | 2.5 |
| 42 | DI | 67 | GLY | 2.5 |
| 59 | BZ | 586 | GLY | 2.5 |
| 1 | AA | 2181 | G | 2.5 |
| 58 | DY | 24 | G | 2.5 |
| 59 | BZ | 229 | LEU | 2.5 |
| 35 | BB | 123 | ALA | 2.5 |
| 35 | DB | 226 | ARG | 2.4 |
| 3 | AC | 179 | ALA | 2.4 |
| 3 | CC | 27 | ALA | 2.4 |
| 34 | BA | 1032 | G | 2.4 |
| 34 | DA | 80 | G | 2.4 |
| 59 | BZ | 509 | HIS | 2.4 |
| 1 | AA | 943 | C | 2.4 |
| 56 | DW | 61 | C | 2.4 |
| 3 | AC | 223 | VAL | 2.4 |
| 35 | DB | 227 | GLY | 2.4 |
| 59 | BZ | 588 | MET | 2.4 |
| 3 | AC | 196 | ALA | 2.4 |
| 9 | CK | 104 | ILE | 2.4 |
| 42 | DI | 15 | ALA | 2.4 |
| 49 | BP | 38 | TYR | 2.4 |
| 59 | BZ | 450 | ILE | 2.4 |
| 55 | BV | 13 | A | 2.4 |
| 1 | AA | 697 | C | 2.4 |
| 48 | BO | 88 | ARG | 2.4 |
| 59 | BZ | 545 | GLY | 2.4 |
| 17 | AT | 1 | MET | 2.4 |
| 3 | CC | 55 | SER | 2.4 |
| 59 | BZ | 448 | GLN | 2.4 |
| 59 | BZ | -4 | ALA | 2.4 |
| 59 | DZ | 556 | ILE | 2.4 |
| 1 | AA | 1105 | G | 2.4 |
| 56 | BW | 18 | G | 2.4 |
| 59 | DZ | 570 | GLY | 2.4 |
| 7 | CG | 49 | ASP | 2.4 |
| 51 | BR | 23 | LYS | 2.4 |
| 51 | DR | 22 | VAL | 2.4 |
| 3 | CC | 224 | ARG | 2.4 |
| 42 | DI | 29 | ASN | 2.4 |
| 56 | DW | 45 | U | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 59 | DZ | 449 | THR | 2.4 |
| 4 | AD | 275 | LYS | 2.4 |
| 8 | CH | 123 | PHE | 2.4 |
| 9 | CK | 114 | GLY | 2.4 |
| 46 | BM | 115 | LYS | 2.4 |
| 47 | DN | 16 | PHE | 2.4 |
| 52 | DS | 10 | PHE | 2.4 |
| 23 | CZ | 140 | ASP | 2.4 |
| 42 | BI | 46 | ALA | 2.4 |
| 31 | A7 | 48 | LYS | 2.4 |
| 59 | BZ | 570 | GLY | 2.4 |
| 52 | DS | 47 | HIS | 2.4 |
| 1 | CA | 1060 | U | 2.4 |
| 34 | BA | 1006 | C | 2.4 |
| 34 | BA | 1137 | C | 2.4 |
| 7 | AG | 50 | ALA | 2.4 |
| 49 | DP | 19 | ILE | 2.4 |
| 59 | BZ | 446 | THR | 2.4 |
| 1 | CA | 2169 | A | 2.4 |
| 10 | AL | 104 | VAL | 2.4 |
| 42 | DI | 128 | ARG | 2.4 |
| 59 | BZ | 87 | HIS | 2.4 |
| 1 | CA | 2152 | G | 2.4 |
| 47 | DN | 8 | GLU | 2.4 |
| 59 | DZ | 535 | PRO | 2.4 |
| 7 | CG | 181 | ARG | 2.4 |
| 54 | DU | 10 | ARG | 2.4 |
| 8 | CH | 44 | VAL | 2.4 |
| 59 | BZ | 611 | THR | 2.4 |
| 9 | CK | 117 | LEU | 2.4 |
| 56 | BW | 45 | U | 2.4 |
| 10 | AL | 112 | MET | 2.4 |
| 8 | CH | 119 | GLU | 2.4 |
| 35 | BB | 228 | GLY | 2.4 |
| 41 | BH | 122 | ARG | 2.4 |
| 59 | DZ | 497 | PHE | 2.4 |
| 35 | BB | 229 | VAL | 2.4 |
| 23 | CZ | 170 | THR | 2.4 |
| 59 | BZ | 492 | ASP | 2.4 |
| 1 | AA | 2139 | A | 2.3 |
| 1 | CA | 1057 | A | 2.3 |
| 1 | CA | 2170 | A | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | CH | 105 | LEU | 2.3 |
| 9 | CK | 32 | LEU | 2.3 |
| 10 | AL | 129 | GLY | 2.3 |
| 35 | BB | 222 | ILE | 2.3 |
| 3 | AC | 183 | PRO | 2.3 |
| 9 | AK | 102 | LYS | 2.3 |
| 1 | CA | 2123 | G | 2.3 |
| 58 | BY | 19 | G | 2.3 |
| 1 | AA | 2803 | A | 2.3 |
| 26 | A2 | 12 | GLU | 2.3 |
| 59 | BZ | 590 | ILE | 2.3 |
| 51 | BR | 29 | PHE | 2.3 |
| 58 | DY | 61 | C | 2.3 |
| 59 | DZ | 525 | PHE | 2.3 |
| 1 | CA | 2132 | U | 2.3 |
| 22 | CY | 45 | VAL | 2.3 |
| 59 | BZ | 401 | SER | 2.3 |
| 1 | CA | 2134 | A | 2.3 |
| 10 | CL | 100 | THR | 2.3 |
| 34 | BA | 1044 | A | 2.3 |
| 56 | DW | 36 | A | 2.3 |
| 7 | CG | 77 | ILE | 2.3 |
| 35 | DB | 222 | ILE | 2.3 |
| 59 | BZ | 539 | ILE | 2.3 |
| 59 | DZ | 498 | ILE | 2.3 |
| 35 | BB | 122 | PHE | 2.3 |
| 9 | AK | 74 | LEU | 2.3 |
| 9 | CK | 108 | LYS | 2.3 |
| 45 | DL | 64 | TYR | 2.3 |
| 47 | DN | 32 | SER | 2.3 |
| 36 | BC | 171 | GLY | 2.3 |
| 1 | AA | 2187 | G | 2.3 |
| 34 | BA | 1027 | C | 2.3 |
| 35 | BB | 232 | PRO | 2.3 |
| 3 | AC | 168 | LYS | 2.3 |
| 40 | DG | 86 | GLN | 2.3 |
| 36 | DC | 6 | HIS | 2.3 |
| 52 | BS | 61 | TYR | 2.3 |
| 59 | BZ | 506 | GLN | 2.3 |
| 9 | CK | 48 | GLY | 2.3 |
| 24 | C0 | 2 | ALA | 2.3 |
| 59 | DZ | 671 | MET | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 3 | CC | 194 | ILE | 2.3 |
| 59 | DZ | 227 | ILE | 2.3 |
| 8 | CH | 46 | GLU | 2.3 |
| 40 | DG | 85 | TYR | 2.3 |
| 54 | BU | 15 | ARG | 2.3 |
| 59 | BZ | 340 | TYR | 2.3 |
| 52 | DS | 79 | THR | 2.3 |
| 56 | DW | 9 | A | 2.3 |
| 59 | DZ | 558 | PHE | 2.3 |
| 52 | DS | 17 | GLU | 2.3 |
| 23 | AZ | 141 | VAL | 2.3 |
| 59 | BZ | 476 | VAL | 2.3 |
| 1 | AA | 2190 | G | 2.3 |
| 59 | BZ | 628 | ARG | 2.3 |
| 59 | DZ | 466 | LEU | 2.3 |
| 1 | CA | 652(V) | C | 2.3 |
| 36 | DC | 81 | GLY | 2.3 |
| 3 | AC | 8 | TYR | 2.3 |
| 59 | DZ | 7 | ASN | 2.3 |
| 59 | DZ | 582 | PHE | 2.3 |
| 1 | AA | 933 | C | 2.3 |
| 1 | AA | 2173 | G | 2.3 |
| 34 | DA | 79 | G | 2.3 |
| 58 | DY | 22 | G | 2.3 |
| 59 | BZ | 672 | PHE | 2.3 |
| 58 | DY | 58 | A | 2.3 |
| 42 | DI | 103 | THR | 2.3 |
| 59 | DZ | 566 | THR | 2.3 |
| 27 | C3 | 2 | PRO | 2.3 |
| 42 | DI | 124 | GLN | 2.3 |
| 34 | BA | 91 | C | 2.2 |
| 1 | CA | 881 | G | 2.2 |
| 35 | BB | 37 | ASN | 2.2 |
| 37 | DD | 179 | GLU | 2.2 |
| 40 | BG | 153 | HIS | 2.2 |
| 34 | BA | 161 | A | 2.2 |
| 47 | BN | 17 | LYS | 2.2 |
| 3 | CC | 218 | THR | 2.2 |
| 35 | DB | 95 | GLN | 2.2 |
| 42 | DI | 115 | GLY | 2.2 |
| 43 | DJ | 65 | LEU | 2.2 |
| 38 | DE | 21 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | CH | 32 | GLU | 2.2 |
| 43 | DJ | 46 | ARG | 2.2 |
| 59 | BZ | 669 | PHE | 2.2 |
| 52 | DS | 28 | LYS | 2.2 |
| 1 | CA | 878 | A | 2.2 |
| 35 | DB | 165 | VAL | 2.2 |
| 24 | A0 | 7 | LEU | 2.2 |
| 59 | DZ | 189 | GLY | 2.2 |
| 59 | DZ | 516 | PRO | 2.2 |
| 9 | AK | 52 | PHE | 2.2 |
| 59 | BZ | 529 | ILE | 2.2 |
| 59 | DZ | 643 | ILE | 2.2 |
| 10 | AL | 75 | SER | 2.2 |
| 45 | DL | 69 | TYR | 2.2 |
| 20 | CW | 112 | GLY | 2.2 |
| 52 | DS | 56 | GLN | 2.2 |
| 30 | C6 | 54 | ILE | 2.2 |
| 52 | DS | 40 | ILE | 2.2 |
| 1 | CA | 2161 | C | 2.2 |
| 23 | CZ | 153 | SER | 2.2 |
| 34 | DA | 1029 | C | 2.2 |
| 35 | BB | 148 | TYR | 2.2 |
| 59 | DZ | 509 | HIS | 2.2 |
| 56 | BW | 48 | C | 2.2 |
| 59 | DZ | 550 | MET | 2.2 |
| 35 | DB | 38 | GLY | 2.2 |
| 35 | DB | 137 | ARG | 2.2 |
| 37 | BD | 3 | ARG | 2.2 |
| 42 | BI | 41 | VAL | 2.2 |
| 54 | DU | 9 | ARG | 2.2 |
| 34 | DA | 1261 | A | 2.2 |
| 58 | DY | 21 | A | 2.2 |
| 59 | BZ | 687 | LEU | 2.2 |
| 1 | AA | 694 | G | 2.2 |
| 1 | AA | 2146 | G | 2.2 |
| 1 | CA | 1062 | G | 2.2 |
| 43 | DJ | 99 | LYS | 2.2 |
| 42 | DI | 59 | PHE | 2.2 |
| 47 | DN | 37 | PHE | 2.2 |
| 46 | DM | 88 | ARG | 2.2 |
| 1 | AA | 2133 | C | 2.2 |
| 59 | DZ | 545 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 169 | THR | 2.2 |
| 34 | DA | 1017 | G | 2.2 |
| 54 | BU | 17 | THR | 2.2 |
| 40 | DG | 120 | ILE | 2.2 |
| 9 | CK | 64 | LYS | 2.2 |
| 18 | CU | 89 | GLU | 2.2 |
| 36 | DC | 194 | GLY | 2.2 |
| 35 | BB | 45 | GLN | 2.2 |
| 56 | BW | 25 | C | 2.2 |
| 58 | BY | 36 | A | 2.2 |
| 52 | DS | 78 | ARG | 2.2 |
| 22 | CY | 4 | LYS | 2.2 |
| 43 | DJ | 7 | LYS | 2.2 |
| 35 | DB | 7 | VAL | 2.2 |
| 59 | DZ | 212 | TYR | 2.2 |
| 55 | BV | 14 | A | 2.2 |
| 52 | BS | 21 | GLU | 2.2 |
| 59 | DZ | 233 | GLU | 2.2 |
| 3 | CC | 169 | THR | 2.2 |
| 13 | CP | 88 | LEU | 2.2 |
| 22 | CY | 90 | LEU | 2.2 |
| 36 | DC | 195 | VAL | 2.2 |
| 27 | C3 | 5 | LYS | 2.1 |
| 52 | BS | 4 | SER | 2.1 |
| 52 | DS | 38 | SER | 2.1 |
| 1 | CA | 2135 | A | 2.1 |
| 55 | DV | 15 | A | 2.1 |
| 47 | BN | 51 | GLY | 2.1 |
| 43 | BJ | 34 | VAL | 2.1 |
| 59 | DZ | 652 | MET | 2.1 |
| 1 | CA | 1063 | G | 2.1 |
| 1 | CA | 2137 | C | 2.1 |
| 8 | AH | 174 | GLY | 2.1 |
| 59 | DZ | 450 | ILE | 2.1 |
| 59 | BZ | 657 | THR | 2.1 |
| 16 | CS | 29 | PHE | 2.1 |
| 48 | BO | 6 | GLU | 2.1 |
| 1 | CA | 2833 | G | 2.1 |
| 34 | DA | 1024 | G | 2.1 |
| 56 | DW | 34 | G | 2.1 |
| 1 | CA | 1847 | A | 2.1 |
| 56 | DW | 50 | U | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 59 | BZ | 532 | GLY | 2.1 |
| 9 | CK | 102 | LYS | 2.1 |
| 47 | DN | 33 | VAL | 2.1 |
| 9 | AK | 130 | THR | 2.1 |
| 9 | CK | 130 | THR | 2.1 |
| 43 | BJ | 100 | THR | 2.1 |
| 16 | CS | 3 | ARG | 2.1 |
| 52 | DS | 37 | ARG | 2.1 |
| 59 | DZ | -10 | ARG | 2.1 |
| 59 | DZ | 93 | GLU | 2.1 |
| 36 | DC | 62 | ASP | 2.1 |
| 40 | DG | 18 | TYR | 2.1 |
| 59 | BZ | 464 | ASP | 2.1 |
| 35 | DB | 124 | SER | 2.1 |
| 40 | DG | 42 | ILE | 2.1 |
| 52 | BS | 85 | LYS | 2.1 |
| 54 | DU | 2 | GLY | 2.1 |
| 1 | AA | 2191 | A | 2.1 |
| 1 | CA | 897 | C | 2.1 |
| 34 | DA | 994 | A | 2.1 |
| 35 | BB | 165 | VAL | 2.1 |
| 28 | A4 | 62 | ARG | 2.1 |
| 36 | BC | 89 | GLU | 2.1 |
| 43 | BJ | 97 | GLU | 2.1 |
| 46 | DM | 91 | ARG | 2.1 |
| 54 | BU | 9 | ARG | 2.1 |
| 59 | DZ | 659 | LEU | 2.1 |
| 59 | DZ | 589 | ALA | 2.1 |
| 43 | DJ | 69 | ASN | 2.1 |
| 59 | DZ | 536 | LYS | 2.1 |
| 1 | AA | 2130 | C | 2.1 |
| 34 | BA | 1257 | U | 2.1 |
| 1 | CA | 2165 | G | 2.1 |
| 1 | CA | 2802 | G | 2.1 |
| 23 | CZ | 141 | VAL | 2.1 |
| 46 | DM | 93 | ARG | 2.1 |
| 58 | BY | 5 | G | 2.1 |
| 47 | DN | 15 | LYS | 2.1 |
| 53 | DT | 40 | ALA | 2.1 |
| 59 | BZ | 496 | LYS | 2.1 |
| 3 | AC | 18 | ASN | 2.1 |
| 52 | DS | 49 | ILE | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | C7 | 47 | ARG | 2.1 |
| 47 | DN | 31 | ARG | 2.1 |
| 1 | CA | 2119 | A | 2.1 |
| 3 | AC | 42 | VAL | 2.1 |
| 8 | CH | 113 | VAL | 2.1 |
| 59 | DZ | 225 | GLU | 2.1 |
| 42 | DI | 61 | ALA | 2.1 |
| 9 | CK | 38 | HIS | 2.1 |
| 17 | AT | 37 | GLY | 2.1 |
| 52 | DS | 83 | HIS | 2.1 |
| 42 | BI | 64 | THR | 2.1 |
| 43 | DJ | 100 | THR | 2.1 |
| 52 | BS | 49 | ILE | 2.1 |
| 56 | DW | 12 | U | 2.1 |
| 3 | CC | 30 | VAL | 2.1 |
| 13 | CP | 95 | VAL | 2.1 |
| 29 | C5 | 60 | VAL | 2.1 |
| 42 | BI | 50 | LEU | 2.1 |
| 59 | DZ | 479 | PRO | 2.1 |
| 59 | BZ | 528 | ALA | 2.1 |
| 59 | BZ | 593 | ALA | 2.1 |
| 1 | AA | 2182 | G | 2.1 |
| 52 | DS | 62 | ILE | 2.1 |
| 59 | BZ | 544 | LYS | 2.1 |
| 7 | CG | 41 | GLN | 2.1 |
| 35 | BB | 95 | GLN | 2.1 |
| 43 | DJ | 35 | SER | 2.1 |
| 52 | DS | 60 | VAL | 2.1 |
| 59 | BZ | 571 | SER | 2.1 |
| 7 | CG | 43 | LEU | 2.1 |
| 34 | DA | 1044 | A | 2.1 |
| 59 | BZ | 466 | LEU | 2.1 |
| 35 | DB | 97 | TRP | 2.1 |
| 9 | AK | 31 | GLY | 2.0 |
| 9 | CK | 131 | MET | 2.0 |
| 34 | DA | 204 | U | 2.0 |
| 59 | DZ | 544 | LYS | 2.0 |
| 1 | AA | 2137 | G | 2.0 |
| 34 | BA | 1023 | G | 2.0 |
| 58 | BY | 44 | G | 2.0 |
| 59 | BZ | 572 | TYR | 2.0 |
| 24 | C0 | 63 | VAL | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 41 | DH | 129 | VAL | 2.0 |
| 43 | DJ | 70 | ARG | 2.0 |
| 59 | DZ | 533 | VAL | 2.0 |
| 1 | AA | 2195 | A | 2.0 |
| 42 | BI | 106 | ALA | 2.0 |
| 9 | AK | 73 | GLY | 2.0 |
| 59 | BZ | 409 | ILE | 2.0 |
| 34 | DA | 1040 | U | 2.0 |
| 54 | DU | 18 | TYR | 2.0 |
| 58 | DY | 1 | G | 2.0 |
| 59 | DZ | 229 | LEU | 2.0 |
| 36 | DC | 147 | LYS | 2.0 |
| 36 | DC | 154 | SER | 2.0 |
| 1 | CA | 2117 | A | 2.0 |
| 9 | AK | 103 | GLY | 2.0 |
| 34 | BA | 1004 | A | 2.0 |
| 59 | BZ | 580 | MET | 2.0 |
| 9 | CK | 95 | GLN | 2.0 |
| 39 | DF | 100 | ASN | 2.0 |
| 52 | BS | 30 | LEU | 2.0 |
| 52 | BS | 41 | VAL | 2.0 |
| 1 | CA | 652(E) | G | 2.0 |
| 1 | CA | 2133 | G | 2.0 |
| 9 | CK | 110 | GLY | 2.0 |
| 59 | BZ | 667 | GLY | 2.0 |
| 59 | DZ | 557 | GLY | 2.0 |
| 1 | AA | 1144 | A | 2.0 |
| 28 | C4 | 18 | CYS | 2.0 |
| 34 | BA | 1531 | A | 2.0 |
| 35 | DB | 141 | GLU | 2.0 |
| 10 | AL | 126 | MET | 2.0 |
| 49 | BP | 68 | ASP | 2.0 |
| 23 | CZ | 124 | ILE | 2.0 |
| 59 | BZ | 573 | HIS | 2.0 |
| 35 | DB | 148 | TYR | 2.0 |
| 3 | CC | 207 | GLY | 2.0 |
| 28 | C4 | 66 | SER | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 56 | PSU | BW | 39 | 20/21 | 0.90 | 0.23 | - | 96,96,96,96 | 0 |
| 58 | MIA | BY | 37 | 22/30 | 0.85 | 0.18 | - | 118,118,118,118 | 0 |
| 56 | 4SU | BW | 8 | 20/21 | 0.64 | 0.28 | - | 200,200,200,200 | 0 |
| 58 | 5MU | DY | 54 | 21/22 | 0.73 | 0.36 | - | 200,200,200,200 | 0 |
| 56 | PSU | BW | 55 | 20/21 | 0.73 | 0.31 | - | 113,113,113,113 | 0 |
| 58 | 4SU | BY | 8 | 20/21 | 0.71 | 0.21 | - | 191,191,191,191 | 0 |
| 58 | PSU | DY | 32 | 20/21 | 0.82 | 0.20 | - | 154,154,154,154 | 0 |
| 57 | PSU | BX | 55 | 20/21 | 0.94 | 0.13 | - | 74,74,74,74 | 0 |
| 58 | PSU | BY | 55 | 20/21 | 0.64 | 0.24 | - | 205,205,205,205 | 0 |
| 58 | MIA | DY | 37 | 22/30 | 0.68 | 0.29 | - | 156,156,156,156 | 0 |
| 57 | 5MU | DX | 54 | 21/22 | 0.94 | 0.18 | - | 108,108,108,108 | 0 |
| 57 | 31H | BX | 76 | 32/33 | 0.94 | 0.26 | - | 58,58,58,58 | 4 |
| 56 | 5MU | BW | 54 | 21/22 | 0.89 | 0.25 | - | 89,89,89,89 | 0 |
| 58 | PSU | DY | 55 | 20/21 | 0.51 | 0.53 | - | 222,222,222,222 | 0 |
| 58 | 7MG | BY | 46 | 24/25 | 0.71 | 0.21 | - | 200,200,200,200 | 0 |
| 57 | 5MC | BX | 32 | 21/22 | 0.95 | 0.17 | - | 65,65,65,65 | 0 |
| 56 | 7MG | DW | 46 | 24/25 | 0.65 | 0.34 | - | 244,244,244,244 | 0 |
| 56 | PSU | BW | 32 | 20/21 | 0.92 | 0.21 | - | 110,110,110,110 | 0 |
| 57 | 31H | DX | 76 | 32/33 | 0.87 | 0.31 | - | 58,58,58,58 | 4 |
| 56 | PSU | DW | 32 | 20/21 | 0.89 | 0.36 | - | 139,139,139,139 | 0 |
| 56 | PSU | DW | 55 | 20/21 | 0.52 | 0.44 | - | 190,190,190,190 | 0 |
| 58 | PSU | BY | 32 | 20/21 | 0.84 | 0.20 | - | 126,126,126,126 | 0 |
| 56 | 5MU | DW | 54 | 21/22 | 0.87 | 0.22 | - | 118,118,118,118 | 0 |
| 58 | 4SU | DY | 8 | 20/21 | 0.62 | 0.21 | - | 193,193,193,193 | 0 |
| 56 | MIA | DW | 37 | 22/30 | 0.90 | 0.27 | - | 116,116,116,116 | 0 |
| 57 | 4SU | BX | 8 | 20/21 | 0.93 | 0.14 | - | 70,70,70,70 | 1 |
| 56 | F3N | BW | 76 | 33/34 | 0.96 | 0.25 | - | 54,54,54,54 | 1 |
| 58 | 7MG | DY | 46 | 24/25 | 0.64 | 0.24 | - | 206,206,206,206 | 0 |
| 56 | 7MG | BW | 46 | 24/25 | 0.72 | 0.27 | - | 203,203,203,203 | 0 |
| 56 | 4SU | DW | 8 | 20/21 | 0.58 | 0.49 | - | 225,225,225,225 | 0 |
| 56 | PSU | DW | 39 | 20/21 | 0.89 | 0.24 | - | 118,118,118,118 | 0 |
| 57 | 5MU | BX | 54 | 21/22 | 0.93 | 0.17 | - | 85,85,85,85 | 0 |
| 58 | PSU | DY | 39 | 20/21 | 0.84 | 0.21 | - | 138,138,138,138 | 0 |
| 57 | 4SU | DX | 8 | 20/21 | 0.90 | 0.14 | - | 96,96,96,96 | 0 |
| 56 | MIA | BW | 37 | 29/30 | 0.90 | 0.30 | - | 95,95,95,95 | 1 |
| 56 | F3N | DW | 76 | 33/34 | 0.91 | 0.35 | - | 75,75,75,75 | 1 |
| 58 | 5MU | BY | 54 | 21/22 | 0.30 | 0.33 | - | 217,217,217,217 | 0 |
| 57 | 5MC | DX | 32 | 21/22 | 0.93 | 0.20 | - | 86,86,86,86 | 0 |
| 58 | PSU | BY | 39 | 20/21 | 0.91 | 0.17 | - | 106,106,106,106 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 57 | PSU | DX | 55 | 20/21 | 0.91 | 0.13 | - | 95,95,95,95 | 0 |

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(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|----------------------------|-------|
| 60 | MG | AA | 3110 | 1/1 | 0.80 | 0.49 | 130.27 | 57,57,57,57 | 0 |
| 60 | MG | CE | 304 | 1/1 | 0.86 | 0.75 | 95.16 | 74,74,74,74 | 0 |
| 60 | MG | CA | 3182 | 1/1 | 0.97 | 0.58 | 89.51 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3183 | 1/1 | 0.72 | 0.97 | 88.23 | 89,89,89,89 | 0 |
| 60 | MG | AA | 3240 | 1/1 | 0.91 | 0.51 | 83.99 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3170 | 1/1 | 0.91 | 0.57 | 77.69 | 44,44,44,44 | 1 |
| 60 | MG | AA | 3770 | 1/1 | 0.45 | 0.80 | 73.21 | 57,57,57,57 | 1 |
| 60 | MG | AA | 3671 | 1/1 | 0.86 | 0.58 | 65.39 | 31,31,31,31 | 1 |
| 60 | MG | AA | 3121 | 1/1 | 0.85 | 0.30 | 61.99 | 63,63,63,63 | 0 |
| 60 | MG | AA | 3806 | 1/1 | 0.86 | 0.55 | 46.27 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3115 | 1/1 | 0.97 | 0.47 | 45.73 | 44,44,44,44 | 0 |
| 60 | MG | AA | 3018 | 1/1 | 0.81 | 0.66 | 45.66 | 55,55,55,55 | 0 |
| 60 | MG | AA | 3196 | 1/1 | 0.97 | 0.34 | 45.12 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3134 | 1/1 | 0.94 | 0.52 | 45.11 | 49,49,49,49 | 0 |
| 60 | MG | AA | 3705 | 1/1 | 0.91 | 0.44 | 44.42 | 29,29,29,29 | 1 |
| 60 | MG | CA | 3218 | 1/1 | 0.83 | 0.88 | 43.83 | 63,63,63,63 | 0 |
| 60 | MG | AA | 3817 | 1/1 | 0.96 | 0.46 | 41.72 | 40,40,40,40 | 0 |
| 60 | MG | AA | 3739 | 1/1 | 0.60 | 0.42 | 40.61 | 90,90,90,90 | 0 |
| 60 | MG | AH | 201 | 1/1 | 0.83 | 1.24 | 40.42 | 83,83,83,83 | 0 |
| 60 | MG | AA | 3101 | 1/1 | 0.89 | 0.47 | 38.58 | 68,68,68,68 | 0 |
| 60 | MG | C5 | 101 | 1/1 | 0.90 | 0.43 | 36.58 | 64,64,64,64 | 0 |
| 60 | MG | CA | 3641 | 1/1 | 0.95 | 0.54 | 35.93 | 59,59,59,59 | 0 |
| 60 | MG | CF | 302 | 1/1 | 0.91 | 0.32 | 33.58 | 64,64,64,64 | 0 |
| 60 | MG | CF | 306 | 1/1 | 0.74 | 0.94 | 33.26 | 85,85,85,85 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 60 | MG | CA | 3595 | 1/1 | 0.92 | 0.26 | 32.98 | 67,67,67,67 | 0 |
| 60 | MG | AA | 3160 | 1/1 | 0.85 | 0.48 | 32.92 | 96,96,96,96 | 0 |
| 60 | MG | AA | 3213 | 1/1 | 0.93 | 0.61 | 32.67 | 49,49,49,49 | 0 |
| 60 | MG | DA | 1667 | 1/1 | 0.89 | 0.43 | 32.45 | 70,70,70,70 | 0 |
| 60 | MG | AA | 3060 | 1/1 | 0.94 | 0.34 | 31.97 | 23,23,23,23 | 0 |
| 60 | MG | CA | 3099 | 1/1 | 0.97 | 0.46 | 30.72 | 55,55,55,55 | 0 |
| 60 | MG | AA | 3044 | 1/1 | 0.95 | 0.36 | 30.69 | 62,62,62,62 | 0 |
| 60 | MG | CA | 3022 | 1/1 | 0.92 | 0.62 | 30.67 | 76,76,76,76 | 0 |
| 60 | MG | AA | 3822 | 1/1 | 0.90 | 0.60 | 30.59 | 67,67,67,67 | 0 |
| 60 | MG | CA | 3165 | 1/1 | 0.92 | 0.52 | 30.20 | 58,58,58,58 | 0 |
| 60 | MG | CA | 3496 | 1/1 | 0.82 | 0.55 | 30.19 | 58,58,58,58 | 0 |
| 60 | MG | AA | 3231 | 1/1 | 0.92 | 0.49 | 29.73 | 87,87,87,87 | 0 |
| 60 | MG | CE | 301 | 1/1 | 0.86 | 0.60 | 29.57 | 54,54,54,54 | 0 |
| 60 | MG | AA | 3038 | 1/1 | 0.93 | 0.40 | 29.24 | 42,42,42,42 | 0 |
| 60 | MG | AA | 3082 | 1/1 | 0.98 | 0.58 | 28.14 | 57,57,57,57 | 1 |
| 60 | MG | AA | 3818 | 1/1 | 0.98 | 0.36 | 27.88 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3302 | 1/1 | 0.95 | 0.34 | 27.53 | 58,58,58,58 | 0 |
| 60 | MG | CA | 3312 | 1/1 | 0.89 | 0.38 | 27.15 | 52,52,52,52 | 0 |
| 60 | MG | CF | 301 | 1/1 | 0.83 | 0.45 | 27.00 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3133 | 1/1 | 0.95 | 0.47 | 26.48 | 92,92,92,92 | 1 |
| 60 | MG | AA | 3772 | 1/1 | 0.93 | 0.53 | 26.40 | 37,37,37,37 | 0 |
| 60 | MG | AA | 3803 | 1/1 | 0.95 | 0.33 | 26.15 | 37,37,37,37 | 0 |
| 60 | MG | CA | 3500 | 1/1 | 0.88 | 0.47 | 25.81 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3144 | 1/1 | 0.97 | 0.49 | 25.72 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3769 | 1/1 | 0.88 | 0.45 | 25.71 | 48,48,48,48 | 1 |
| 60 | MG | CA | 3655 | 1/1 | 0.91 | 0.47 | 25.45 | 69,69,69,69 | 0 |
| 60 | MG | CE | 303 | 1/1 | 0.73 | 0.39 | 25.27 | 55,55,55,55 | 0 |
| 60 | MG | AU | 201 | 1/1 | 0.89 | 0.53 | 25.21 | 72,72,72,72 | 0 |
| 60 | MG | AA | 3300 | 1/1 | 0.81 | 0.30 | 25.14 | 43,43,43,43 | 0 |
| 60 | MG | CA | 3656 | 1/1 | 0.92 | 0.54 | 25.05 | 75,75,75,75 | 0 |
| 60 | MG | AA | 3829 | 1/1 | 0.82 | 0.39 | 25.01 | 89,89,89,89 | 0 |
| 60 | MG | BA | 1687 | 1/1 | 0.92 | 0.59 | 24.67 | 73,73,73,73 | 0 |
| 60 | MG | AA | 3043 | 1/1 | 0.92 | 0.29 | 24.61 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3178 | 1/1 | 0.99 | 0.43 | 24.24 | 50,50,50,50 | 0 |
| 60 | MG | AF | 303 | 1/1 | 0.87 | 0.56 | 23.85 | 54,54,54,54 | 0 |
| 60 | MG | AA | 3167 | 1/1 | 0.91 | 0.29 | 23.74 | 69,69,69,69 | 0 |
| 60 | MG | CA | 3282 | 1/1 | 0.73 | 0.38 | 22.31 | 75,75,75,75 | 0 |
| 60 | MG | AA | 3211 | 1/1 | 0.93 | 0.59 | 21.98 | 53,53,53,53 | 0 |
| 60 | MG | AA | 3706 | 1/1 | 0.99 | 0.35 | 21.68 | 26,26,26,26 | 1 |
| 60 | MG | AA | 3034 | 1/1 | 0.94 | 0.34 | 21.60 | 84,84,84,84 | 0 |
| 60 | MG | CA | 3035 | 1/1 | 0.87 | 0.36 | 21.53 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | CA | 3662 | 1/1 | 0.90 | 0.37 | 21.52 | 60,60,60,60 | 0 |
| 60 | MG | AB | 3008 | 1/1 | 0.95 | 0.39 | 21.39 | 46,46,46,46 | 0 |
| 60 | MG | CA | 3463 | 1/1 | 0.95 | 0.43 | 21.07 | 75,75,75,75 | 0 |
| 60 | MG | CA | 3115 | 1/1 | 0.84 | 0.54 | 20.69 | 71,71,71,71 | 0 |
| 60 | MG | CA | 3464 | 1/1 | 0.87 | 0.61 | 20.51 | 78,78,78,78 | 0 |
| 60 | MG | CU | 201 | 1/1 | 0.95 | 0.51 | 20.51 | 62,62,62,62 | 0 |
| 60 | MG | CA | 3028 | 1/1 | 0.97 | 0.64 | 20.12 | 60,60,60,60 | 0 |
| 60 | MG | AA | 3129 | 1/1 | 0.95 | 0.26 | 20.00 | 52,52,52,52 | 0 |
| 60 | MG | CA | 3026 | 1/1 | 0.96 | 0.47 | 19.94 | 55,55,55,55 | 0 |
| 60 | MG | AA | 3354 | 1/1 | 0.93 | 0.29 | 19.84 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3033 | 1/1 | 0.88 | 0.41 | 19.83 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3692 | 1/1 | 0.67 | 0.48 | 19.80 | 86,86,86,86 | 0 |
| 60 | MG | AA | 3250 | 1/1 | 0.86 | 0.45 | 19.51 | 46,46,46,46 | 1 |
| 60 | MG | AA | 3212 | 1/1 | 0.99 | 0.40 | 19.29 | 43,43,43,43 | 0 |
| 60 | MG | CD | 301 | 1/1 | 0.92 | 0.35 | 18.88 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3662 | 1/1 | 0.95 | 0.33 | 18.83 | 60,60,60,60 | 0 |
| 60 | MG | AU | 204 | 1/1 | 0.95 | 0.45 | 18.69 | 55,55,55,55 | 0 |
| 60 | MG | CA | 3084 | 1/1 | 0.93 | 0.39 | 18.69 | 73,73,73,73 | 0 |
| 60 | MG | BA | 1757 | 1/1 | 0.79 | 0.35 | 18.61 | 63,63,63,63 | 0 |
| 60 | MG | CA | 3102 | 1/1 | 0.92 | 0.34 | 18.51 | 50,50,50,50 | 0 |
| 60 | MG | AE | 305 | 1/1 | 0.88 | 0.42 | 18.43 | 44,44,44,44 | 0 |
