



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:04 PM GMT

PDB ID : 4V8J
Title : Crystal structure of the bacterial ribosome ram mutation G347U.
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2011-12-20
Resolution : 3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

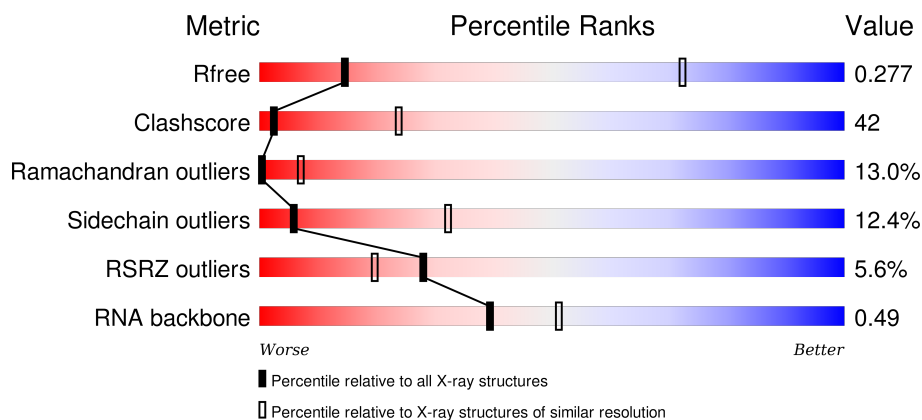
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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 | 1014 (4.28-3.52) |
| Clashscore | 102246 | 1031 (4.24-3.56) |
| Ramachandran outliers | 100387 | 1012 (4.26-3.54) |
| Sidechain outliers | 100360 | 1004 (4.26-3.54) |
| RSRZ outliers | 91569 | 1018 (4.28-3.52) |
| RNA backbone | 2183 | 1078 (5.00-2.80) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AA | 1522 | <div> <div>4%</div> <div>35%</div> <div>52%</div> <div>12%</div> <div>..</div> </div> |
| 1 | CA | 1522 | <div> <div>3%</div> <div>34%</div> <div>51%</div> <div>13%</div> <div>..</div> </div> |
| 2 | AB | 256 | <div> <div>4%</div> <div>20%</div> <div>57%</div> <div>14%</div> <div>8%</div> </div> |
| 2 | CB | 256 | <div> <div>4%</div> <div>18%</div> <div>60%</div> <div>13%</div> <div>8%</div> </div> |

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CO | 89 | |
| 16 | AP | 88 | |
| 16 | CP | 88 | |
| 17 | AQ | 105 | |
| 17 | CQ | 105 | |
| 18 | AR | 88 | |
| 18 | CR | 88 | |
| 19 | AS | 93 | |
| 19 | CS | 93 | |
| 20 | AT | 106 | |
| 20 | CT | 106 | |
| 21 | AU | 27 | |
| 21 | CU | 27 | |
| 22 | AW | 76 | |
| 22 | AY | 76 | |
| 22 | CW | 76 | |
| 22 | CY | 76 | |
| 23 | AV | 77 | |
| 23 | CV | 77 | |
| 24 | AX | 24 | |
| 24 | CX | 24 | |
| 25 | BA | 2916 | |
| 25 | DA | 2916 | |
| 26 | BB | 122 | |
| 26 | DB | 122 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27 | BC | 229 | |
| 27 | DC | 229 | |
| 28 | BD | 276 | |
| 28 | DD | 276 | |
| 29 | BE | 206 | |
| 29 | DE | 206 | |
| 30 | BF | 210 | |
| 30 | DF | 210 | |
| 31 | BG | 182 | |
| 31 | DG | 182 | |
| 32 | BH | 180 | |
| 32 | DH | 180 | |
| 33 | BI | 148 | |
| 33 | DI | 148 | |
| 34 | BN | 140 | |
| 34 | DN | 140 | |
| 35 | BO | 122 | |
| 35 | DO | 122 | |
| 36 | BP | 150 | |
| 36 | DP | 150 | |
| 37 | BQ | 141 | |
| 37 | DQ | 141 | |
| 38 | BR | 118 | |
| 38 | DR | 118 | |
| 39 | BS | 112 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39 | DS | 112 | |
| 40 | BT | 146 | |
| 40 | DT | 146 | |
| 41 | BU | 118 | |
| 41 | DU | 118 | |
| 42 | BV | 101 | |
| 42 | DV | 101 | |
| 43 | BW | 113 | |
| 43 | DW | 113 | |
| 44 | BX | 96 | |
| 44 | DX | 96 | |
| 45 | BY | 110 | |
| 45 | DY | 110 | |
| 46 | BZ | 206 | |
| 46 | DZ | 206 | |
| 47 | B0 | 85 | |
| 47 | D0 | 85 | |
| 48 | B1 | 98 | |
| 48 | D1 | 98 | |
| 49 | B2 | 72 | |
| 49 | D2 | 72 | |
| 50 | B3 | 60 | |
| 50 | D3 | 60 | |
| 51 | B4 | 71 | |
| 51 | D4 | 71 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52 | B5 | 60 | |
| 52 | D5 | 60 | |
| 53 | B6 | 54 | |
| 53 | D6 | 54 | |
| 54 | B7 | 49 | |
| 54 | D7 | 49 | |
| 55 | B8 | 65 | |
| 55 | D8 | 65 | |
| 56 | B9 | 37 | |
| 56 | D9 | 37 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | AA | 1604 | - | - | - | X |
| 57 | MG | AA | 1606 | - | - | - | X |
| 57 | MG | AA | 1609 | - | - | - | X |
| 57 | MG | AA | 1611 | - | - | - | X |
| 57 | MG | AA | 1615 | - | - | - | X |
| 57 | MG | AA | 1616 | - | - | - | X |
| 57 | MG | AA | 1617 | - | - | - | X |
| 57 | MG | AA | 1624 | - | - | - | X |
| 57 | MG | AA | 1635 | - | - | - | X |
| 57 | MG | AA | 1639 | - | - | - | X |
| 57 | MG | AA | 1644 | - | - | - | X |
| 57 | MG | AA | 1650 | - | - | - | X |
| 57 | MG | AA | 1653 | - | - | - | X |
| 57 | MG | AA | 1657 | - | - | - | X |
| 57 | MG | AA | 1664 | - | - | - | X |
| 57 | MG | AA | 1667 | - | - | - | X |
| 57 | MG | AA | 1671 | - | - | - | X |
| 57 | MG | AA | 1691 | - | - | - | X |
| 57 | MG | AA | 1692 | - | - | - | X |
| 57 | MG | BA | 3002 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | BA | 3003 | - | - | - | X |
| 57 | MG | BA | 3007 | - | - | - | X |
| 57 | MG | BA | 3019 | - | - | - | X |
| 57 | MG | BA | 3020 | - | - | - | X |
| 57 | MG | BA | 3035 | - | - | - | X |
| 57 | MG | BA | 3036 | - | - | - | X |
| 57 | MG | BA | 3046 | - | - | - | X |
| 57 | MG | BA | 3047 | - | - | - | X |
| 57 | MG | BA | 3048 | - | - | - | X |
| 57 | MG | BA | 3051 | - | - | - | X |
| 57 | MG | BA | 3053 | - | - | - | X |
| 57 | MG | BA | 3055 | - | - | - | X |
| 57 | MG | BA | 3061 | - | - | X | - |
| 57 | MG | BA | 3062 | - | - | X | - |
| 57 | MG | BA | 3067 | - | - | - | X |
| 57 | MG | BA | 3070 | - | - | - | X |
| 57 | MG | BA | 3074 | - | - | - | X |
| 57 | MG | BA | 3075 | - | - | - | X |
| 57 | MG | BA | 3079 | - | - | - | X |
| 57 | MG | BA | 3081 | - | - | - | X |
| 57 | MG | BA | 3089 | - | - | - | X |
| 57 | MG | BA | 3091 | - | - | - | X |
| 57 | MG | BA | 3093 | - | - | - | X |
| 57 | MG | BA | 3094 | - | - | - | X |
| 57 | MG | BA | 3095 | - | - | - | X |
| 57 | MG | BA | 3103 | - | - | - | X |
| 57 | MG | BA | 3104 | - | - | - | X |
| 57 | MG | BA | 3113 | - | - | - | X |
| 57 | MG | BA | 3114 | - | - | - | X |
| 57 | MG | BA | 3117 | - | - | - | X |
| 57 | MG | BA | 3125 | - | - | - | X |
| 57 | MG | BA | 3138 | - | - | - | X |
| 57 | MG | BA | 3139 | - | - | - | X |
| 57 | MG | BA | 3140 | - | - | - | X |
| 57 | MG | BA | 3141 | - | - | - | X |
| 57 | MG | BA | 3142 | - | - | - | X |
| 57 | MG | BA | 3146 | - | - | - | X |
| 57 | MG | BA | 3150 | - | - | - | X |
| 57 | MG | BA | 3151 | - | - | - | X |
| 57 | MG | BA | 3152 | - | - | - | X |
| 57 | MG | BA | 3157 | - | - | - | X |
| 57 | MG | BA | 3161 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | BA | 3166 | - | - | - | X |
| 57 | MG | BA | 3173 | - | - | - | X |
| 57 | MG | BA | 3174 | - | - | - | X |
| 57 | MG | BA | 3183 | - | - | - | X |
| 57 | MG | BA | 3194 | - | - | - | X |
| 57 | MG | BA | 3197 | - | - | - | X |
| 57 | MG | BA | 3201 | - | - | - | X |
| 57 | MG | BA | 3214 | - | - | - | X |
| 57 | MG | BA | 3215 | - | - | - | X |
| 57 | MG | BA | 3221 | - | - | X | - |
| 57 | MG | BA | 3227 | - | - | - | X |
| 57 | MG | BA | 3233 | - | - | - | X |
| 57 | MG | BA | 3239 | - | - | - | X |
| 57 | MG | BA | 3240 | - | - | - | X |
| 57 | MG | BA | 3247 | - | - | - | X |
| 57 | MG | BA | 3251 | - | - | - | X |
| 57 | MG | BA | 3257 | - | - | - | X |
| 57 | MG | BU | 201 | - | - | - | X |
| 57 | MG | CA | 1602 | - | - | - | X |
| 57 | MG | CA | 1603 | - | - | - | X |
| 57 | MG | CA | 1613 | - | - | - | X |
| 57 | MG | CA | 1615 | - | - | - | X |
| 57 | MG | CA | 1619 | - | - | - | X |
| 57 | MG | CA | 1620 | - | - | - | X |
| 57 | MG | CA | 1622 | - | - | - | X |
| 57 | MG | CA | 1626 | - | - | - | X |
| 57 | MG | CA | 1629 | - | - | - | X |
| 57 | MG | CA | 1640 | - | - | - | X |
| 57 | MG | CA | 1648 | - | - | - | X |
| 57 | MG | CA | 1650 | - | - | - | X |
| 57 | MG | CA | 1651 | - | - | - | X |
| 57 | MG | CA | 1652 | - | - | - | X |
| 57 | MG | CA | 1653 | - | - | - | X |
| 57 | MG | CA | 1659 | - | - | - | X |
| 57 | MG | CA | 1663 | - | - | - | X |
| 57 | MG | CA | 1666 | - | - | - | X |
| 57 | MG | CA | 1670 | - | - | - | X |
| 57 | MG | CA | 1673 | - | - | - | X |
| 57 | MG | CA | 1689 | - | - | - | X |
| 57 | MG | CA | 1690 | - | - | - | X |
| 57 | MG | CA | 1694 | - | - | - | X |
| 57 | MG | D0 | 101 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | D5 | 102 | - | - | - | X |
| 57 | MG | DA | 3004 | - | - | - | X |
| 57 | MG | DA | 3005 | - | - | - | X |
| 57 | MG | DA | 3007 | - | - | - | X |
| 57 | MG | DA | 3009 | - | - | - | X |
| 57 | MG | DA | 3018 | - | - | - | X |
| 57 | MG | DA | 3019 | - | - | - | X |
| 57 | MG | DA | 3020 | - | - | - | X |
| 57 | MG | DA | 3023 | - | - | - | X |
| 57 | MG | DA | 3033 | - | - | - | X |
| 57 | MG | DA | 3035 | - | - | - | X |
| 57 | MG | DA | 3043 | - | - | - | X |
| 57 | MG | DA | 3044 | - | - | - | X |
| 57 | MG | DA | 3045 | - | - | - | X |
| 57 | MG | DA | 3046 | - | - | - | X |
| 57 | MG | DA | 3047 | - | - | - | X |
| 57 | MG | DA | 3048 | - | - | - | X |
| 57 | MG | DA | 3050 | - | - | - | X |
| 57 | MG | DA | 3051 | - | - | - | X |
| 57 | MG | DA | 3055 | - | - | - | X |
| 57 | MG | DA | 3056 | - | - | - | X |
| 57 | MG | DA | 3059 | - | - | - | X |
| 57 | MG | DA | 3061 | - | - | - | X |
| 57 | MG | DA | 3062 | - | - | - | X |
| 57 | MG | DA | 3063 | - | - | - | X |
| 57 | MG | DA | 3064 | - | - | - | X |
| 57 | MG | DA | 3068 | - | - | - | X |
| 57 | MG | DA | 3070 | - | - | - | X |
| 57 | MG | DA | 3072 | - | - | - | X |
| 57 | MG | DA | 3073 | - | - | - | X |
| 57 | MG | DA | 3080 | - | - | - | X |
| 57 | MG | DA | 3082 | - | - | - | X |
| 57 | MG | DA | 3084 | - | - | - | X |
| 57 | MG | DA | 3086 | - | - | - | X |
| 57 | MG | DA | 3087 | - | - | - | X |
| 57 | MG | DA | 3088 | - | - | - | X |
| 57 | MG | DA | 3092 | - | - | - | X |
| 57 | MG | DA | 3098 | - | - | - | X |
| 57 | MG | DA | 3099 | - | - | - | X |
| 57 | MG | DA | 3100 | - | - | - | X |
| 57 | MG | DA | 3103 | - | - | - | X |
| 57 | MG | DA | 3107 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | DA | 3108 | - | - | - | X |
| 57 | MG | DA | 3109 | - | - | - | X |
| 57 | MG | DA | 3112 | - | - | - | X |
| 57 | MG | DA | 3114 | - | - | - | X |
| 57 | MG | DA | 3117 | - | - | - | X |
| 57 | MG | DA | 3119 | - | - | - | X |
| 57 | MG | DA | 3120 | - | - | - | X |
| 57 | MG | DA | 3122 | - | - | - | X |
| 57 | MG | DA | 3123 | - | - | - | X |
| 57 | MG | DA | 3127 | - | - | - | X |
| 57 | MG | DA | 3128 | - | - | - | X |
| 57 | MG | DA | 3129 | - | - | - | X |
| 57 | MG | DA | 3135 | - | - | - | X |
| 57 | MG | DA | 3138 | - | - | - | X |
| 57 | MG | DA | 3141 | - | - | - | X |
| 57 | MG | DA | 3144 | - | - | - | X |
| 57 | MG | DA | 3145 | - | - | - | X |
| 57 | MG | DA | 3146 | - | - | - | X |
| 57 | MG | DA | 3149 | - | - | - | X |
| 57 | MG | DA | 3155 | - | - | - | X |
| 57 | MG | DA | 3158 | - | - | - | X |
| 57 | MG | DA | 3161 | - | - | - | X |
| 57 | MG | DA | 3169 | - | - | - | X |
| 57 | MG | DA | 3170 | - | - | - | X |
| 57 | MG | DA | 3173 | - | - | - | X |
| 57 | MG | DA | 3174 | - | - | - | X |
| 57 | MG | DA | 3177 | - | - | - | X |
| 57 | MG | DA | 3182 | - | - | - | X |
| 57 | MG | DA | 3183 | - | - | - | X |
| 57 | MG | DA | 3189 | - | - | - | X |
| 57 | MG | DA | 3191 | - | - | - | X |
| 57 | MG | DA | 3194 | - | - | - | X |
| 57 | MG | DA | 3196 | - | - | - | X |
| 57 | MG | DA | 3197 | - | - | - | X |
| 57 | MG | DA | 3201 | - | - | - | X |
| 57 | MG | DA | 3205 | - | - | - | X |
| 57 | MG | DA | 3209 | - | - | - | X |
| 57 | MG | DA | 3211 | - | - | - | X |
| 57 | MG | DA | 3225 | - | - | - | X |
| 57 | MG | DA | 3227 | - | - | - | X |
| 57 | MG | DA | 3228 | - | - | - | X |
| 57 | MG | DA | 3232 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | DA | 3235 | - | - | - | X |
| 57 | MG | DA | 3238 | - | - | - | X |
| 57 | MG | DA | 3245 | - | - | - | X |
| 57 | MG | DA | 3248 | - | - | - | X |
| 57 | MG | DA | 3250 | - | - | - | X |
| 57 | MG | DA | 3251 | - | - | - | X |
| 57 | MG | DA | 3258 | - | - | - | X |
| 57 | MG | DA | 3259 | - | - | - | X |
| 57 | MG | DA | 3262 | - | - | - | X |
| 58 | PAR | AA | 1694 | - | - | - | X |
| 58 | PAR | CA | 1695 | - | - | - | X |
| 59 | ZN | AN | 101 | - | - | X | - |