| 60 | MG | AA | 3116 | 1/1 | 0.97 | 0.32 | 18.32 | 36,36,36,36 | 0 |
| 60 | MG | AA | 3702 | 1/1 | 0.80 | 0.45 | 18.27 | 45,45,45,45 | 1 |
| 60 | MG | AD | 310 | 1/1 | 0.92 | 0.49 | 18.20 | 63,63,63,63 | 0 |
| 60 | MG | CA | 3438 | 1/1 | 0.97 | 0.29 | 18.15 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3347 | 1/1 | 0.74 | 0.32 | 18.07 | 63,63,63,63 | 0 |
| 60 | MG | DA | 1686 | 1/1 | 0.21 | 0.36 | 18.06 | 102,102,102,102 | 0 |
| 60 | MG | CA | 3460 | 1/1 | 0.90 | 0.28 | 18.05 | 57,57,57,57 | 0 |
| 60 | MG | AA | 3698 | 1/1 | 0.90 | 0.31 | 17.97 | 51,51,51,51 | 1 |
| 60 | MG | AA | 3810 | 1/1 | 0.92 | 0.34 | 17.94 | 49,49,49,49 | 0 |
| 60 | MG | AA | 3210 | 1/1 | 0.79 | 0.55 | 17.48 | 106,106,106,106 | 0 |
| 60 | MG | CQ | 201 | 1/1 | 0.58 | 0.76 | 17.37 | 85,85,85,85 | 0 |
| 60 | MG | CA | 3121 | 1/1 | 0.95 | 0.32 | 17.22 | 78,78,78,78 | 0 |
| 60 | MG | AA | 3460 | 1/1 | 0.90 | 0.30 | 17.19 | 81,81,81,81 | 0 |
| 60 | MG | AA | 3339 | 1/1 | 0.94 | 0.29 | 17.12 | 18,18,18,18 | 0 |
| 60 | MG | AA | 3824 | 1/1 | 0.88 | 0.33 | 17.01 | 53,53,53,53 | 0 |
| 60 | MG | CA | 3541 | 1/1 | 0.97 | 0.34 | 16.99 | 58,58,58,58 | 0 |
| 60 | MG | CA | 3215 | 1/1 | 0.91 | 0.43 | 16.78 | 50,50,50,50 | 0 |
| 60 | MG | CA | 3653 | 1/1 | 0.40 | 0.52 | 16.76 | 102,102,102,102 | 0 |
| 60 | MG | BA | 1724 | 1/1 | 0.88 | 0.31 | 16.59 | 60,60,60,60 | 0 |
| 60 | MG | AA | 3281 | 1/1 | 0.96 | 0.43 | 16.45 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | CA | 3226 | 1/1 | 0.82 | 0.37 | 16.37 | 56,56,56,56 | 0 |
| 60 | MG | CA | 3220 | 1/1 | 0.90 | 0.50 | 16.33 | 89,89,89,89 | 0 |
| 60 | MG | CA | 3156 | 1/1 | 0.81 | 1.42 | 16.19 | 92,92,92,92 | 0 |
| 60 | MG | AA | 3581 | 1/1 | 0.92 | 0.26 | 16.10 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3507 | 1/1 | 0.91 | 0.25 | 16.04 | 53,53,53,53 | 0 |
| 60 | MG | BA | 1804 | 1/1 | 0.75 | 0.47 | 15.74 | 94,94,94,94 | 0 |
| 60 | MG | AA | 3050 | 1/1 | 0.94 | 0.25 | 15.59 | 29,29,29,29 | 0 |
| 60 | MG | AA | 3767 | 1/1 | 0.83 | 0.29 | 15.51 | 75,75,75,75 | 0 |
| 60 | MG | CA | 3601 | 1/1 | 0.92 | 0.36 | 15.19 | 61,61,61,61 | 0 |
| 60 | MG | CA | 3346 | 1/1 | 0.92 | 0.31 | 15.13 | 48,48,48,48 | 0 |
| 60 | MG | CA | 3576 | 1/1 | 0.81 | 0.35 | 15.13 | 91,91,91,91 | 0 |
| 60 | MG | AA | 3740 | 1/1 | 0.89 | 0.26 | 15.11 | 54,54,54,54 | 0 |
| 60 | MG | C7 | 101 | 1/1 | 0.91 | 0.43 | 14.99 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3596 | 1/1 | 0.93 | 0.21 | 14.95 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3461 | 1/1 | 0.92 | 0.22 | 14.94 | 57,57,57,57 | 0 |
| 60 | MG | AA | 3127 | 1/1 | 0.83 | 0.45 | 14.93 | 83,83,83,83 | 0 |
| 60 | MG | AA | 3258 | 1/1 | 0.87 | 0.26 | 14.92 | 32,32,32,32 | 0 |
| 60 | MG | CA | 3418 | 1/1 | 0.89 | 0.31 | 14.73 | 53,53,53,53 | 0 |
| 60 | MG | AA | 3828 | 1/1 | 0.71 | 0.55 | 14.71 | 68,68,68,68 | 0 |
| 60 | MG | AX | 102 | 1/1 | 0.77 | 0.37 | 14.48 | 78,78,78,78 | 0 |
| 60 | MG | CA | 3233 | 1/1 | 0.97 | 0.30 | 14.24 | 52,52,52,52 | 0 |
| 60 | MG | AA | 3200 | 1/1 | 0.87 | 0.28 | 14.19 | 73,73,73,73 | 0 |
| 60 | MG | AA | 3181 | 1/1 | 0.83 | 0.40 | 14.19 | 55,55,55,55 | 0 |
| 60 | MG | CA | 3163 | 1/1 | 0.94 | 0.31 | 14.05 | 41,41,41,41 | 0 |
| 60 | MG | AD | 305 | 1/1 | 0.92 | 0.55 | 14.03 | 75,75,75,75 | 0 |
| 60 | MG | AA | 3296 | 1/1 | 0.98 | 0.27 | 14.01 | 40,40,40,40 | 0 |
| 60 | MG | AA | 3228 | 1/1 | 0.88 | 0.32 | 14.01 | 63,63,63,63 | 0 |
| 60 | MG | AP | 201 | 1/1 | 0.97 | 0.31 | 13.63 | 35,35,35,35 | 0 |
| 60 | MG | CA | 3439 | 1/1 | 0.97 | 0.23 | 13.58 | 47,47,47,47 | 0 |
| 60 | MG | CA | 3181 | 1/1 | 0.88 | 0.31 | 13.47 | 68,68,68,68 | 0 |
| 60 | MG | CA | 3619 | 1/1 | 0.75 | 0.35 | 13.19 | 78,78,78,78 | 0 |
| 60 | MG | CA | 3122 | 1/1 | 0.79 | 0.33 | 13.09 | 95,95,95,95 | 0 |
| 60 | MG | CA | 3320 | 1/1 | 0.97 | 0.25 | 13.07 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3137 | 1/1 | 0.92 | 0.36 | 13.03 | 55,55,55,55 | 0 |
| 60 | MG | AA | 3036 | 1/1 | 0.83 | 0.20 | 13.02 | 63,63,63,63 | 0 |
| 60 | MG | CA | 3110 | 1/1 | 0.96 | 0.33 | 12.80 | 35,35,35,35 | 0 |
| 60 | MG | AA | 3819 | 1/1 | 0.97 | 0.37 | 12.77 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3112 | 1/1 | 0.98 | 0.36 | 12.74 | 44,44,44,44 | 0 |
| 60 | MG | BA | 1705 | 1/1 | 0.95 | 0.30 | 12.67 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3039 | 1/1 | 0.96 | 0.25 | 12.66 | 34,34,34,34 | 0 |
| 60 | MG | DA | 1767 | 1/1 | 0.84 | 0.56 | 12.51 | 88,88,88,88 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | AA | 3376 | 1/1 | 0.95 | 0.21 | 12.41 | 39,39,39,39 | 0 |
| 60 | MG | CA | 3032 | 1/1 | 0.77 | 0.43 | 12.40 | 67,67,67,67 | 0 |
| 60 | MG | BA | 1629 | 1/1 | 0.78 | 0.25 | 12.30 | 71,71,71,71 | 0 |
| 60 | MG | AA | 3525 | 1/1 | 0.92 | 0.21 | 11.87 | 45,45,45,45 | 0 |
| 60 | MG | CA | 3279 | 1/1 | 0.97 | 0.26 | 11.79 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3047 | 1/1 | 0.94 | 0.30 | 11.58 | 40,40,40,40 | 0 |
| 60 | MG | AA | 3510 | 1/1 | 0.96 | 0.22 | 11.56 | 13,13,13,13 | 0 |
| 60 | MG | AA | 3589 | 1/1 | 0.87 | 0.33 | 11.53 | 31,31,31,31 | 1 |
| 60 | MG | AA | 3131 | 1/1 | 0.96 | 0.29 | 11.46 | 39,39,39,39 | 0 |
| 60 | MG | CA | 3529 | 1/1 | 0.73 | 0.31 | 11.40 | 69,69,69,69 | 0 |
| 60 | MG | AA | 3248 | 1/1 | 0.88 | 0.49 | 10.92 | 79,79,79,79 | 0 |
| 60 | MG | CA | 3154 | 1/1 | 0.92 | 0.22 | 10.90 | 68,68,68,68 | 0 |
| 60 | MG | AA | 3582 | 1/1 | 0.76 | 0.35 | 10.87 | 78,78,78,78 | 0 |
| 60 | MG | AA | 3289 | 1/1 | 0.91 | 0.19 | 10.79 | 47,47,47,47 | 0 |
| 60 | MG | BA | 1671 | 1/1 | 0.80 | 0.36 | 10.78 | 71,71,71,71 | 0 |
| 60 | MG | CA | 3179 | 1/1 | 0.95 | 0.27 | 10.78 | 27,27,27,27 | 0 |
| 60 | MG | AA | 3717 | 1/1 | 0.97 | 0.23 | 10.74 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3714 | 1/1 | 0.94 | 0.24 | 10.73 | 44,44,44,44 | 0 |
| 60 | MG | AA | 3120 | 1/1 | 0.89 | 0.26 | 10.63 | 54,54,54,54 | 0 |
| 60 | MG | AA | 3564 | 1/1 | 0.97 | 0.23 | 10.61 | 17,17,17,17 | 0 |
| 60 | MG | CA | 3288 | 1/1 | 0.90 | 0.34 | 10.53 | 39,39,39,39 | 0 |
| 60 | MG | DA | 1619 | 1/1 | 0.93 | 0.36 | 10.48 | 50,50,50,50 | 0 |
| 60 | MG | CA | 3214 | 1/1 | 0.91 | 0.28 | 10.41 | 50,50,50,50 | 0 |
| 60 | MG | BA | 1686 | 1/1 | 0.98 | 0.25 | 10.38 | 58,58,58,58 | 0 |
| 60 | MG | CA | 3106 | 1/1 | 0.93 | 0.27 | 10.21 | 45,45,45,45 | 0 |
| 60 | MG | AD | 302 | 1/1 | 0.94 | 0.39 | 10.18 | 31,31,31,31 | 0 |
| 60 | MG | AA | 3206 | 1/1 | 0.96 | 0.19 | 9.95 | 55,55,55,55 | 0 |
| 60 | MG | AA | 3109 | 1/1 | 0.84 | 0.35 | 9.81 | 75,75,75,75 | 0 |
| 60 | MG | AA | 3797 | 1/1 | 0.91 | 0.31 | 9.79 | 60,60,60,60 | 0 |
| 60 | MG | AA | 3825 | 1/1 | 0.96 | 0.29 | 9.74 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3524 | 1/1 | 0.85 | 0.30 | 9.72 | 41,41,41,41 | 0 |
| 60 | MG | CA | 3408 | 1/1 | 0.94 | 0.27 | 9.32 | 35,35,35,35 | 0 |
| 60 | MG | CA | 3160 | 1/1 | 0.95 | 0.27 | 9.21 | 33,33,33,33 | 0 |
| 60 | MG | AA | 3830 | 1/1 | 0.94 | 0.30 | 9.02 | 75,75,75,75 | 0 |
| 60 | MG | CA | 3209 | 1/1 | 0.91 | 0.27 | 9.01 | 101,101,101,101 | 0 |
| 60 | MG | CA | 3184 | 1/1 | 0.87 | 0.26 | 8.92 | 43,43,43,43 | 0 |
| 60 | MG | CA | 3311 | 1/1 | 0.72 | 0.29 | 8.85 | 54,54,54,54 | 0 |
| 60 | MG | AA | 3827 | 1/1 | 0.91 | 0.29 | 8.75 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3604 | 1/1 | 0.89 | 0.23 | 8.73 | 44,44,44,44 | 1 |
| 60 | MG | AA | 3823 | 1/1 | 0.94 | 0.34 | 8.70 | 51,51,51,51 | 0 |
| 60 | MG | CA | 3293 | 1/1 | 0.85 | 0.31 | 8.64 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | DA | 1638 | 1/1 | 0.81 | 0.28 | 8.48 | 60,60,60,60 | 0 |
| 60 | MG | AA | 3019 | 1/1 | 0.89 | 0.26 | 8.42 | 53,53,53,53 | 0 |
| 60 | MG | AA | 3708 | 1/1 | 0.86 | 0.30 | 8.40 | 71,71,71,71 | 0 |
| 60 | MG | AD | 301 | 1/1 | 0.97 | 0.34 | 8.33 | 46,46,46,46 | 0 |
| 60 | MG | DA | 1650 | 1/1 | 0.92 | 0.31 | 8.22 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3686 | 1/1 | 0.96 | 0.24 | 8.18 | 62,62,62,62 | 0 |
| 60 | MG | CV | 202 | 1/1 | 0.95 | 0.35 | 8.16 | 82,82,82,82 | 0 |
| 60 | MG | CA | 3236 | 1/1 | 0.85 | 0.30 | 8.11 | 80,80,80,80 | 0 |
| 60 | MG | CA | 3366 | 1/1 | 0.85 | 0.24 | 8.10 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3330 | 1/1 | 0.92 | 0.27 | 8.03 | 37,37,37,37 | 0 |
| 60 | MG | CA | 3450 | 1/1 | 0.98 | 0.24 | 8.01 | 38,38,38,38 | 0 |
| 60 | MG | AA | 3149 | 1/1 | 0.98 | 0.25 | 7.95 | 15,15,15,15 | 0 |
| 60 | MG | BA | 1658 | 1/1 | 0.91 | 0.55 | 7.88 | 68,68,68,68 | 0 |
| 60 | MG | DA | 1637 | 1/1 | 0.94 | 0.37 | 7.87 | 61,61,61,61 | 0 |
| 60 | MG | CA | 3157 | 1/1 | 0.97 | 0.23 | 7.84 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3539 | 1/1 | 0.95 | 0.23 | 7.82 | 42,42,42,42 | 0 |
| 60 | MG | CA | 3083 | 1/1 | 0.76 | 0.22 | 7.79 | 80,80,80,80 | 0 |
| 60 | MG | CA | 3227 | 1/1 | 0.95 | 0.25 | 7.73 | 30,30,30,30 | 0 |
| 60 | MG | AD | 304 | 1/1 | 0.97 | 0.34 | 7.68 | 49,49,49,49 | 0 |
| 60 | MG | AA | 3173 | 1/1 | 0.94 | 0.26 | 7.52 | 74,74,74,74 | 0 |
| 60 | MG | DA | 1696 | 1/1 | 0.95 | 0.26 | 7.49 | 65,65,65,65 | 0 |
| 60 | MG | AA | 3517 | 1/1 | 0.96 | 0.31 | 7.44 | 44,44,44,44 | 0 |
| 60 | MG | CA | 3430 | 1/1 | 0.94 | 0.22 | 7.37 | 38,38,38,38 | 0 |
| 60 | MG | CA | 3407 | 1/1 | 0.80 | 0.28 | 7.36 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3711 | 1/1 | 0.95 | 0.37 | 7.34 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3020 | 1/1 | 0.96 | 0.18 | 7.29 | 25,25,25,25 | 0 |
| 60 | MG | AA | 3654 | 1/1 | 0.84 | 0.25 | 7.27 | 81,81,81,81 | 0 |
| 60 | MG | DA | 1646 | 1/1 | 0.96 | 0.30 | 7.24 | 51,51,51,51 | 0 |
| 60 | MG | CA | 3659 | 1/1 | 0.80 | 0.35 | 7.21 | 72,72,72,72 | 0 |
| 60 | MG | CA | 3187 | 1/1 | 0.78 | 0.32 | 7.18 | 70,70,70,70 | 0 |
| 60 | MG | AA | 3721 | 1/1 | 0.90 | 0.20 | 7.08 | 21,21,21,21 | 0 |
| 60 | MG | CA | 3143 | 1/1 | 0.90 | 0.23 | 7.02 | 62,62,62,62 | 0 |
| 60 | MG | AA | 3119 | 1/1 | 0.89 | 0.22 | 7.01 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3514 | 1/1 | 0.97 | 0.21 | 7.00 | 32,32,32,32 | 0 |
| 60 | MG | AA | 3669 | 1/1 | 0.97 | 0.21 | 6.98 | 36,36,36,36 | 0 |
| 60 | MG | AA | 3516 | 1/1 | 0.90 | 0.27 | 6.98 | 38,38,38,38 | 0 |
| 60 | MG | AA | 3251 | 1/1 | 0.93 | 0.26 | 6.94 | 50,50,50,50 | 0 |
| 60 | MG | AW | 3003 | 1/1 | 0.95 | 0.33 | 6.93 | 38,38,38,38 | 0 |
| 60 | MG | CA | 3455 | 1/1 | 0.97 | 0.27 | 6.82 | 37,37,37,37 | 0 |
| 60 | MG | AA | 3602 | 1/1 | 0.95 | 0.21 | 6.82 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3834 | 1/1 | 0.93 | 0.29 | 6.70 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3102 | 1/1 | 0.95 | 0.24 | 6.66 | 38,38,38,38 | 0 |
| 60 | MG | A0 | 101 | 1/1 | 0.79 | 0.23 | 6.65 | 88,88,88,88 | 0 |
| 60 | MG | AA | 3816 | 1/1 | 0.96 | 0.24 | 6.65 | 64,64,64,64 | 0 |
| 60 | MG | AA | 3001 | 1/1 | 0.94 | 0.21 | 6.58 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3833 | 1/1 | 0.97 | 0.24 | 6.58 | 39,39,39,39 | 0 |
| 60 | MG | CA | 3013 | 1/1 | 0.87 | 0.32 | 6.57 | 52,52,52,52 | 0 |
| 60 | MG | AD | 309 | 1/1 | 0.80 | 0.34 | 6.52 | 58,58,58,58 | 0 |
| 60 | MG | BA | 1615 | 1/1 | 0.94 | 0.30 | 6.52 | 65,65,65,65 | 0 |
| 60 | MG | CA | 3324 | 1/1 | 0.97 | 0.22 | 6.45 | 31,31,31,31 | 0 |
| 60 | MG | AA | 3220 | 1/1 | 0.95 | 0.19 | 6.32 | 65,65,65,65 | 0 |
| 60 | MG | AA | 3408 | 1/1 | 0.82 | 0.26 | 6.29 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3369 | 1/1 | 0.84 | 0.19 | 6.24 | 59,59,59,59 | 0 |
| 60 | MG | AA | 3023 | 1/1 | 0.98 | 0.46 | 6.22 | 40,40,40,40 | 1 |
| 60 | MG | AA | 3310 | 1/1 | 0.92 | 0.17 | 6.21 | 37,37,37,37 | 0 |
| 60 | MG | CA | 3413 | 1/1 | 0.94 | 0.25 | 6.21 | 38,38,38,38 | 0 |
| 60 | MG | CA | 3087 | 1/1 | 0.79 | 0.41 | 6.16 | 107,107,107,107 | 0 |
| 60 | MG | AA | 3315 | 1/1 | 0.95 | 0.21 | 6.10 | 56,56,56,56 | 0 |
| 60 | MG | DA | 1694 | 1/1 | 0.92 | 0.27 | 6.08 | 60,60,60,60 | 0 |
| 60 | MG | AA | 3417 | 1/1 | 0.93 | 0.19 | 6.04 | 16,16,16,16 | 0 |
| 60 | MG | BA | 1662 | 1/1 | 0.90 | 0.17 | 6.01 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3222 | 1/1 | 0.92 | 0.26 | 5.97 | 58,58,58,58 | 0 |
| 60 | MG | AA | 3141 | 1/1 | 0.91 | 0.20 | 5.96 | 46,46,46,46 | 0 |
| 60 | MG | CA | 3356 | 1/1 | 0.95 | 0.24 | 5.95 | 28,28,28,28 | 0 |
| 60 | MG | AB | 3014 | 1/1 | 0.72 | 0.23 | 5.92 | 70,70,70,70 | 0 |
| 60 | MG | CA | 3598 | 1/1 | 0.88 | 0.21 | 5.87 | 66,66,66,66 | 0 |
| 60 | MG | AU | 202 | 1/1 | 0.92 | 0.27 | 5.84 | 65,65,65,65 | 0 |
| 60 | MG | BA | 1626 | 1/1 | 0.92 | 0.25 | 5.80 | 72,72,72,72 | 0 |
| 60 | MG | AA | 3451 | 1/1 | 0.96 | 0.18 | 5.80 | 43,43,43,43 | 0 |
| 60 | MG | AA | 3415 | 1/1 | 0.99 | 0.20 | 5.68 | 29,29,29,29 | 0 |
| 60 | MG | AA | 3185 | 1/1 | 0.97 | 0.20 | 5.65 | 35,35,35,35 | 0 |
| 60 | MG | AA | 3257 | 1/1 | 0.91 | 0.22 | 5.63 | 18,18,18,18 | 0 |
| 60 | MG | AQ | 3001 | 1/1 | 0.86 | 0.26 | 5.60 | 56,56,56,56 | 0 |
| 60 | MG | CA | 3129 | 1/1 | 0.83 | 0.30 | 5.58 | 76,76,76,76 | 0 |
| 60 | MG | AA | 3035 | 1/1 | 0.96 | 0.22 | 5.56 | 69,69,69,69 | 0 |
| 60 | MG | AA | 3735 | 1/1 | 0.92 | 0.27 | 5.46 | 30,30,30,30 | 0 |
| 60 | MG | CA | 3549 | 1/1 | 0.89 | 0.18 | 5.42 | 29,29,29,29 | 0 |
| 60 | MG | AA | 3352 | 1/1 | 0.92 | 0.18 | 5.29 | 64,64,64,64 | 0 |
| 60 | MG | AA | 3790 | 1/1 | 0.97 | 0.23 | 5.28 | 11,11,11,11 | 0 |
| 60 | MG | CA | 3411 | 1/1 | 0.73 | 0.24 | 5.26 | 49,49,49,49 | 0 |
| 60 | MG | AA | 3021 | 1/1 | 0.90 | 0.20 | 5.24 | 49,49,49,49 | 0 |
| 60 | MG | CA | 3652 | 1/1 | 0.75 | 0.23 | 5.22 | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | DA | 1742 | 1/1 | 0.88 | 0.25 | 5.17 | 52,52,52,52 | 0 |
| 60 | MG | AA | 3218 | 1/1 | 0.98 | 0.20 | 5.16 | 10,10,10,10 | 0 |
| 60 | MG | AA | 3274 | 1/1 | 0.92 | 0.49 | 5.13 | 48,48,48,48 | 1 |
| 60 | MG | AA | 3529 | 1/1 | 0.94 | 0.19 | 5.13 | 12,12,12,12 | 1 |
| 60 | MG | AA | 3045 | 1/1 | 0.97 | 0.33 | 5.09 | 58,58,58,58 | 0 |
| 60 | MG | AA | 3309 | 1/1 | 0.91 | 0.18 | 5.07 | 72,72,72,72 | 0 |
| 60 | MG | AA | 3387 | 1/1 | 0.96 | 0.21 | 5.03 | 34,34,34,34 | 0 |
| 60 | MG | AN | 3002 | 1/1 | 0.90 | 0.20 | 5.01 | 76,76,76,76 | 0 |
| 60 | MG | CA | 3264 | 1/1 | 0.96 | 0.20 | 4.96 | 54,54,54,54 | 0 |
| 60 | MG | AA | 3241 | 1/1 | 0.96 | 0.26 | 4.93 | 29,29,29,29 | 0 |
| 60 | MG | DA | 1651 | 1/1 | 0.65 | 0.26 | 4.92 | 86,86,86,86 | 0 |
| 60 | MG | CA | 3002 | 1/1 | 0.93 | 0.24 | 4.88 | 32,32,32,32 | 0 |
| 60 | MG | CA | 3210 | 1/1 | 0.88 | 0.23 | 4.87 | 44,44,44,44 | 0 |
| 60 | MG | AA | 3528 | 1/1 | 0.96 | 0.19 | 4.87 | 26,26,26,26 | 0 |
| 60 | MG | BA | 1683 | 1/1 | 0.91 | 0.24 | 4.83 | 50,50,50,50 | 0 |
| 60 | MG | CA | 3558 | 1/1 | 0.96 | 0.20 | 4.82 | 49,49,49,49 | 1 |
| 60 | MG | BA | 1765 | 1/1 | 0.98 | 0.30 | 4.82 | 67,67,67,67 | 0 |
| 60 | MG | AA | 3437 | 1/1 | 0.91 | 0.20 | 4.77 | 25,25,25,25 | 0 |
| 60 | MG | CA | 3307 | 1/1 | 0.98 | 0.21 | 4.75 | 31,31,31,31 | 0 |
| 60 | MG | CA | 3315 | 1/1 | 0.91 | 0.21 | 4.71 | 44,44,44,44 | 0 |
| 60 | MG | CA | 3274 | 1/1 | 0.95 | 0.18 | 4.68 | 64,64,64,64 | 0 |
| 60 | MG | AA | 3401 | 1/1 | 0.92 | 0.22 | 4.66 | 26,26,26,26 | 0 |
| 60 | MG | AA | 3323 | 1/1 | 0.97 | 0.18 | 4.65 | 42,42,42,42 | 0 |
| 60 | MG | DA | 1679 | 1/1 | 0.95 | 0.38 | 4.64 | 70,70,70,70 | 0 |
| 60 | MG | AA | 3398 | 1/1 | 0.95 | 0.19 | 4.62 | 29,29,29,29 | 0 |
| 60 | MG | C3 | 101 | 1/1 | 0.84 | 0.46 | 4.60 | 91,91,91,91 | 0 |
| 60 | MG | AA | 3486 | 1/1 | 0.80 | 0.21 | 4.60 | 34,34,34,34 | 0 |
| 60 | MG | CA | 3446 | 1/1 | 0.97 | 0.24 | 4.60 | 37,37,37,37 | 0 |
| 60 | MG | AA | 3385 | 1/1 | 0.96 | 0.20 | 4.59 | 24,24,24,24 | 0 |
| 60 | MG | CA | 3198 | 1/1 | 0.96 | 0.25 | 4.58 | 49,49,49,49 | 0 |
| 60 | MG | AA | 3826 | 1/1 | 0.98 | 0.22 | 4.58 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3357 | 1/1 | 0.96 | 0.18 | 4.53 | 52,52,52,52 | 0 |
| 60 | MG | AA | 3741 | 1/1 | 0.95 | 0.27 | 4.48 | 47,47,47,47 | 0 |
| 60 | MG | AN | 3001 | 1/1 | 0.86 | 0.47 | 4.47 | 64,64,64,64 | 0 |
| 60 | MG | CA | 3166 | 1/1 | 0.98 | 0.20 | 4.46 | 31,31,31,31 | 0 |
| 60 | MG | AA | 3559 | 1/1 | 0.90 | 0.21 | 4.45 | 37,37,37,37 | 0 |
| 60 | MG | CA | 3265 | 1/1 | 0.86 | 0.20 | 4.44 | 66,66,66,66 | 0 |
| 60 | MG | AA | 3430 | 1/1 | 0.97 | 0.24 | 4.37 | 23,23,23,23 | 0 |
| 60 | MG | AA | 3454 | 1/1 | 0.95 | 0.16 | 4.27 | 27,27,27,27 | 0 |
| 60 | MG | DE | 201 | 1/1 | 0.78 | 0.31 | 4.25 | 93,93,93,93 | 0 |
| 60 | MG | DA | 1714 | 1/1 | 0.90 | 0.39 | 4.24 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3792 | 1/1 | 0.95 | 0.26 | 4.21 | 35,35,35,35 | 0 |
| 60 | MG | AA | 3513 | 1/1 | 0.93 | 0.22 | 4.20 | 37,37,37,37 | 0 |
| 60 | MG | CA | 3449 | 1/1 | 0.97 | 0.21 | 4.16 | 52,52,52,52 | 0 |
| 60 | MG | CA | 3082 | 1/1 | 0.96 | 0.21 | 4.12 | 31,31,31,31 | 0 |
| 60 | MG | AA | 3438 | 1/1 | 0.86 | 0.21 | 4.11 | 75,75,75,75 | 0 |
| 60 | MG | CA | 3359 | 1/1 | 0.97 | 0.22 | 4.06 | 44,44,44,44 | 0 |
| 60 | MG | AA | 3378 | 1/1 | 0.86 | 0.21 | 4.04 | 24,24,24,24 | 0 |
| 60 | MG | BA | 1655 | 1/1 | 0.95 | 0.26 | 4.04 | 65,65,65,65 | 0 |
| 60 | MG | BA | 1630 | 1/1 | 0.80 | 0.19 | 3.89 | 61,61,61,61 | 0 |
| 60 | MG | DA | 1674 | 1/1 | 0.93 | 0.28 | 3.86 | 60,60,60,60 | 0 |
| 60 | MG | DA | 1611 | 1/1 | 0.74 | 0.23 | 3.86 | 80,80,80,80 | 0 |
| 60 | MG | AA | 3180 | 1/1 | 0.86 | 0.25 | 3.84 | 53,53,53,53 | 0 |
| 60 | MG | AA | 3518 | 1/1 | 0.94 | 0.18 | 3.82 | 28,28,28,28 | 0 |
| 60 | MG | CA | 3381 | 1/1 | 0.97 | 0.22 | 3.82 | 37,37,37,37 | 0 |
| 60 | MG | AA | 3565 | 1/1 | 0.97 | 0.21 | 3.78 | 26,26,26,26 | 0 |
| 60 | MG | AA | 3541 | 1/1 | 0.78 | 0.20 | 3.77 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3712 | 1/1 | 0.92 | 0.20 | 3.73 | 50,50,50,50 | 0 |
| 60 | MG | AA | 3052 | 1/1 | 0.96 | 0.20 | 3.68 | 15,15,15,15 | 0 |
| 60 | MG | AA | 3556 | 1/1 | 0.94 | 0.17 | 3.67 | 54,54,54,54 | 0 |
| 60 | MG | DA | 1631 | 1/1 | 0.77 | 0.22 | 3.65 | 55,55,55,55 | 0 |
| 60 | MG | AA | 3386 | 1/1 | 0.97 | 0.21 | 3.63 | 19,19,19,19 | 0 |
| 60 | MG | AA | 3506 | 1/1 | 0.97 | 0.20 | 3.59 | 19,19,19,19 | 0 |
| 60 | MG | AA | 3505 | 1/1 | 0.97 | 0.23 | 3.55 | 29,29,29,29 | 0 |
| 60 | MG | BA | 1749 | 1/1 | 0.99 | 0.27 | 3.53 | 52,52,52,52 | 0 |
| 60 | MG | BA | 1778 | 1/1 | 0.98 | 0.26 | 3.53 | 52,52,52,52 | 0 |
| 60 | MG | CA | 3114 | 1/1 | 0.86 | 0.20 | 3.50 | 59,59,59,59 | 0 |
| 60 | MG | DA | 1719 | 1/1 | 0.85 | 0.22 | 3.49 | 87,87,87,87 | 0 |
| 60 | MG | AA | 3523 | 1/1 | 0.98 | 0.17 | 3.42 | 35,35,35,35 | 0 |
| 60 | MG | CA | 3617 | 1/1 | 0.86 | 0.38 | 3.42 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3042 | 1/1 | 0.97 | 0.20 | 3.39 | 43,43,43,43 | 0 |
| 60 | MG | AA | 3184 | 1/1 | 0.95 | 0.20 | 3.39 | 39,39,39,39 | 0 |
| 60 | MG | CA | 3249 | 1/1 | 0.80 | 0.18 | 3.32 | 67,67,67,67 | 0 |
| 60 | MG | AA | 3551 | 1/1 | 0.95 | 0.17 | 3.28 | 58,58,58,58 | 0 |
| 60 | MG | AA | 3832 | 1/1 | 0.96 | 0.21 | 3.26 | 52,52,52,52 | 0 |
| 60 | MG | CV | 201 | 1/1 | 0.95 | 0.36 | 3.25 | 84,84,84,84 | 0 |
| 60 | MG | AU | 203 | 1/1 | 0.89 | 0.24 | 3.17 | 55,55,55,55 | 0 |
| 60 | MG | CA | 3038 | 1/1 | 0.96 | 0.21 | 3.13 | 26,26,26,26 | 0 |
| 60 | MG | AA | 3313 | 1/1 | 0.92 | 0.17 | 3.13 | 31,31,31,31 | 0 |
| 60 | MG | AA | 3330 | 1/1 | 0.97 | 0.21 | 3.13 | 33,33,33,33 | 0 |
| 60 | MG | BA | 1785 | 1/1 | 0.89 | 0.19 | 3.12 | 69,69,69,69 | 0 |
| 60 | MG | BA | 1675 | 1/1 | 0.93 | 0.19 | 3.12 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3068 | 1/1 | 0.84 | 0.19 | 3.08 | 73,73,73,73 | 0 |
| 60 | MG | AD | 308 | 1/1 | 0.97 | 0.36 | 3.08 | 49,49,49,49 | 0 |
| 60 | MG | AA | 3253 | 1/1 | 0.95 | 0.19 | 3.07 | 42,42,42,42 | 0 |
| 60 | MG | BA | 1601 | 1/1 | 0.82 | 0.19 | 3.06 | 66,66,66,66 | 0 |
| 60 | MG | BA | 1701 | 1/1 | 0.94 | 0.21 | 3.05 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3217 | 1/1 | 0.92 | 0.16 | 3.04 | 50,50,50,50 | 0 |
| 60 | MG | DA | 1688 | 1/1 | 0.88 | 0.20 | 2.99 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3172 | 1/1 | 0.97 | 0.18 | 2.95 | 50,50,50,50 | 0 |
| 60 | MG | AA | 3294 | 1/1 | 0.90 | 0.19 | 2.92 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3277 | 1/1 | 0.91 | 0.19 | 2.92 | 48,48,48,48 | 0 |
| 60 | MG | CQ | 202 | 1/1 | 0.92 | 0.25 | 2.85 | 56,56,56,56 | 0 |
| 60 | MG | DA | 1706 | 1/1 | 0.94 | 0.19 | 2.81 | 70,70,70,70 | 0 |
| 60 | MG | AA | 3535 | 1/1 | 0.94 | 0.18 | 2.79 | 37,37,37,37 | 0 |
| 60 | MG | CA | 3423 | 1/1 | 0.96 | 0.17 | 2.79 | 57,57,57,57 | 0 |
| 60 | MG | AA | 3187 | 1/1 | 0.89 | 0.17 | 2.79 | 29,29,29,29 | 0 |
| 60 | MG | AA | 3540 | 1/1 | 0.92 | 0.20 | 2.77 | 28,28,28,28 | 0 |
| 60 | MG | CA | 3018 | 1/1 | 0.78 | 0.18 | 2.72 | 59,59,59,59 | 0 |
| 60 | MG | AF | 301 | 1/1 | 0.85 | 0.20 | 2.68 | 49,49,49,49 | 0 |
| 60 | MG | CA | 3473 | 1/1 | 0.93 | 0.24 | 2.67 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3272 | 1/1 | 0.93 | 0.41 | 2.64 | 74,74,74,74 | 0 |