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 292667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1504 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32326 | 14389 | 5989 | 10445 | 1503 | | | |
| 1 | CA | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32304 | 14379 | 5984 | 10439 | 1502 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|---------------|
| AA | 342 | U | G | ENGINEERED MUTATION | GB AP008226.1 |
| CA | 342 | U | G | ENGINEERED MUTATION | GB AP008226.1 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 235 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1901 | 1213 | 342 | 341 | 5 | | | |
| 2 | CB | 235 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1901 | 1213 | 342 | 341 | 5 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 281 | 1 | | | |
| 3 | CC | 207 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1613 | 1016 | 315 | 281 | 1 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | AD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1703 | 1066 | 339 | 291 | 7 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |
| 5 | CE | 151 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1147 | 724 | 218 | 201 | 4 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |
| 6 | CF | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 843 | 531 | 155 | 154 | 3 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |
| 7 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1257 | 781 | 252 | 218 | 6 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |
| 8 | CH | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1116 | 705 | 215 | 193 | 3 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9 | AI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |
| 9 | CI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1010 | 639 | 197 | 174 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 795 | 499 | 157 | 138 | 1 | | | |
| 10 | CJ | 99 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 795 | 499 | 157 | 138 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |
| 11 | CK | 119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 885 | 549 | 168 | 165 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | | |
| 12 | CL | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 971 | 611 | 196 | 163 | 1 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 988 | 611 | 206 | 169 | 2 | | | |
| 13 | CM | 125 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 988 | 611 | 206 | 169 | 2 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14 | AN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |
| 14 | CN | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 492 | 312 | 104 | 72 | 4 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |
| 15 | CO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 734 | 459 | 147 | 126 | 2 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |
| 16 | CP | 84 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 701 | 443 | 140 | 117 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 100 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |
| 17 | CQ | 100 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 824 | 528 | 152 | 142 | 2 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | AR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 18 | CR | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 79 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 630 | 403 | 115 | 110 | 2 | | | |
| 19 | CS | 79 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 630 | 403 | 115 | 110 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | CT | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 470 | 162 | 129 | 2 | | | |

- Molecule 21 is a protein called 30S ribosomal protein THX.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21 | AU | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |
| 21 | CU | 25 | Total | C | N | O | 0 | 0 | 1 |
| | | | 209 | 128 | 51 | 30 | | | |

- Molecule 22 is a RNA chain called tRNA-Phe.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | AW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1619 | 723 | 290 | 531 | 75 | | | |
| 22 | AY | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 365 | 163 | 68 | 117 | 17 | | | |
| 22 | CW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1619 | 723 | 290 | 531 | 75 | | | |
| 22 | CY | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 365 | 163 | 68 | 117 | 17 | | | |

- Molecule 23 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23 | AV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |
| 23 | CV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1644 | 732 | 297 | 538 | 77 | | | |

- Molecule 24 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 24 | AX | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 169 | 76 | 29 | 56 | 8 | | | |
| 24 | CX | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 210 | 96 | 39 | 66 | 9 | | | |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|------------|------------|-----------|---------|---------|-------|
| 25 | BA | 2803 | Total 60378 | C 26870 | N 11297 | O 19409 | P 2802 | 0 | 0 | 0 |
| 25 | DA | 2803 | Total 60378 | C 26870 | N 11297 | O 19409 | P 2802 | 0 | 0 | 0 |

- Molecule 26 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|---------|-------|
| 26 | BB | 119 | Total 2551 | C 1136 | N 471 | O 826 | P 118 | 0 | 0 | 0 |
| 26 | DB | 119 | Total 2551 | C 1136 | N 471 | O 826 | P 118 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|-------|
| 27 | BC | 191 | Total 1142 | C 691 | N 221 | O 230 | 0 | 0 | 1 |
| 27 | DC | 191 | Total 1142 | C 691 | N 221 | O 230 | 0 | 0 | 1 |

- Molecule 28 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 28 | BD | 272 | Total 2105 | C 1329 | N 417 | O 356 | S 3 | 0 | 0 | 1 |
| 28 | DD | 272 | Total 2105 | C 1329 | N 417 | O 356 | S 3 | 0 | 0 | 1 |

- Molecule 29 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| 29 | BE | 205 | Total 1564 | C 988 | N 300 | O 270 | S 6 | 0 | 0 | 1 |
| 29 | DE | 205 | Total 1564 | C 988 | N 300 | O 270 | S 6 | 0 | 0 | 1 |

- Molecule 30 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 30 | BF | 208 | Total 1624 | C 1035 | N 304 | O 282 | S 3 | 0 | 0 | 1 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30 | DF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 31 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BH | 160 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1223 | 773 | 229 | 220 | 1 | | | |
| 32 | DH | 160 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1223 | 773 | 229 | 220 | 1 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BI | 146 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1132 | 723 | 201 | 207 | 1 | | | |
| 33 | DI | 146 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1132 | 723 | 201 | 207 | 1 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |
| 34 | DN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 35 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |
| 36 | DP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |
| 37 | DQ | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 38 | BR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 38 | DR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39 | BS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |
| 39 | DS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BT | 138 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1142 | 710 | 235 | 196 | 1 | | | |
| 40 | DT | 138 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1142 | 710 | 235 | 196 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 202 | 151 | 1 | | | |
| 41 | DU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 202 | 151 | 1 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 42 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 896 | 563 | 176 | 155 | 2 | | | |
| 43 | DW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 896 | 563 | 176 | 155 | 2 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 44 | BX | 93 | Total | C | N | O | | 0 | 0 | 1 |
| | | | 726 | 471 | 132 | 123 | | | | |
| 44 | DX | 93 | Total | C | N | O | | 0 | 0 | 1 |
| | | | 726 | 471 | 132 | 123 | | | | |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BY | 101 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 776 | 500 | 149 | 123 | 4 | | | |
| 45 | DY | 101 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 776 | 500 | 149 | 123 | 4 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BZ | 177 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1404 | 897 | 253 | 252 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | DZ | 177 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1404 | 897 | 253 | 252 | 2 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | B0 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |
| 47 | D0 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | B1 | 94 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 732 | 460 | 146 | 125 | 1 | | | |
| 48 | D1 | 94 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 732 | 460 | 146 | 125 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | B2 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 370 | 121 | 106 | 1 | | | |
| 49 | D2 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 598 | 370 | 121 | 106 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | B3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |
| 50 | D3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B4 | 31 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 226 | 142 | 37 | 43 | 4 | | | |
| 51 | D4 | 31 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 226 | 142 | 37 | 43 | 4 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 52 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 53 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | B6 | 45 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 381 | 235 | 78 | 64 | 4 | | | |
| 53 | D6 | 45 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 381 | 235 | 78 | 64 | 4 | | | |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | B7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |
| 54 | D7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |
| 55 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |

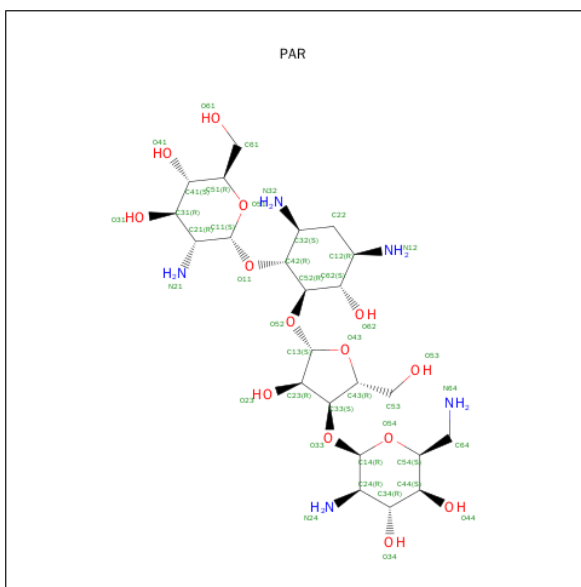
- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 56 | B9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 299 | 183 | 67 | 46 | 3 | | | |
| 56 | D9 | 36 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 299 | 183 | 67 | 46 | 3 | | | |

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 57 | BU | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | BB | 4 | Total 4 Mg 4 | 0 | 0 |
| 57 | BO | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | BA | 261 | Total 261 Mg 261 | 0 | 0 |
| 57 | CA | 94 | Total 94 Mg 94 | 0 | 0 |
| 57 | D0 | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | CV | 2 | Total 2 Mg 2 | 0 | 0 |
| 57 | BF | 2 | Total 2 Mg 2 | 0 | 0 |
| 57 | B3 | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | B5 | 2 | Total 2 Mg 2 | 0 | 0 |
| 57 | BE | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | D5 | 2 | Total 2 Mg 2 | 0 | 0 |
| 57 | AA | 93 | Total 93 Mg 93 | 0 | 0 |
| 57 | B1 | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | DE | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | DA | 268 | Total 268 Mg 268 | 0 | 0 |
| 57 | AX | 2 | Total 2 Mg 2 | 0 | 0 |
| 57 | DD | 1 | Total 1 Mg 1 | 0 | 0 |
| 57 | DB | 2 | Total 2 Mg 2 | 0 | 0 |

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 58 | AA | 1 | Total 42 | C 23 | N 5 | O 14 | 0 | 0 |
| 58 | CA | 1 | Total 42 | C 23 | N 5 | O 14 | 0 | 0 |

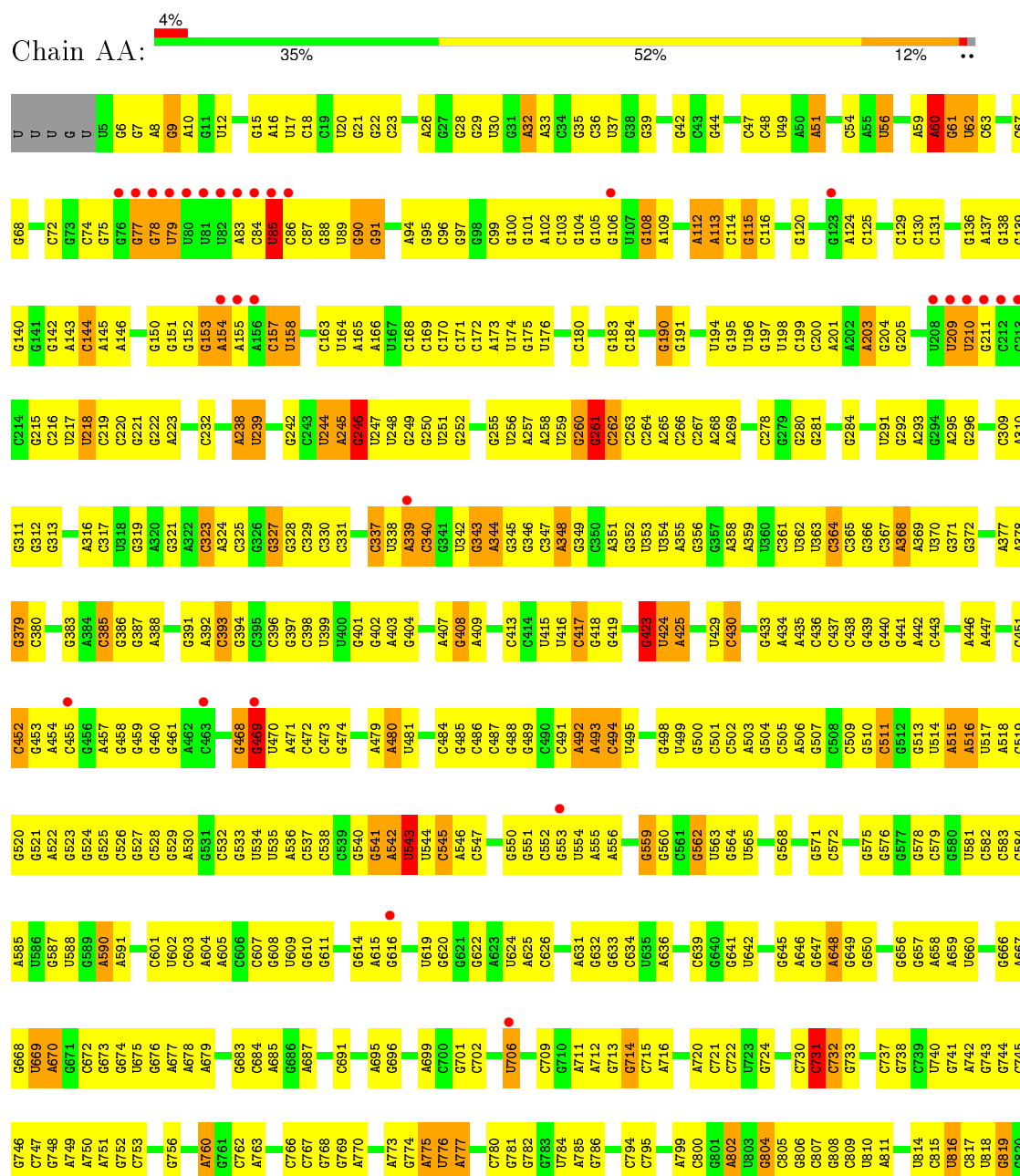
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

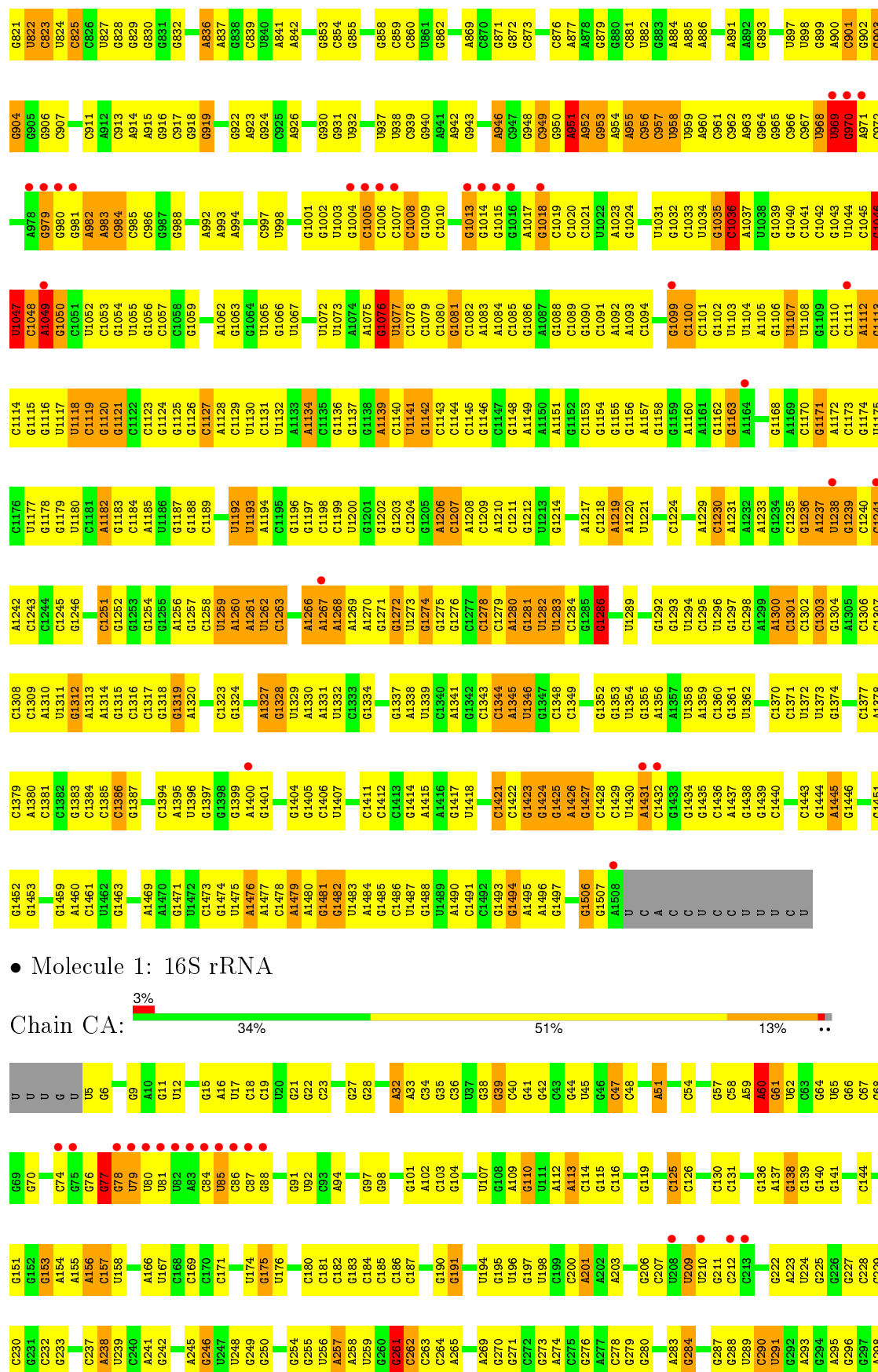
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 59 | CN | 1 | Total Zn 1 1 | 0 | 0 |
| 59 | AD | 1 | Total Zn 1 1 | 0 | 0 |
| 59 | CD | 1 | Total Zn 1 1 | 0 | 0 |
| 59 | AN | 1 | Total Zn 1 1 | 0 | 0 |