| 60 | MG | BB | 3001 | 1/1 | 0.96 | 0.23 | 2.63 | 67,67,67,67 | 0 |
| 60 | MG | CA | 3431 | 1/1 | 0.78 | 0.17 | 2.61 | 80,80,80,80 | 0 |
| 60 | MG | BA | 1679 | 1/1 | 0.92 | 0.20 | 2.59 | 51,51,51,51 | 0 |
| 60 | MG | AA | 3532 | 1/1 | 0.97 | 0.18 | 2.55 | 20,20,20,20 | 0 |
| 60 | MG | CA | 3625 | 1/1 | 0.98 | 0.23 | 2.49 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3168 | 1/1 | 0.93 | 0.20 | 2.47 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3100 | 1/1 | 0.96 | 0.17 | 2.46 | 75,75,75,75 | 0 |
| 60 | MG | DA | 1602 | 1/1 | 0.80 | 0.22 | 2.45 | 65,65,65,65 | 0 |
| 60 | MG | AA | 3471 | 1/1 | 0.99 | 0.18 | 2.33 | 24,24,24,24 | 0 |
| 60 | MG | CA | 3454 | 1/1 | 0.98 | 0.23 | 2.31 | 43,43,43,43 | 0 |
| 60 | MG | AA | 3190 | 1/1 | 0.95 | 0.18 | 2.27 | 51,51,51,51 | 0 |
| 60 | MG | CA | 3004 | 1/1 | 0.97 | 0.18 | 2.25 | 43,43,43,43 | 0 |
| 60 | MG | AA | 3008 | 1/1 | 0.98 | 0.17 | 2.22 | 28,28,28,28 | 0 |
| 60 | MG | AB | 3016 | 1/1 | 0.87 | 0.14 | 2.21 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3384 | 1/1 | 0.95 | 0.16 | 2.20 | 26,26,26,26 | 0 |
| 60 | MG | CA | 3103 | 1/1 | 0.77 | 0.19 | 2.18 | 80,80,80,80 | 0 |
| 60 | MG | BA | 1648 | 1/1 | 0.95 | 0.18 | 2.15 | 28,28,28,28 | 0 |
| 60 | MG | AA | 3796 | 1/1 | 0.99 | 0.24 | 2.11 | 45,45,45,45 | 0 |
| 60 | MG | CA | 3488 | 1/1 | 0.94 | 0.17 | 2.11 | 58,58,58,58 | 0 |
| 60 | MG | AA | 3572 | 1/1 | 0.90 | 0.16 | 2.07 | 51,51,51,51 | 0 |
| 60 | MG | AD | 306 | 1/1 | 0.80 | 0.22 | 1.99 | 108,108,108,108 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3661 | 1/1 | 0.93 | 0.18 | 1.95 | 78,78,78,78 | 0 |
| 60 | MG | CA | 3224 | 1/1 | 0.97 | 0.18 | 1.94 | 32,32,32,32 | 0 |
| 60 | MG | CA | 3426 | 1/1 | 0.95 | 0.16 | 1.94 | 46,46,46,46 | 0 |
| 60 | MG | DA | 1763 | 1/1 | 0.86 | 0.15 | 1.92 | 61,61,61,61 | 0 |
| 60 | MG | CA | 3134 | 1/1 | 0.94 | 0.18 | 1.91 | 64,64,64,64 | 0 |
| 60 | MG | BA | 1678 | 1/1 | 0.95 | 0.22 | 1.89 | 52,52,52,52 | 0 |
| 60 | MG | CA | 3452 | 1/1 | 0.94 | 0.17 | 1.79 | 37,37,37,37 | 0 |
| 60 | MG | AA | 3723 | 1/1 | 0.98 | 0.16 | 1.79 | 30,30,30,30 | 0 |
| 60 | MG | BA | 1791 | 1/1 | 0.92 | 0.18 | 1.78 | 58,58,58,58 | 0 |
| 60 | MG | CA | 3297 | 1/1 | 0.96 | 0.16 | 1.77 | 55,55,55,55 | 0 |
| 60 | MG | CA | 3316 | 1/1 | 0.97 | 0.19 | 1.72 | 34,34,34,34 | 0 |
| 60 | MG | AA | 3484 | 1/1 | 0.92 | 0.23 | 1.65 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3407 | 1/1 | 0.96 | 0.19 | 1.64 | 22,22,22,22 | 0 |
| 60 | MG | AA | 3835 | 1/1 | 0.94 | 0.23 | 1.63 | 34,34,34,34 | 1 |
| 60 | MG | AA | 3809 | 1/1 | 0.96 | 0.25 | 1.63 | 46,46,46,46 | 0 |
| 60 | MG | CA | 3650 | 1/1 | 0.91 | 0.17 | 1.57 | 42,42,42,42 | 0 |
| 60 | MG | CA | 3495 | 1/1 | 0.91 | 0.18 | 1.52 | 64,64,64,64 | 0 |
| 60 | MG | AA | 3457 | 1/1 | 0.96 | 0.17 | 1.45 | 18,18,18,18 | 0 |
| 60 | MG | AA | 3501 | 1/1 | 0.92 | 0.16 | 1.40 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3801 | 1/1 | 0.95 | 0.16 | 1.29 | 39,39,39,39 | 0 |
| 60 | MG | CA | 3040 | 1/1 | 0.94 | 0.18 | 1.24 | 63,63,63,63 | 0 |
| 60 | MG | AA | 3432 | 1/1 | 0.99 | 0.16 | 1.24 | 24,24,24,24 | 0 |
| 60 | MG | AA | 3527 | 1/1 | 0.97 | 0.16 | 1.24 | 20,20,20,20 | 0 |
| 60 | MG | CB | 3007 | 1/1 | 0.90 | 0.14 | 1.22 | 57,57,57,57 | 0 |
| 60 | MG | A9 | 502 | 1/1 | 0.93 | 0.28 | 1.20 | 52,52,52,52 | 0 |
| 60 | MG | AA | 3820 | 1/1 | 0.94 | 0.21 | 1.19 | 31,31,31,31 | 0 |
| 60 | MG | CA | 3657 | 1/1 | 0.94 | 0.24 | 1.16 | 34,34,34,34 | 0 |
| 60 | MG | CA | 3422 | 1/1 | 0.98 | 0.18 | 1.15 | 43,43,43,43 | 0 |
| 60 | MG | CA | 3344 | 1/1 | 0.96 | 0.18 | 1.15 | 27,27,27,27 | 0 |
| 60 | MG | DA | 1740 | 1/1 | 0.98 | 0.17 | 1.13 | 56,56,56,56 | 0 |
| 60 | MG | AA | 3328 | 1/1 | 0.98 | 0.22 | 1.12 | 21,21,21,21 | 0 |
| 60 | MG | DA | 1685 | 1/1 | 0.96 | 0.20 | 1.10 | 49,49,49,49 | 0 |
| 60 | MG | DA | 1668 | 1/1 | 0.87 | 0.27 | 1.07 | 68,68,68,68 | 0 |
| 60 | MG | AA | 3606 | 1/1 | 0.96 | 0.18 | 1.07 | 62,62,62,62 | 0 |
| 60 | MG | BA | 1640 | 1/1 | 0.90 | 0.19 | 1.02 | 56,56,56,56 | 0 |
| 60 | MG | DA | 1601 | 1/1 | 0.93 | 0.17 | 0.99 | 59,59,59,59 | 0 |
| 60 | MG | AA | 3791 | 1/1 | 0.94 | 0.23 | 0.99 | 48,48,48,48 | 0 |
| 60 | MG | BA | 1690 | 1/1 | 0.93 | 0.19 | 0.96 | 59,59,59,59 | 0 |
| 60 | MG | AA | 3012 | 1/1 | 0.94 | 0.17 | 0.96 | 38,38,38,38 | 0 |
| 60 | MG | AA | 3298 | 1/1 | 0.94 | 0.15 | 0.95 | 28,28,28,28 | 0 |
| 60 | MG | CA | 3328 | 1/1 | 0.95 | 0.17 | 0.95 | 40,40,40,40 | 0 |
| 60 | MG | CA | 3361 | 1/1 | 0.87 | 0.14 | 0.93 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | CA | 3357 | 1/1 | 0.85 | 0.17 | 0.92 | 34,34,34,34 | 0 |
| 60 | MG | CA | 3425 | 1/1 | 0.93 | 0.15 | 0.92 | 45,45,45,45 | 0 |
| 60 | MG | CA | 3223 | 1/1 | 0.98 | 0.18 | 0.85 | 46,46,46,46 | 0 |
| 60 | MG | BA | 1775 | 1/1 | 0.99 | 0.22 | 0.83 | 47,47,47,47 | 0 |
| 60 | MG | DA | 1657 | 1/1 | 0.87 | 0.14 | 0.81 | 75,75,75,75 | 0 |
| 60 | MG | DA | 1644 | 1/1 | 0.96 | 0.18 | 0.77 | 49,49,49,49 | 0 |
| 60 | MG | BA | 1603 | 1/1 | 0.85 | 0.20 | 0.75 | 65,65,65,65 | 0 |
| 60 | MG | AA | 3224 | 1/1 | 0.98 | 0.19 | 0.74 | 26,26,26,26 | 0 |
| 60 | MG | CA | 3589 | 1/1 | 0.85 | 0.16 | 0.73 | 67,67,67,67 | 0 |
| 60 | MG | AA | 3393 | 1/1 | 0.93 | 0.17 | 0.72 | 18,18,18,18 | 0 |
| 60 | MG | CA | 3304 | 1/1 | 0.95 | 0.15 | 0.69 | 48,48,48,48 | 0 |
| 60 | MG | CA | 3390 | 1/1 | 0.87 | 0.21 | 0.66 | 42,42,42,42 | 0 |
| 60 | MG | CA | 3097 | 1/1 | 0.88 | 0.17 | 0.66 | 79,79,79,79 | 0 |
| 60 | MG | CA | 3280 | 1/1 | 0.82 | 0.17 | 0.63 | 43,43,43,43 | 0 |
| 60 | MG | BA | 1684 | 1/1 | 0.91 | 0.21 | 0.62 | 64,64,64,64 | 0 |
| 60 | MG | CD | 304 | 1/1 | 0.94 | 0.23 | 0.58 | 32,32,32,32 | 0 |
| 60 | MG | CA | 3651 | 1/1 | 0.97 | 0.17 | 0.57 | 41,41,41,41 | 0 |
| 60 | MG | CA | 3615 | 1/1 | 0.95 | 0.15 | 0.52 | 33,33,33,33 | 0 |
| 60 | MG | DA | 1765 | 1/1 | 0.72 | 0.26 | 0.50 | 66,66,66,66 | 0 |
| 60 | MG | DT | 3001 | 1/1 | 0.83 | 0.25 | 0.48 | 59,59,59,59 | 0 |
| 60 | MG | CA | 3417 | 1/1 | 0.93 | 0.18 | 0.47 | 58,58,58,58 | 0 |
| 60 | MG | AA | 3053 | 1/1 | 0.98 | 0.15 | 0.47 | 21,21,21,21 | 0 |
| 60 | MG | DA | 1642 | 1/1 | 0.85 | 0.17 | 0.46 | 67,67,67,67 | 0 |
| 60 | MG | CA | 3649 | 1/1 | 0.97 | 0.19 | 0.45 | 15,15,15,15 | 0 |
| 60 | MG | BT | 3001 | 1/1 | 0.92 | 0.27 | 0.41 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3504 | 1/1 | 0.90 | 0.13 | 0.32 | 44,44,44,44 | 0 |
| 60 | MG | AA | 3585 | 1/1 | 0.82 | 0.15 | 0.31 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3554 | 1/1 | 0.94 | 0.16 | 0.24 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3318 | 1/1 | 0.97 | 0.16 | 0.21 | 31,31,31,31 | 0 |
| 60 | MG | CF | 305 | 1/1 | 0.96 | 0.20 | 0.20 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3312 | 1/1 | 0.95 | 0.14 | 0.19 | 25,25,25,25 | 0 |
| 60 | MG | BN | 503 | 1/1 | 0.78 | 0.22 | 0.17 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3574 | 1/1 | 0.98 | 0.15 | 0.16 | 26,26,26,26 | 0 |
| 60 | MG | AA | 3483 | 1/1 | 0.90 | 0.18 | 0.13 | 21,21,21,21 | 0 |
| 60 | MG | DA | 1693 | 1/1 | 0.94 | 0.15 | 0.11 | 50,50,50,50 | 0 |
| 60 | MG | CA | 3266 | 1/1 | 0.95 | 0.15 | 0.11 | 67,67,67,67 | 0 |
| 62 | ZN | A5 | 101 | 1/1 | 1.00 | 0.13 | 0.08 | 40,40,40,40 | 0 |
| 60 | MG | CA | 3518 | 1/1 | 0.95 | 0.18 | 0.03 | 72,72,72,72 | 0 |
| 60 | MG | AA | 3333 | 1/1 | 0.93 | 0.15 | 0.03 | 33,33,33,33 | 0 |
| 60 | MG | AA | 3380 | 1/1 | 0.91 | 0.18 | -0.01 | 75,75,75,75 | 0 |
| 60 | MG | CA | 3211 | 1/1 | 0.98 | 0.14 | -0.17 | 19,19,19,19 | 0 |
| 60 | MG | CA | 3415 | 1/1 | 0.97 | 0.18 | -0.19 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | CA | 3044 | 1/1 | 0.93 | 0.14 | -0.26 | 64,64,64,64 | 0 |
| 60 | MG | CA | 3017 | 1/1 | 0.98 | 0.15 | -0.26 | 28,28,28,28 | 0 |
| 60 | MG | CG | 3001 | 1/1 | 0.93 | 0.19 | -0.28 | 66,66,66,66 | 0 |
| 60 | MG | CA | 3335 | 1/1 | 0.91 | 0.16 | -0.30 | 38,38,38,38 | 0 |
| 60 | MG | AA | 3620 | 1/1 | 0.96 | 0.14 | -0.31 | 49,49,49,49 | 0 |
| 60 | MG | CA | 3660 | 1/1 | 0.83 | 0.14 | -0.32 | 65,65,65,65 | 0 |
| 60 | MG | CA | 3300 | 1/1 | 0.94 | 0.15 | -0.33 | 56,56,56,56 | 0 |
| 60 | MG | BA | 1813 | 1/1 | 0.88 | 0.17 | -0.38 | 66,66,66,66 | 0 |
| 60 | MG | BA | 1741 | 1/1 | 0.96 | 0.15 | -0.38 | 49,49,49,49 | 0 |
| 60 | MG | BA | 1759 | 1/1 | 0.85 | 0.14 | -0.42 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3034 | 1/1 | 0.94 | 0.15 | -0.45 | 51,51,51,51 | 0 |
| 60 | MG | AA | 3622 | 1/1 | 0.89 | 0.13 | -0.46 | 52,52,52,52 | 0 |
| 60 | MG | AA | 3617 | 1/1 | 0.97 | 0.12 | -0.47 | 32,32,32,32 | 0 |
| 60 | MG | AA | 3405 | 1/1 | 0.97 | 0.15 | -0.49 | 27,27,27,27 | 0 |
| 60 | MG | CA | 3486 | 1/1 | 0.86 | 0.14 | -0.54 | 48,48,48,48 | 0 |
| 64 | GDP | BZ | 702 | 28/28 | 0.97 | 0.14 | -0.55 | 57,57,57,57 | 1 |
| 60 | MG | CA | 3313 | 1/1 | 0.98 | 0.14 | -0.55 | 54,54,54,54 | 0 |
| 60 | MG | AD | 303 | 1/1 | 0.90 | 0.13 | -0.58 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3759 | 1/1 | 0.94 | 0.13 | -0.60 | 29,29,29,29 | 0 |
| 60 | MG | DE | 202 | 1/1 | 0.83 | 0.17 | -0.70 | 92,92,92,92 | 0 |
| 60 | MG | AA | 3799 | 1/1 | 0.94 | 0.12 | -0.70 | 45,45,45,45 | 0 |
| 60 | MG | DA | 1681 | 1/1 | 0.96 | 0.14 | -0.71 | 44,44,44,44 | 0 |
| 60 | MG | CA | 3208 | 1/1 | 0.94 | 0.12 | -0.71 | 24,24,24,24 | 0 |
| 60 | MG | AA | 3374 | 1/1 | 0.97 | 0.15 | -0.71 | 22,22,22,22 | 0 |
| 60 | MG | AA | 3058 | 1/1 | 0.91 | 0.12 | -0.71 | 38,38,38,38 | 0 |
| 60 | MG | BA | 1617 | 1/1 | 0.86 | 0.16 | -0.74 | 64,64,64,64 | 0 |
| 60 | MG | AA | 3355 | 1/1 | 0.97 | 0.14 | -0.83 | 19,19,19,19 | 0 |
| 60 | MG | CA | 3351 | 1/1 | 0.92 | 0.13 | -0.84 | 50,50,50,50 | 0 |
| 62 | ZN | A6 | 102 | 1/1 | 0.99 | 0.10 | -0.84 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3390 | 1/1 | 0.96 | 0.14 | -0.89 | 23,23,23,23 | 0 |
| 60 | MG | CA | 3337 | 1/1 | 0.99 | 0.13 | -0.91 | 27,27,27,27 | 0 |
| 60 | MG | DA | 1665 | 1/1 | 0.93 | 0.15 | -0.93 | 57,57,57,57 | 0 |
| 60 | MG | BA | 1717 | 1/1 | 0.92 | 0.15 | -0.94 | 77,77,77,77 | 0 |
| 60 | MG | AA | 3382 | 1/1 | 0.93 | 0.13 | -0.94 | 29,29,29,29 | 0 |
| 62 | ZN | A9 | 501 | 1/1 | 0.99 | 0.11 | -0.98 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3395 | 1/1 | 0.98 | 0.14 | -0.99 | 21,21,21,21 | 0 |
| 60 | MG | CA | 3175 | 1/1 | 0.89 | 0.14 | -1.00 | 59,59,59,59 | 0 |
| 60 | MG | CA | 3101 | 1/1 | 0.64 | 0.11 | -1.00 | 86,86,86,86 | 0 |
| 60 | MG | AA | 3202 | 1/1 | 0.85 | 0.12 | -1.02 | 46,46,46,46 | 0 |
| 64 | GDP | DZ | 702 | 28/28 | 0.96 | 0.13 | -1.09 | 69,69,69,69 | 0 |
| 60 | MG | BA | 1811 | 1/1 | 0.94 | 0.14 | -1.09 | 52,52,52,52 | 0 |
| 60 | MG | DA | 1606 | 1/1 | 0.94 | 0.17 | -1.10 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | DA | 1768 | 1/1 | 0.90 | 0.10 | -1.11 | 57,57,57,57 | 0 |
| 60 | MG | CA | 3436 | 1/1 | 0.96 | 0.15 | -1.11 | 34,34,34,34 | 0 |
| 60 | MG | CA | 3368 | 1/1 | 0.97 | 0.12 | -1.15 | 45,45,45,45 | 0 |
| 60 | MG | CA | 3459 | 1/1 | 0.82 | 0.12 | -1.22 | 46,46,46,46 | 0 |
| 60 | MG | DA | 1720 | 1/1 | 0.87 | 0.12 | -1.25 | 61,61,61,61 | 0 |
| 60 | MG | CO | 202 | 1/1 | 0.97 | 0.13 | -1.26 | 53,53,53,53 | 0 |
| 60 | MG | CA | 3559 | 1/1 | 0.96 | 0.14 | -1.26 | 30,30,30,30 | 0 |
| 60 | MG | BA | 1810 | 1/1 | 0.97 | 0.13 | -1.27 | 39,39,39,39 | 0 |
| 60 | MG | AX | 101 | 1/1 | 0.97 | 0.11 | -1.29 | 37,37,37,37 | 0 |
| 60 | MG | BX | 102 | 1/1 | 0.84 | 0.10 | -1.31 | 78,78,78,78 | 0 |
| 60 | MG | CA | 3309 | 1/1 | 0.88 | 0.11 | -1.31 | 50,50,50,50 | 0 |
| 62 | ZN | C9 | 501 | 1/1 | 0.99 | 0.07 | -1.32 | 70,70,70,70 | 0 |
| 60 | MG | AA | 3084 | 1/1 | 0.95 | 0.10 | -1.34 | 27,27,27,27 | 0 |
| 60 | MG | DA | 1622 | 1/1 | 0.91 | 0.15 | -1.36 | 43,43,43,43 | 0 |
| 60 | MG | AA | 3776 | 1/1 | 0.96 | 0.12 | -1.41 | 21,21,21,21 | 0 |
| 60 | MG | BA | 1729 | 1/1 | 0.97 | 0.13 | -1.43 | 38,38,38,38 | 0 |
| 60 | MG | CA | 3358 | 1/1 | 0.95 | 0.13 | -1.44 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3345 | 1/1 | 0.94 | 0.10 | -1.47 | 34,34,34,34 | 0 |
| 60 | MG | BA | 1619 | 1/1 | 0.90 | 0.13 | -1.50 | 54,54,54,54 | 0 |
| 60 | MG | DA | 1766 | 1/1 | 0.98 | 0.07 | -1.53 | 41,41,41,41 | 0 |
| 60 | MG | CE | 302 | 1/1 | 0.94 | 0.13 | -1.55 | 31,31,31,31 | 0 |
| 60 | MG | CA | 3054 | 1/1 | 0.89 | 0.13 | -1.56 | 50,50,50,50 | 0 |
| 60 | MG | AA | 3037 | 1/1 | 0.98 | 0.12 | -1.63 | 12,12,12,12 | 0 |
| 62 | ZN | C6 | 501 | 1/1 | 0.98 | 0.09 | -1.65 | 66,66,66,66 | 0 |
| 60 | MG | CA | 3395 | 1/1 | 0.95 | 0.12 | -1.70 | 60,60,60,60 | 0 |
| 62 | ZN | BN | 501 | 1/1 | 0.98 | 0.09 | -1.75 | 83,83,83,83 | 0 |
| 63 | SF4 | DD | 501 | 8/8 | 0.98 | 0.11 | -1.75 | 71,71,71,71 | 0 |
| 60 | MG | BA | 1753 | 1/1 | 0.96 | 0.14 | -1.75 | 48,48,48,48 | 0 |
| 60 | MG | CA | 3263 | 1/1 | 0.91 | 0.12 | -1.76 | 50,50,50,50 | 0 |
| 60 | MG | A1 | 101 | 1/1 | 0.93 | 0.10 | -1.77 | 58,58,58,58 | 0 |
| 60 | MG | BA | 1696 | 1/1 | 0.84 | 0.14 | -1.79 | 84,84,84,84 | 0 |
| 60 | MG | AA | 3375 | 1/1 | 0.96 | 0.13 | -1.82 | 16,16,16,16 | 0 |
| 60 | MG | BM | 201 | 1/1 | 0.89 | 0.06 | -1.83 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3105 | 1/1 | 0.92 | 0.12 | -1.85 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3049 | 1/1 | 0.92 | 0.14 | -1.85 | 35,35,35,35 | 0 |
| 62 | ZN | A4 | 501 | 1/1 | 0.95 | 0.08 | -1.88 | 120,120,120,120 | 0 |
| 63 | SF4 | BD | 501 | 8/8 | 0.99 | 0.11 | -1.90 | 67,67,67,67 | 0 |
| 60 | MG | AA | 3492 | 1/1 | 0.92 | 0.12 | -1.92 | 41,41,41,41 | 0 |
| 60 | MG | AA | 3391 | 1/1 | 0.96 | 0.13 | -1.95 | 27,27,27,27 | 0 |
| 62 | ZN | C4 | 501 | 1/1 | 0.95 | 0.07 | -1.95 | 163,163,163,163 | 0 |
| 60 | MG | BA | 1612 | 1/1 | 0.89 | 0.14 | -1.96 | 79,79,79,79 | 0 |
| 60 | MG | CA | 3010 | 1/1 | 0.94 | 0.13 | -1.96 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | AG | 201 | 1/1 | 0.98 | 0.05 | -2.02 | 41,41,41,41 | 0 |
| 60 | MG | CA | 3186 | 1/1 | 0.98 | 0.07 | -2.03 | 49,49,49,49 | 0 |
| 60 | MG | CB | 3004 | 1/1 | 0.94 | 0.13 | -2.04 | 70,70,70,70 | 0 |
| 60 | MG | AB | 3003 | 1/1 | 0.93 | 0.12 | -2.08 | 40,40,40,40 | 0 |
| 60 | MG | CA | 3261 | 1/1 | 0.84 | 0.12 | -2.10 | 50,50,50,50 | 0 |
| 60 | MG | CA | 3019 | 1/1 | 0.94 | 0.14 | -2.12 | 23,23,23,23 | 0 |
| 60 | MG | AA | 3613 | 1/1 | 0.91 | 0.12 | -2.15 | 96,96,96,96 | 0 |
| 60 | MG | CA | 3567 | 1/1 | 0.98 | 0.12 | -2.18 | 42,42,42,42 | 0 |
| 60 | MG | DA | 1625 | 1/1 | 0.97 | 0.12 | -2.20 | 38,38,38,38 | 0 |
| 60 | MG | AA | 3342 | 1/1 | 0.89 | 0.11 | -2.24 | 77,77,77,77 | 0 |
| 60 | MG | AG | 202 | 1/1 | 0.86 | 0.08 | -2.25 | 69,69,69,69 | 0 |
| 60 | MG | CA | 3271 | 1/1 | 0.90 | 0.12 | -2.42 | 59,59,59,59 | 0 |
| 62 | ZN | AY | 501 | 1/1 | 0.99 | 0.06 | -2.45 | 68,68,68,68 | 0 |
| 60 | MG | CA | 3520 | 1/1 | 0.92 | 0.10 | -2.46 | 27,27,27,27 | 0 |
| 60 | MG | CA | 3340 | 1/1 | 0.98 | 0.13 | -2.47 | 38,38,38,38 | 0 |
| 60 | MG | CA | 3120 | 1/1 | 0.97 | 0.12 | -2.47 | 47,47,47,47 | 0 |
| 62 | ZN | CY | 501 | 1/1 | 0.98 | 0.05 | -2.52 | 92,92,92,92 | 0 |
| 60 | MG | AA | 3007 | 1/1 | 0.98 | 0.10 | -2.55 | 18,18,18,18 | 0 |
| 60 | MG | AA | 3734 | 1/1 | 0.96 | 0.12 | -2.56 | 23,23,23,23 | 0 |
| 60 | MG | CA | 3370 | 1/1 | 0.99 | 0.13 | -2.59 | 31,31,31,31 | 0 |
| 60 | MG | CA | 3240 | 1/1 | 0.83 | 0.14 | -2.65 | 49,49,49,49 | 0 |
| 62 | ZN | C5 | 102 | 1/1 | 0.99 | 0.07 | -2.74 | 66,66,66,66 | 0 |
| 60 | MG | AF | 302 | 1/1 | 0.95 | 0.09 | -2.80 | 42,42,42,42 | 0 |
| 62 | ZN | DN | 501 | 1/1 | 0.97 | 0.07 | -2.82 | 120,120,120,120 | 0 |
| 60 | MG | AA | 3009 | 1/1 | 0.96 | 0.09 | -2.85 | 26,26,26,26 | 0 |
| 60 | MG | AA | 3754 | 1/1 | 0.96 | 0.09 | -2.95 | 25,25,25,25 | 0 |
| 60 | MG | AB | 3020 | 1/1 | 0.93 | 0.09 | -2.95 | 66,66,66,66 | 0 |
| 60 | MG | AB | 3007 | 1/1 | 0.98 | 0.07 | -2.97 | 37,37,37,37 | 0 |
| 60 | MG | BA | 1616 | 1/1 | 0.95 | 0.11 | -3.05 | 69,69,69,69 | 0 |
| 60 | MG | CA | 3523 | 1/1 | 0.89 | 0.09 | -3.12 | 77,77,77,77 | 0 |
| 60 | MG | BX | 105 | 1/1 | 0.85 | 0.09 | -3.14 | 87,87,87,87 | 0 |
| 60 | MG | CA | 3189 | 1/1 | 0.96 | 0.07 | -3.16 | 40,40,40,40 | 0 |
| 60 | MG | BA | 1654 | 1/1 | 0.95 | 0.12 | -3.21 | 45,45,45,45 | 0 |
| 60 | MG | CA | 3602 | 1/1 | 0.93 | 0.07 | -3.21 | 49,49,49,49 | 0 |
| 60 | MG | BA | 1607 | 1/1 | 0.86 | 0.11 | -3.27 | 64,64,64,64 | 0 |
| 60 | MG | AA | 3623 | 1/1 | 0.93 | 0.10 | -3.30 | 58,58,58,58 | 0 |
| 60 | MG | CA | 3174 | 1/1 | 0.98 | 0.12 | -3.30 | 31,31,31,31 | 0 |
| 60 | MG | CA | 3047 | 1/1 | 0.96 | 0.06 | -3.37 | 54,54,54,54 | 0 |
| 60 | MG | AA | 3542 | 1/1 | 0.87 | 0.10 | -3.38 | 47,47,47,47 | 0 |
| 60 | MG | AA | 3306 | 1/1 | 0.98 | 0.15 | -3.47 | 3,3,3,3 | 0 |
| 60 | MG | AA | 3069 | 1/1 | 0.91 | 0.08 | -3.52 | 32,32,32,32 | 0 |
| 60 | MG | BA | 1734 | 1/1 | 0.97 | 0.13 | -3.53 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 60 | MG | AA | 3079 | 1/1 | 0.90 | 0.10 | -3.59 | 27,27,27,27 | 0 |
| 60 | MG | AA | 3750 | 1/1 | 0.99 | 0.10 | -3.73 | 26,26,26,26 | 0 |
| 60 | MG | AA | 3099 | 1/1 | 0.92 | 0.08 | -3.78 | 48,48,48,48 | 0 |
| 60 | MG | AA | 3616 | 1/1 | 0.98 | 0.10 | -3.78 | 33,33,33,33 | 0 |
| 60 | MG | BA | 1685 | 1/1 | 0.93 | 0.11 | -3.79 | 41,41,41,41 | 0 |
| 60 | MG | BA | 1736 | 1/1 | 0.92 | 0.10 | -3.83 | 66,66,66,66 | 0 |
| 60 | MG | AA | 3410 | 1/1 | 0.98 | 0.13 | -3.85 | 19,19,19,19 | 0 |
| 60 | MG | AA | 3571 | 1/1 | 0.72 | 0.11 | -3.86 | 53,53,53,53 | 0 |
| 60 | MG | AA | 3446 | 1/1 | 0.93 | 0.11 | -3.91 | 25,25,25,25 | 0 |
| 60 | MG | AA | 3583 | 1/1 | 0.98 | 0.12 | -3.94 | 18,18,18,18 | 0 |
| 60 | MG | AB | 3017 | 1/1 | 0.95 | 0.07 | -3.97 | 76,76,76,76 | 0 |
| 60 | MG | DA | 1653 | 1/1 | 0.97 | 0.08 | -4.09 | 29,29,29,29 | 0 |
| 60 | MG | CA | 3289 | 1/1 | 0.96 | 0.13 | -4.12 | 23,23,23,23 | 0 |
| 60 | MG | CA | 3461 | 1/1 | 0.98 | 0.10 | -4.17 | 46,46,46,46 | 0 |
| 60 | MG | AA | 3683 | 1/1 | 0.91 | 0.10 | -4.28 | 40,40,40,40 | 0 |
| 60 | MG | AA | 3668 | 1/1 | 0.97 | 0.10 | -4.30 | 25,25,25,25 | 0 |
| 60 | MG | CA | 3135 | 1/1 | 0.88 | 0.11 | -4.30 | 73,73,73,73 | 0 |
| 60 | MG | CA | 3626 | 1/1 | 0.90 | 0.09 | -4.46 | 52,52,52,52 | 0 |
| 60 | MG | AA | 3308 | 1/1 | 0.95 | 0.11 | -4.65 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3774 | 1/1 | 0.96 | 0.10 | -4.66 | 44,44,44,44 | 0 |
| 60 | MG | BA | 1680 | 1/1 | 0.94 | 0.08 | -4.73 | 50,50,50,50 | 0 |
| 60 | MG | BA | 1620 | 1/1 | 0.92 | 0.09 | -4.74 | 60,60,60,60 | 0 |
| 60 | MG | CA | 3062 | 1/1 | 0.90 | 0.09 | -5.04 | 41,41,41,41 | 0 |
| 60 | MG | BA | 1674 | 1/1 | 0.68 | 0.08 | -5.07 | 78,78,78,78 | 0 |
| 60 | MG | AA | 3236 | 1/1 | 0.88 | 0.10 | -5.13 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3381 | 1/1 | 0.89 | 0.12 | -5.14 | 34,34,34,34 | 0 |
| 60 | MG | AA | 3619 | 1/1 | 0.92 | 0.12 | -5.18 | 39,39,39,39 | 0 |
| 60 | MG | AA | 3497 | 1/1 | 0.92 | 0.10 | -5.31 | 36,36,36,36 | 0 |
| 60 | MG | CA | 3012 | 1/1 | 0.93 | 0.09 | -5.32 | 41,41,41,41 | 0 |
| 60 | MG | DA | 1618 | 1/1 | 0.88 | 0.08 | -5.38 | 51,51,51,51 | 0 |
| 60 | MG | CA | 3574 | 1/1 | 0.94 | 0.11 | -5.48 | 31,31,31,31 | 0 |
| 60 | MG | CA | 3525 | 1/1 | 0.92 | 0.07 | -5.49 | 30,30,30,30 | 0 |
| 60 | MG | AA | 3214 | 1/1 | 0.94 | 0.08 | -5.80 | 47,47,47,47 | 0 |
| 60 | MG | CA | 3272 | 1/1 | 0.94 | 0.05 | -6.22 | 56,56,56,56 | 0 |
| 60 | MG | BA | 1643 | 1/1 | 0.91 | 0.09 | -6.35 | 56,56,56,56 | 0 |
| 60 | MG | BA | 1742 | 1/1 | 0.96 | 0.09 | -6.45 | 45,45,45,45 | 0 |
| 60 | MG | AA | 3340 | 1/1 | 0.99 | 0.10 | -6.50 | 3,3,3,3 | 0 |
| 60 | MG | CA | 3577 | 1/1 | 0.96 | 0.12 | -6.86 | 52,52,52,52 | 0 |
| 60 | MG | CA | 3362 | 1/1 | 0.95 | 0.11 | -7.14 | 20,20,20,20 | 0 |
| 60 | MG | AA | 3400 | 1/1 | 0.97 | 0.07 | -7.23 | 19,19,19,19 | 0 |
| 60 | MG | AA | 3072 | 1/1 | 0.92 | 0.08 | -7.39 | 20,20,20,20 | 0 |
| 60 | MG | AA | 3371 | 1/1 | 0.98 | 0.07 | -7.44 | 21,21,21,21 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 60 | MG | CA | 3027 | 1/1 | 0.98 | 0.05 | -7.88 | 29,29,29,29 | 0 |
| 60 | MG | AA | 3547 | 1/1 | 0.93 | 0.06 | -8.12 | 50,50,50,50 | 0 |
| 60 | MG | CA | 3009 | 1/1 | 0.95 | 0.05 | -8.50 | 24,24,24,24 | 0 |
| 60 | MG | BA | 1792 | 1/1 | 0.92 | 0.07 | -8.55 | 61,61,61,61 | 0 |
| 60 | MG | AA | 3011 | 1/1 | 0.97 | 0.10 | -9.47 | 27,27,27,27 | 0 |
| 60 | MG | BA | 1611 | 1/1 | 0.97 | 0.09 | -10.17 | 31,31,31,31 | 0 |
| 60 | MG | AA | 3022 | 1/1 | 0.96 | 0.09 | -12.93 | 19,19,19,19 | 0 |
| 60 | MG | BA | 1613 | 1/1 | 0.88 | 0.07 | -13.74 | 92,92,92,92 | 0 |
| 60 | MG | CA | 3319 | 1/1 | 0.95 | 0.07 | -15.86 | 32,32,32,32 | 0 |
| 60 | MG | CA | 3479 | 1/1 | 0.95 | 0.16 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3199 | 1/1 | 0.88 | 0.22 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3169 | 1/1 | 0.97 | 0.26 | - | 36,36,36,36 | 0 |
| 60 | MG | BA | 1739 | 1/1 | 0.88 | 0.18 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3061 | 1/1 | 0.95 | 0.15 | - | 36,36,36,36 | 0 |
| 60 | MG | AA | 3356 | 1/1 | 0.94 | 0.12 | - | 51,51,51,51 | 0 |
| 60 | MG | AA | 3146 | 1/1 | 0.79 | 0.20 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3585 | 1/1 | 0.96 | 0.11 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3597 | 1/1 | 0.97 | 0.12 | - | 58,58,58,58 | 0 |
| 60 | MG | BA | 1660 | 1/1 | 0.92 | 0.32 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3080 | 1/1 | 0.79 | 0.58 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3325 | 1/1 | 0.92 | 0.11 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3232 | 1/1 | 0.97 | 0.22 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3481 | 1/1 | 0.90 | 0.06 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3111 | 1/1 | 0.87 | 0.31 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3112 | 1/1 | 0.82 | 0.47 | - | 76,76,76,76 | 0 |
| 60 | MG | CA | 3136 | 1/1 | 0.89 | 0.20 | - | 112,112,112,112 | 0 |
| 60 | MG | AA | 3068 | 1/1 | 0.93 | 0.34 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3422 | 1/1 | 0.96 | 0.19 | - | 22,22,22,22 | 0 |
| 60 | MG | CA | 3624 | 1/1 | 0.94 | 0.22 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3459 | 1/1 | 0.95 | 0.47 | - | 65,65,65,65 | 0 |
| 60 | MG | DD | 502 | 1/1 | 0.82 | 0.50 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3442 | 1/1 | 0.84 | 0.13 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3522 | 1/1 | 0.96 | 0.16 | - | 31,31,31,31 | 0 |
| 60 | MG | CA | 3089 | 1/1 | 0.69 | 0.71 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3468 | 1/1 | 0.95 | 0.12 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3488 | 1/1 | 0.90 | 0.09 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3531 | 1/1 | 0.93 | 0.15 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3675 | 1/1 | 0.94 | 0.16 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3059 | 1/1 | 0.73 | 0.38 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3447 | 1/1 | 0.87 | 0.19 | - | 44,44,44,44 | 0 |
| 60 | MG | CA | 3033 | 1/1 | 0.89 | 0.12 | - | 47,47,47,47 | 0 |
| 60 | MG | AA | 3618 | 1/1 | 0.91 | 0.13 | - | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3497 | 1/1 | 0.86 | 0.18 | - | 85,85,85,85 | 0 |
| 60 | MG | CA | 3338 | 1/1 | 0.86 | 0.15 | - | 58,58,58,58 | 0 |
| 60 | MG | CB | 3010 | 1/1 | 0.80 | 0.16 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3365 | 1/1 | 0.93 | 0.40 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3713 | 1/1 | 0.75 | 0.52 | - | 48,48,48,48 | 0 |
| 60 | MG | A8 | 5001 | 1/1 | 0.88 | 0.31 | - | 66,66,66,66 | 0 |
| 60 | MG | BA | 1714 | 1/1 | 0.99 | 0.16 | - | 44,44,44,44 | 0 |
| 60 | MG | DA | 1735 | 1/1 | 0.78 | 0.10 | - | 75,75,75,75 | 0 |
| 60 | MG | DX | 3001 | 1/1 | 0.59 | 0.41 | - | 75,75,75,75 | 0 |
| 60 | MG | DA | 1691 | 1/1 | 0.90 | 0.18 | - | 66,66,66,66 | 0 |
| 60 | MG | DA | 1628 | 1/1 | 0.87 | 0.20 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3219 | 1/1 | 0.93 | 0.22 | - | 38,38,38,38 | 0 |
| 60 | MG | CA | 3648 | 1/1 | 0.88 | 0.60 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3302 | 1/1 | 0.89 | 0.11 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3153 | 1/1 | 0.89 | 0.31 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3245 | 1/1 | 0.71 | 0.30 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3043 | 1/1 | 0.81 | 0.19 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3231 | 1/1 | 0.94 | 0.26 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3190 | 1/1 | 0.92 | 0.30 | - | 77,77,77,77 | 0 |
| 60 | MG | AA | 3242 | 1/1 | 0.62 | 0.20 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3633 | 1/1 | 0.79 | 0.19 | - | 85,85,85,85 | 0 |
| 60 | MG | CA | 3334 | 1/1 | 0.92 | 0.09 | - | 56,56,56,56 | 0 |
| 60 | MG | DA | 1709 | 1/1 | 0.96 | 0.22 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3075 | 1/1 | 0.86 | 0.15 | - | 51,51,51,51 | 0 |
| 60 | MG | AB | 3006 | 1/1 | 0.86 | 0.21 | - | 84,84,84,84 | 0 |
| 60 | MG | AA | 3189 | 1/1 | 0.97 | 0.26 | - | 31,31,31,31 | 0 |
| 60 | MG | BA | 1625 | 1/1 | 0.90 | 0.24 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3764 | 1/1 | 0.84 | 0.37 | - | 48,48,48,48 | 0 |
| 60 | MG | CA | 3530 | 1/1 | 0.89 | 0.15 | - | 68,68,68,68 | 0 |
| 60 | MG | C8 | 5001 | 1/1 | 0.94 | 0.29 | - | 43,43,43,43 | 0 |
| 60 | MG | AA | 3720 | 1/1 | 0.94 | 0.35 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3191 | 1/1 | 0.89 | 0.29 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3473 | 1/1 | 0.88 | 0.14 | - | 57,57,57,57 | 0 |
| 60 | MG | CN | 5001 | 1/1 | 0.98 | 0.10 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3618 | 1/1 | 0.95 | 0.21 | - | 79,79,79,79 | 0 |
| 60 | MG | BA | 1735 | 1/1 | 0.93 | 0.14 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3738 | 1/1 | 0.87 | 0.14 | - | 73,73,73,73 | 0 |
| 60 | MG | CA | 3515 | 1/1 | 0.91 | 0.11 | - | 72,72,72,72 | 0 |
| 60 | MG | DA | 1658 | 1/1 | 0.86 | 0.13 | - | 89,89,89,89 | 0 |
| 60 | MG | AA | 3661 | 1/1 | 0.85 | 0.17 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3667 | 1/1 | 0.91 | 0.14 | - | 45,45,45,45 | 0 |
| 60 | MG | AB | 3001 | 1/1 | 0.88 | 0.18 | - | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3251 | 1/1 | 0.97 | 0.15 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3081 | 1/1 | 0.85 | 0.40 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3329 | 1/1 | 0.88 | 0.23 | - | 82,82,82,82 | 0 |
| 60 | MG | CA | 3587 | 1/1 | 0.88 | 0.14 | - | 72,72,72,72 | 0 |
| 60 | MG | DA | 1705 | 1/1 | 0.91 | 0.17 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3348 | 1/1 | 0.69 | 0.15 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3531 | 1/1 | 0.93 | 0.13 | - | 67,67,67,67 | 0 |
| 60 | MG | BA | 1691 | 1/1 | 0.67 | 0.34 | - | 98,98,98,98 | 0 |
| 60 | MG | AA | 3107 | 1/1 | 0.88 | 0.17 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3550 | 1/1 | 0.39 | 0.36 | - | 88,88,88,88 | 0 |
| 60 | MG | AA | 3320 | 1/1 | 0.94 | 0.24 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3203 | 1/1 | 0.94 | 0.32 | - | 45,45,45,45 | 0 |
| 60 | MG | CA | 3085 | 1/1 | 0.62 | 0.53 | - | 82,82,82,82 | 0 |
| 60 | MG | CA | 3256 | 1/1 | 0.96 | 0.29 | - | 73,73,73,73 | 0 |
| 60 | MG | CA | 3572 | 1/1 | 0.92 | 0.22 | - | 82,82,82,82 | 0 |
| 60 | MG | AB | 3021 | 1/1 | 0.85 | 0.14 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3802 | 1/1 | 0.88 | 0.27 | - | 55,55,55,55 | 0 |
| 60 | MG | BA | 1755 | 1/1 | 0.83 | 0.18 | - | 92,92,92,92 | 0 |
| 60 | MG | AA | 3123 | 1/1 | 0.93 | 0.48 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3246 | 1/1 | 0.91 | 0.28 | - | 79,79,79,79 | 0 |
| 60 | MG | DA | 1702 | 1/1 | 0.78 | 0.27 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3746 | 1/1 | 0.93 | 0.43 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3798 | 1/1 | 0.92 | 0.10 | - | 34,34,34,34 | 0 |
| 60 | MG | CA | 3126 | 1/1 | 0.91 | 0.54 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3758 | 1/1 | 0.81 | 0.35 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3601 | 1/1 | 0.93 | 0.28 | - | 44,44,44,44 | 0 |
| 60 | MG | BF | 3001 | 1/1 | 0.91 | 0.15 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3243 | 1/1 | 0.83 | 0.29 | - | 79,79,79,79 | 0 |
| 60 | MG | AA | 3025 | 1/1 | 0.86 | 0.44 | - | 60,60,60,60 | 0 |
| 60 | MG | CA | 3571 | 1/1 | 0.93 | 0.15 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3485 | 1/1 | 0.98 | 0.17 | - | 34,34,34,34 | 0 |
| 60 | MG | CA | 3560 | 1/1 | 0.83 | 0.16 | - | 103,103,103,103 | 0 |
| 60 | MG | CA | 3508 | 1/1 | 0.94 | 0.14 | - | 74,74,74,74 | 0 |
| 60 | MG | CD | 302 | 1/1 | 0.89 | 0.43 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3130 | 1/1 | 0.96 | 0.17 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3588 | 1/1 | 0.57 | 0.19 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3261 | 1/1 | 0.92 | 0.27 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3679 | 1/1 | 0.91 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | CB | 3013 | 1/1 | 0.90 | 0.12 | - | 90,90,90,90 | 0 |
| 60 | MG | AA | 3140 | 1/1 | 0.87 | 0.90 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3079 | 1/1 | 0.52 | 0.57 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3815 | 1/1 | 0.95 | 0.46 | - | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3502 | 1/1 | 0.96 | 0.09 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3783 | 1/1 | 0.71 | 0.39 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3727 | 1/1 | 0.86 | 0.16 | - | 64,64,64,64 | 0 |
| 60 | MG | DA | 1675 | 1/1 | 0.91 | 0.13 | - | 61,61,61,61 | 0 |
| 60 | MG | BA | 1628 | 1/1 | 0.91 | 0.30 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3090 | 1/1 | 0.60 | 0.46 | - | 98,98,98,98 | 0 |
| 60 | MG | CA | 3332 | 1/1 | 0.97 | 0.24 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3145 | 1/1 | 0.94 | 0.33 | - | 65,65,65,65 | 0 |
| 60 | MG | DA | 1684 | 1/1 | 0.93 | 0.29 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3118 | 1/1 | 0.93 | 0.11 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3278 | 1/1 | 0.92 | 0.24 | - | 38,38,38,38 | 0 |
| 60 | MG | CA | 3467 | 1/1 | 0.78 | 0.45 | - | 99,99,99,99 | 0 |
| 60 | MG | AA | 3570 | 1/1 | 0.93 | 0.14 | - | 22,22,22,22 | 0 |
| 60 | MG | CA | 3663 | 1/1 | 0.88 | 0.26 | - | 74,74,74,74 | 0 |
| 60 | MG | BA | 1799 | 1/1 | 0.88 | 0.07 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3659 | 1/1 | 0.92 | 0.10 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3195 | 1/1 | 0.74 | 0.18 | - | 36,36,36,36 | 0 |
| 60 | MG | AA | 3425 | 1/1 | 0.86 | 0.17 | - | 40,40,40,40 | 0 |
| 60 | MG | BA | 1621 | 1/1 | 0.78 | 0.66 | - | 78,78,78,78 | 0 |
| 60 | MG | DA | 1680 | 1/1 | 0.95 | 0.17 | - | 40,40,40,40 | 0 |
| 60 | MG | DA | 1728 | 1/1 | 0.96 | 0.09 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3609 | 1/1 | 0.95 | 0.21 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3017 | 1/1 | 0.87 | 0.11 | - | 71,71,71,71 | 0 |
| 60 | MG | CY | 502 | 1/1 | 0.97 | 0.14 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3074 | 1/1 | 0.96 | 0.37 | - | 26,26,26,26 | 0 |
| 60 | MG | AA | 3279 | 1/1 | 0.82 | 0.55 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3676 | 1/1 | 0.95 | 0.17 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3428 | 1/1 | 0.93 | 0.14 | - | 36,36,36,36 | 0 |
| 60 | MG | CA | 3643 | 1/1 | 0.88 | 0.33 | - | 83,83,83,83 | 0 |
| 60 | MG | AA | 3321 | 1/1 | 0.81 | 0.08 | - | 45,45,45,45 | 0 |
| 60 | MG | AA | 3373 | 1/1 | 0.95 | 0.22 | - | 23,23,23,23 | 0 |
| 60 | MG | CA | 3582 | 1/1 | 0.93 | 0.15 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3681 | 1/1 | 0.93 | 0.21 | - | 52,52,52,52 | 0 |
| 60 | MG | CQ | 204 | 1/1 | 0.93 | 0.28 | - | 74,74,74,74 | 0 |
| 60 | MG | DA | 1727 | 1/1 | 0.95 | 0.17 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3646 | 1/1 | 0.87 | 0.28 | - | 82,82,82,82 | 0 |
| 60 | MG | BA | 1709 | 1/1 | 0.59 | 0.27 | - | 96,96,96,96 | 0 |
| 60 | MG | AA | 3080 | 1/1 | 0.89 | 0.36 | - | 54,54,54,54 | 0 |
| 60 | MG | DA | 1643 | 1/1 | 0.98 | 0.14 | - | 51,51,51,51 | 0 |
| 60 | MG | AA | 3448 | 1/1 | 0.93 | 0.27 | - | 74,74,74,74 | 0 |
| 60 | MG | DA | 1614 | 1/1 | 0.82 | 0.15 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3097 | 1/1 | 0.99 | 0.26 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3354 | 1/1 | 0.94 | 0.18 | - | 40,40,40,40 | 0 |
| 60 | MG | AA | 3487 | 1/1 | 0.76 | 0.10 | - | 66,66,66,66 | 0 |
| 60 | MG | DA | 1672 | 1/1 | 0.90 | 0.16 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3050 | 1/1 | 0.91 | 0.65 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3485 | 1/1 | 0.87 | 0.24 | - | 76,76,76,76 | 0 |
| 60 | MG | CA | 3242 | 1/1 | 0.89 | 0.33 | - | 48,48,48,48 | 0 |
| 60 | MG | DA | 1753 | 1/1 | 0.61 | 0.26 | - | 85,85,85,85 | 0 |
| 60 | MG | AA | 3731 | 1/1 | 0.98 | 0.14 | - | 34,34,34,34 | 0 |
| 60 | MG | BA | 1704 | 1/1 | 0.95 | 0.26 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3172 | 1/1 | 0.96 | 0.17 | - | 41,41,41,41 | 0 |
| 60 | MG | DA | 1612 | 1/1 | 0.98 | 0.13 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3087 | 1/1 | 0.88 | 0.31 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3605 | 1/1 | 0.95 | 0.19 | - | 72,72,72,72 | 0 |
| 60 | MG | AA | 3106 | 1/1 | 0.85 | 0.19 | - | 43,43,43,43 | 0 |
| 60 | MG | CA | 3622 | 1/1 | 0.64 | 0.17 | - | 106,106,106,106 | 0 |
| 60 | MG | AA | 3245 | 1/1 | 0.75 | 0.22 | - | 79,79,79,79 | 0 |
| 60 | MG | AA | 3538 | 1/1 | 0.82 | 0.20 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3595 | 1/1 | 0.86 | 0.18 | - | 60,60,60,60 | 0 |
| 60 | MG | DA | 1692 | 1/1 | 0.94 | 0.26 | - | 49,49,49,49 | 0 |
| 60 | MG | CA | 3171 | 1/1 | 0.97 | 0.43 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3268 | 1/1 | 0.87 | 0.23 | - | 80,80,80,80 | 0 |
| 60 | MG | AW | 3002 | 1/1 | 0.89 | 0.19 | - | 59,59,59,59 | 0 |
| 60 | MG | DA | 1722 | 1/1 | 0.87 | 0.19 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3282 | 1/1 | 0.96 | 0.39 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3441 | 1/1 | 0.93 | 0.16 | - | 37,37,37,37 | 0 |
| 60 | MG | CA | 3132 | 1/1 | 0.83 | 0.19 | - | 67,67,67,67 | 0 |
| 60 | MG | DA | 1738 | 1/1 | 0.85 | 0.25 | - | 100,100,100,100 | 0 |
| 60 | MG | AN | 3003 | 1/1 | 0.89 | 0.07 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3065 | 1/1 | 0.90 | 0.15 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3339 | 1/1 | 0.93 | 0.33 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3545 | 1/1 | 0.84 | 0.11 | - | 93,93,93,93 | 0 |
| 60 | MG | CA | 3158 | 1/1 | 0.99 | 0.33 | - | 54,54,54,54 | 0 |
| 60 | MG | BA | 1768 | 1/1 | 0.97 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3384 | 1/1 | 0.87 | 0.20 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3379 | 1/1 | 0.88 | 0.22 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3036 | 1/1 | 0.89 | 0.26 | - | 65,65,65,65 | 0 |
| 60 | MG | BE | 3001 | 1/1 | 0.97 | 0.08 | - | 83,83,83,83 | 0 |
| 60 | MG | A1 | 102 | 1/1 | 0.95 | 0.16 | - | 46,46,46,46 | 0 |
| 60 | MG | CA | 3470 | 1/1 | 0.91 | 0.11 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3360 | 1/1 | 0.89 | 0.44 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3493 | 1/1 | 0.94 | 0.22 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3553 | 1/1 | 0.97 | 0.14 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3475 | 1/1 | 0.94 | 0.15 | - | 73,73,73,73 | 0 |
| 60 | MG | DA | 1682 | 1/1 | 0.94 | 0.30 | - | 60,60,60,60 | 0 |
| 60 | MG | BA | 1786 | 1/1 | 0.78 | 0.33 | - | 79,79,79,79 | 0 |
| 60 | MG | AA | 3318 | 1/1 | 0.97 | 0.16 | - | 64,64,64,64 | 0 |
| 60 | MG | DA | 1613 | 1/1 | 0.90 | 0.25 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3469 | 1/1 | 0.95 | 0.20 | - | 37,37,37,37 | 0 |
| 60 | MG | CA | 3021 | 1/1 | 0.86 | 0.33 | - | 91,91,91,91 | 0 |
| 60 | MG | BA | 1746 | 1/1 | 0.96 | 0.16 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3552 | 1/1 | 0.93 | 0.14 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3633 | 1/1 | 0.96 | 0.25 | - | 51,51,51,51 | 0 |
| 60 | MG | DA | 1708 | 1/1 | 0.97 | 0.10 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3780 | 1/1 | 0.87 | 0.35 | - | 51,51,51,51 | 1 |
| 60 | MG | CA | 3453 | 1/1 | 0.93 | 0.08 | - | 43,43,43,43 | 0 |
| 60 | MG | AA | 3733 | 1/1 | 0.97 | 0.13 | - | 40,40,40,40 | 0 |
| 60 | MG | CA | 3092 | 1/1 | 0.66 | 0.49 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3760 | 1/1 | 0.95 | 0.34 | - | 50,50,50,50 | 0 |
| 60 | MG | AQ | 3003 | 1/1 | 0.98 | 0.34 | - | 37,37,37,37 | 0 |
| 60 | MG | BA | 1805 | 1/1 | 0.95 | 0.10 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3611 | 1/1 | 0.89 | 0.30 | - | 64,64,64,64 | 0 |
| 60 | MG | DA | 1695 | 1/1 | 0.87 | 0.18 | - | 79,79,79,79 | 0 |
| 60 | MG | DA | 1689 | 1/1 | 0.91 | 0.24 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3612 | 1/1 | 0.84 | 0.20 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3650 | 1/1 | 0.83 | 0.29 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3491 | 1/1 | 0.27 | 0.61 | - | 99,99,99,99 | 0 |
| 60 | MG | AB | 3023 | 1/1 | 0.92 | 0.26 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3401 | 1/1 | 0.86 | 0.07 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3725 | 1/1 | 0.62 | 0.27 | - | 42,42,42,42 | 0 |
| 60 | MG | CA | 3088 | 1/1 | 0.90 | 0.43 | - | 85,85,85,85 | 0 |
| 60 | MG | AA | 3794 | 1/1 | 0.91 | 0.20 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3394 | 1/1 | 0.86 | 0.26 | - | 54,54,54,54 | 0 |
| 60 | MG | AD | 307 | 1/1 | 0.74 | 0.20 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3041 | 1/1 | 0.88 | 0.47 | - | 67,67,67,67 | 0 |
| 60 | MG | DA | 1656 | 1/1 | 0.95 | 0.07 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3143 | 1/1 | 0.96 | 0.05 | - | 37,37,37,37 | 0 |
| 60 | MG | CA | 3094 | 1/1 | 0.76 | 0.35 | - | 92,92,92,92 | 0 |
| 60 | MG | BA | 1783 | 1/1 | 0.94 | 0.15 | - | 61,61,61,61 | 0 |
| 60 | MG | DA | 1729 | 1/1 | 0.86 | 0.10 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3685 | 1/1 | 0.96 | 0.15 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3673 | 1/1 | 0.97 | 0.24 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3342 | 1/1 | 0.92 | 0.17 | - | 84,84,84,84 | 0 |
| 60 | MG | CA | 3489 | 1/1 | 0.93 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3386 | 1/1 | 0.86 | 0.14 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3014 | 1/1 | 0.96 | 0.14 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3046 | 1/1 | 0.91 | 0.36 | - | 47,47,47,47 | 0 |
| 60 | MG | AA | 3249 | 1/1 | 0.71 | 0.45 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1807 | 1/1 | 0.89 | 0.21 | - | 72,72,72,72 | 0 |
| 60 | MG | AA | 3409 | 1/1 | 0.97 | 0.19 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3555 | 1/1 | 0.81 | 0.08 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3812 | 1/1 | 0.90 | 0.20 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3301 | 1/1 | 0.94 | 0.43 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3404 | 1/1 | 0.90 | 0.11 | - | 46,46,46,46 | 0 |
| 60 | MG | CA | 3107 | 1/1 | 0.95 | 0.11 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3188 | 1/1 | 0.96 | 0.16 | - | 15,15,15,15 | 0 |
| 60 | MG | BA | 1681 | 1/1 | 0.87 | 0.65 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3285 | 1/1 | 0.97 | 0.07 | - | 41,41,41,41 | 0 |
| 60 | MG | BA | 1706 | 1/1 | 0.65 | 0.25 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3057 | 1/1 | 0.96 | 0.29 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3607 | 1/1 | 0.95 | 0.15 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3207 | 1/1 | 0.94 | 0.34 | - | 67,67,67,67 | 0 |
| 60 | MG | BA | 1737 | 1/1 | 0.72 | 0.28 | - | 87,87,87,87 | 0 |
| 60 | MG | AA | 3394 | 1/1 | 0.91 | 0.13 | - | 22,22,22,22 | 0 |
| 60 | MG | AA | 3349 | 1/1 | 0.94 | 0.13 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3230 | 1/1 | 0.83 | 0.34 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3290 | 1/1 | 0.94 | 0.15 | - | 61,61,61,61 | 0 |
| 60 | MG | AV | 201 | 1/1 | 0.97 | 0.27 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3358 | 1/1 | 0.96 | 0.06 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3503 | 1/1 | 0.85 | 0.09 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3023 | 1/1 | 0.92 | 0.20 | - | 56,56,56,56 | 0 |
| 60 | MG | DA | 1629 | 1/1 | 0.90 | 0.80 | - | 79,79,79,79 | 0 |
| 60 | MG | DA | 1627 | 1/1 | 0.95 | 0.36 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3458 | 1/1 | 0.92 | 0.20 | - | 79,79,79,79 | 0 |
| 60 | MG | CA | 3573 | 1/1 | 0.85 | 0.12 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3299 | 1/1 | 0.82 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1798 | 1/1 | 0.92 | 0.38 | - | 62,62,62,62 | 0 |
| 60 | MG | AB | 3018 | 1/1 | 0.85 | 0.14 | - | 76,76,76,76 | 0 |
| 60 | MG | CA | 3658 | 1/1 | 0.88 | 0.19 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3194 | 1/1 | 0.88 | 0.35 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3449 | 1/1 | 0.95 | 0.20 | - | 46,46,46,46 | 0 |
| 60 | MG | CA | 3104 | 1/1 | 0.93 | 0.15 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3709 | 1/1 | 0.99 | 0.47 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3465 | 1/1 | 0.99 | 0.05 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3024 | 1/1 | 0.86 | 0.13 | - | 60,60,60,60 | 0 |
| 60 | MG | BA | 1793 | 1/1 | 0.88 | 0.10 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3331 | 1/1 | 0.96 | 0.47 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3687 | 1/1 | 0.91 | 0.11 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3660 | 1/1 | 0.98 | 0.34 | - | 58,58,58,58 | 0 |