3 Residue-property plots

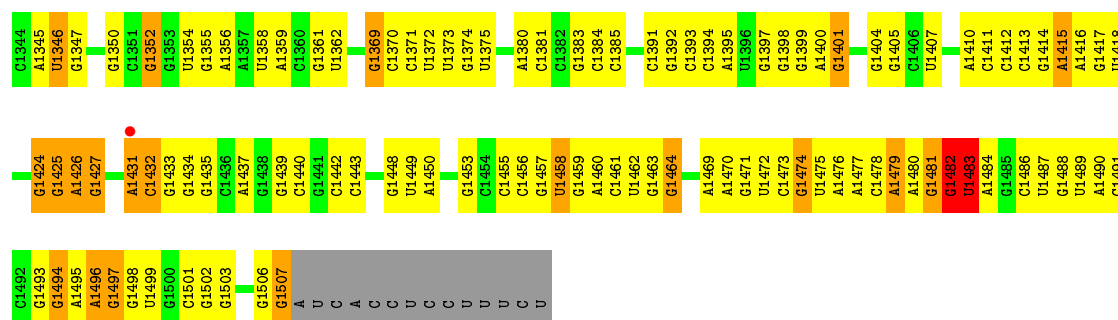
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

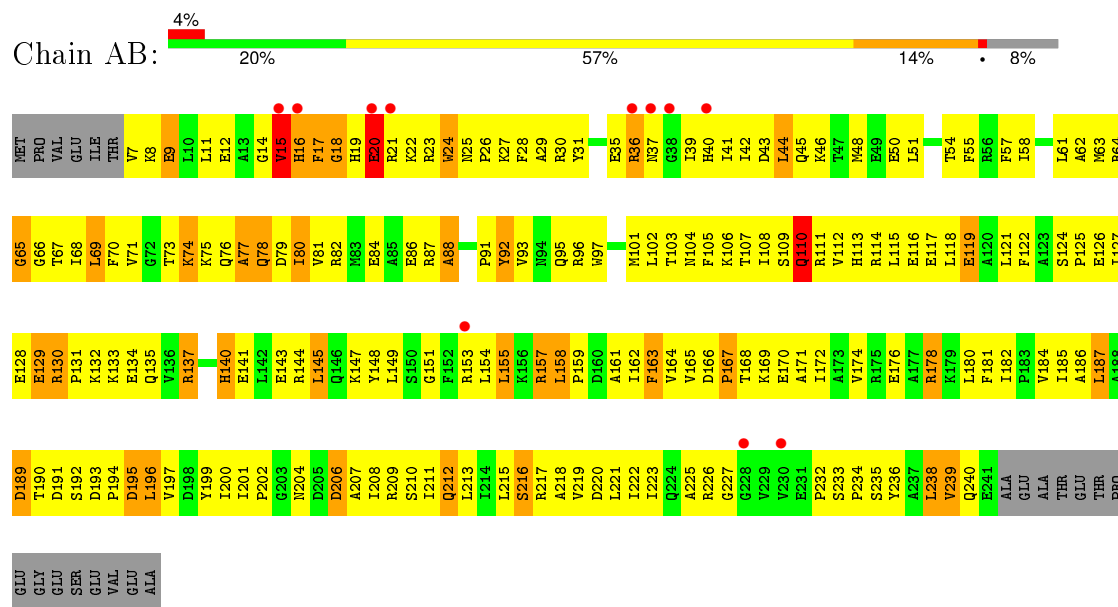




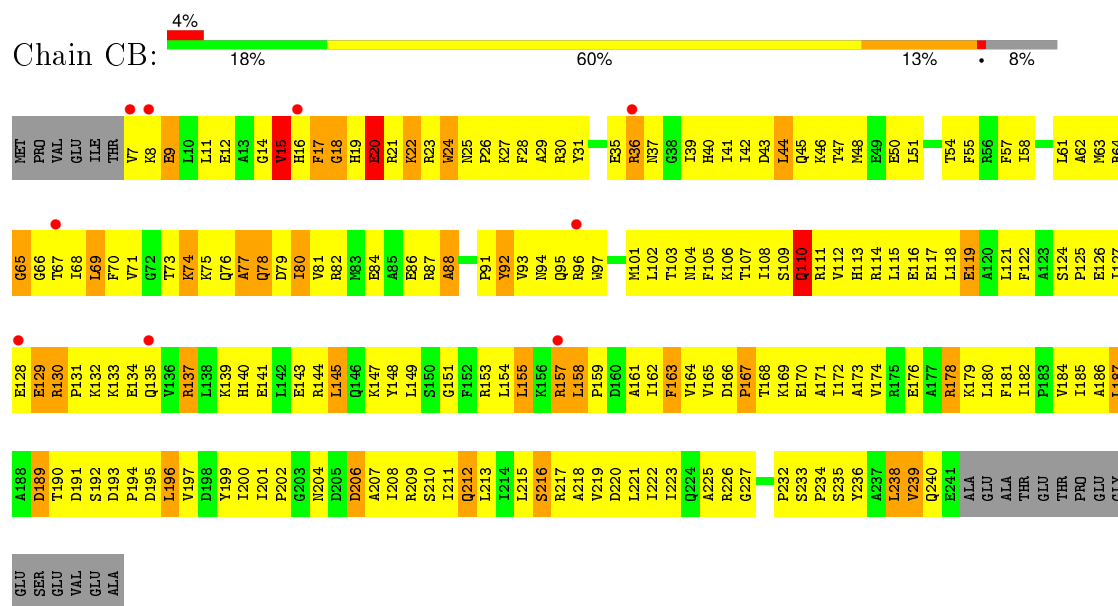
| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|
| C1279 | A1208 | U1141 | A1074 | G1011 | A946 | A884 | G806 | C737 | G665 | C583 | U514 | C443 | G371 | U299 |
| A1280 | C1209 | G1142 | A1075 | A1012 | C947 | A885 | G810 | G738 | G666 | C584 | A515 | A446 | G375 | G300 |
| G1281 | G1143 | C1144 | U1076 | G1013 | G948 | A886 | U810 | C739 | G666 | A516 | U517 | A447 | G376 | G304 |
| U1283 | U1212 | U1213 | U1077 | G1014 | C949 | C987 | G811 | U740 | U669 | A518 | C519 | C451 | A378 | C306 |
| G1286 | C1214 | C1145 | C1078 | G1015 | G950 | U888 | G812 | G741 | A670 | A519 | G520 | C452 | A379 | C307 |
| A1287 | C1215 | G1146 | C1079 | G1016 | A951 | C989 | U816 | A742 | G671 | A590 | G521 | C453 | G380 | A308 |
| U1288 | U1216 | G1147 | A1083 | A1017 | A952 | A890 | U817 | G743 | G672 | A597 | G522 | A454 | C385 | C309 |
| A1289 | A1217 | G1148 | A1084 | C1018 | G953 | A891 | C817 | G744 | G673 | A598 | A522 | C455 | A310 | G311 |
| U1290 | C1218 | A1149 | A954 | C1019 | A954 | A892 | U818 | C745 | G674 | C601 | G523 | C456 | G386 | G312 |
| G1291 | A1150 | A1151 | G1086 | G1020 | A955 | G893 | G819 | G746 | G675 | U602 | G524 | C457 | G387 | G313 |
| A1292 | G1152 | G1087 | A1087 | G1021 | C956 | G894 | G820 | G747 | G676 | C607 | G525 | G458 | G391 | G314 |
| G1293 | C1153 | C1088 | U1022 | U1022 | G957 | A895 | G821 | G748 | A677 | G608 | G526 | G459 | A392 | C315 |
| U1294 | G1154 | C1089 | U1023 | A1024 | U958 | U897 | U822 | A750 | A685 | U609 | G527 | G460 | C393 | A316 |
| C1295 | A1160 | G1090 | C1025 | C1026 | A960 | U898 | C823 | A751 | G686 | U610 | C528 | A466 | C394 | G317 |
| U1296 | A1161 | C1095 | A1026 | A1026 | G961 | G899 | U824 | G752 | A687 | G611 | G530 | A467 | C395 | U318 |
| G1297 | G1162 | C1096 | C1027 | C1027 | G962 | A900 | G828 | G756 | U688 | G612 | G533 | G468 | C396 | G319 |
| C1298 | G1163 | C1096 | A963 | G1028 | G963 | G901 | G829 | G757 | A689 | G613 | U534 | G469 | G397 | A320 |
| A1299 | A1164 | G1099 | G964 | G1029 | G964 | G902 | G830 | G758 | C690 | G614 | U535 | G470 | C398 | G321 |
| C1300 | G1165 | C1100 | G965 | G1030 | G965 | G903 | G831 | G759 | C691 | A615 | A536 | A471 | U399 | A322 |
| G1301 | G1166 | C1101 | C966 | G1031 | G966 | G904 | G832 | A760 | G692 | G616 | C537 | G476 | U400 | C323 |
| A1302 | G1167 | C1101 | C967 | G1032 | G967 | G905 | G833 | G761 | G696 | G617 | C538 | G477 | G401 | G324 |
| G1303 | G1168 | U1104 | U968 | G1035 | G969 | C909 | A836 | G762 | G697 | G618 | C539 | G478 | G402 | G326 |
| G1304 | A1169 | A1105 | G970 | C1036 | G970 | G910 | A837 | A763 | G697 | U619 | C540 | U478 | A483 | G327 |
| C1307 | G1170 | G1106 | A971 | A1037 | A971 | C911 | G838 | A764 | A698 | G620 | A542 | A479 | G404 | G328 |
| U1308 | A1171 | U1107 | C972 | U1038 | G972 | A912 | G844 | G765 | A699 | G621 | A543 | A480 | G405 | C329 |
| C1309 | C1172 | U1108 | A973 | G1039 | G973 | C913 | C845 | G766 | C700 | A625 | U544 | A481 | A406 | G334 |
| G1310 | C1173 | G1109 | U974 | G1040 | U974 | A914 | C846 | G767 | G701 | G626 | U545 | A482 | A407 | U335 |
| A1311 | G1174 | C1110 | G975 | G1041 | G975 | A915 | C847 | G768 | G701 | G627 | C545 | G483 | G408 | C336 |
| U1312 | C1175 | C1111 | C976 | G1042 | C976 | G916 | U847 | G769 | A705 | G628 | A546 | C484 | A409 | U337 |
| G1313 | C1176 | C1112 | U977 | G1043 | U977 | C917 | U848 | G773 | U706 | G629 | C547 | G485 | G487 | C337 |
| C1314 | U1177 | G1113 | A978 | U1044 | A978 | G918 | A849 | A774 | G708 | C630 | U548 | C486 | C413 | U338 |
| G1315 | G1178 | C1114 | G980 | C1045 | G980 | G919 | A850 | A775 | G711 | U635 | G551 | C487 | C414 | A339 |
| C1316 | G1179 | G1115 | G981 | U1046 | G981 | G920 | G851 | A776 | A712 | A636 | C552 | U415 | U416 | G340 |
| G1317 | U1180 | G1116 | G982 | U1047 | G982 | G921 | C852 | A777 | G713 | G637 | G553 | G421 | G417 | G341 |
| U1318 | C1181 | U1117 | A983 | C1048 | A983 | A923 | C854 | G783 | G714 | A638 | U554 | A492 | A491 | U342 |
| G1319 | A1182 | U1118 | C984 | G1050 | C984 | G924 | G855 | U784 | C715 | G639 | A555 | A493 | A344 | G343 |
| C1320 | G1183 | C1119 | C985 | U1051 | C985 | G925 | C856 | A785 | G716 | U642 | A556 | C494 | U422 | G345 |
| G1321 | A1185 | G1120 | C986 | C1052 | C986 | A926 | C857 | G786 | G717 | G643 | A557 | U495 | U423 | G346 |
| U1322 | G1186 | C1121 | G989 | C1053 | U927 | U927 | C858 | U787 | C718 | G644 | G558 | C496 | U424 | C347 |
| C1323 | G1187 | G1122 | U990 | G1054 | G989 | G928 | C859 | A790 | C719 | G645 | G559 | C497 | U425 | A348 |
| G1324 | U1192 | C1123 | U991 | U1055 | U990 | U929 | C860 | C791 | A720 | G646 | C561 | C498 | U426 | G349 |
| A1261 | U1193 | G1124 | A992 | C1056 | G991 | G930 | U861 | G792 | G721 | U647 | C562 | U499 | A427 | C350 |
| U1262 | C1194 | C1125 | G1000 | C1057 | A992 | G931 | G864 | C793 | G722 | G648 | U563 | C501 | U429 | A351 |
| C1263 | G1195 | G1126 | G1001 | G1063 | G1001 | A936 | C870 | U796 | G723 | G649 | U564 | C502 | U430 | G357 |
| A1266 | C1196 | A1128 | G1002 | G1066 | G1002 | U937 | G871 | A797 | C724 | G650 | G564 | C503 | C430 | U360 |
| U1267 | G1197 | G1129 | G1003 | U1067 | G999 | U938 | G872 | A798 | U725 | G651 | U565 | G504 | G433 | A361 |
| A1268 | C1198 | U1130 | U1004 | G1068 | U999 | U939 | G873 | A799 | G726 | G652 | U566 | C505 | A434 | U362 |
| A1269 | C1199 | C1131 | G1005 | U1069 | G1000 | U940 | G874 | C800 | U727 | G653 | G576 | A506 | A435 | U363 |
| C1332 | U1200 | U1132 | C1006 | G1068 | G1001 | C939 | G875 | G801 | C731 | G654 | G577 | G507 | C436 | C365 |
| G1333 | G1201 | A1133 | G1007 | U1068 | G1002 | C940 | G876 | G802 | G732 | G655 | G578 | C508 | C437 | G366 |
| C1335 | C1135 | G1136 | C1008 | G1069 | G1003 | G941 | G877 | A803 | G733 | G656 | G579 | C509 | C438 | C367 |
| U1338 | G1203 | G1137 | C1007 | G1070 | C1007 | A942 | G878 | A802 | G734 | G657 | C580 | G510 | C439 | C368 |
| U1339 | C1204 | G1138 | C1008 | U1071 | C1007 | A943 | G879 | A803 | G735 | A658 | G581 | G511 | G440 | A369 |
| C1340 | A1205 | U1139 | G1009 | G1072 | C1008 | G944 | G880 | G804 | A736 | U660 | U581 | G512 | G441 | A370 |
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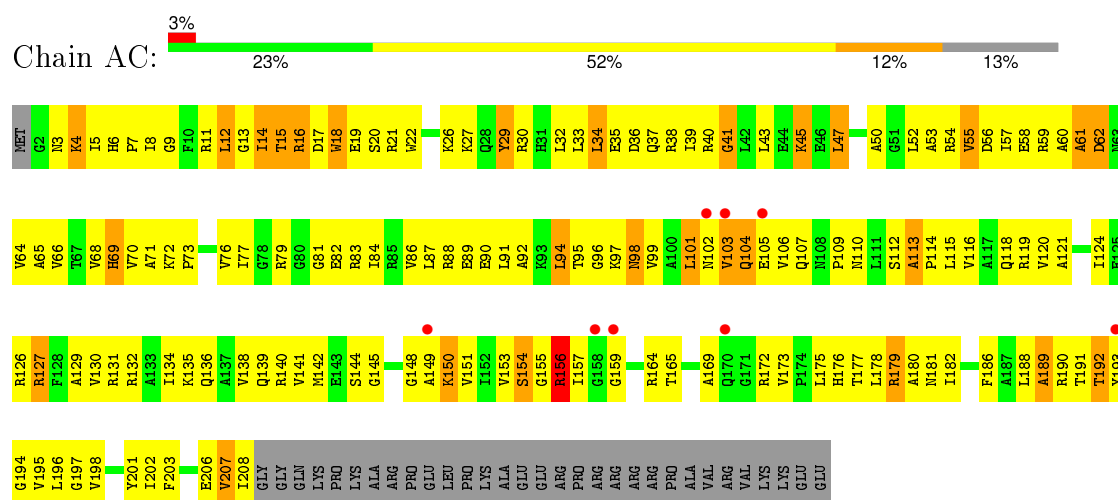
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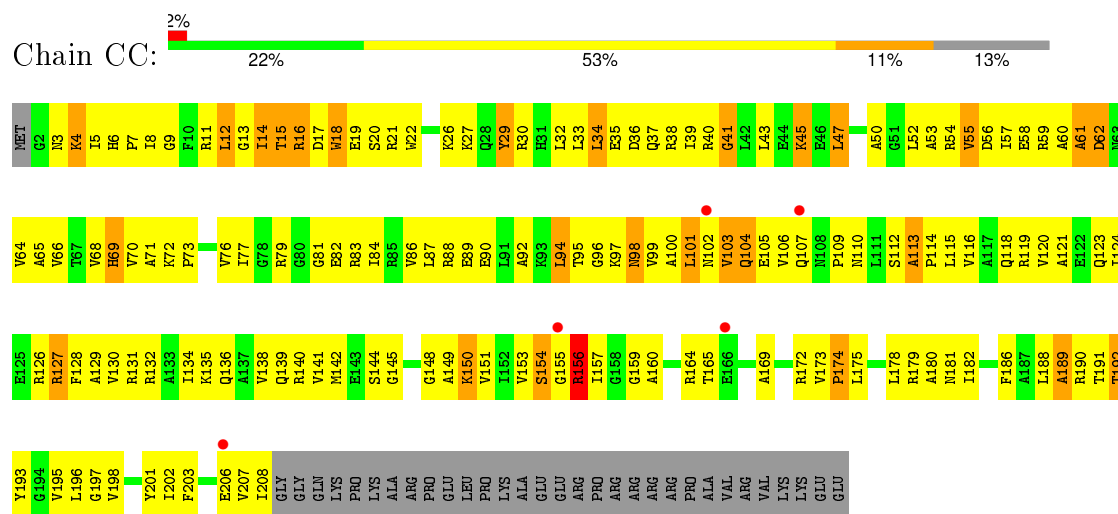
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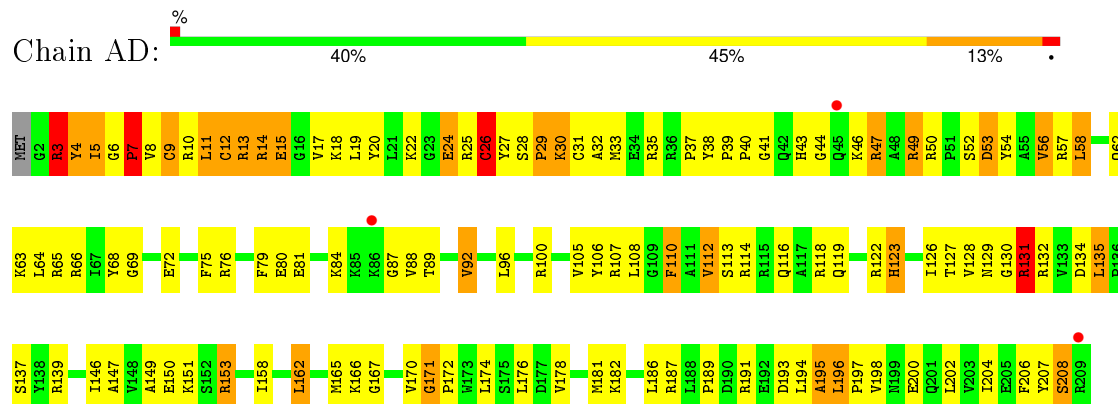
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• Molecule 3: 30S ribosomal protein S3

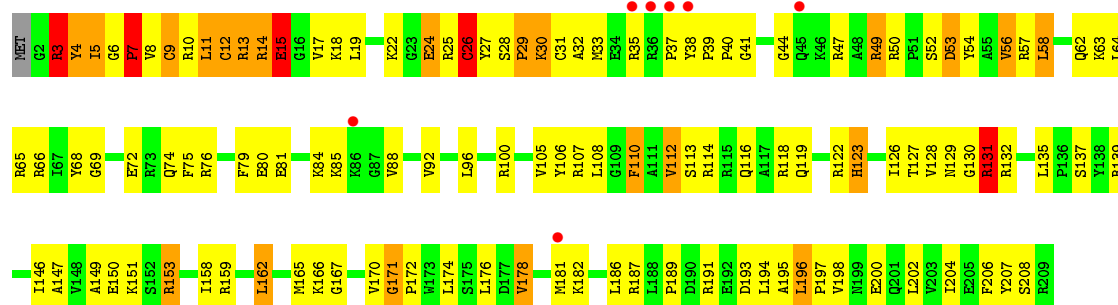


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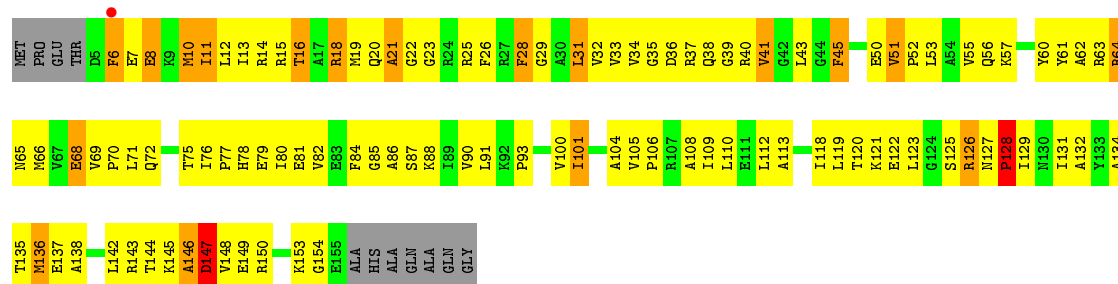


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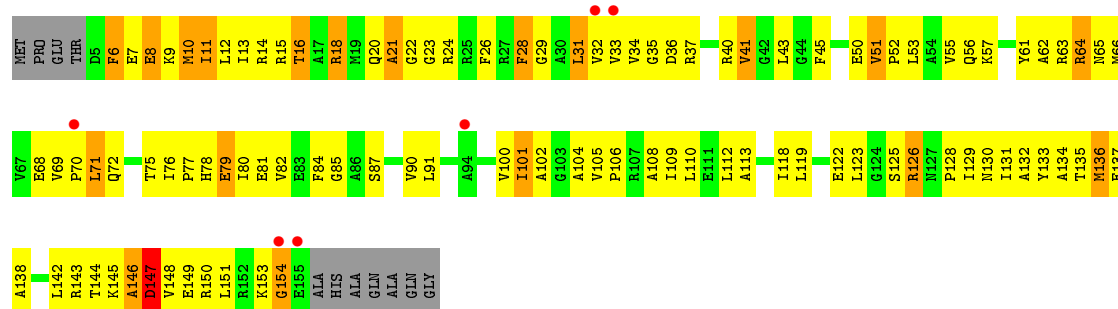




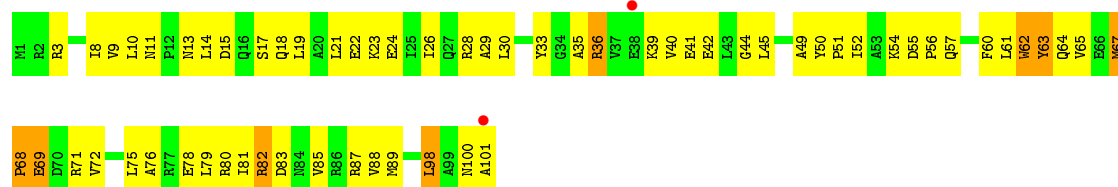
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• Molecule 5: 30S ribosomal protein S5

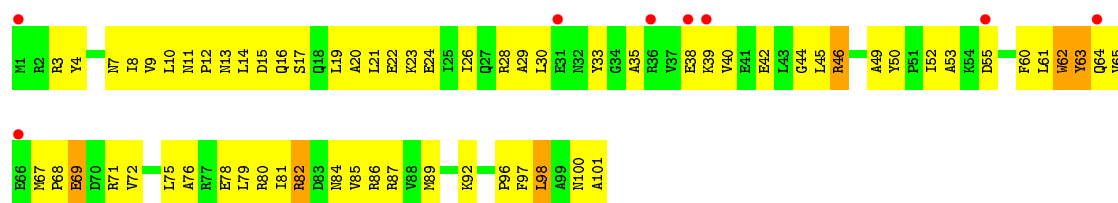


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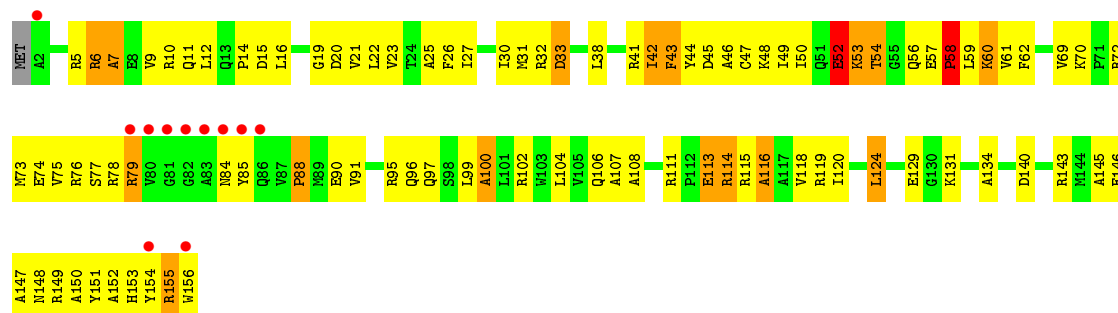


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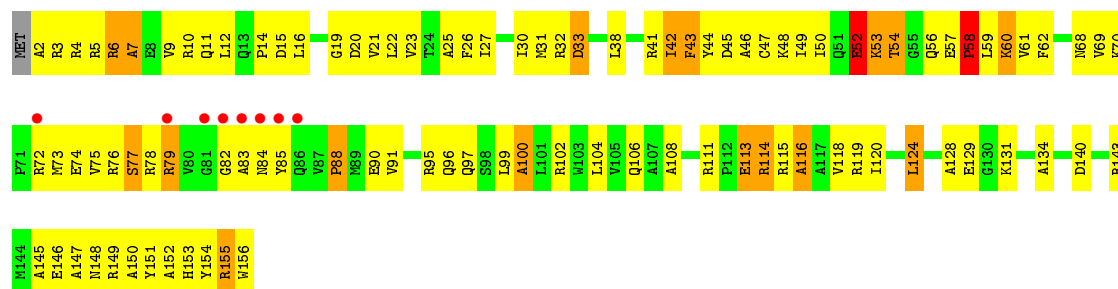




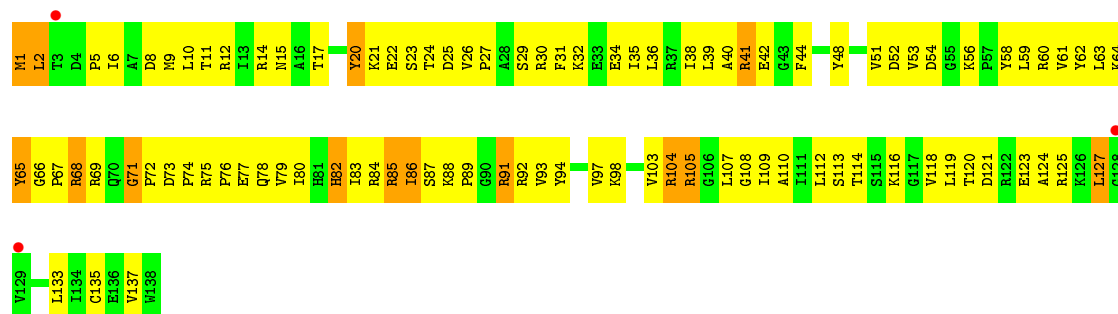
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7

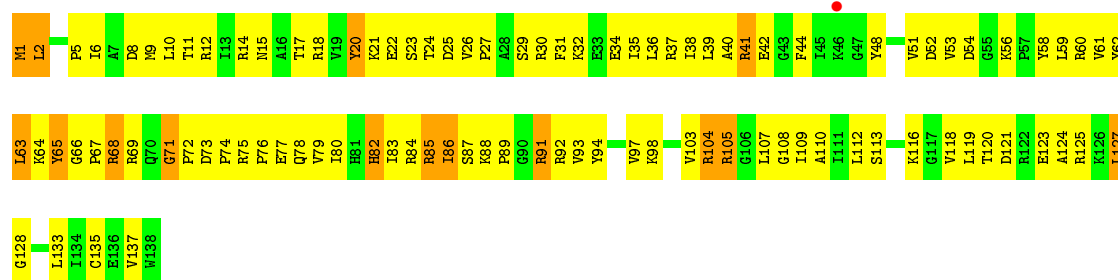


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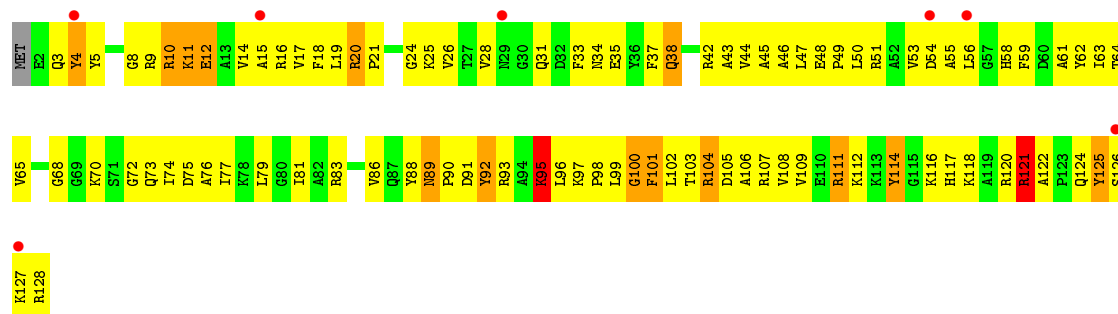


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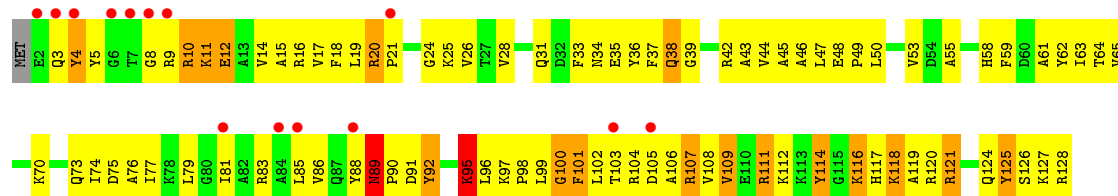




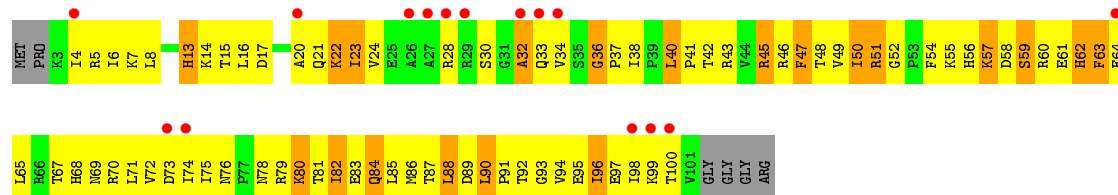
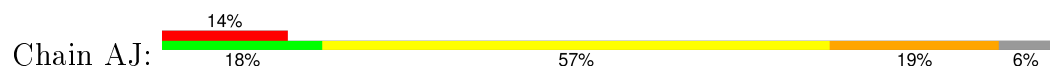
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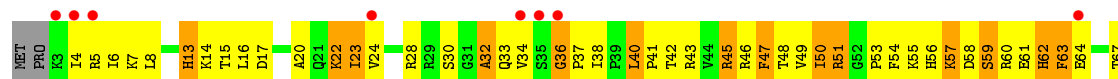
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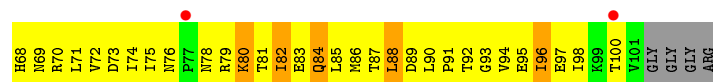


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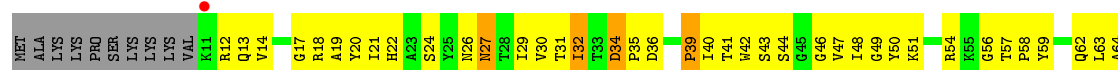