| 60 | MG | AB | 3011 | 1/1 | 0.88 | 0.17 | - | 47,47,47,47 | 0 |
| 60 | MG | BA | 1682 | 1/1 | 0.93 | 0.11 | - | 71,71,71,71 | 0 |
| 60 | MG | DA | 1659 | 1/1 | 0.94 | 0.35 | - | 79,79,79,79 | 0 |
| 60 | MG | BA | 1651 | 1/1 | 0.94 | 0.12 | - | 69,69,69,69 | 0 |
| 60 | MG | DA | 1761 | 1/1 | 0.86 | 0.08 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3526 | 1/1 | 0.67 | 0.13 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3130 | 1/1 | 0.87 | 0.33 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3678 | 1/1 | 0.87 | 0.13 | - | 62,62,62,62 | 0 |
| 60 | MG | CB | 3005 | 1/1 | 0.94 | 0.23 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3628 | 1/1 | 0.81 | 0.11 | - | 76,76,76,76 | 0 |
| 60 | MG | CA | 3569 | 1/1 | 0.88 | 0.16 | - | 71,71,71,71 | 0 |
| 60 | MG | CA | 3260 | 1/1 | 0.91 | 0.13 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3149 | 1/1 | 0.92 | 0.22 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3512 | 1/1 | 0.91 | 0.13 | - | 32,32,32,32 | 0 |
| 60 | MG | CA | 3552 | 1/1 | 0.87 | 0.09 | - | 60,60,60,60 | 0 |
| 60 | MG | CA | 3419 | 1/1 | 0.93 | 0.18 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3069 | 1/1 | 0.84 | 0.28 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3360 | 1/1 | 0.94 | 0.17 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3447 | 1/1 | 0.96 | 0.12 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3695 | 1/1 | 0.94 | 0.29 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3059 | 1/1 | 0.73 | 0.52 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3389 | 1/1 | 0.91 | 0.09 | - | 55,55,55,55 | 0 |
| 60 | MG | DA | 1617 | 1/1 | 0.88 | 0.18 | - | 47,47,47,47 | 0 |
| 60 | MG | BA | 1609 | 1/1 | 0.85 | 0.20 | - | 77,77,77,77 | 0 |
| 60 | MG | BA | 1647 | 1/1 | 0.91 | 0.09 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3443 | 1/1 | 0.96 | 0.31 | - | 40,40,40,40 | 0 |
| 60 | MG | AA | 3132 | 1/1 | 0.86 | 0.45 | - | 43,43,43,43 | 0 |
| 60 | MG | CA | 3270 | 1/1 | 0.96 | 0.33 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3111 | 1/1 | 0.64 | 0.20 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3205 | 1/1 | 0.96 | 0.31 | - | 45,45,45,45 | 0 |
| 60 | MG | BA | 1645 | 1/1 | 0.88 | 0.76 | - | 58,58,58,58 | 0 |
| 60 | MG | DA | 1609 | 1/1 | 0.86 | 0.18 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3290 | 1/1 | 0.97 | 0.16 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3367 | 1/1 | 0.95 | 0.11 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3353 | 1/1 | 0.93 | 0.13 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3773 | 1/1 | 0.71 | 0.20 | - | 77,77,77,77 | 0 |
| 60 | MG | AA | 3789 | 1/1 | 0.85 | 0.21 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3397 | 1/1 | 0.97 | 0.36 | - | 41,41,41,41 | 0 |
| 60 | MG | DA | 1747 | 1/1 | 0.88 | 0.11 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3637 | 1/1 | 0.87 | 0.24 | - | 78,78,78,78 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3788 | 1/1 | 0.91 | 0.17 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3631 | 1/1 | 0.75 | 0.29 | - | 88,88,88,88 | 0 |
| 60 | MG | CA | 3213 | 1/1 | 0.83 | 0.34 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3563 | 1/1 | 0.93 | 0.29 | - | 30,30,30,30 | 0 |
| 60 | MG | CA | 3512 | 1/1 | 0.93 | 0.12 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3680 | 1/1 | 0.94 | 0.12 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3398 | 1/1 | 0.94 | 0.20 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3267 | 1/1 | 0.95 | 0.31 | - | 43,43,43,43 | 0 |
| 60 | MG | AA | 3694 | 1/1 | 0.61 | 0.17 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3090 | 1/1 | 0.94 | 0.27 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3037 | 1/1 | 0.91 | 0.19 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3064 | 1/1 | 0.88 | 0.20 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3275 | 1/1 | 0.84 | 0.13 | - | 73,73,73,73 | 0 |
| 60 | MG | BA | 1740 | 1/1 | 0.52 | 0.12 | - | 89,89,89,89 | 0 |
| 60 | MG | CA | 3363 | 1/1 | 0.91 | 0.18 | - | 55,55,55,55 | 0 |
| 60 | MG | DA | 1624 | 1/1 | 0.87 | 0.07 | - | 83,83,83,83 | 0 |
| 60 | MG | DA | 1639 | 1/1 | 0.91 | 0.10 | - | 59,59,59,59 | 0 |
| 60 | MG | DA | 1630 | 1/1 | 0.87 | 0.27 | - | 51,51,51,51 | 0 |
| 60 | MG | AA | 3259 | 1/1 | 0.96 | 0.36 | - | 27,27,27,27 | 0 |
| 60 | MG | AA | 3337 | 1/1 | 0.84 | 0.22 | - | 52,52,52,52 | 0 |
| 60 | MG | BA | 1794 | 1/1 | 0.93 | 0.15 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3349 | 1/1 | 0.92 | 0.15 | - | 36,36,36,36 | 0 |
| 60 | MG | AA | 3377 | 1/1 | 0.90 | 0.15 | - | 19,19,19,19 | 0 |
| 60 | MG | AA | 3549 | 1/1 | 0.94 | 0.12 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3491 | 1/1 | 0.89 | 0.30 | - | 40,40,40,40 | 0 |
| 60 | MG | AA | 3563 | 1/1 | 0.89 | 0.07 | - | 37,37,37,37 | 1 |
| 60 | MG | CA | 3176 | 1/1 | 0.95 | 0.35 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3591 | 1/1 | 0.93 | 0.23 | - | 61,61,61,61 | 0 |
| 60 | MG | DK | 201 | 1/1 | 0.93 | 0.23 | - | 55,55,55,55 | 0 |
| 60 | MG | BA | 1669 | 1/1 | 0.86 | 0.18 | - | 70,70,70,70 | 0 |
| 60 | MG | BA | 1673 | 1/1 | 0.90 | 0.72 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3284 | 1/1 | 0.93 | 0.22 | - | 49,49,49,49 | 0 |
| 60 | MG | CA | 3127 | 1/1 | 0.90 | 0.16 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3691 | 1/1 | 0.96 | 0.09 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3193 | 1/1 | 0.98 | 0.36 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3519 | 1/1 | 0.90 | 0.20 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3051 | 1/1 | 0.59 | 0.69 | - | 84,84,84,84 | 0 |
| 60 | MG | AA | 3420 | 1/1 | 0.91 | 0.13 | - | 26,26,26,26 | 0 |
| 60 | MG | AA | 3346 | 1/1 | 0.83 | 0.23 | - | 32,32,32,32 | 0 |
| 60 | MG | BA | 1767 | 1/1 | 0.72 | 0.27 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3747 | 1/1 | 0.84 | 0.33 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3327 | 1/1 | 0.94 | 0.22 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | DA | 1610 | 1/1 | 0.66 | 0.29 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3577 | 1/1 | 0.93 | 0.13 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3074 | 1/1 | 0.90 | 0.31 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3159 | 1/1 | 0.98 | 0.42 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3590 | 1/1 | 0.93 | 0.19 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3297 | 1/1 | 0.87 | 0.08 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3753 | 1/1 | 0.81 | 0.15 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3682 | 1/1 | 0.95 | 0.20 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3653 | 1/1 | 0.96 | 0.12 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3409 | 1/1 | 0.88 | 0.32 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3259 | 1/1 | 0.98 | 0.17 | - | 19,19,19,19 | 0 |
| 60 | MG | AA | 3136 | 1/1 | 0.42 | 0.46 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3238 | 1/1 | 0.86 | 0.13 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3361 | 1/1 | 0.99 | 0.17 | - | 33,33,33,33 | 0 |
| 60 | MG | BA | 1722 | 1/1 | 0.67 | 0.29 | - | 86,86,86,86 | 0 |
| 60 | MG | CA | 3474 | 1/1 | 0.79 | 0.14 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3540 | 1/1 | 0.86 | 0.24 | - | 71,71,71,71 | 0 |
| 60 | MG | DA | 1699 | 1/1 | 0.93 | 0.20 | - | 79,79,79,79 | 0 |
| 60 | MG | BA | 1790 | 1/1 | 0.73 | 0.32 | - | 87,87,87,87 | 0 |
| 60 | MG | CA | 3424 | 1/1 | 0.95 | 0.25 | - | 40,40,40,40 | 0 |
| 60 | MG | BA | 1699 | 1/1 | 0.73 | 0.19 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3658 | 1/1 | 0.94 | 0.22 | - | 25,25,25,25 | 0 |
| 60 | MG | DA | 1669 | 1/1 | 0.98 | 0.20 | - | 63,63,63,63 | 0 |
| 60 | MG | DA | 1713 | 1/1 | 0.95 | 0.15 | - | 59,59,59,59 | 0 |
| 60 | MG | BA | 1637 | 1/1 | 0.94 | 0.19 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3427 | 1/1 | 0.98 | 0.12 | - | 34,34,34,34 | 0 |
| 60 | MG | BX | 112 | 1/1 | 0.68 | 0.21 | - | 78,78,78,78 | 0 |
| 60 | MG | DA | 1711 | 1/1 | 0.96 | 0.10 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3116 | 1/1 | 0.94 | 0.45 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3341 | 1/1 | 0.84 | 0.19 | - | 35,35,35,35 | 0 |
| 60 | MG | CA | 3621 | 1/1 | 0.94 | 0.22 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3167 | 1/1 | 0.82 | 0.32 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3456 | 1/1 | 0.96 | 0.15 | - | 37,37,37,37 | 0 |
| 60 | MG | AA | 3472 | 1/1 | 0.95 | 0.23 | - | 37,37,37,37 | 0 |
| 60 | MG | BA | 1663 | 1/1 | 0.96 | 0.13 | - | 66,66,66,66 | 0 |
| 60 | MG | BA | 1672 | 1/1 | 0.83 | 0.22 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3423 | 1/1 | 0.97 | 0.22 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3131 | 1/1 | 0.95 | 0.28 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3451 | 1/1 | 0.97 | 0.12 | - | 78,78,78,78 | 0 |
| 60 | MG | BA | 1730 | 1/1 | 0.93 | 0.21 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3377 | 1/1 | 0.83 | 0.14 | - | 53,53,53,53 | 0 |
| 60 | MG | DA | 1707 | 1/1 | 0.90 | 0.09 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | BA | 1636 | 1/1 | 0.92 | 0.27 | - | 66,66,66,66 | 0 |
| 60 | MG | A0 | 102 | 1/1 | 0.97 | 0.06 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3334 | 1/1 | 0.96 | 0.21 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3614 | 1/1 | 0.91 | 0.14 | - | 66,66,66,66 | 0 |
| 60 | MG | BA | 1707 | 1/1 | 0.93 | 0.24 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3155 | 1/1 | 0.96 | 0.24 | - | 31,31,31,31 | 0 |
| 60 | MG | AA | 3441 | 1/1 | 0.85 | 0.18 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3005 | 1/1 | 0.82 | 0.20 | - | 63,63,63,63 | 0 |
| 60 | MG | BA | 1634 | 1/1 | 0.91 | 0.21 | - | 71,71,71,71 | 0 |
| 60 | MG | DA | 1745 | 1/1 | 0.96 | 0.23 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3781 | 1/1 | 0.95 | 0.17 | - | 49,49,49,49 | 0 |
| 60 | MG | CA | 3402 | 1/1 | 0.91 | 0.16 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3048 | 1/1 | 0.82 | 0.16 | - | 39,39,39,39 | 0 |
| 60 | MG | CA | 3627 | 1/1 | 0.95 | 0.07 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3696 | 1/1 | 0.95 | 0.20 | - | 62,62,62,62 | 0 |
| 60 | MG | BA | 1716 | 1/1 | 0.96 | 0.27 | - | 71,71,71,71 | 0 |
| 60 | MG | CA | 3269 | 1/1 | 0.94 | 0.40 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3388 | 1/1 | 0.86 | 0.18 | - | 97,97,97,97 | 0 |
| 60 | MG | CA | 3646 | 1/1 | 0.83 | 0.10 | - | 90,90,90,90 | 0 |
| 60 | MG | BA | 1693 | 1/1 | 0.94 | 0.14 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3503 | 1/1 | 0.94 | 0.14 | - | 41,41,41,41 | 0 |
| 60 | MG | CA | 3299 | 1/1 | 0.95 | 0.23 | - | 42,42,42,42 | 0 |
| 60 | MG | CA | 3565 | 1/1 | 0.95 | 0.14 | - | 36,36,36,36 | 0 |
| 60 | MG | AA | 3104 | 1/1 | 0.91 | 0.25 | - | 55,55,55,55 | 0 |
| 60 | MG | BN | 502 | 1/1 | 0.94 | 0.29 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3636 | 1/1 | 0.91 | 0.32 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3478 | 1/1 | 0.95 | 0.07 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3537 | 1/1 | 0.94 | 0.10 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3108 | 1/1 | 0.90 | 0.18 | - | 84,84,84,84 | 0 |
| 60 | MG | AA | 3763 | 1/1 | 0.75 | 0.26 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3142 | 1/1 | 0.85 | 0.26 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3029 | 1/1 | 0.86 | 0.20 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3233 | 1/1 | 0.92 | 0.28 | - | 85,85,85,85 | 0 |
| 60 | MG | CA | 3535 | 1/1 | 0.73 | 0.19 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3180 | 1/1 | 0.95 | 0.17 | - | 46,46,46,46 | 0 |
| 60 | MG | DA | 1764 | 1/1 | 0.58 | 0.41 | - | 94,94,94,94 | 0 |
| 60 | MG | BA | 1800 | 1/1 | 0.09 | 0.56 | - | 116,116,116,116 | 0 |
| 60 | MG | AA | 3399 | 1/1 | 0.97 | 0.24 | - | 51,51,51,51 | 0 |
| 60 | MG | BY | 3001 | 1/1 | 0.88 | 0.06 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3373 | 1/1 | 0.96 | 0.38 | - | 71,71,71,71 | 0 |
| 60 | MG | BA | 1602 | 1/1 | 0.84 | 0.20 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3238 | 1/1 | 0.91 | 0.34 | - | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | DA | 1655 | 1/1 | 0.84 | 0.22 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3235 | 1/1 | 0.80 | 0.37 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3500 | 1/1 | 0.89 | 0.14 | - | 27,27,27,27 | 0 |
| 60 | MG | AA | 3156 | 1/1 | 0.88 | 0.23 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3113 | 1/1 | 0.92 | 0.23 | - | 41,41,41,41 | 0 |
| 60 | MG | AF | 305 | 1/1 | 0.97 | 0.09 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3509 | 1/1 | 0.87 | 0.26 | - | 51,51,51,51 | 0 |
| 60 | MG | A4 | 502 | 1/1 | 0.86 | 0.18 | - | 81,81,81,81 | 0 |
| 60 | MG | AA | 3576 | 1/1 | 0.97 | 0.29 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3343 | 1/1 | 0.94 | 0.07 | - | 60,60,60,60 | 0 |
| 60 | MG | CA | 3039 | 1/1 | 0.88 | 0.39 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3175 | 1/1 | 0.84 | 0.33 | - | 50,50,50,50 | 1 |
| 60 | MG | CO | 201 | 1/1 | 0.87 | 0.16 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3178 | 1/1 | 0.98 | 0.21 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3566 | 1/1 | 0.96 | 0.19 | - | 26,26,26,26 | 0 |
| 60 | MG | AA | 3700 | 1/1 | 0.76 | 0.21 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3317 | 1/1 | 0.94 | 0.19 | - | 56,56,56,56 | 0 |
| 60 | MG | BA | 1788 | 1/1 | 0.81 | 0.17 | - | 79,79,79,79 | 0 |
| 60 | MG | DA | 1677 | 1/1 | 0.82 | 0.38 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3636 | 1/1 | 0.94 | 0.21 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3640 | 1/1 | 0.79 | 0.49 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3455 | 1/1 | 0.88 | 0.23 | - | 80,80,80,80 | 0 |
| 60 | MG | BX | 107 | 1/1 | 0.87 | 0.11 | - | 69,69,69,69 | 0 |
| 60 | MG | DA | 1662 | 1/1 | 0.86 | 0.10 | - | 51,51,51,51 | 0 |
| 60 | MG | DA | 1671 | 1/1 | 0.60 | 0.65 | - | 77,77,77,77 | 0 |
| 60 | MG | CA | 3647 | 1/1 | 0.94 | 0.38 | - | 61,61,61,61 | 0 |
| 60 | MG | BA | 1763 | 1/1 | 0.70 | 0.08 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3730 | 1/1 | 0.96 | 0.27 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3624 | 1/1 | 0.84 | 0.27 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3546 | 1/1 | 0.95 | 0.17 | - | 59,59,59,59 | 0 |
| 60 | MG | AZ | 5001 | 1/1 | 0.79 | 0.11 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3355 | 1/1 | 0.84 | 0.12 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3338 | 1/1 | 0.95 | 0.12 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3341 | 1/1 | 0.93 | 0.14 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3490 | 1/1 | 0.43 | 0.52 | - | 87,87,87,87 | 0 |
| 60 | MG | A7 | 101 | 1/1 | 0.96 | 0.10 | - | 57,57,57,57 | 0 |
| 60 | MG | BA | 1751 | 1/1 | 0.94 | 0.30 | - | 49,49,49,49 | 0 |
| 60 | MG | CA | 3221 | 1/1 | 0.92 | 0.56 | - | 60,60,60,60 | 0 |
| 60 | MG | CA | 3584 | 1/1 | 0.84 | 0.27 | - | 91,91,91,91 | 0 |
| 60 | MG | CA | 3133 | 1/1 | 0.89 | 0.20 | - | 72,72,72,72 | 0 |
| 60 | MG | BA | 1758 | 1/1 | 0.83 | 0.18 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3060 | 1/1 | 0.94 | 0.28 | - | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3177 | 1/1 | 0.86 | 0.21 | - | 43,43,43,43 | 0 |
| 60 | MG | DA | 1733 | 1/1 | 0.92 | 0.09 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3464 | 1/1 | 0.95 | 0.09 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3634 | 1/1 | 0.95 | 0.25 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3075 | 1/1 | 0.96 | 0.28 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3306 | 1/1 | 0.99 | 0.11 | - | 39,39,39,39 | 0 |
| 60 | MG | CA | 3607 | 1/1 | 0.85 | 0.18 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3693 | 1/1 | 0.92 | 0.19 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3216 | 1/1 | 0.96 | 0.25 | - | 32,32,32,32 | 0 |
| 60 | MG | AB | 3009 | 1/1 | 0.94 | 0.10 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3583 | 1/1 | 0.83 | 0.28 | - | 114,114,114,114 | 0 |
| 60 | MG | CA | 3568 | 1/1 | 0.94 | 0.24 | - | 71,71,71,71 | 0 |
| 60 | MG | CA | 3086 | 1/1 | 0.84 | 0.15 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3103 | 1/1 | 0.97 | 0.12 | - | 11,11,11,11 | 0 |
| 60 | MG | AA | 3065 | 1/1 | 0.97 | 0.41 | - | 51,51,51,51 | 0 |
| 60 | MG | BA | 1649 | 1/1 | 0.87 | 0.34 | - | 56,56,56,56 | 0 |
| 60 | MG | A0 | 103 | 1/1 | 0.94 | 0.12 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3521 | 1/1 | 0.97 | 0.19 | - | 30,30,30,30 | 0 |
| 60 | MG | CA | 3664 | 1/1 | 0.70 | 0.31 | - | 69,69,69,69 | 0 |
| 60 | MG | BA | 1720 | 1/1 | 0.91 | 0.14 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3482 | 1/1 | 0.67 | 0.29 | - | 89,89,89,89 | 0 |
| 60 | MG | BW | 102 | 1/1 | 0.79 | 0.20 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3031 | 1/1 | 0.98 | 0.25 | - | 29,29,29,29 | 1 |
| 60 | MG | AA | 3368 | 1/1 | 0.96 | 0.30 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3336 | 1/1 | 0.99 | 0.12 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3225 | 1/1 | 0.56 | 0.89 | - | 91,91,91,91 | 0 |
| 60 | MG | CA | 3049 | 1/1 | 0.63 | 0.29 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3652 | 1/1 | 0.86 | 0.44 | - | 87,87,87,87 | 0 |
| 60 | MG | AA | 3688 | 1/1 | 0.83 | 0.16 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3587 | 1/1 | 0.91 | 0.17 | - | 44,44,44,44 | 0 |
| 60 | MG | A6 | 101 | 1/1 | 0.90 | 0.20 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3222 | 1/1 | 0.79 | 0.70 | - | 81,81,81,81 | 0 |
| 60 | MG | CA | 3173 | 1/1 | 0.94 | 0.53 | - | 72,72,72,72 | 0 |
| 60 | MG | CB | 3012 | 1/1 | 0.78 | 0.16 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3437 | 1/1 | 0.90 | 0.25 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3412 | 1/1 | 0.85 | 0.16 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3737 | 1/1 | 0.98 | 0.15 | - | 25,25,25,25 | 0 |
| 60 | MG | DA | 1704 | 1/1 | 0.68 | 0.31 | - | 83,83,83,83 | 0 |
| 60 | MG | BA | 1692 | 1/1 | 0.95 | 0.31 | - | 69,69,69,69 | 0 |
| 60 | MG | AY | 502 | 1/1 | 0.89 | 0.24 | - | 54,54,54,54 | 0 |
| 60 | MG | DA | 1721 | 1/1 | 0.89 | 0.32 | - | 60,60,60,60 | 0 |
| 60 | MG | BA | 1779 | 1/1 | 0.55 | 0.33 | - | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | A2 | 3001 | 1/1 | 0.78 | 0.25 | - | 62,62,62,62 | 0 |
| 60 | MG | BA | 1719 | 1/1 | 0.90 | 0.27 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3777 | 1/1 | 0.90 | 0.32 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3626 | 1/1 | 0.96 | 0.23 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3155 | 1/1 | 0.79 | 0.48 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3561 | 1/1 | 0.90 | 0.17 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3635 | 1/1 | 0.94 | 0.15 | - | 33,33,33,33 | 0 |
| 60 | MG | AA | 3093 | 1/1 | 0.79 | 0.85 | - | 81,81,81,81 | 0 |
| 60 | MG | DA | 1623 | 1/1 | 0.65 | 0.38 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3197 | 1/1 | 0.93 | 0.28 | - | 48,48,48,48 | 0 |
| 60 | MG | BA | 1710 | 1/1 | 0.92 | 0.10 | - | 83,83,83,83 | 0 |
| 60 | MG | CB | 3001 | 1/1 | 0.91 | 0.21 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3276 | 1/1 | 0.95 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | BX | 111 | 1/1 | 0.86 | 0.14 | - | 67,67,67,67 | 0 |
| 60 | MG | AB | 3012 | 1/1 | 0.97 | 0.14 | - | 24,24,24,24 | 1 |
| 60 | MG | CA | 3536 | 1/1 | 0.87 | 0.13 | - | 95,95,95,95 | 0 |
| 60 | MG | CA | 3468 | 1/1 | 0.96 | 0.17 | - | 37,37,37,37 | 0 |
| 60 | MG | AA | 3748 | 1/1 | 0.96 | 0.18 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3273 | 1/1 | 0.91 | 0.27 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3067 | 1/1 | 0.75 | 0.60 | - | 82,82,82,82 | 0 |
| 60 | MG | CA | 3253 | 1/1 | 0.96 | 0.38 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3070 | 1/1 | 0.57 | 0.57 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3123 | 1/1 | 0.89 | 0.26 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3654 | 1/1 | 0.93 | 0.63 | - | 76,76,76,76 | 0 |
| 60 | MG | BA | 1713 | 1/1 | 0.94 | 0.24 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3003 | 1/1 | 0.96 | 0.07 | - | 14,14,14,14 | 0 |
| 60 | MG | CA | 3207 | 1/1 | 0.94 | 0.48 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3808 | 1/1 | 0.93 | 0.16 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3113 | 1/1 | 0.76 | 0.47 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3229 | 1/1 | 0.93 | 0.21 | - | 48,48,48,48 | 0 |