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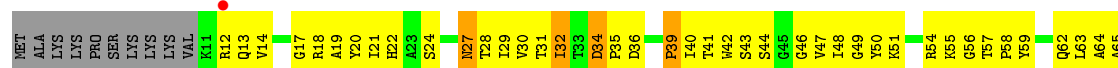




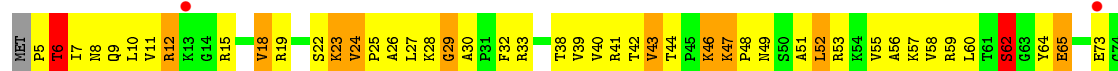
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

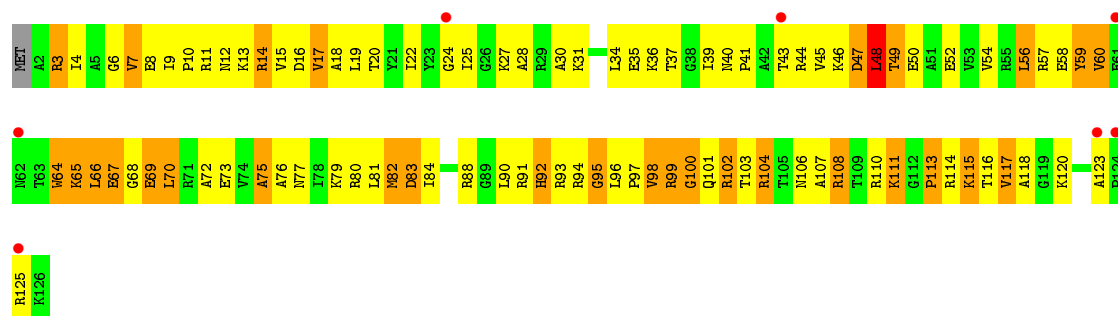


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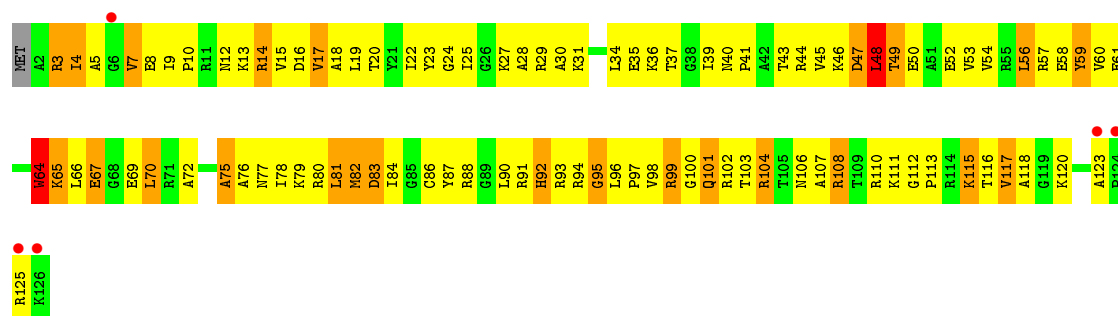


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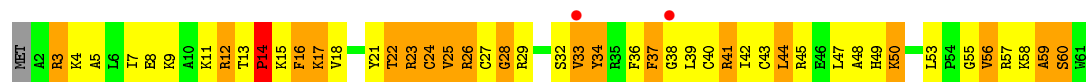
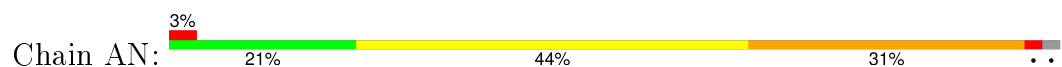




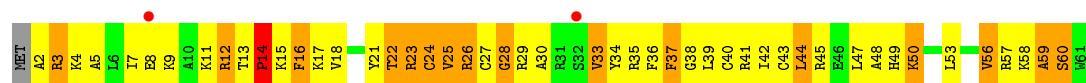
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



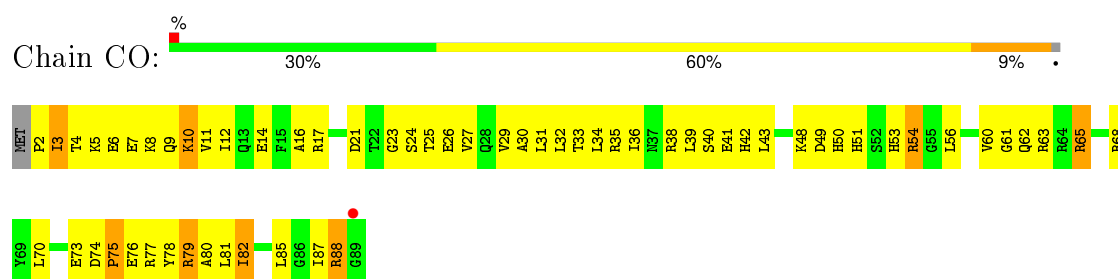
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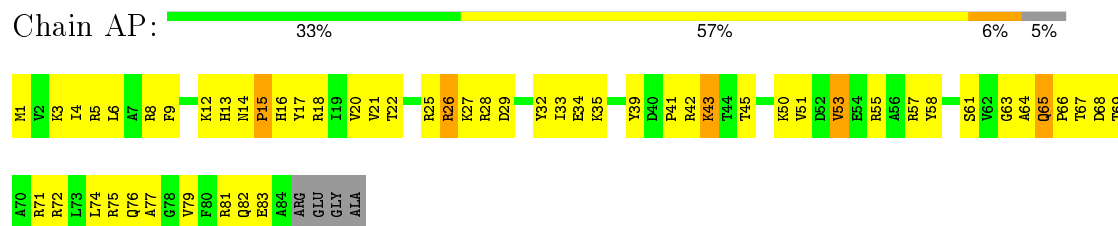
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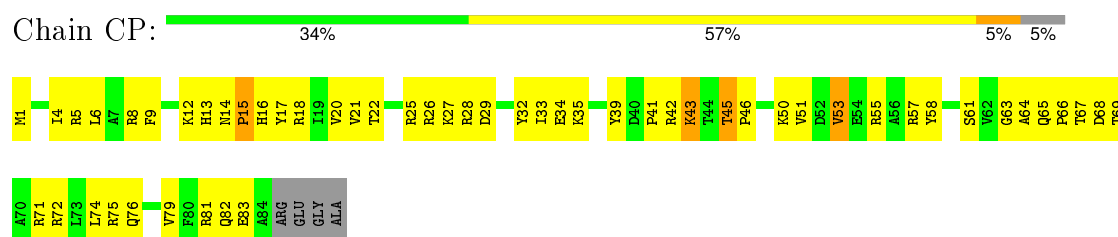
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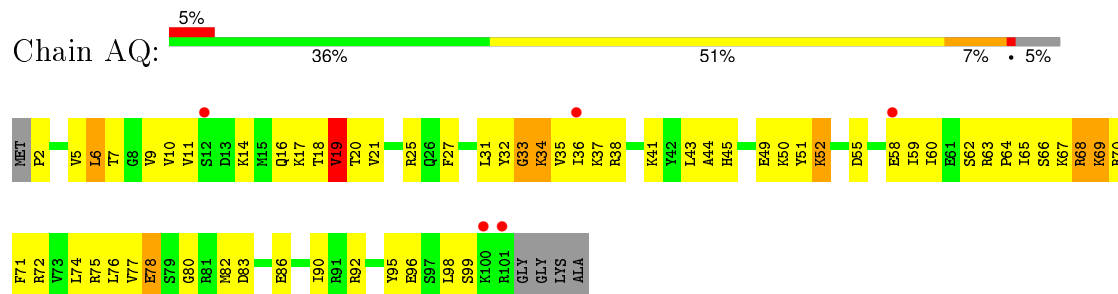
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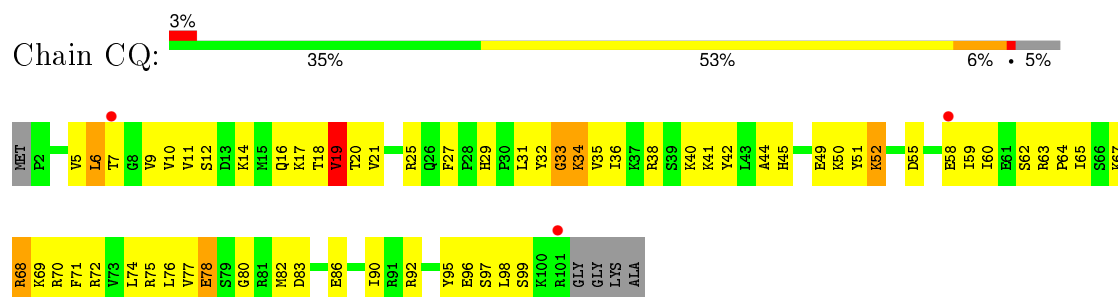
- Molecule 16: 30S ribosomal protein S16



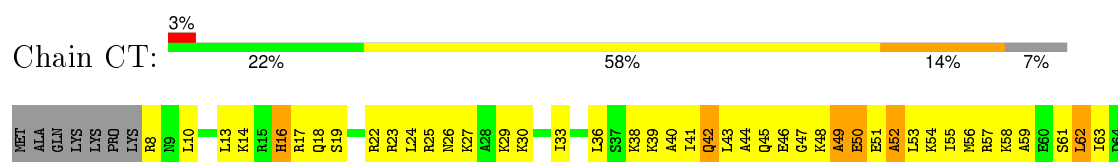
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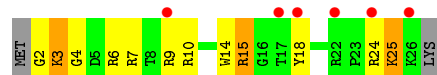
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- Molecule 18: 30S ribosomal protein S18



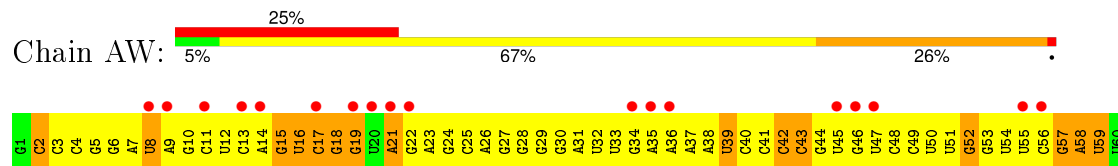
- Molecule 21: 30S ribosomal protein THX



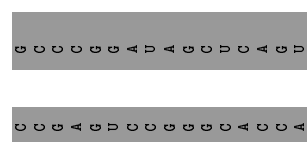
- Molecule 21: 30S ribosomal protein THX



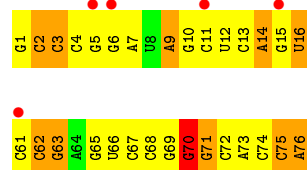
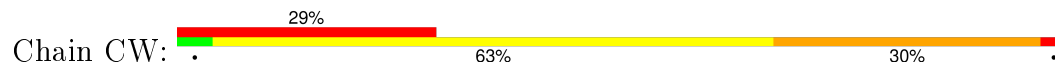
- Molecule 22: tRNA-Phe



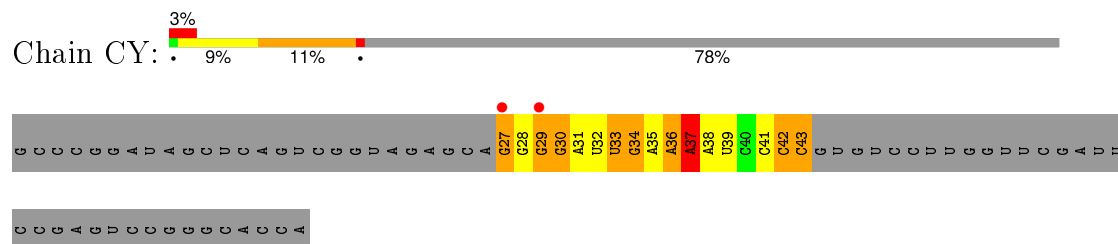
- Molecule 22: tRNA-Phe



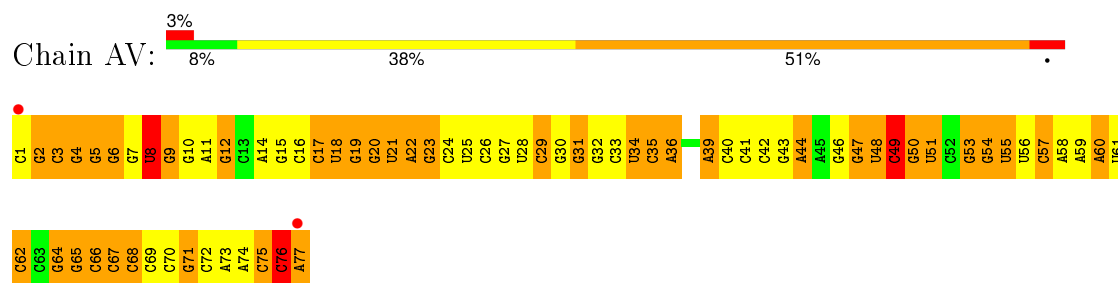
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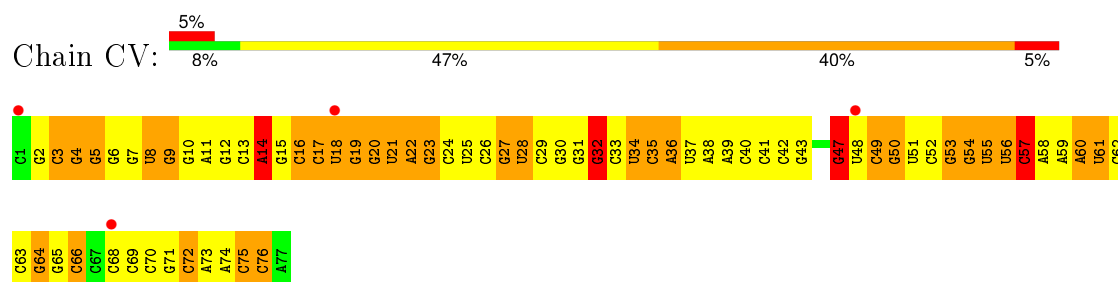
- Molecule 22: tRNA-Phe



- Molecule 23: tRNA-fMet



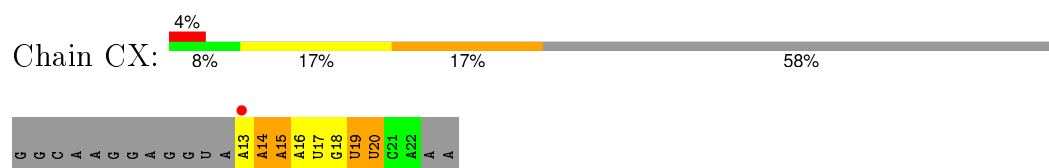
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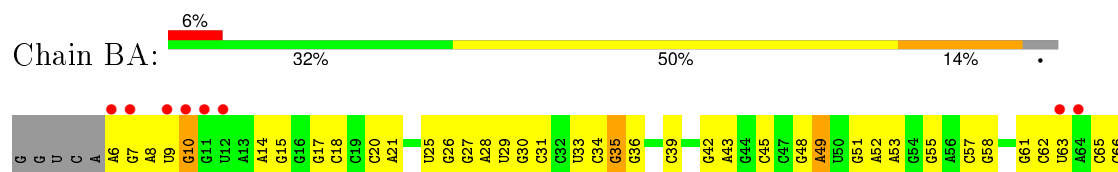
- Molecule 24: messenger RNA



- Molecule 24: messenger RNA

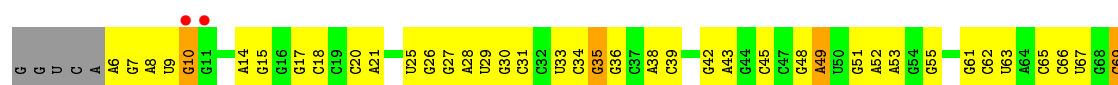


- Molecule 25: 23S rRNA





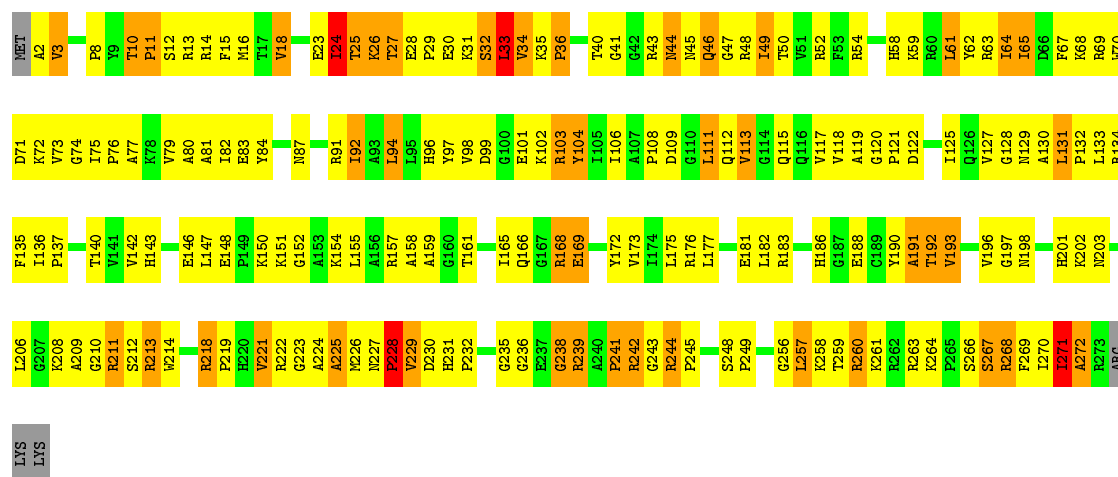
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| C2066 | A1986 | C1902 | G1814 | C1743 | G1647 | U1570 | U1503 | A1439 | A1373 | A1308 | G1230 | G1160 | C |
| U2068 | G1987 | G2067 | A1815 | C1744 | C1648 | A1571 | C1504 | G1440 | G1374 | G1309 | G1231 | G1161 | G |
| G2069 | C1988 | G1903 | G1816 | G1745 | C1648 | A1572 | U1505 | G1441 | G1374 | G1310 | G1232 | G1162 | U |
| G2070 | A1990 | G1906 | G1817 | G1746 | G1651 | A1573 | C1506 | G1442 | A1378 | G1311 | G1233 | G1163 | A |
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| G2078 | C1994 | A1914 | A1821 | A1749 | C1657 | A1579 | A1509B | C1446 | A1384 | C1314 | G1238 | U1167 | G |
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| A2013 | A2013 | G1930 | U1941 | G1763 | C1675 | G1591 | U1523 | A1459 | A1396 | G1325 | U1249 | G1178 | U |
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| A2015 | A2015 | A1937 | C1844 | U1766 | G1678 | G1594 | G1526 | C1462 | G1400 | U1328 | G1252 | A1183 | U |
| U2016 | U2016 | U1938 | G1845 | C1767 | G1678 | G1595 | G1527 | C1463 | G1401 | U1329 | A1253 | G1184 | U |
| U2017 | U2017 | A1946 | A1846 | C1771 | G1681 | C1598 | A1528 | C1464 | C1402 | C1330 | G1256 | G1186 | U |
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| G2106 | G2106 | G1857 | U1696 | A1785 | U1696 | G1541 | G1541 | G1475 | A1412 | U1341 | A1268 | U1198 | U |
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| U2109 | U2109 | G1859 | G1697 | A1786 | G1697 | C1543 | C1543 | G1479 | G1414 | G1345 | G1271 | C1200 | U |
| G2035 | G2035 | G1863 | C1698 | A1789 | A1698 | A1544 | A1544 | G1480 | U1415 | C1346 | A1272 | C1201 | U |
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| G2039 | G2039 | U1864 | A1701 | A1791 | A1701 | C1546 | C1546 | G1482 | C1417 | G1348 | A1274 | G1203 | U |
| C2040 | C2040 | G1865 | C1708 | U1794 | C1708 | C1547 | C1547 | G1484 | A1418 | A1349 | A1275 | A1204 | U |
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| A2042 | A2042 | A1876 | U1796 | U1796 | U1796 | C1551 | C1551 | G1486 | U1420 | C1351 | A1278 | C1208 | U |
| G2043 | G2043 | G1878 | C1710 | C1797 | C1710 | G1519 | G1519 | G1487 | G1421 | U1352 | G1281 | U1141 | U |
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| U2118 | U2118 | A1880 | C1712 | G1799 | C1712 | G1525 | A1554 | U1489 | G1425 | A1354 | A1287 | A1143 | U |
| A2119 | A2119 | C1881 | U1713 | C1800 | U1713 | G1526 | G1555 | A1490 | G1426 | G1355 | A1287 | U1144 | U |
| G2120 | G2120 | G1882 | G1714 | C1800 | G1714 | G1527 | C1556 | A1491 | A1427 | G1356 | U1288 | G1145 | U |
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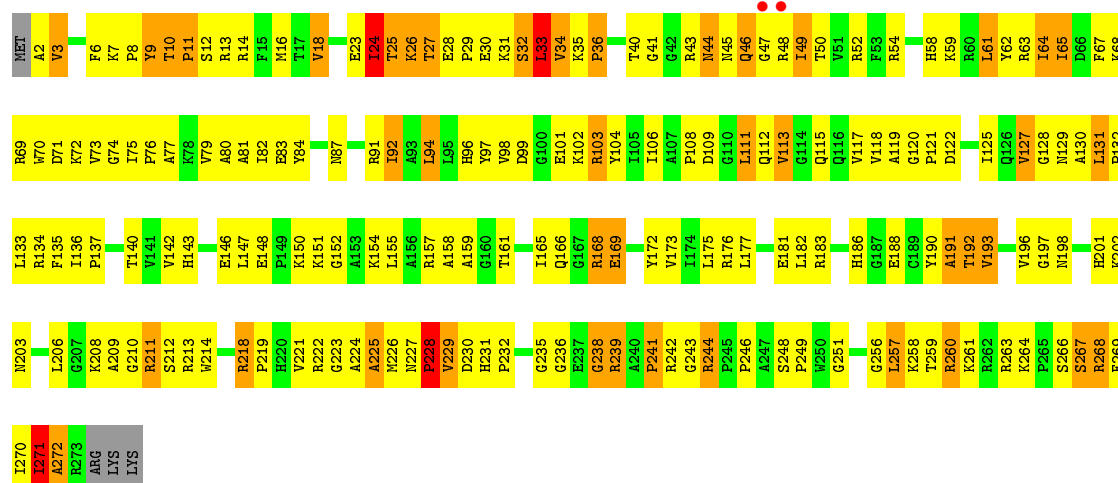
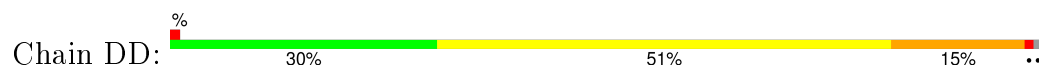


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| C2063 | A1986 | G1906 | G1814 | C1743 | G1647 | G1568 | C1501 | U1438 | G1369 | | G1224 | G1154 | U |
| C2064 | G1907 | A1815 | A1815 | C1744 | C1648 | A1569 | G1502 | A1439 | | U1300 | | A1155 | G |
| C2065 | C1987 | C1908 | G1816 | G1745 | | A1570 | U1503 | G1440 | A1373 | A1301 | | A1156 | C |
| C2066 | C1988 | C1909 | G1817 | G1746A | G1651 | A1571 | U1504 | G1441 | G1374 | A1302 | G1227 | G1157 | G |
| G2067 | G1989 | | U1818 | G1747 | A1652 | A1572 | C1505 | G1442 | | | | G1158 | U |
| U2068 | C1990 | A1912 | A1819 | G1747A | G1653 | G1573 | A1506 | G1443 | A1378 | A1308 | C1230 | G1159 | A |
| G2069 | U1991 | A1913 | U1820 | | A1654 | C1574 | A1507 | G1444 | A1379 | G1309 | G1232 | G1160 | A |
| G2070 | G1992 | C1914 | A1821 | G1748 | A1655 | | A1508 | A1445 | G1380 | G1310 | G1233 | C1161 | U |
| | U1993 | A1915 | | A1749 | C1656 | | C1509 | C1445A | | G1311 | U1234 | G1162 | A |
| C2073 | C1994 | | G1826 | A1750 | C1657 | | A1509A | C1446 | A1384 | U1312 | G1235 | G1163 | G |
| U2074 | U1995 | A1919 | C1827 | G1750 | A1657 | U1578 | A1509B | G1447 | G1385 | U1313 | G1236 | G1164 | U |
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| G2087 | U2011 | G1935 | C1843 | C1767 | | G1591 | U1523 | G1459 | A1247 | | A1247 | A1176 | U |
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| U2091 | A2014 | A1937 | G1846 | G1772 | G1681 | G1594 | G1526 | G1462 | G1400 | U1327 | U1249 | C1179 | U |
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| C2095 | | | | U1778 | C1886 | C1598 | A1528A | | U1405 | A1331 | A1253 | G1183 | |
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| G2097 | G2023 | C1947 | C1852 | A1780 | U1688 | C1468 | C1532 | A1469 | U1406 | | G1256 | G1188 | |
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| C2025 | C2025 | | A1854 | C1782 | U1602 | G1601 | U | A1471 | C1408 | A1336 | G1269 | G1122 | |
| C2026 | C2026 | A1952 | | A1783 | A1603 | U1603 | A | A1472 | C1409 | G1337 | G1260 | G1123 | |
| | | A1953 | G1858 | U1692 | U1693 | | C | G1473 | G1410 | G1338 | | G1124 | |
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| G2032 | C2105 | C1957 | G1865 | A1789 | A1699 | A1610 | A1542 | G1478 | U1415 | | G1270 | A1128 | |
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| U2034 | G2035 | A1959 | A1876 | A1791 | A1701 | G1615 | A1544 | G1480 | C1417 | G1346 | A1272 | U1130 | |
| C2108 | C2036 | C1961 | G1878 | | G1702 | A1616 | A1545 | U1481 | G1418 | G1347 | U1273 | G1131 | |
| U2109 | | C1962 | C1879 | C1795 | | C1617 | A1546 | G1482 | A1419 | G1348 | G1274 | A1132 | |
| G2110 | | U1963 | C1880 | U1796 | | A1618 | C1547 | G1483 | U1420 | A1349 | A1275 | U1133 | |
| C2111 | C2039 | G1964 | C1881 | C1797 | U1709 | G1619 | | G1485 | G1421 | C1350 | A1276 | G1135 | |
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| G2115 | C2043 | A1969 | C1885 | C1801 | U1713 | G1626 | A1554 | G1488 | G1425 | A1354 | G1281 | U1141 | |
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| G2121 | C2055 | C1974 | | | U1720 | | G1559 | A1494 | U1431 | A1358 | C1289 | G1144 | |
| U2122 | G2056 | G1975 | G1899 | U1808 | G1721 | U1639 | | A1495 | C1432 | A1359 | | C1145 | |
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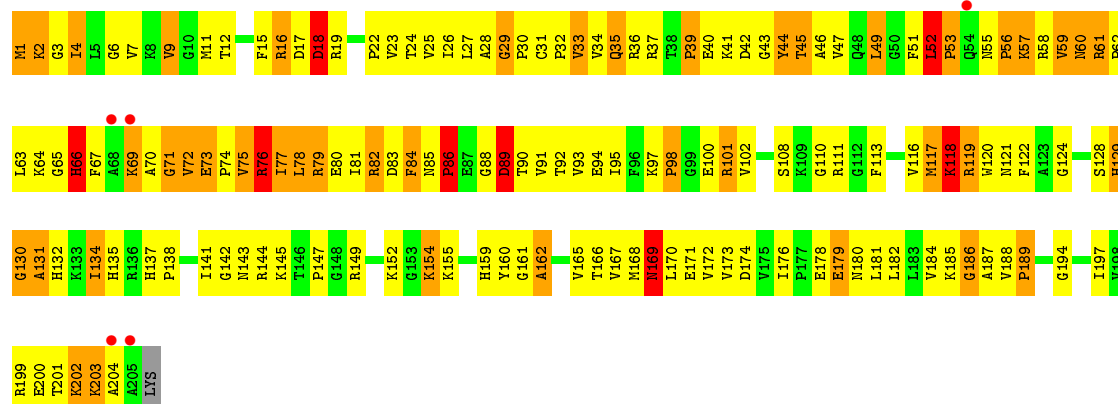




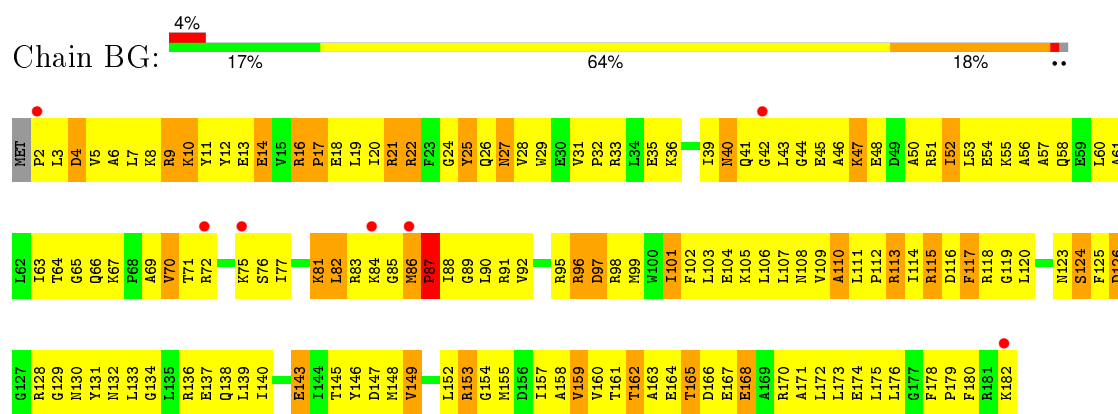
• Molecule 28: 50S ribosomal protein L2



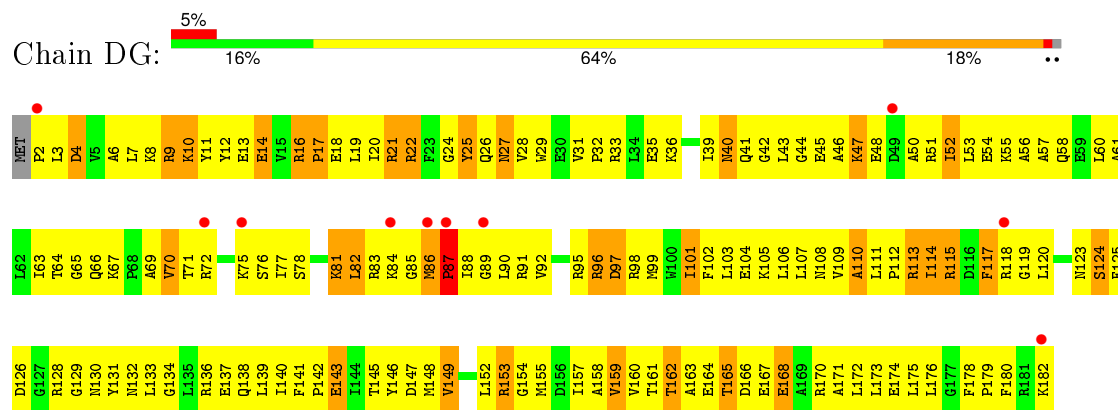
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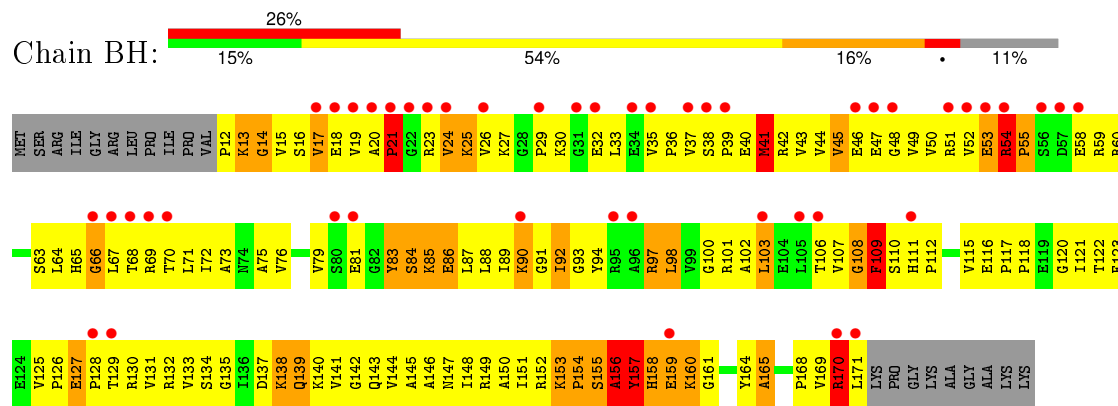