| 60 | MG | BA | 1752 | 1/1 | 0.78 | 0.07 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3778 | 1/1 | 0.90 | 0.10 | - | 68,68,68,68 | 0 |
| 60 | MG | AB | 3015 | 1/1 | 0.87 | 0.12 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3367 | 1/1 | 0.96 | 0.13 | - | 39,39,39,39 | 0 |
| 60 | MG | CA | 3117 | 1/1 | 0.96 | 0.13 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3768 | 1/1 | 0.84 | 0.35 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3616 | 1/1 | 0.73 | 0.34 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3429 | 1/1 | 0.86 | 0.22 | - | 58,58,58,58 | 0 |
| 60 | MG | BX | 113 | 1/1 | 0.87 | 0.20 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3369 | 1/1 | 0.96 | 0.17 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3689 | 1/1 | 0.72 | 0.16 | - | 84,84,84,84 | 0 |
| 60 | MG | AA | 3766 | 1/1 | 0.71 | 0.22 | - | 69,69,69,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AE | 302 | 1/1 | 0.96 | 0.18 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3672 | 1/1 | 0.93 | 0.07 | - | 71,71,71,71 | 0 |
| 60 | MG | CA | 3071 | 1/1 | 0.82 | 0.31 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3761 | 1/1 | 0.95 | 0.19 | - | 72,72,72,72 | 0 |
| 60 | MG | AA | 3718 | 1/1 | 0.97 | 0.14 | - | 40,40,40,40 | 0 |
| 60 | MG | AB | 3019 | 1/1 | 0.77 | 0.18 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3057 | 1/1 | 0.78 | 0.71 | - | 77,77,77,77 | 0 |
| 60 | MG | AA | 3494 | 1/1 | 0.90 | 0.14 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3534 | 1/1 | 0.90 | 0.12 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3592 | 1/1 | 0.89 | 0.26 | - | 67,67,67,67 | 0 |
| 60 | MG | BA | 1624 | 1/1 | 0.59 | 0.21 | - | 75,75,75,75 | 0 |
| 60 | MG | BK | 3101 | 1/1 | 0.51 | 0.56 | - | 95,95,95,95 | 0 |
| 60 | MG | CA | 3630 | 1/1 | 0.88 | 0.21 | - | 91,91,91,91 | 0 |
| 60 | MG | CA | 3562 | 1/1 | 0.87 | 0.17 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3291 | 1/1 | 0.79 | 0.17 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3440 | 1/1 | 0.82 | 0.18 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3509 | 1/1 | 0.78 | 0.19 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3138 | 1/1 | 0.88 | 0.28 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3501 | 1/1 | 0.96 | 0.17 | - | 78,78,78,78 | 0 |
| 60 | MG | BV | 101 | 1/1 | 0.81 | 0.16 | - | 78,78,78,78 | 0 |
| 60 | MG | BA | 1677 | 1/1 | 0.95 | 0.32 | - | 57,57,57,57 | 0 |
| 60 | MG | CB | 3011 | 1/1 | 0.88 | 0.27 | - | 51,51,51,51 | 0 |
| 60 | MG | AA | 3331 | 1/1 | 0.95 | 0.20 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3151 | 1/1 | 0.85 | 0.32 | - | 63,63,63,63 | 0 |
| 60 | MG | BA | 1604 | 1/1 | 0.91 | 0.16 | - | 85,85,85,85 | 0 |
| 60 | MG | CA | 3188 | 1/1 | 0.92 | 0.27 | - | 55,55,55,55 | 0 |
| 60 | MG | DA | 1750 | 1/1 | 0.89 | 0.18 | - | 86,86,86,86 | 0 |
| 60 | MG | AA | 3445 | 1/1 | 0.90 | 0.06 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3664 | 1/1 | 0.66 | 0.21 | - | 94,94,94,94 | 0 |
| 60 | MG | BX | 115 | 1/1 | 0.93 | 0.20 | - | 44,44,44,44 | 0 |
| 60 | MG | CR | 202 | 1/1 | 0.88 | 0.39 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3081 | 1/1 | 0.90 | 0.20 | - | 38,38,38,38 | 0 |
| 60 | MG | AA | 3729 | 1/1 | 0.92 | 0.07 | - | 40,40,40,40 | 0 |
| 60 | MG | CA | 3325 | 1/1 | 0.94 | 0.25 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3608 | 1/1 | 0.89 | 0.15 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3062 | 1/1 | 0.87 | 0.36 | - | 60,60,60,60 | 0 |
| 60 | MG | CA | 3499 | 1/1 | 0.92 | 0.21 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3431 | 1/1 | 0.95 | 0.15 | - | 25,25,25,25 | 0 |
| 60 | MG | A5 | 102 | 1/1 | 0.92 | 0.25 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3067 | 1/1 | 0.94 | 0.62 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3216 | 1/1 | 0.97 | 0.17 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3140 | 1/1 | 0.93 | 0.55 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3268 | 1/1 | 0.91 | 0.21 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3550 | 1/1 | 0.90 | 0.21 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3273 | 1/1 | 0.77 | 0.21 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3027 | 1/1 | 0.82 | 0.55 | - | 85,85,85,85 | 0 |
| 60 | MG | CA | 3376 | 1/1 | 0.62 | 0.17 | - | 94,94,94,94 | 0 |
| 60 | MG | CA | 3579 | 1/1 | 0.96 | 0.07 | - | 58,58,58,58 | 0 |
| 60 | MG | DA | 1603 | 1/1 | 0.97 | 0.07 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3329 | 1/1 | 0.81 | 0.22 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3374 | 1/1 | 0.72 | 0.15 | - | 74,74,74,74 | 0 |
| 60 | MG | AF | 304 | 1/1 | 0.76 | 0.43 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3164 | 1/1 | 0.95 | 0.13 | - | 38,38,38,38 | 0 |
| 60 | MG | BA | 1773 | 1/1 | 0.92 | 0.24 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3416 | 1/1 | 0.97 | 0.28 | - | 33,33,33,33 | 0 |
| 60 | MG | DA | 1621 | 1/1 | 0.84 | 0.08 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3600 | 1/1 | 0.93 | 0.39 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3551 | 1/1 | 0.91 | 0.15 | - | 76,76,76,76 | 0 |
| 60 | MG | CA | 3248 | 1/1 | 0.96 | 0.08 | - | 58,58,58,58 | 0 |
| 60 | MG | BA | 1633 | 1/1 | 0.88 | 0.36 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3613 | 1/1 | 0.64 | 0.31 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3244 | 1/1 | 0.98 | 0.39 | - | 42,42,42,42 | 0 |
| 60 | MG | DA | 1616 | 1/1 | 0.98 | 0.41 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3016 | 1/1 | 0.87 | 0.31 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3765 | 1/1 | 0.91 | 0.20 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3096 | 1/1 | 0.90 | 0.22 | - | 54,54,54,54 | 0 |
| 60 | MG | DA | 1645 | 1/1 | 0.98 | 0.34 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3521 | 1/1 | 0.80 | 0.34 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3530 | 1/1 | 0.90 | 0.10 | - | 60,60,60,60 | 0 |
| 60 | MG | C0 | 102 | 1/1 | 0.86 | 0.08 | - | 56,56,56,56 | 0 |
| 60 | MG | BA | 1727 | 1/1 | 0.97 | 0.28 | - | 53,53,53,53 | 0 |
| 60 | MG | BA | 1652 | 1/1 | 0.92 | 0.10 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3296 | 1/1 | 0.81 | 0.14 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3124 | 1/1 | 0.93 | 0.38 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3176 | 1/1 | 0.93 | 0.21 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3052 | 1/1 | 0.94 | 0.33 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3350 | 1/1 | 0.97 | 0.16 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3364 | 1/1 | 0.88 | 0.24 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3326 | 1/1 | 0.93 | 0.21 | - | 54,54,54,54 | 0 |
| 60 | MG | CE | 306 | 1/1 | 0.88 | 0.09 | - | 69,69,69,69 | 0 |
| 60 | MG | DA | 1758 | 1/1 | 0.85 | 0.35 | - | 80,80,80,80 | 0 |
| 60 | MG | AA | 3477 | 1/1 | 0.89 | 0.15 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3343 | 1/1 | 0.94 | 0.15 | - | 37,37,37,37 | 0 |
| 60 | MG | CA | 3492 | 1/1 | 0.93 | 0.26 | - | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3294 | 1/1 | 0.98 | 0.31 | - | 40,40,40,40 | 0 |
| 60 | MG | AA | 3322 | 1/1 | 0.94 | 0.19 | - | 37,37,37,37 | 0 |
| 60 | MG | BA | 1697 | 1/1 | 0.94 | 0.47 | - | 80,80,80,80 | 0 |
| 60 | MG | CA | 3465 | 1/1 | 0.94 | 0.08 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3472 | 1/1 | 0.95 | 0.28 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3757 | 1/1 | 0.93 | 0.29 | - | 67,67,67,67 | 0 |
| 60 | MG | DA | 1731 | 1/1 | 0.97 | 0.19 | - | 51,51,51,51 | 0 |
| 60 | MG | BA | 1635 | 1/1 | 0.93 | 0.29 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3545 | 1/1 | 0.93 | 0.06 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1688 | 1/1 | 0.86 | 0.29 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3284 | 1/1 | 0.97 | 0.39 | - | 45,45,45,45 | 0 |
| 60 | MG | CA | 3237 | 1/1 | 0.94 | 0.34 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3235 | 1/1 | 0.90 | 0.27 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3336 | 1/1 | 0.96 | 0.27 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3502 | 1/1 | 0.55 | 0.14 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3644 | 1/1 | 0.92 | 0.17 | - | 60,60,60,60 | 0 |
| 60 | MG | BA | 1650 | 1/1 | 0.92 | 0.22 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3139 | 1/1 | 0.92 | 0.25 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3128 | 1/1 | 0.95 | 0.22 | - | 31,31,31,31 | 0 |
| 60 | MG | AA | 3118 | 1/1 | 0.95 | 0.30 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3547 | 1/1 | 0.97 | 0.06 | - | 57,57,57,57 | 1 |
| 60 | MG | AA | 3264 | 1/1 | 0.96 | 0.09 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3285 | 1/1 | 0.88 | 0.22 | - | 72,72,72,72 | 0 |
| 60 | MG | BA | 1808 | 1/1 | 0.80 | 0.16 | - | 80,80,80,80 | 0 |
| 60 | MG | BA | 1750 | 1/1 | 0.97 | 0.10 | - | 54,54,54,54 | 0 |
| 60 | MG | BA | 1698 | 1/1 | 0.90 | 0.31 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3548 | 1/1 | 0.85 | 0.12 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3480 | 1/1 | 0.89 | 0.14 | - | 61,61,61,61 | 0 |
| 60 | MG | BA | 1644 | 1/1 | 0.91 | 0.27 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3095 | 1/1 | 0.91 | 0.09 | - | 92,92,92,92 | 0 |
| 60 | MG | CA | 3011 | 1/1 | 0.84 | 0.25 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3212 | 1/1 | 0.67 | 0.10 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3088 | 1/1 | 0.75 | 0.53 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3208 | 1/1 | 0.83 | 0.27 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3732 | 1/1 | 0.78 | 0.18 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3076 | 1/1 | 0.97 | 0.13 | - | 6,6,6,6 | 0 |
| 60 | MG | CB | 3008 | 1/1 | 0.47 | 0.26 | - | 87,87,87,87 | 0 |
| 60 | MG | CA | 3639 | 1/1 | 0.97 | 0.31 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3246 | 1/1 | 0.54 | 0.60 | - | 86,86,86,86 | 0 |
| 60 | MG | BA | 1627 | 1/1 | 0.77 | 0.21 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3024 | 1/1 | 0.96 | 0.62 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3015 | 1/1 | 0.79 | 0.49 | - | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3745 | 1/1 | 0.85 | 0.28 | - | 42,42,42,42 | 0 |
| 60 | MG | BA | 1731 | 1/1 | 0.92 | 0.06 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3283 | 1/1 | 0.93 | 0.31 | - | 48,48,48,48 | 0 |
| 60 | MG | DA | 1703 | 1/1 | 0.98 | 0.06 | - | 59,59,59,59 | 0 |
| 60 | MG | DA | 1701 | 1/1 | 0.94 | 0.14 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3122 | 1/1 | 0.94 | 0.29 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3089 | 1/1 | 0.81 | 0.39 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3490 | 1/1 | 0.85 | 0.41 | - | 81,81,81,81 | 0 |
| 60 | MG | AA | 3656 | 1/1 | 0.87 | 0.24 | - | 62,62,62,62 | 1 |
| 60 | MG | AA | 3637 | 1/1 | 0.88 | 0.19 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3201 | 1/1 | 0.91 | 0.31 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3752 | 1/1 | 0.90 | 0.63 | - | 75,75,75,75 | 0 |
| 60 | MG | DK | 202 | 1/1 | 0.89 | 0.23 | - | 80,80,80,80 | 0 |
| 60 | MG | CA | 3510 | 1/1 | 0.88 | 0.17 | - | 71,71,71,71 | 0 |
| 60 | MG | CA | 3243 | 1/1 | 0.92 | 0.35 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3333 | 1/1 | 0.90 | 0.20 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3588 | 1/1 | 0.97 | 0.15 | - | 33,33,33,33 | 0 |
| 60 | MG | AA | 3091 | 1/1 | 0.95 | 0.48 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3042 | 1/1 | 0.52 | 0.89 | - | 84,84,84,84 | 0 |
| 60 | MG | CA | 3191 | 1/1 | 0.86 | 0.27 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3154 | 1/1 | 0.89 | 0.16 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3305 | 1/1 | 0.92 | 0.16 | - | 38,38,38,38 | 0 |
| 60 | MG | CA | 3614 | 1/1 | 0.89 | 0.28 | - | 79,79,79,79 | 0 |
| 60 | MG | CA | 3109 | 1/1 | 0.95 | 0.18 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3666 | 1/1 | 0.95 | 0.29 | - | 28,28,28,28 | 0 |
| 60 | MG | AA | 3663 | 1/1 | 0.97 | 0.20 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3015 | 1/1 | 0.71 | 0.46 | - | 74,74,74,74 | 0 |
| 60 | MG | BA | 1664 | 1/1 | 0.93 | 0.57 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3030 | 1/1 | 0.97 | 0.34 | - | 44,44,44,44 | 1 |
| 60 | MG | CA | 3252 | 1/1 | 0.96 | 0.25 | - | 30,30,30,30 | 0 |
| 60 | MG | AA | 3291 | 1/1 | 0.87 | 0.13 | - | 84,84,84,84 | 0 |
| 60 | MG | CA | 3487 | 1/1 | 0.82 | 0.29 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1657 | 1/1 | 0.77 | 0.47 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3498 | 1/1 | 0.85 | 0.33 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3793 | 1/1 | 0.79 | 0.35 | - | 76,76,76,76 | 0 |
| 60 | MG | BA | 1711 | 1/1 | 0.94 | 0.37 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3533 | 1/1 | 0.94 | 0.12 | - | 20,20,20,20 | 0 |
| 60 | MG | BL | 202 | 1/1 | 0.97 | 0.14 | - | 56,56,56,56 | 0 |
| 60 | MG | BA | 1762 | 1/1 | 0.90 | 0.07 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3323 | 1/1 | 0.90 | 0.16 | - | 32,32,32,32 | 0 |
| 60 | MG | AA | 3493 | 1/1 | 0.94 | 0.22 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3119 | 1/1 | 0.92 | 0.69 | - | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | DA | 1739 | 1/1 | 0.67 | 0.43 | - | 85,85,85,85 | 0 |
| 60 | MG | AA | 3782 | 1/1 | 0.91 | 0.17 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3114 | 1/1 | 0.93 | 0.34 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3125 | 1/1 | 0.91 | 0.35 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3326 | 1/1 | 0.96 | 0.14 | - | 22,22,22,22 | 0 |
| 60 | MG | BA | 1789 | 1/1 | 0.88 | 0.11 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3645 | 1/1 | 0.96 | 0.10 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3298 | 1/1 | 0.76 | 0.21 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3142 | 1/1 | 0.90 | 0.27 | - | 50,50,50,50 | 0 |
| 60 | MG | CA | 3152 | 1/1 | 0.70 | 0.16 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3591 | 1/1 | 0.95 | 0.14 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3554 | 1/1 | 0.95 | 0.07 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3234 | 1/1 | 0.75 | 0.41 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3066 | 1/1 | 0.91 | 0.19 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3185 | 1/1 | 0.93 | 0.32 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3557 | 1/1 | 0.89 | 0.25 | - | 76,76,76,76 | 0 |
| 60 | MG | CA | 3006 | 1/1 | 0.97 | 0.09 | - | 24,24,24,24 | 0 |
| 60 | MG | CA | 3305 | 1/1 | 0.88 | 0.31 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3440 | 1/1 | 0.94 | 0.41 | - | 69,69,69,69 | 0 |
| 60 | MG | DA | 1752 | 1/1 | 0.92 | 0.32 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3605 | 1/1 | 0.80 | 0.11 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3228 | 1/1 | 0.90 | 0.71 | - | 68,68,68,68 | 0 |
| 60 | MG | BA | 1642 | 1/1 | 0.86 | 0.18 | - | 59,59,59,59 | 0 |
| 60 | MG | DZ | 701 | 1/1 | 0.97 | 0.24 | - | 47,47,47,47 | 0 |
| 60 | MG | AA | 3456 | 1/1 | 0.99 | 0.12 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3303 | 1/1 | 0.89 | 0.21 | - | 30,30,30,30 | 0 |
| 60 | MG | AB | 3002 | 1/1 | 0.98 | 0.22 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3147 | 1/1 | 0.96 | 0.12 | - | 51,51,51,51 | 0 |
| 60 | MG | DA | 1717 | 1/1 | 0.94 | 0.16 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3784 | 1/1 | 0.90 | 0.15 | - | 69,69,69,69 | 0 |
| 60 | MG | DA | 1734 | 1/1 | 0.70 | 0.28 | - | 75,75,75,75 | 0 |
| 60 | MG | BA | 1667 | 1/1 | 0.91 | 0.15 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3388 | 1/1 | 0.88 | 0.16 | - | 55,55,55,55 | 0 |
| 60 | MG | BA | 1797 | 1/1 | 0.96 | 0.15 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3202 | 1/1 | 0.78 | 0.32 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3596 | 1/1 | 0.89 | 0.10 | - | 75,75,75,75 | 0 |
| 60 | MG | DA | 1710 | 1/1 | 0.92 | 0.23 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3634 | 1/1 | 0.85 | 0.21 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3690 | 1/1 | 0.91 | 0.11 | - | 58,58,58,58 | 0 |
| 60 | MG | BA | 1638 | 1/1 | 0.84 | 0.64 | - | 83,83,83,83 | 0 |
| 60 | MG | DA | 1670 | 1/1 | 0.87 | 0.25 | - | 74,74,74,74 | 0 |
| 60 | MG | BA | 1641 | 1/1 | 0.95 | 0.29 | - | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3586 | 1/1 | 0.94 | 0.25 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3005 | 1/1 | 0.86 | 0.18 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3025 | 1/1 | 0.95 | 0.50 | - | 32,32,32,32 | 1 |
| 60 | MG | C0 | 101 | 1/1 | 0.92 | 0.07 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3742 | 1/1 | 0.95 | 0.20 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3061 | 1/1 | 0.81 | 0.77 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3580 | 1/1 | 0.96 | 0.12 | - | 37,37,37,37 | 0 |
| 60 | MG | CA | 3053 | 1/1 | 0.93 | 0.19 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3426 | 1/1 | 0.94 | 0.20 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3250 | 1/1 | 0.83 | 0.17 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3628 | 1/1 | 0.97 | 0.18 | - | 62,62,62,62 | 0 |
| 60 | MG | DA | 1741 | 1/1 | 0.92 | 0.32 | - | 81,81,81,81 | 0 |
| 60 | MG | CA | 3542 | 1/1 | 0.74 | 0.20 | - | 82,82,82,82 | 0 |
| 60 | MG | BA | 1689 | 1/1 | 0.80 | 0.29 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3314 | 1/1 | 0.90 | 0.15 | - | 41,41,41,41 | 0 |
| 60 | MG | BA | 1756 | 1/1 | 0.95 | 0.25 | - | 43,43,43,43 | 0 |
| 60 | MG | AA | 3179 | 1/1 | 0.91 | 0.23 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3002 | 1/1 | 0.77 | 0.24 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3055 | 1/1 | 0.90 | 0.17 | - | 61,61,61,61 | 0 |
| 60 | MG | AA | 3642 | 1/1 | 0.94 | 0.23 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3041 | 1/1 | 0.93 | 0.33 | - | 41,41,41,41 | 0 |
| 60 | MG | BA | 1606 | 1/1 | 0.97 | 0.28 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3785 | 1/1 | 0.91 | 0.21 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3599 | 1/1 | 0.66 | 0.43 | - | 113,113,113,113 | 0 |
| 60 | MG | AB | 3005 | 1/1 | 0.81 | 0.17 | - | 70,70,70,70 | 0 |
| 60 | MG | DA | 1726 | 1/1 | 0.93 | 0.16 | - | 58,58,58,58 | 0 |
| 60 | MG | BA | 1670 | 1/1 | 0.76 | 0.30 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3192 | 1/1 | 0.69 | 0.42 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3308 | 1/1 | 0.93 | 0.19 | - | 35,35,35,35 | 0 |
| 60 | MG | CA | 3638 | 1/1 | 0.94 | 0.48 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3070 | 1/1 | 0.66 | 0.35 | - | 68,68,68,68 | 0 |
| 60 | MG | BX | 106 | 1/1 | 0.80 | 0.17 | - | 85,85,85,85 | 0 |
| 60 | MG | CA | 3405 | 1/1 | 0.96 | 0.15 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3648 | 1/1 | 0.70 | 0.17 | - | 80,80,80,80 | 0 |
| 60 | MG | BA | 1780 | 1/1 | 0.97 | 0.07 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3463 | 1/1 | 0.95 | 0.19 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3161 | 1/1 | 0.79 | 0.57 | - | 89,89,89,89 | 0 |
| 60 | MG | AA | 3078 | 1/1 | 0.88 | 0.26 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3428 | 1/1 | 0.93 | 0.36 | - | 50,50,50,50 | 0 |
| 60 | MG | A0 | 104 | 1/1 | 0.73 | 0.80 | - | 81,81,81,81 | 0 |
| 60 | MG | AA | 3553 | 1/1 | 0.94 | 0.17 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3200 | 1/1 | 0.89 | 0.15 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | BA | 1760 | 1/1 | 0.93 | 0.18 | - | 68,68,68,68 | 0 |
| 60 | MG | AB | 3022 | 1/1 | 0.94 | 0.06 | - | 79,79,79,79 | 0 |
| 60 | MG | BA | 1721 | 1/1 | 0.98 | 0.26 | - | 60,60,60,60 | 0 |
| 60 | MG | BX | 114 | 1/1 | 0.93 | 0.26 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3146 | 1/1 | 0.83 | 0.31 | - | 79,79,79,79 | 0 |
| 60 | MG | CB | 3009 | 1/1 | 0.92 | 0.16 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3645 | 1/1 | 0.78 | 0.13 | - | 78,78,78,78 | 0 |
| 60 | MG | DA | 1716 | 1/1 | 0.91 | 0.27 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3171 | 1/1 | 0.86 | 0.51 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3174 | 1/1 | 0.94 | 0.27 | - | 39,39,39,39 | 0 |
| 60 | MG | CA | 3051 | 1/1 | 0.82 | 0.18 | - | 52,52,52,52 | 0 |
| 60 | MG | BA | 1776 | 1/1 | 0.83 | 0.10 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3610 | 1/1 | 0.95 | 0.10 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3476 | 1/1 | 0.89 | 0.10 | - | 50,50,50,50 | 0 |
| 60 | MG | CA | 3183 | 1/1 | 0.75 | 0.43 | - | 83,83,83,83 | 0 |