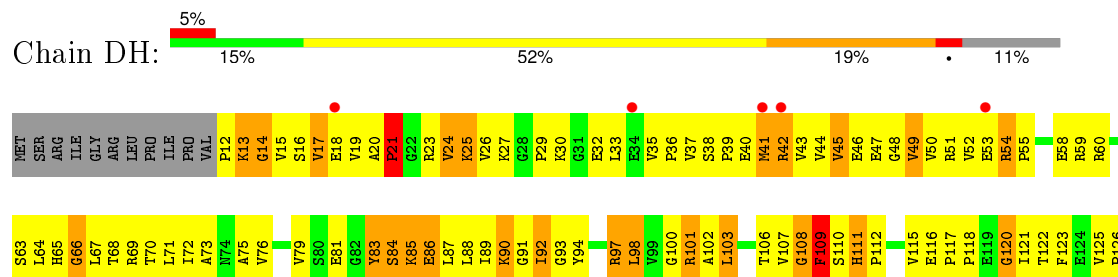
• Molecule 31: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L6

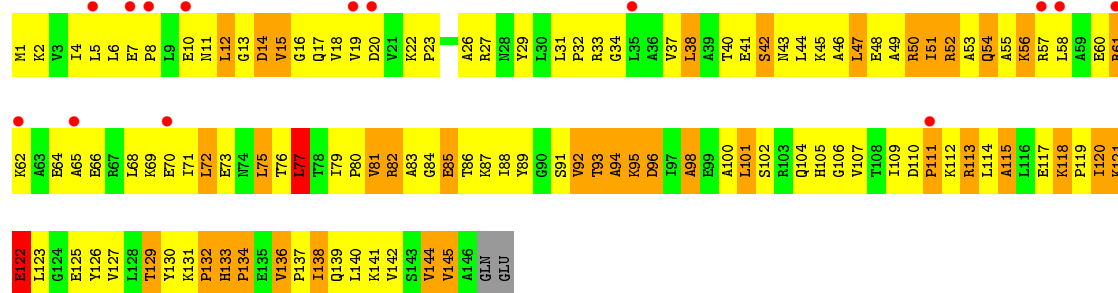
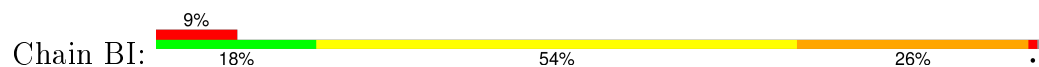


• Molecule 32: 50S ribosomal protein L6

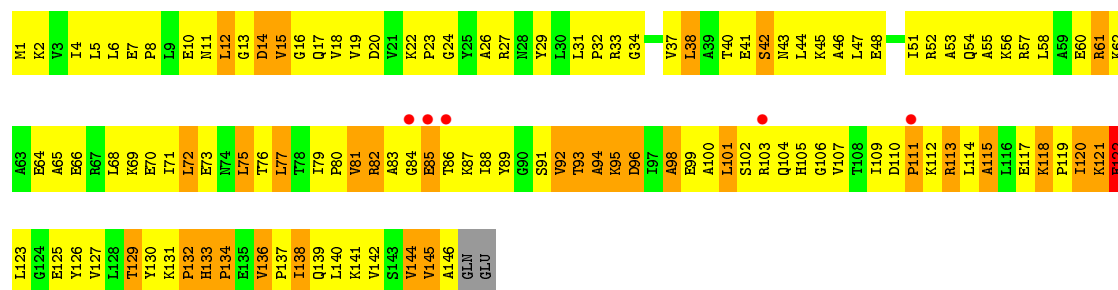




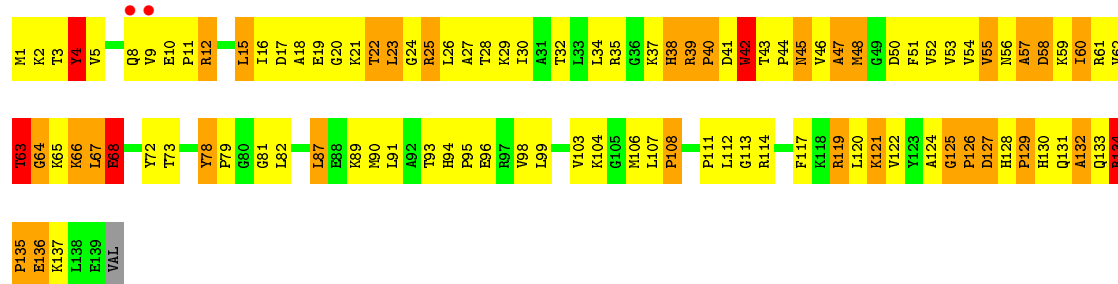
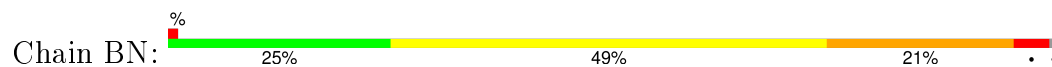
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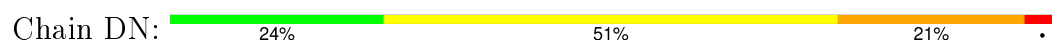
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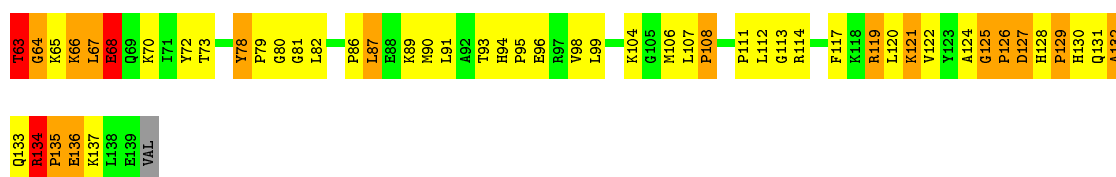


• Molecule 34: 50S ribosomal protein L13



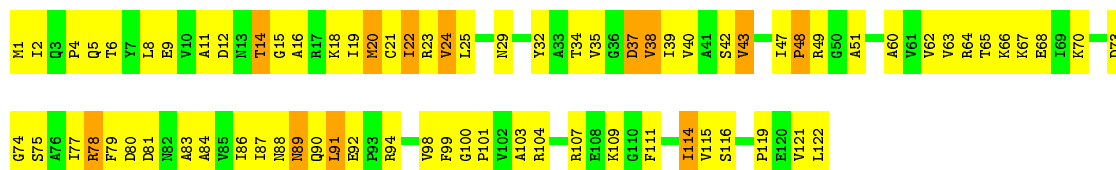
• Molecule 34: 50S ribosomal protein L13





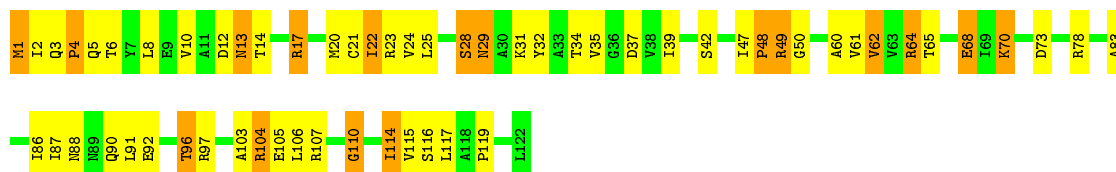
- Molecule 35: 50S ribosomal protein L14

Chain BO: 38% 52% 10%



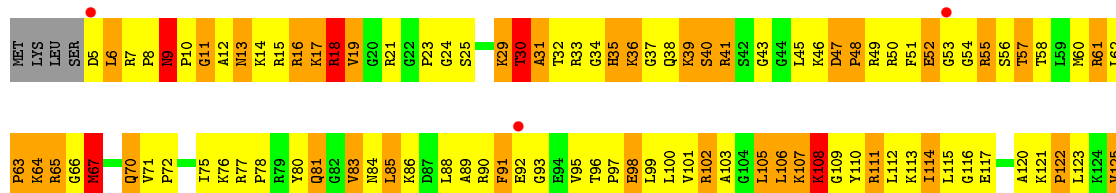
- Molecule 35: 50S ribosomal protein L14

Chain DO: 51% 35% 14%



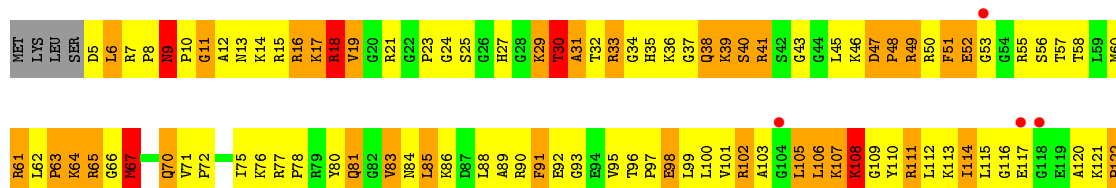
- Molecule 36: 50S ribosomal protein L15

Chain BP: 3% 17% 49% 28%



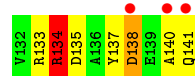
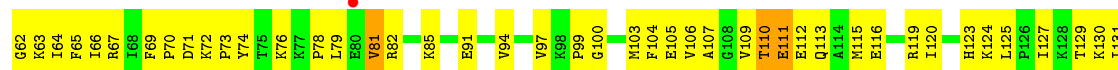
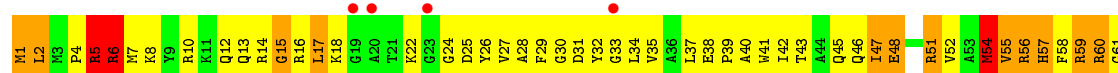
- Molecule 36: 50S ribosomal protein L15

Chain DP: 3% 19% 48% 27%

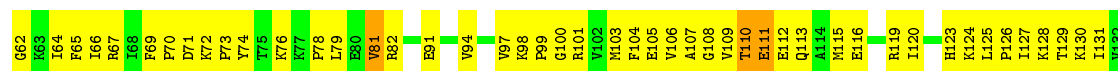
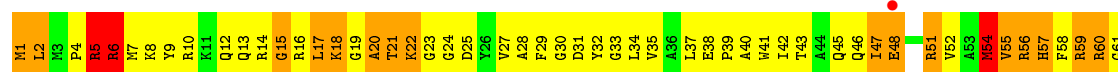




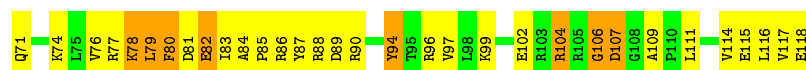
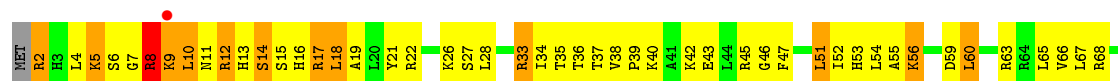
- Molecule 37: 50S ribosomal protein L16



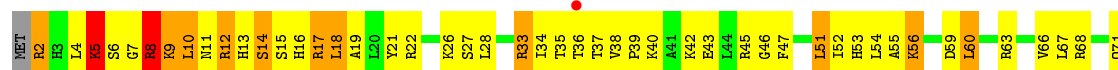
- Molecule 37: 50S ribosomal protein L16



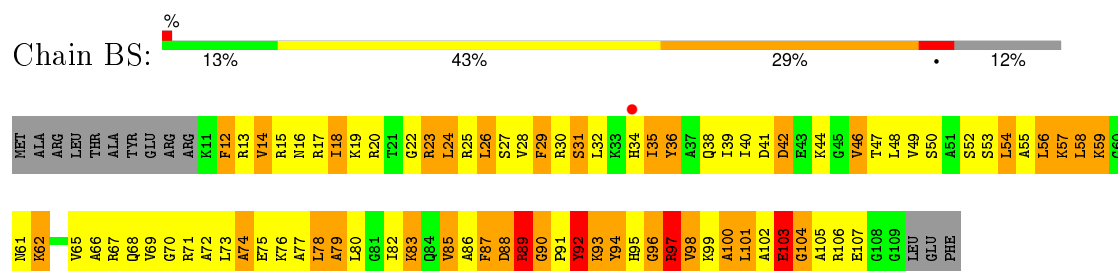
- Molecule 38: 50S ribosomal protein L17



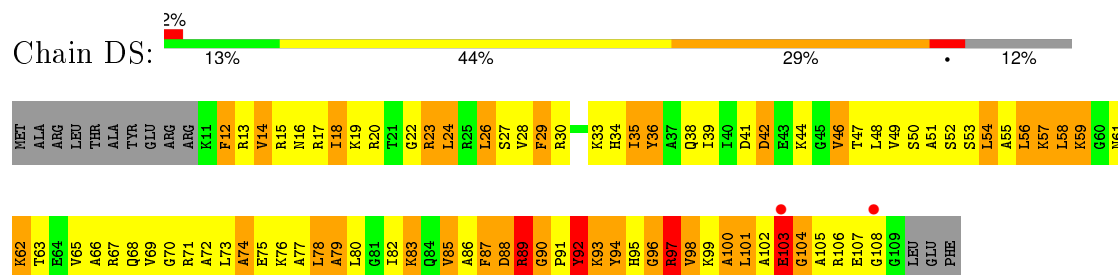
- Molecule 38: 50S ribosomal protein L17



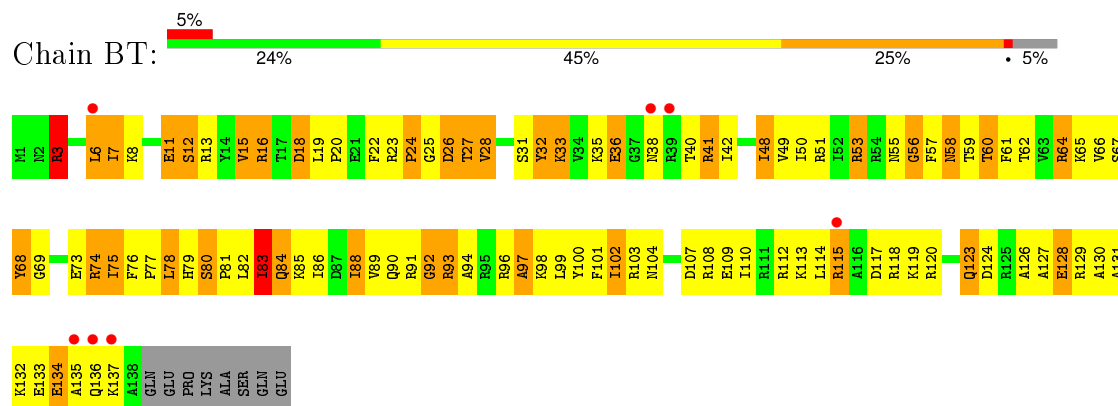
- Molecule 39: 50S ribosomal protein L18



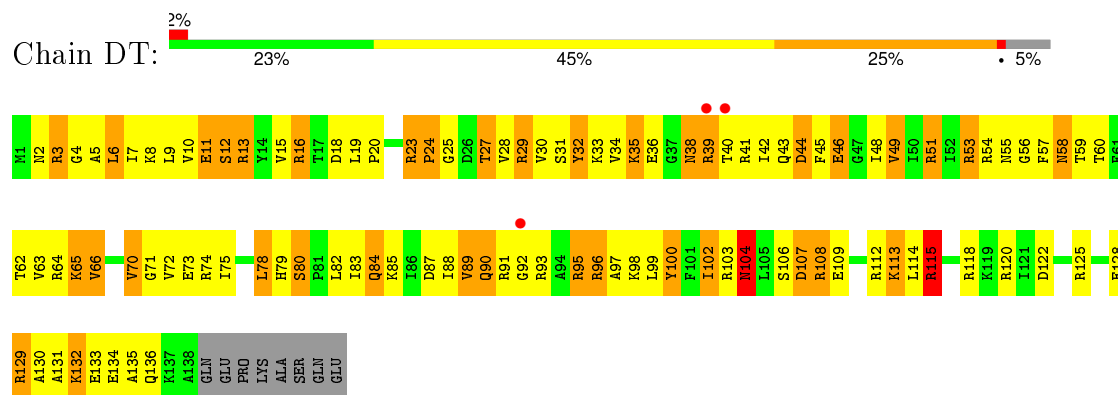
- Molecule 39: 50S ribosomal protein L18