| 60 | MG | AA | 3804 | 1/1 | 0.91 | 0.38 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3562 | 1/1 | 0.91 | 0.06 | - | 45,45,45,45 | 0 |
| 60 | MG | BA | 1732 | 1/1 | 0.88 | 0.25 | - | 65,65,65,65 | 0 |
| 60 | MG | DA | 1751 | 1/1 | 0.88 | 0.25 | - | 84,84,84,84 | 0 |
| 60 | MG | CA | 3392 | 1/1 | 0.96 | 0.09 | - | 66,66,66,66 | 0 |
| 60 | MG | DA | 1636 | 1/1 | 0.90 | 0.32 | - | 77,77,77,77 | 0 |
| 60 | MG | AA | 3795 | 1/1 | 0.85 | 0.28 | - | 26,26,26,26 | 1 |
| 60 | MG | CE | 305 | 1/1 | 0.81 | 0.26 | - | 37,37,37,37 | 0 |
| 60 | MG | BA | 1676 | 1/1 | 0.93 | 0.24 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3152 | 1/1 | 0.78 | 0.41 | - | 80,80,80,80 | 0 |
| 60 | MG | AA | 3787 | 1/1 | 0.94 | 0.27 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3598 | 1/1 | 0.88 | 0.20 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3403 | 1/1 | 0.97 | 0.14 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3539 | 1/1 | 0.89 | 0.31 | - | 72,72,72,72 | 0 |
| 60 | MG | DA | 1615 | 1/1 | 0.51 | 0.52 | - | 87,87,87,87 | 0 |
| 60 | MG | CA | 3597 | 1/1 | 0.50 | 0.47 | - | 108,108,108,108 | 0 |
| 60 | MG | DA | 1737 | 1/1 | 0.82 | 0.40 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3744 | 1/1 | 0.79 | 0.15 | - | 79,79,79,79 | 0 |
| 60 | MG | AA | 3579 | 1/1 | 0.65 | 0.14 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3635 | 1/1 | 0.92 | 0.30 | - | 77,77,77,77 | 0 |
| 60 | MG | AA | 3813 | 1/1 | 0.91 | 0.21 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3643 | 1/1 | 0.97 | 0.14 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3169 | 1/1 | 0.82 | 0.28 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3310 | 1/1 | 0.95 | 0.21 | - | 45,45,45,45 | 0 |
| 60 | MG | CA | 3434 | 1/1 | 0.93 | 0.17 | - | 67,67,67,67 | 0 |
| 60 | MG | BA | 1656 | 1/1 | 0.84 | 0.19 | - | 83,83,83,83 | 0 |
| 60 | MG | CA | 3148 | 1/1 | 0.92 | 0.15 | - | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3467 | 1/1 | 0.96 | 0.13 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3295 | 1/1 | 0.90 | 0.29 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3286 | 1/1 | 0.98 | 0.25 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3756 | 1/1 | 0.86 | 0.24 | - | 57,57,57,57 | 0 |
| 60 | MG | DA | 1698 | 1/1 | 0.92 | 0.15 | - | 75,75,75,75 | 0 |
| 60 | MG | AE | 304 | 1/1 | 0.86 | 0.53 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3347 | 1/1 | 0.98 | 0.14 | - | 37,37,37,37 | 0 |
| 60 | MG | BA | 1694 | 1/1 | 0.87 | 0.23 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3418 | 1/1 | 0.95 | 0.17 | - | 22,22,22,22 | 0 |
| 60 | MG | AR | 5001 | 1/1 | 0.97 | 0.14 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3166 | 1/1 | 0.98 | 0.12 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3359 | 1/1 | 0.97 | 0.18 | - | 31,31,31,31 | 0 |
| 60 | MG | AA | 3396 | 1/1 | 0.99 | 0.14 | - | 22,22,22,22 | 0 |
| 60 | MG | CA | 3283 | 1/1 | 0.90 | 0.23 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3707 | 1/1 | 0.94 | 0.43 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3186 | 1/1 | 0.95 | 0.24 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3623 | 1/1 | 0.93 | 0.58 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3575 | 1/1 | 0.87 | 0.16 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3254 | 1/1 | 0.89 | 0.15 | - | 35,35,35,35 | 0 |
| 60 | MG | AA | 3135 | 1/1 | 0.95 | 0.16 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3382 | 1/1 | 0.86 | 0.18 | - | 70,70,70,70 | 0 |
| 60 | MG | DA | 1757 | 1/1 | 0.81 | 0.13 | - | 77,77,77,77 | 0 |
| 60 | MG | AE | 301 | 1/1 | 0.85 | 0.40 | - | 65,65,65,65 | 0 |
| 60 | MG | BD | 502 | 1/1 | 0.87 | 0.42 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3629 | 1/1 | 0.86 | 0.14 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3270 | 1/1 | 0.88 | 0.20 | - | 92,92,92,92 | 0 |
| 60 | MG | BX | 103 | 1/1 | 0.82 | 0.08 | - | 88,88,88,88 | 0 |
| 60 | MG | CA | 3098 | 1/1 | 0.45 | 1.04 | - | 90,90,90,90 | 0 |
| 60 | MG | CA | 3475 | 1/1 | 0.73 | 0.17 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3275 | 1/1 | 0.96 | 0.39 | - | 56,56,56,56 | 0 |
| 60 | MG | BA | 1700 | 1/1 | 0.94 | 0.11 | - | 62,62,62,62 | 0 |
| 60 | MG | CP | 201 | 1/1 | 0.96 | 0.13 | - | 57,57,57,57 | 0 |
| 60 | MG | CQ | 203 | 1/1 | 0.86 | 0.28 | - | 62,62,62,62 | 0 |
| 60 | MG | DA | 1664 | 1/1 | 0.87 | 0.24 | - | 49,49,49,49 | 0 |
| 60 | MG | AA | 3749 | 1/1 | 0.94 | 0.14 | - | 30,30,30,30 | 0 |
| 60 | MG | CA | 3196 | 1/1 | 0.95 | 0.28 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3703 | 1/1 | 0.97 | 0.07 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3586 | 1/1 | 0.94 | 0.19 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3599 | 1/1 | 0.80 | 0.09 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3280 | 1/1 | 0.91 | 0.20 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3638 | 1/1 | 0.76 | 0.36 | - | 72,72,72,72 | 0 |
| 60 | MG | BA | 1608 | 1/1 | 0.92 | 0.35 | - | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3400 | 1/1 | 0.98 | 0.10 | - | 48,48,48,48 | 0 |
| 60 | MG | CA | 3528 | 1/1 | 0.87 | 0.07 | - | 51,51,51,51 | 1 |
| 60 | MG | AA | 3470 | 1/1 | 0.98 | 0.13 | - | 24,24,24,24 | 0 |
| 60 | MG | CA | 3524 | 1/1 | 0.75 | 0.29 | - | 87,87,87,87 | 0 |
| 60 | MG | AA | 3153 | 1/1 | 0.93 | 0.27 | - | 47,47,47,47 | 0 |
| 60 | MG | BA | 1708 | 1/1 | 0.90 | 0.27 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3592 | 1/1 | 0.66 | 0.23 | - | 87,87,87,87 | 0 |
| 60 | MG | CB | 3002 | 1/1 | 0.92 | 0.13 | - | 78,78,78,78 | 0 |
| 60 | MG | DA | 1723 | 1/1 | 0.94 | 0.28 | - | 53,53,53,53 | 0 |
| 60 | MG | BA | 1771 | 1/1 | 0.97 | 0.13 | - | 48,48,48,48 | 0 |
| 60 | MG | BA | 1618 | 1/1 | 0.85 | 0.52 | - | 54,54,54,54 | 0 |
| 60 | MG | CA | 3556 | 1/1 | 0.95 | 0.05 | - | 77,77,77,77 | 0 |
| 60 | MG | DA | 1678 | 1/1 | 0.92 | 0.40 | - | 66,66,66,66 | 0 |
| 60 | MG | DA | 1640 | 1/1 | 0.91 | 0.35 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3223 | 1/1 | 0.93 | 0.17 | - | 21,21,21,21 | 0 |
| 60 | MG | CA | 3578 | 1/1 | 0.57 | 0.12 | - | 96,96,96,96 | 0 |
| 60 | MG | BA | 1623 | 1/1 | 0.90 | 0.25 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3269 | 1/1 | 0.91 | 0.54 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3380 | 1/1 | 0.94 | 0.16 | - | 37,37,37,37 | 0 |
| 60 | MG | BA | 1781 | 1/1 | 0.93 | 0.14 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3137 | 1/1 | 0.97 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3076 | 1/1 | 0.91 | 0.32 | - | 48,48,48,48 | 0 |
| 60 | MG | CA | 3511 | 1/1 | 0.76 | 0.34 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3288 | 1/1 | 0.90 | 0.13 | - | 39,39,39,39 | 0 |
| 60 | MG | CA | 3139 | 1/1 | 0.49 | 0.53 | - | 83,83,83,83 | 0 |
| 60 | MG | CA | 3620 | 1/1 | 0.92 | 0.22 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3404 | 1/1 | 0.97 | 0.10 | - | 50,50,50,50 | 0 |
| 60 | MG | BA | 1796 | 1/1 | 0.94 | 0.18 | - | 75,75,75,75 | 0 |
| 60 | MG | BA | 1801 | 1/1 | 0.91 | 0.12 | - | 55,55,55,55 | 0 |
| 60 | MG | DA | 1673 | 1/1 | 0.83 | 0.40 | - | 68,68,68,68 | 0 |
| 60 | MG | BA | 1712 | 1/1 | 0.83 | 0.60 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3219 | 1/1 | 0.85 | 0.32 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3701 | 1/1 | 0.95 | 0.56 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3508 | 1/1 | 0.98 | 0.13 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3543 | 1/1 | 0.84 | 0.17 | - | 84,84,84,84 | 0 |
| 60 | MG | AA | 3807 | 1/1 | 0.95 | 0.20 | - | 62,62,62,62 | 0 |
| 60 | MG | DA | 1647 | 1/1 | 0.97 | 0.14 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3496 | 1/1 | 0.97 | 0.05 | - | 43,43,43,43 | 0 |
| 60 | MG | AA | 3719 | 1/1 | 0.95 | 0.09 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3138 | 1/1 | 0.93 | 0.14 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3316 | 1/1 | 0.85 | 0.20 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1718 | 1/1 | 0.93 | 0.16 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3762 | 1/1 | 0.96 | 0.26 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3578 | 1/1 | 0.74 | 0.37 | - | 71,71,71,71 | 0 |
| 60 | MG | DA | 1755 | 1/1 | 0.96 | 0.14 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3406 | 1/1 | 0.93 | 0.14 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3434 | 1/1 | 0.86 | 0.27 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3197 | 1/1 | 0.94 | 0.32 | - | 42,42,42,42 | 0 |
| 60 | MG | CA | 3317 | 1/1 | 0.90 | 0.16 | - | 61,61,61,61 | 0 |
| 60 | MG | AE | 303 | 1/1 | 0.97 | 0.19 | - | 23,23,23,23 | 0 |
| 60 | MG | AA | 3073 | 1/1 | 0.93 | 0.22 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3287 | 1/1 | 0.89 | 0.35 | - | 43,43,43,43 | 0 |
| 60 | MG | CA | 3205 | 1/1 | 0.92 | 0.31 | - | 66,66,66,66 | 0 |
| 60 | MG | DF | 3001 | 1/1 | 0.93 | 0.12 | - | 53,53,53,53 | 0 |
| 60 | MG | BA | 1754 | 1/1 | 0.94 | 0.05 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3278 | 1/1 | 0.92 | 0.35 | - | 58,58,58,58 | 0 |
| 60 | MG | BA | 1605 | 1/1 | 0.91 | 0.11 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3548 | 1/1 | 0.77 | 0.13 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3073 | 1/1 | 0.38 | 0.73 | - | 94,94,94,94 | 0 |
| 60 | MG | BA | 1726 | 1/1 | 0.94 | 0.17 | - | 59,59,59,59 | 0 |
| 60 | MG | BW | 101 | 1/1 | 0.64 | 0.47 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3771 | 1/1 | 0.94 | 0.18 | - | 40,40,40,40 | 0 |
| 60 | MG | AA | 3071 | 1/1 | 0.94 | 0.73 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3227 | 1/1 | 0.99 | 0.25 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3443 | 1/1 | 0.83 | 0.21 | - | 58,58,58,58 | 0 |
| 60 | MG | AB | 3013 | 1/1 | 0.94 | 0.13 | - | 55,55,55,55 | 0 |
| 60 | MG | BA | 1770 | 1/1 | 0.73 | 0.12 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3277 | 1/1 | 0.98 | 0.18 | - | 43,43,43,43 | 0 |
| 60 | MG | BL | 201 | 1/1 | 0.89 | 0.20 | - | 104,104,104,104 | 0 |
| 60 | MG | BA | 1806 | 1/1 | 0.92 | 0.17 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3435 | 1/1 | 0.93 | 0.16 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3148 | 1/1 | 0.99 | 0.24 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3775 | 1/1 | 0.95 | 0.18 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3715 | 1/1 | 0.91 | 0.09 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3092 | 1/1 | 0.90 | 0.23 | - | 41,41,41,41 | 0 |
| 60 | MG | BX | 101 | 1/1 | 0.93 | 0.30 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3433 | 1/1 | 0.95 | 0.28 | - | 50,50,50,50 | 0 |
| 60 | MG | CA | 3003 | 1/1 | 0.97 | 0.31 | - | 49,49,49,49 | 0 |
| 60 | MG | CA | 3544 | 1/1 | 0.90 | 0.18 | - | 74,74,74,74 | 0 |
| 60 | MG | BA | 1803 | 1/1 | 0.58 | 0.22 | - | 79,79,79,79 | 0 |
| 60 | MG | DA | 1743 | 1/1 | 0.73 | 0.13 | - | 83,83,83,83 | 0 |
| 60 | MG | A0 | 105 | 1/1 | 0.87 | 0.08 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3499 | 1/1 | 0.91 | 0.11 | - | 46,46,46,46 | 0 |
| 60 | MG | DA | 1604 | 1/1 | 0.95 | 0.12 | - | 90,90,90,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | BA | 1653 | 1/1 | 0.93 | 0.23 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3609 | 1/1 | 0.92 | 0.21 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3014 | 1/1 | 0.91 | 0.17 | - | 45,45,45,45 | 0 |
| 60 | MG | BA | 1745 | 1/1 | 0.93 | 0.09 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3677 | 1/1 | 0.99 | 0.20 | - | 26,26,26,26 | 0 |
| 60 | MG | AA | 3335 | 1/1 | 0.97 | 0.19 | - | 14,14,14,14 | 0 |
| 60 | MG | CA | 3483 | 1/1 | 0.79 | 0.17 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3419 | 1/1 | 0.89 | 0.05 | - | 88,88,88,88 | 0 |
| 60 | MG | AA | 3670 | 1/1 | 0.94 | 0.17 | - | 66,66,66,66 | 0 |
| 60 | MG | BA | 1782 | 1/1 | 0.88 | 0.29 | - | 72,72,72,72 | 0 |
| 60 | MG | DA | 1620 | 1/1 | 0.77 | 0.23 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3424 | 1/1 | 0.95 | 0.11 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3265 | 1/1 | 0.83 | 0.36 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3247 | 1/1 | 0.87 | 0.42 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3831 | 1/1 | 0.95 | 0.38 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3704 | 1/1 | 0.95 | 0.17 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3641 | 1/1 | 0.98 | 0.14 | - | 45,45,45,45 | 0 |
| 60 | MG | DA | 1712 | 1/1 | 0.88 | 0.17 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3004 | 1/1 | 0.92 | 0.14 | - | 30,30,30,30 | 0 |
| 60 | MG | CA | 3077 | 1/1 | 0.82 | 0.28 | - | 62,62,62,62 | 0 |
| 60 | MG | BA | 1728 | 1/1 | 0.94 | 0.18 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3584 | 1/1 | 0.97 | 0.12 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3640 | 1/1 | 0.86 | 0.24 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3096 | 1/1 | 0.77 | 0.28 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3286 | 1/1 | 0.89 | 0.21 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3462 | 1/1 | 0.81 | 0.34 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3450 | 1/1 | 0.92 | 0.27 | - | 71,71,71,71 | 0 |
| 60 | MG | CA | 3007 | 1/1 | 0.88 | 0.24 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3010 | 1/1 | 0.87 | 0.29 | - | 68,68,68,68 | 0 |
| 60 | MG | BA | 1777 | 1/1 | 0.95 | 0.12 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3226 | 1/1 | 0.90 | 0.27 | - | 51,51,51,51 | 0 |
| 60 | MG | BA | 1646 | 1/1 | 0.75 | 0.52 | - | 71,71,71,71 | 0 |
| 60 | MG | AA | 3558 | 1/1 | 0.94 | 0.14 | - | 72,72,72,72 | 0 |
| 60 | MG | DA | 1746 | 1/1 | 0.87 | 0.28 | - | 67,67,67,67 | 0 |
| 60 | MG | CR | 201 | 1/1 | 0.89 | 0.36 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3462 | 1/1 | 0.95 | 0.06 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3630 | 1/1 | 0.90 | 0.15 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3255 | 1/1 | 0.95 | 0.28 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1661 | 1/1 | 0.88 | 0.45 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3534 | 1/1 | 0.96 | 0.20 | - | 34,34,34,34 | 0 |
| 60 | MG | DA | 1663 | 1/1 | 0.95 | 0.10 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3399 | 1/1 | 0.97 | 0.18 | - | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | BA | 1703 | 1/1 | 0.67 | 0.22 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3372 | 1/1 | 0.91 | 0.29 | - | 63,63,63,63 | 0 |
| 60 | MG | DA | 1654 | 1/1 | 0.92 | 0.40 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3444 | 1/1 | 0.80 | 0.09 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3469 | 1/1 | 0.94 | 0.58 | - | 76,76,76,76 | 0 |
| 60 | MG | DA | 1759 | 1/1 | 0.96 | 0.42 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3321 | 1/1 | 0.95 | 0.13 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3281 | 1/1 | 0.82 | 0.20 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3389 | 1/1 | 0.95 | 0.18 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3649 | 1/1 | 0.80 | 0.07 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3543 | 1/1 | 0.16 | 0.55 | - | 114,114,114,114 | 0 |
| 60 | MG | DA | 1744 | 1/1 | 0.96 | 0.14 | - | 57,57,57,57 | 0 |
| 60 | MG | CF | 303 | 1/1 | 0.90 | 0.28 | - | 63,63,63,63 | 0 |
| 60 | MG | AB | 3004 | 1/1 | 0.90 | 0.29 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3144 | 1/1 | 0.89 | 0.29 | - | 84,84,84,84 | 0 |
| 60 | MG | CF | 304 | 1/1 | 0.97 | 0.15 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3631 | 1/1 | 0.86 | 0.39 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3414 | 1/1 | 0.95 | 0.17 | - | 43,43,43,43 | 0 |
| 60 | MG | BA | 1631 | 1/1 | 0.92 | 0.09 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3147 | 1/1 | 0.92 | 0.51 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3504 | 1/1 | 0.96 | 0.11 | - | 77,77,77,77 | 0 |
| 60 | MG | A8 | 5002 | 1/1 | 0.95 | 0.25 | - | 45,45,45,45 | 0 |
| 60 | MG | CA | 3258 | 1/1 | 0.97 | 0.17 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3779 | 1/1 | 0.95 | 0.28 | - | 41,41,41,41 | 0 |
| 60 | MG | AA | 3593 | 1/1 | 0.94 | 0.14 | - | 49,49,49,49 | 0 |
| 60 | MG | DA | 1648 | 1/1 | 0.84 | 0.46 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3478 | 1/1 | 0.41 | 0.29 | - | 91,91,91,91 | 0 |
| 60 | MG | AA | 3126 | 1/1 | 0.97 | 0.24 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3410 | 1/1 | 0.85 | 0.19 | - | 72,72,72,72 | 0 |
| 60 | MG | AA | 3026 | 1/1 | 0.64 | 0.38 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3420 | 1/1 | 0.93 | 0.26 | - | 50,50,50,50 | 0 |
| 60 | MG | CA | 3230 | 1/1 | 0.88 | 0.11 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3366 | 1/1 | 0.94 | 0.18 | - | 35,35,35,35 | 0 |
| 60 | MG | CA | 3217 | 1/1 | 0.94 | 0.13 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3621 | 1/1 | 0.86 | 0.12 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3453 | 1/1 | 0.97 | 0.11 | - | 51,51,51,51 | 0 |
| 60 | MG | BA | 1665 | 1/1 | 0.94 | 0.41 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3098 | 1/1 | 0.81 | 0.29 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3267 | 1/1 | 0.91 | 0.24 | - | 110,110,110,110 | 0 |
| 60 | MG | CA | 3371 | 1/1 | 0.81 | 0.61 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3471 | 1/1 | 0.95 | 0.21 | - | 59,59,59,59 | 0 |
| 60 | MG | DA | 1635 | 1/1 | 0.91 | 0.44 | - | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | BA | 1723 | 1/1 | 0.91 | 0.27 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3393 | 1/1 | 0.92 | 0.35 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3403 | 1/1 | 0.94 | 0.19 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3484 | 1/1 | 0.91 | 0.26 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3352 | 1/1 | 0.98 | 0.23 | - | 40,40,40,40 | 0 |
| 60 | MG | CA | 3029 | 1/1 | 0.93 | 0.11 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3001 | 1/1 | 0.86 | 0.17 | - | 81,81,81,81 | 0 |
| 60 | MG | DA | 1641 | 1/1 | 0.94 | 0.13 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3466 | 1/1 | 0.98 | 0.14 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3751 | 1/1 | 0.75 | 0.20 | - | 76,76,76,76 | 0 |
| 60 | MG | AA | 3755 | 1/1 | 0.74 | 0.23 | - | 77,77,77,77 | 0 |
| 60 | MG | CA | 3365 | 1/1 | 0.94 | 0.18 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3266 | 1/1 | 0.84 | 0.28 | - | 55,55,55,55 | 0 |
| 60 | MG | CB | 3006 | 1/1 | 0.67 | 0.19 | - | 82,82,82,82 | 0 |
| 60 | MG | BA | 1747 | 1/1 | 0.97 | 0.14 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3498 | 1/1 | 0.90 | 0.17 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3229 | 1/1 | 0.96 | 0.13 | - | 33,33,33,33 | 0 |
| 60 | MG | AA | 3697 | 1/1 | 0.96 | 0.15 | - | 71,71,71,71 | 0 |
| 60 | MG | AO | 5001 | 1/1 | 0.99 | 0.10 | - | 43,43,43,43 | 0 |
| 60 | MG | CA | 3458 | 1/1 | 0.91 | 0.14 | - | 28,28,28,28 | 0 |
| 60 | MG | CA | 3517 | 1/1 | 0.86 | 0.21 | - | 75,75,75,75 | 0 |
| 60 | MG | AP | 202 | 1/1 | 0.93 | 0.26 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3526 | 1/1 | 0.94 | 0.15 | - | 26,26,26,26 | 0 |
| 60 | MG | DA | 1724 | 1/1 | 0.90 | 0.19 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3262 | 1/1 | 0.97 | 0.28 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3332 | 1/1 | 0.92 | 0.18 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3391 | 1/1 | 0.93 | 0.10 | - | 67,67,67,67 | 0 |
| 60 | MG | AA | 3145 | 1/1 | 0.92 | 0.32 | - | 41,41,41,41 | 1 |
| 60 | MG | AA | 3627 | 1/1 | 0.93 | 0.14 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3736 | 1/1 | 0.53 | 0.37 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3031 | 1/1 | 0.48 | 0.72 | - | 102,102,102,102 | 0 |
| 60 | MG | AA | 3544 | 1/1 | 0.85 | 0.18 | - | 16,16,16,16 | 0 |
| 60 | MG | CA | 3594 | 1/1 | 0.96 | 0.16 | - | 62,62,62,62 | 0 |
| 60 | MG | AA | 3293 | 1/1 | 0.95 | 0.14 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3287 | 1/1 | 0.88 | 0.20 | - | 25,25,25,25 | 0 |
| 60 | MG | AA | 3162 | 1/1 | 0.95 | 0.32 | - | 35,35,35,35 | 0 |
| 60 | MG | AA | 3262 | 1/1 | 0.92 | 0.58 | - | 70,70,70,70 | 0 |
| 60 | MG | DA | 1700 | 1/1 | 0.82 | 0.21 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3444 | 1/1 | 0.96 | 0.24 | - | 70,70,70,70 | 0 |
| 60 | MG | DJ | 5001 | 1/1 | 0.88 | 0.17 | - | 94,94,94,94 | 0 |
| 60 | MG | BA | 1748 | 1/1 | 0.95 | 0.34 | - | 75,75,75,75 | 0 |
| 60 | MG | CA | 3513 | 1/1 | 0.94 | 0.24 | - | 109,109,109,109 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3800 | 1/1 | 0.89 | 0.28 | - | 59,59,59,59 | 0 |
| 60 | MG | DA | 1748 | 1/1 | 0.85 | 0.18 | - | 78,78,78,78 | 0 |
| 60 | MG | BY | 3002 | 1/1 | 0.71 | 0.17 | - | 83,83,83,83 | 0 |
| 60 | MG | AA | 3105 | 1/1 | 0.83 | 0.18 | - | 77,77,77,77 | 0 |
| 60 | MG | CA | 3151 | 1/1 | 0.82 | 0.21 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3201 | 1/1 | 0.86 | 0.32 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3642 | 1/1 | 0.74 | 0.11 | - | 75,75,75,75 | 0 |
| 60 | MG | BA | 1772 | 1/1 | 0.94 | 0.33 | - | 51,51,51,51 | 0 |
| 60 | MG | AA | 3363 | 1/1 | 0.98 | 0.24 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3396 | 1/1 | 0.91 | 0.14 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3414 | 1/1 | 0.93 | 0.18 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3150 | 1/1 | 0.65 | 0.32 | - | 63,63,63,63 | 0 |
| 60 | MG | DA | 1725 | 1/1 | 0.90 | 0.13 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3421 | 1/1 | 0.95 | 0.19 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3198 | 1/1 | 0.89 | 0.09 | - | 47,47,47,47 | 0 |
| 60 | MG | DA | 1608 | 1/1 | 0.70 | 0.50 | - | 79,79,79,79 | 0 |
| 60 | MG | CA | 3162 | 1/1 | 0.91 | 0.27 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3260 | 1/1 | 0.92 | 0.43 | - | 67,67,67,67 | 0 |
| 60 | MG | AB | 3010 | 1/1 | 0.85 | 0.09 | - | 56,56,56,56 | 1 |
| 60 | MG | CA | 3514 | 1/1 | 0.46 | 0.16 | - | 68,68,68,68 | 0 |
| 60 | MG | BA | 1715 | 1/1 | 0.84 | 0.21 | - | 90,90,90,90 | 0 |
| 60 | MG | AA | 3040 | 1/1 | 0.47 | 0.13 | - | 93,93,93,93 | 0 |
| 60 | MG | BA | 1702 | 1/1 | 0.89 | 0.45 | - | 56,56,56,56 | 0 |
| 60 | MG | CA | 3046 | 1/1 | 0.94 | 0.07 | - | 72,72,72,72 | 0 |
| 60 | MG | CA | 3387 | 1/1 | 0.82 | 0.39 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3083 | 1/1 | 0.93 | 0.68 | - | 48,48,48,48 | 1 |
| 60 | MG | DA | 1652 | 1/1 | 0.98 | 0.09 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3495 | 1/1 | 0.91 | 0.20 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3507 | 1/1 | 0.92 | 0.14 | - | 99,99,99,99 | 0 |
| 60 | MG | AA | 3651 | 1/1 | 0.94 | 0.23 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3072 | 1/1 | 0.92 | 0.43 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3032 | 1/1 | 0.93 | 0.54 | - | 62,62,62,62 | 0 |
| 60 | MG | BA | 1784 | 1/1 | 0.85 | 0.18 | - | 59,59,59,59 | 0 |
| 60 | MG | AA | 3086 | 1/1 | 0.96 | 0.35 | - | 43,43,43,43 | 1 |
| 60 | MG | AA | 3722 | 1/1 | 0.95 | 0.17 | - | 31,31,31,31 | 0 |
| 60 | MG | DA | 1634 | 1/1 | 0.78 | 0.34 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3379 | 1/1 | 0.89 | 0.14 | - | 40,40,40,40 | 1 |
| 60 | MG | AA | 3568 | 1/1 | 0.89 | 0.22 | - | 23,23,23,23 | 0 |
| 60 | MG | AA | 3124 | 1/1 | 0.98 | 0.24 | - | 39,39,39,39 | 1 |
| 60 | MG | DA | 1760 | 1/1 | 0.96 | 0.27 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3439 | 1/1 | 0.88 | 0.18 | - | 43,43,43,43 | 0 |
| 60 | MG | DA | 1697 | 1/1 | 0.93 | 0.21 | - | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3255 | 1/1 | 0.94 | 0.35 | - | 61,61,61,61 | 0 |
| 60 | MG | CA | 3093 | 1/1 | 0.89 | 0.34 | - | 77,77,77,77 | 0 |
| 60 | MG | AA | 3436 | 1/1 | 0.96 | 0.13 | - | 31,31,31,31 | 0 |
| 60 | MG | AA | 3716 | 1/1 | 0.82 | 0.20 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3351 | 1/1 | 0.81 | 0.10 | - | 80,80,80,80 | 0 |
| 60 | MG | AA | 3724 | 1/1 | 0.90 | 0.31 | - | 37,37,37,37 | 0 |
| 60 | MG | DA | 1633 | 1/1 | 0.93 | 0.58 | - | 67,67,67,67 | 0 |
| 60 | MG | BX | 109 | 1/1 | 0.96 | 0.22 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3378 | 1/1 | 0.95 | 0.15 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3611 | 1/1 | 0.96 | 0.26 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3608 | 1/1 | 0.89 | 0.11 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3008 | 1/1 | 0.97 | 0.39 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3674 | 1/1 | 0.92 | 0.09 | - | 56,56,56,56 | 0 |
| 60 | MG | DA | 1676 | 1/1 | 0.68 | 0.29 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3612 | 1/1 | 0.95 | 0.13 | - | 59,59,59,59 | 0 |
| 60 | MG | BA | 1733 | 1/1 | 0.85 | 0.09 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3452 | 1/1 | 0.92 | 0.07 | - | 53,53,53,53 | 0 |
| 60 | MG | CA | 3522 | 1/1 | 0.97 | 0.24 | - | 25,25,25,25 | 0 |
| 60 | MG | AA | 3307 | 1/1 | 0.90 | 0.12 | - | 35,35,35,35 | 0 |
| 60 | MG | CA | 3604 | 1/1 | 0.93 | 0.19 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3182 | 1/1 | 0.81 | 0.27 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3165 | 1/1 | 0.80 | 0.41 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3412 | 1/1 | 0.85 | 0.21 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3743 | 1/1 | 0.89 | 0.20 | - | 66,66,66,66 | 0 |
| 60 | MG | BA | 1725 | 1/1 | 0.96 | 0.31 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3684 | 1/1 | 0.93 | 0.17 | - | 47,47,47,47 | 0 |
| 60 | MG | DA | 1683 | 1/1 | 0.96 | 0.42 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3580 | 1/1 | 0.85 | 0.14 | - | 26,26,26,26 | 0 |
| 60 | MG | AA | 3520 | 1/1 | 0.99 | 0.15 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3311 | 1/1 | 0.96 | 0.21 | - | 46,46,46,46 | 0 |
| 60 | MG | AA | 3221 | 1/1 | 0.74 | 0.16 | - | 72,72,72,72 | 0 |
| 60 | MG | AA | 3372 | 1/1 | 0.95 | 0.27 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3170 | 1/1 | 0.89 | 0.36 | - | 68,68,68,68 | 0 |
| 60 | MG | CA | 3232 | 1/1 | 0.92 | 0.24 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3655 | 1/1 | 0.85 | 0.20 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3538 | 1/1 | 0.82 | 0.31 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3055 | 1/1 | 0.85 | 0.29 | - | 77,77,77,77 | 0 |
| 60 | MG | CA | 3206 | 1/1 | 0.37 | 0.66 | - | 109,109,109,109 | 0 |
| 60 | MG | CA | 3448 | 1/1 | 0.96 | 0.09 | - | 64,64,64,64 | 0 |
| 60 | MG | BA | 1787 | 1/1 | 0.82 | 0.13 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3141 | 1/1 | 0.94 | 0.32 | - | 51,51,51,51 | 0 |
| 60 | MG | CA | 3177 | 1/1 | 0.48 | 0.65 | - | 98,98,98,98 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3370 | 1/1 | 0.92 | 0.16 | - | 43,43,43,43 | 0 |
| 60 | MG | CA | 3192 | 1/1 | 0.97 | 0.26 | - | 47,47,47,47 | 0 |
| 60 | MG | AA | 3159 | 1/1 | 0.80 | 0.41 | - | 66,66,66,66 | 0 |
| 60 | MG | BA | 1744 | 1/1 | 0.96 | 0.13 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3292 | 1/1 | 0.95 | 0.18 | - | 31,31,31,31 | 0 |
| 60 | MG | AA | 3479 | 1/1 | 0.83 | 0.14 | - | 66,66,66,66 | 0 |
| 60 | MG | DA | 1607 | 1/1 | 0.92 | 0.83 | - | 63,63,63,63 | 0 |
| 60 | MG | BA | 1632 | 1/1 | 0.87 | 0.23 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3163 | 1/1 | 0.84 | 0.27 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3064 | 1/1 | 0.94 | 0.22 | - | 31,31,31,31 | 0 |
| 60 | MG | DA | 1718 | 1/1 | 0.83 | 0.11 | - | 66,66,66,66 | 0 |
| 60 | MG | AA | 3295 | 1/1 | 0.92 | 0.16 | - | 24,24,24,24 | 0 |
| 60 | MG | CA | 3445 | 1/1 | 0.81 | 0.36 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3215 | 1/1 | 0.92 | 0.18 | - | 48,48,48,48 | 0 |
| 60 | MG | BA | 1622 | 1/1 | 0.80 | 0.63 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3161 | 1/1 | 0.97 | 0.44 | - | 45,45,45,45 | 0 |
| 60 | MG | DA | 1626 | 1/1 | 0.90 | 0.41 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3383 | 1/1 | 0.84 | 0.34 | - | 66,66,66,66 | 0 |
| 60 | MG | CA | 3476 | 1/1 | 0.98 | 0.22 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3710 | 1/1 | 0.94 | 0.17 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3028 | 1/1 | 0.85 | 0.30 | - | 40,40,40,40 | 1 |
| 60 | MG | AA | 3603 | 1/1 | 0.97 | 0.10 | - | 68,68,68,68 | 0 |
| 60 | MG | DA | 1661 | 1/1 | 0.82 | 0.14 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3108 | 1/1 | 0.31 | 0.41 | - | 88,88,88,88 | 0 |
| 60 | MG | AW | 3001 | 1/1 | 0.93 | 0.19 | - | 46,46,46,46 | 0 |
| 60 | MG | CA | 3432 | 1/1 | 0.98 | 0.13 | - | 29,29,29,29 | 0 |
| 60 | MG | AA | 3006 | 1/1 | 0.93 | 0.28 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3164 | 1/1 | 0.78 | 0.21 | - | 106,106,106,106 | 0 |
| 60 | MG | CA | 3241 | 1/1 | 0.74 | 0.19 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3482 | 1/1 | 0.89 | 0.26 | - | 46,46,46,46 | 0 |
| 60 | MG | CA | 3561 | 1/1 | 0.96 | 0.12 | - | 62,62,62,62 | 0 |
| 60 | MG | BA | 1795 | 1/1 | 0.98 | 0.15 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3593 | 1/1 | 0.93 | 0.11 | - | 62,62,62,62 | 0 |
| 60 | MG | CA | 3125 | 1/1 | 0.93 | 0.48 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3537 | 1/1 | 0.70 | 0.12 | - | 90,90,90,90 | 0 |
| 60 | MG | BX | 104 | 1/1 | 0.91 | 0.20 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3397 | 1/1 | 0.85 | 0.10 | - | 80,80,80,80 | 0 |
| 60 | MG | AA | 3786 | 1/1 | 0.97 | 0.19 | - | 57,57,57,57 | 0 |
| 60 | MG | CA | 3168 | 1/1 | 0.91 | 0.23 | - | 65,65,65,65 | 0 |
| 60 | MG | DA | 1749 | 1/1 | 0.83 | 0.23 | - | 72,72,72,72 | 0 |
| 60 | MG | BA | 1764 | 1/1 | 0.97 | 0.16 | - | 55,55,55,55 | 0 |
| 60 | MG | AQ | 3002 | 1/1 | 0.72 | 0.31 | - | 79,79,79,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3532 | 1/1 | 0.82 | 0.16 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3276 | 1/1 | 0.87 | 0.17 | - | 32,32,32,32 | 0 |
| 60 | MG | AA | 3158 | 1/1 | 0.87 | 0.37 | - | 50,50,50,50 | 0 |
| 60 | MG | AA | 3515 | 1/1 | 0.94 | 0.14 | - | 27,27,27,27 | 0 |
| 60 | MG | BA | 1766 | 1/1 | 0.83 | 0.16 | - | 81,81,81,81 | 0 |
| 60 | MG | AA | 3639 | 1/1 | 0.82 | 0.23 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3557 | 1/1 | 0.97 | 0.17 | - | 21,21,21,21 | 0 |
| 60 | MG | CA | 3603 | 1/1 | 0.90 | 0.28 | - | 93,93,93,93 | 0 |
| 60 | MG | BX | 110 | 1/1 | 0.89 | 0.14 | - | 67,67,67,67 | 0 |
| 60 | MG | CA | 3078 | 1/1 | 0.94 | 0.14 | - | 49,49,49,49 | 0 |
| 60 | MG | BA | 1809 | 1/1 | 0.91 | 0.18 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3629 | 1/1 | 0.96 | 0.11 | - | 51,51,51,51 | 0 |
| 60 | MG | DA | 1649 | 1/1 | 0.94 | 0.30 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3195 | 1/1 | 0.86 | 0.20 | - | 55,55,55,55 | 0 |
| 60 | MG | BA | 1639 | 1/1 | 0.98 | 0.37 | - | 42,42,42,42 | 0 |
| 60 | MG | AA | 3193 | 1/1 | 0.97 | 0.20 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3699 | 1/1 | 0.96 | 0.22 | - | 61,61,61,61 | 0 |
| 60 | MG | BZ | 701 | 1/1 | 0.97 | 0.20 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3610 | 1/1 | 0.92 | 0.45 | - | 94,94,94,94 | 0 |
| 60 | MG | AA | 3344 | 1/1 | 0.95 | 0.18 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3466 | 1/1 | 0.91 | 0.17 | - | 48,48,48,48 | 0 |
| 60 | MG | BA | 1774 | 1/1 | 0.88 | 0.09 | - | 79,79,79,79 | 0 |
| 60 | MG | AA | 3536 | 1/1 | 0.96 | 0.09 | - | 36,36,36,36 | 0 |
| 60 | MG | AA | 3632 | 1/1 | 0.70 | 0.27 | - | 97,97,97,97 | 0 |
| 60 | MG | AA | 3013 | 1/1 | 0.97 | 0.14 | - | 38,38,38,38 | 0 |
| 60 | MG | AA | 3821 | 1/1 | 0.93 | 0.13 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3527 | 1/1 | 0.34 | 0.38 | - | 83,83,83,83 | 0 |
| 60 | MG | AA | 3625 | 1/1 | 0.66 | 0.30 | - | 88,88,88,88 | 0 |
| 60 | MG | AA | 3314 | 1/1 | 0.95 | 0.20 | - | 43,43,43,43 | 0 |
| 60 | MG | AA | 3644 | 1/1 | 0.87 | 0.21 | - | 74,74,74,74 | 0 |
| 60 | MG | BA | 1668 | 1/1 | 0.91 | 0.18 | - | 72,72,72,72 | 0 |
| 60 | MG | DA | 1756 | 1/1 | 0.94 | 0.24 | - | 60,60,60,60 | 0 |
| 60 | MG | BA | 1695 | 1/1 | 0.96 | 0.06 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3480 | 1/1 | 0.77 | 0.13 | - | 78,78,78,78 | 0 |
| 60 | MG | AA | 3811 | 1/1 | 0.91 | 0.59 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3474 | 1/1 | 0.94 | 0.14 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3345 | 1/1 | 0.96 | 0.19 | - | 41,41,41,41 | 0 |
| 60 | MG | CA | 3350 | 1/1 | 0.92 | 0.07 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3016 | 1/1 | 0.66 | 0.48 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3481 | 1/1 | 0.51 | 0.24 | - | 86,86,86,86 | 0 |
| 60 | MG | CA | 3150 | 1/1 | 0.92 | 0.12 | - | 52,52,52,52 | 0 |
| 60 | MG | CA | 3056 | 1/1 | 0.93 | 0.34 | - | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3385 | 1/1 | 0.99 | 0.26 | - | 48,48,48,48 | 0 |
| 60 | MG | CA | 3234 | 1/1 | 0.70 | 0.36 | - | 96,96,96,96 | 0 |
| 60 | MG | AA | 3489 | 1/1 | 0.83 | 0.32 | - | 39,39,39,39 | 0 |
| 60 | MG | CA | 3566 | 1/1 | 0.92 | 0.24 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3442 | 1/1 | 0.88 | 0.13 | - | 70,70,70,70 | 0 |
| 60 | MG | AW | 3004 | 1/1 | 0.96 | 0.14 | - | 45,45,45,45 | 0 |
| 60 | MG | DA | 1762 | 1/1 | 0.69 | 0.16 | - | 86,86,86,86 | 0 |
| 60 | MG | AA | 3392 | 1/1 | 0.93 | 0.17 | - | 31,31,31,31 | 0 |
| 60 | MG | CA | 3505 | 1/1 | 0.76 | 0.25 | - | 66,66,66,66 | 0 |
| 60 | MG | BX | 108 | 1/1 | 0.96 | 0.10 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3632 | 1/1 | 0.98 | 0.15 | - | 55,55,55,55 | 0 |
| 60 | MG | CA | 3204 | 1/1 | 0.89 | 0.25 | - | 88,88,88,88 | 0 |
| 60 | MG | DA | 1715 | 1/1 | 0.42 | 0.46 | - | 87,87,87,87 | 0 |
| 60 | MG | AA | 3411 | 1/1 | 0.97 | 0.15 | - | 21,21,21,21 | 0 |
| 60 | MG | AA | 3555 | 1/1 | 0.97 | 0.16 | - | 57,57,57,57 | 0 |
| 60 | MG | AA | 3327 | 1/1 | 0.55 | 0.23 | - | 36,36,36,36 | 0 |
| 60 | MG | CA | 3091 | 1/1 | 0.77 | 0.40 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3567 | 1/1 | 0.92 | 0.14 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3506 | 1/1 | 0.65 | 0.25 | - | 120,120,120,120 | 0 |
| 60 | MG | CA | 3433 | 1/1 | 0.95 | 0.15 | - | 45,45,45,45 | 0 |
| 60 | MG | BA | 1743 | 1/1 | 0.97 | 0.08 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3077 | 1/1 | 0.94 | 0.26 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3383 | 1/1 | 0.93 | 0.21 | - | 31,31,31,31 | 0 |
| 60 | MG | AA | 3519 | 1/1 | 0.97 | 0.13 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3560 | 1/1 | 0.97 | 0.20 | - | 49,49,49,49 | 0 |
| 60 | MG | CB | 3003 | 1/1 | 0.98 | 0.13 | - | 61,61,61,61 | 0 |
| 60 | MG | DA | 1605 | 1/1 | 0.91 | 0.29 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3590 | 1/1 | 0.70 | 0.53 | - | 78,78,78,78 | 0 |
| 60 | MG | CA | 3257 | 1/1 | 0.90 | 0.14 | - | 45,45,45,45 | 0 |
| 60 | MG | AA | 3117 | 1/1 | 0.95 | 0.17 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3030 | 1/1 | 0.82 | 0.43 | - | 52,52,52,52 | 0 |
| 60 | MG | AA | 3304 | 1/1 | 0.99 | 0.17 | - | 44,44,44,44 | 0 |
| 60 | MG | AA | 3204 | 1/1 | 0.81 | 0.45 | - | 83,83,83,83 | 0 |
| 60 | MG | BA | 1610 | 1/1 | 0.95 | 0.14 | - | 112,112,112,112 | 0 |
| 60 | MG | AA | 3271 | 1/1 | 0.58 | 0.28 | - | 81,81,81,81 | 0 |
| 60 | MG | AA | 3435 | 1/1 | 0.91 | 0.27 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3324 | 1/1 | 0.67 | 0.10 | - | 69,69,69,69 | 0 |
| 60 | MG | AA | 3348 | 1/1 | 0.95 | 0.30 | - | 39,39,39,39 | 0 |
| 60 | MG | AA | 3256 | 1/1 | 0.94 | 0.18 | - | 24,24,24,24 | 0 |
| 60 | MG | CA | 3564 | 1/1 | 0.94 | 0.28 | - | 33,33,33,33 | 0 |
| 60 | MG | CA | 3292 | 1/1 | 0.93 | 0.15 | - | 56,56,56,56 | 0 |
| 60 | MG | AA | 3569 | 1/1 | 0.96 | 0.19 | - | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | CA | 3600 | 1/1 | 0.98 | 0.12 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3203 | 1/1 | 0.35 | 1.03 | - | 125,125,125,125 | 0 |
| 60 | MG | CA | 3477 | 1/1 | 0.89 | 0.24 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3254 | 1/1 | 0.91 | 0.29 | - | 47,47,47,47 | 0 |
| 60 | MG | AA | 3319 | 1/1 | 0.98 | 0.17 | - | 28,28,28,28 | 0 |
| 60 | MG | BA | 1659 | 1/1 | 0.92 | 0.32 | - | 68,68,68,68 | 0 |
| 60 | MG | DA | 1660 | 1/1 | 0.95 | 0.29 | - | 81,81,81,81 | 0 |
| 60 | MG | CA | 3045 | 1/1 | 0.87 | 0.23 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3594 | 1/1 | 0.96 | 0.26 | - | 48,48,48,48 | 0 |
| 60 | MG | AA | 3511 | 1/1 | 0.93 | 0.26 | - | 84,84,84,84 | 0 |
| 60 | MG | AA | 3413 | 1/1 | 0.83 | 0.15 | - | 34,34,34,34 | 0 |
| 60 | MG | BA | 1812 | 1/1 | 0.93 | 0.16 | - | 47,47,47,47 | 0 |
| 60 | MG | CA | 3247 | 1/1 | 0.75 | 0.16 | - | 45,45,45,45 | 0 |
| 60 | MG | AA | 3100 | 1/1 | 0.96 | 0.21 | - | 34,34,34,34 | 0 |
| 60 | MG | AA | 3085 | 1/1 | 0.96 | 0.25 | - | 80,80,80,80 | 0 |
| 60 | MG | AA | 3728 | 1/1 | 0.90 | 0.27 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3301 | 1/1 | 0.98 | 0.17 | - | 59,59,59,59 | 0 |
| 60 | MG | CA | 3303 | 1/1 | 0.72 | 0.28 | - | 52,52,52,52 | 0 |
| 60 | MG | DA | 1754 | 1/1 | 0.92 | 0.23 | - | 77,77,77,77 | 0 |
| 60 | MG | BA | 1769 | 1/1 | 0.98 | 0.26 | - | 80,80,80,80 | 0 |
| 60 | MG | DW | 3001 | 1/1 | 0.75 | 0.80 | - | 90,90,90,90 | 0 |
| 60 | MG | AA | 3362 | 1/1 | 0.88 | 0.21 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3199 | 1/1 | 0.67 | 0.57 | - | 92,92,92,92 | 0 |
| 60 | MG | AA | 3805 | 1/1 | 0.38 | 1.55 | - | 117,117,117,117 | 0 |
| 60 | MG | CA | 3244 | 1/1 | 0.69 | 0.32 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3516 | 1/1 | 0.95 | 0.20 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3128 | 1/1 | 0.97 | 0.47 | - | 53,53,53,53 | 1 |
| 60 | MG | DA | 1687 | 1/1 | 0.93 | 0.25 | - | 60,60,60,60 | 0 |
| 60 | MG | AA | 3209 | 1/1 | 0.91 | 0.26 | - | 64,64,64,64 | 0 |
| 60 | MG | AA | 3263 | 1/1 | 0.68 | 0.44 | - | 75,75,75,75 | 0 |
| 60 | MG | AA | 3402 | 1/1 | 0.90 | 0.33 | - | 53,53,53,53 | 0 |
| 60 | MG | AA | 3615 | 1/1 | 0.84 | 0.39 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3194 | 1/1 | 0.74 | 0.55 | - | 87,87,87,87 | 0 |
| 60 | MG | CA | 3606 | 1/1 | 0.89 | 0.27 | - | 58,58,58,58 | 0 |
| 60 | MG | AA | 3726 | 1/1 | 0.96 | 0.13 | - | 74,74,74,74 | 0 |
| 60 | MG | DA | 1666 | 1/1 | 0.89 | 0.19 | - | 45,45,45,45 | 0 |
| 60 | MG | CA | 3063 | 1/1 | 0.66 | 0.71 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3020 | 1/1 | 0.96 | 0.18 | - | 38,38,38,38 | 0 |
| 60 | MG | AA | 3157 | 1/1 | 0.89 | 0.33 | - | 93,93,93,93 | 0 |
| 60 | MG | AA | 3657 | 1/1 | 0.80 | 0.11 | - | 73,73,73,73 | 0 |
| 60 | MG | CA | 3225 | 1/1 | 0.95 | 0.24 | - | 73,73,73,73 | 0 |
| 60 | MG | BA | 1802 | 1/1 | 0.94 | 0.13 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 60 | MG | AA | 3237 | 1/1 | 0.85 | 0.08 | - | 51,51,51,51 | 0 |
| 60 | MG | AA | 3573 | 1/1 | 0.94 | 0.09 | - | 47,47,47,47 | 0 |
| 60 | MG | BA | 1666 | 1/1 | 0.87 | 0.33 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3457 | 1/1 | 0.88 | 0.21 | - | 60,60,60,60 | 0 |
| 60 | MG | CA | 3429 | 1/1 | 0.93 | 0.23 | - | 80,80,80,80 | 0 |
| 60 | MG | AA | 3647 | 1/1 | 0.96 | 0.14 | - | 35,35,35,35 | 0 |
| 60 | MG | DA | 1736 | 1/1 | 0.96 | 0.17 | - | 63,63,63,63 | 0 |
| 60 | MG | DA | 1690 | 1/1 | 0.95 | 0.20 | - | 74,74,74,74 | 0 |
| 60 | MG | CA | 3058 | 1/1 | 0.85 | 0.44 | - | 74,74,74,74 | 0 |
| 60 | MG | AA | 3095 | 1/1 | 0.89 | 0.16 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3375 | 1/1 | 0.96 | 0.09 | - | 65,65,65,65 | 0 |
| 60 | MG | AA | 3063 | 1/1 | 0.89 | 0.17 | - | 46,46,46,46 | 0 |
| 60 | MG | CA | 3406 | 1/1 | 0.93 | 0.08 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3421 | 1/1 | 0.91 | 0.12 | - | 73,73,73,73 | 0 |
| 60 | MG | AA | 3665 | 1/1 | 0.96 | 0.06 | - | 63,63,63,63 | 0 |
| 60 | MG | CA | 3364 | 1/1 | 0.94 | 0.18 | - | 64,64,64,64 | 0 |
| 60 | MG | CA | 3494 | 1/1 | 0.87 | 0.17 | - | 58,58,58,58 | 0 |
| 60 | MG | CA | 3048 | 1/1 | 0.92 | 0.30 | - | 48,48,48,48 | 0 |
| 60 | MG | CA | 3570 | 1/1 | 0.94 | 0.09 | - | 61,61,61,61 | 0 |
| 60 | MG | BA | 1761 | 1/1 | 0.92 | 0.18 | - | 74,74,74,74 | 0 |
| 60 | MG | DA | 1632 | 1/1 | 0.93 | 0.20 | - | 77,77,77,77 | 0 |
| 60 | MG | CA | 3066 | 1/1 | 0.92 | 0.42 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3322 | 1/1 | 0.90 | 0.28 | - | 41,41,41,41 | 0 |
| 60 | MG | CA | 3575 | 1/1 | 0.62 | 0.47 | - | 77,77,77,77 | 0 |
| 60 | MG | DA | 1732 | 1/1 | 0.96 | 0.11 | - | 54,54,54,54 | 0 |
| 60 | MG | AA | 3054 | 1/1 | 0.93 | 0.28 | - | 26,26,26,26 | 0 |
| 60 | MG | CA | 3581 | 1/1 | 0.54 | 0.22 | - | 100,100,100,100 | 0 |
| 61 | K | AA | 3814 | 1/1 | 0.91 | 0.27 | - | 87,87,87,87 | 0 |
| 60 | MG | BA | 1614 | 1/1 | 0.92 | 0.18 | - | 70,70,70,70 | 0 |
| 60 | MG | AA | 3252 | 1/1 | 0.83 | 0.37 | - | 76,76,76,76 | 0 |
| 60 | MG | DA | 1730 | 1/1 | 0.93 | 0.39 | - | 65,65,65,65 | 0 |
| 60 | MG | CA | 3427 | 1/1 | 0.95 | 0.29 | - | 69,69,69,69 | 0 |
| 60 | MG | CA | 3239 | 1/1 | 0.65 | 0.32 | - | 76,76,76,76 | 0 |
| 60 | MG | CD | 303 | 1/1 | 0.90 | 0.14 | - | 70,70,70,70 | 0 |
| 60 | MG | CA | 3533 | 1/1 | 0.84 | 0.14 | - | 63,63,63,63 | 0 |
| 60 | MG | AA | 3546 | 1/1 | 0.95 | 0.17 | - | 36,36,36,36 | 0 |
| 60 | MG | AA | 3056 | 1/1 | 0.82 | 0.49 | - | 72,72,72,72 | 0 |
| 60 | MG | AA | 3094 | 1/1 | 0.96 | 0.31 | - | 82,82,82,82 | 0 |
| 60 | MG | AA | 3239 | 1/1 | 0.96 | 0.21 | - | 63,63,63,63 | 0 |
| 60 | MG | BA | 1738 | 1/1 | 0.91 | 0.23 | - | 55,55,55,55 | 0 |
| 60 | MG | AA | 3353 | 1/1 | 0.88 | 0.11 | - | 68,68,68,68 | 0 |
| 60 | MG | AA | 3416 | 1/1 | 0.95 | 0.19 | - | 31,31,31,31 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.