- Molecule 40: 50S ribosomal protein L19

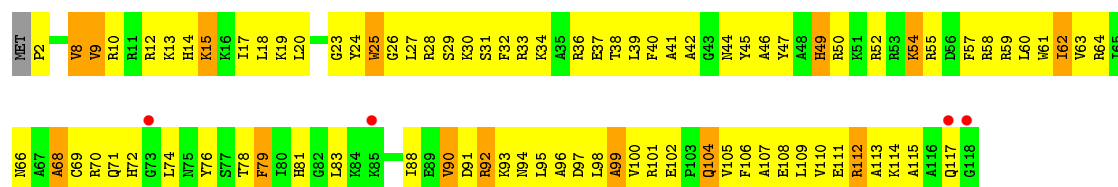


- Molecule 40: 50S ribosomal protein L19



- Molecule 41: 50S ribosomal protein L20





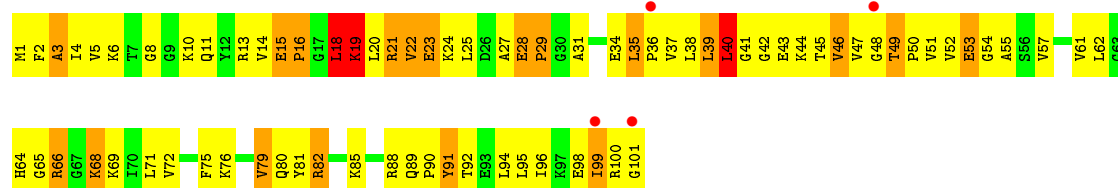
• Molecule 41: 50S ribosomal protein L20

Chain DU: 25% 62% 12%



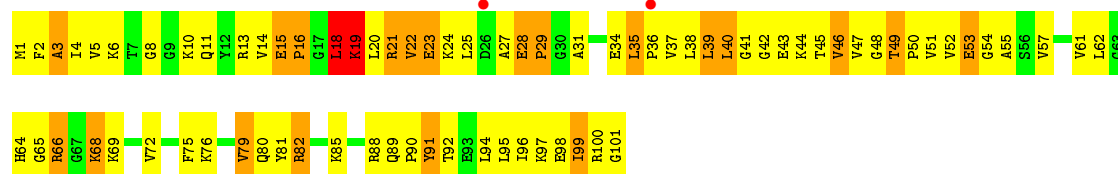
• Molecule 42: 50S ribosomal protein L21

Chain BV: 4% 25% 53% 19%



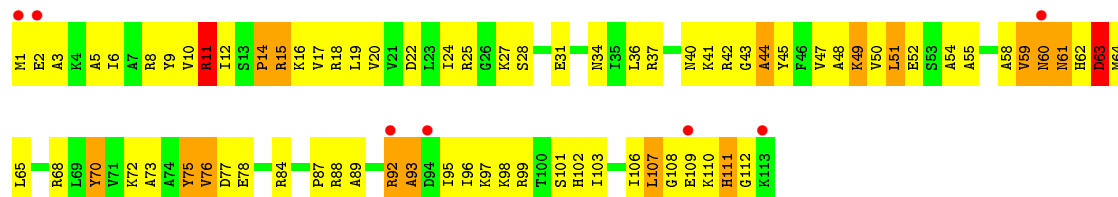
• Molecule 42: 50S ribosomal protein L21

Chain DV: 2% 25% 53% 20%



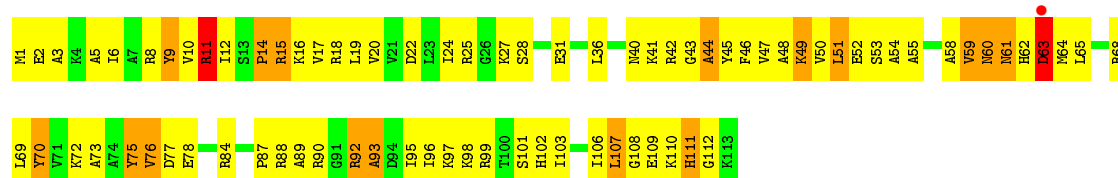
• Molecule 43: 50S ribosomal protein L22

Chain BW: 6% 32% 53% 13%

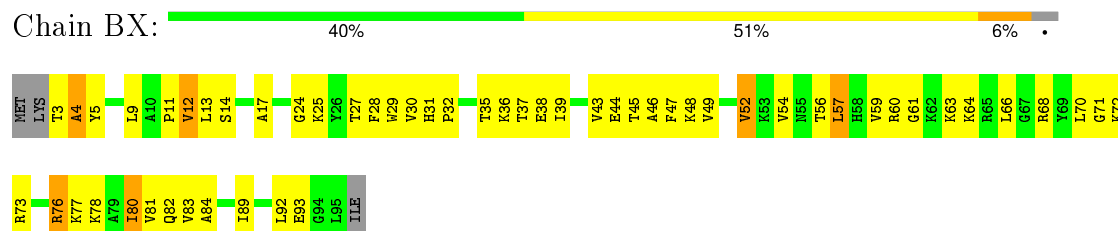


• Molecule 43: 50S ribosomal protein L22

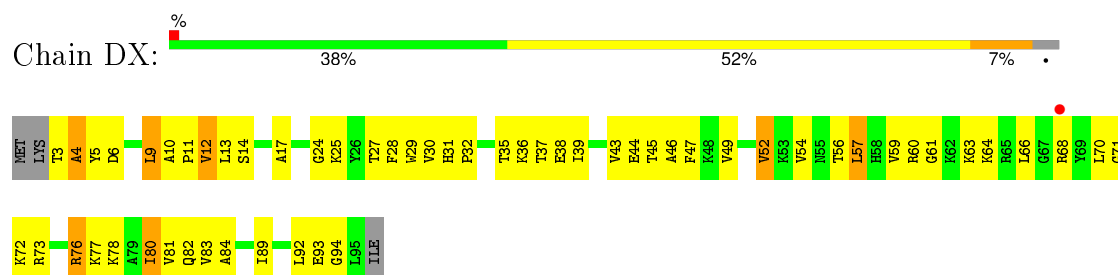
Chain DW: 30% 54% 14%



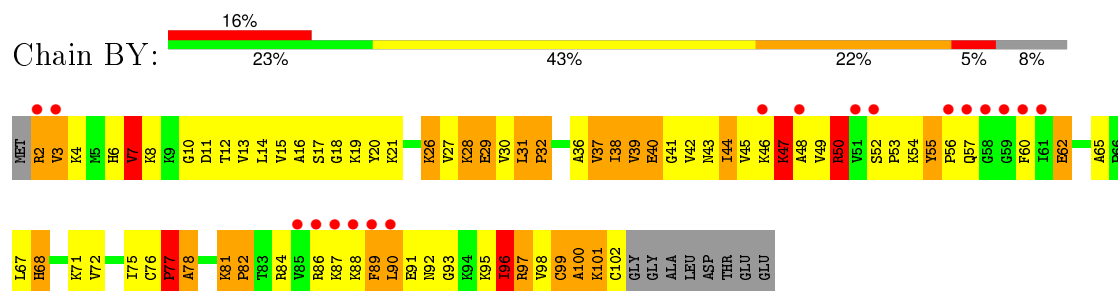
• Molecule 44: 50S ribosomal protein L23



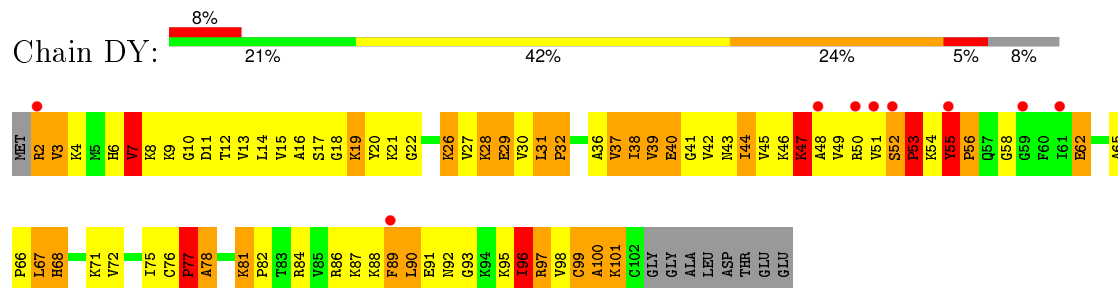
• Molecule 44: 50S ribosomal protein L23



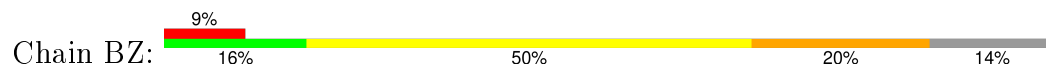
• Molecule 45: 50S ribosomal protein L24

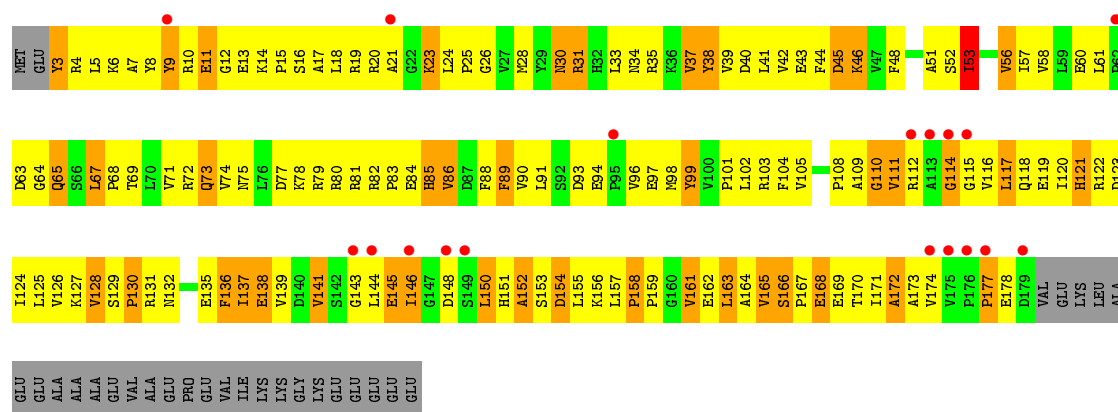


• Molecule 45: 50S ribosomal protein L24

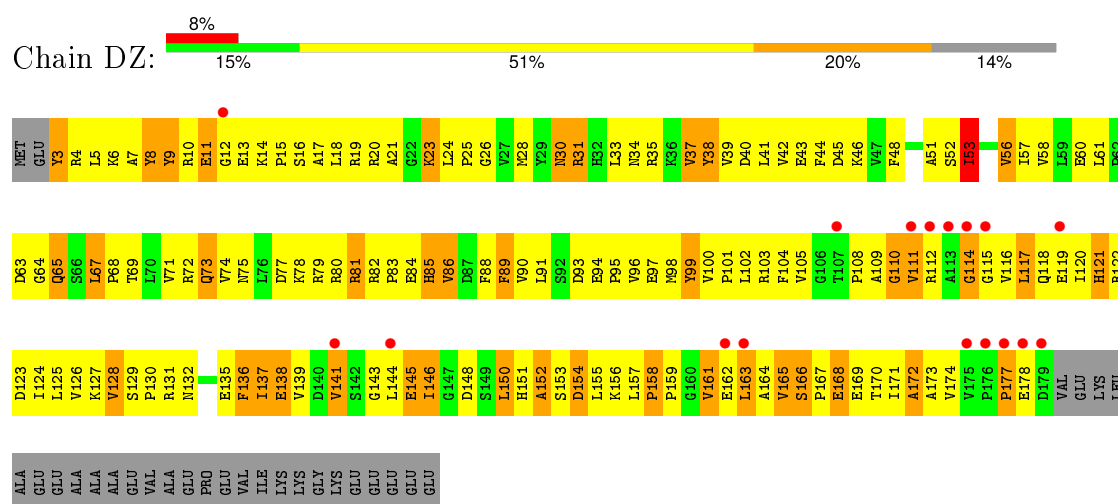


• Molecule 46: 50S ribosomal protein L25

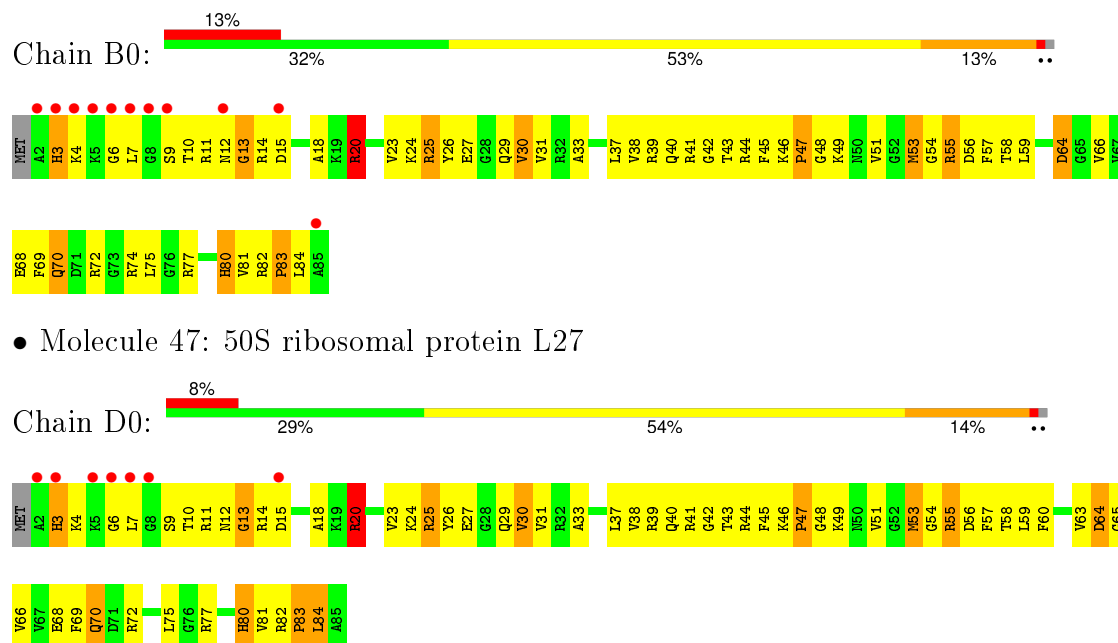




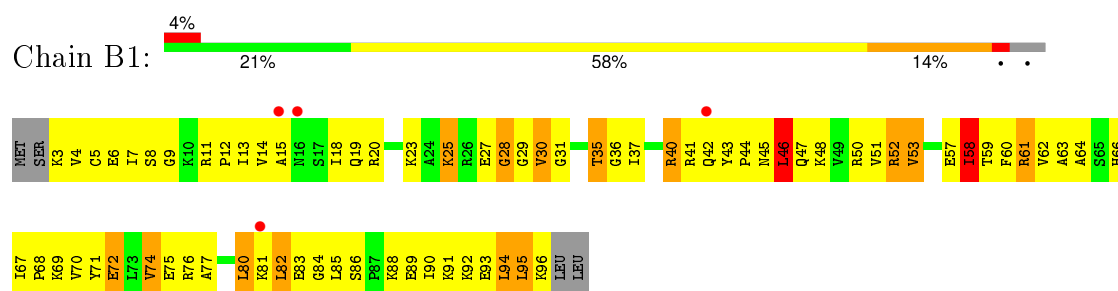
• Molecule 46: 50S ribosomal protein L25



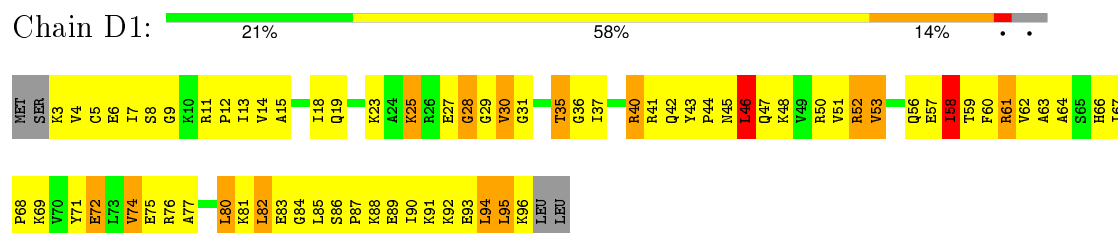
• Molecule 47: 50S ribosomal protein L27



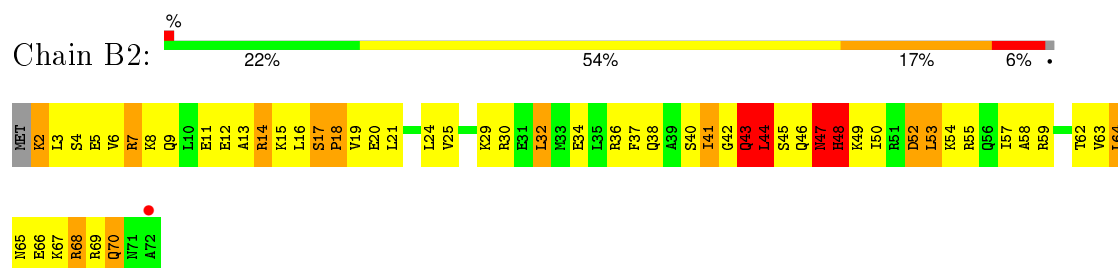
• Molecule 48: 50S ribosomal protein L28



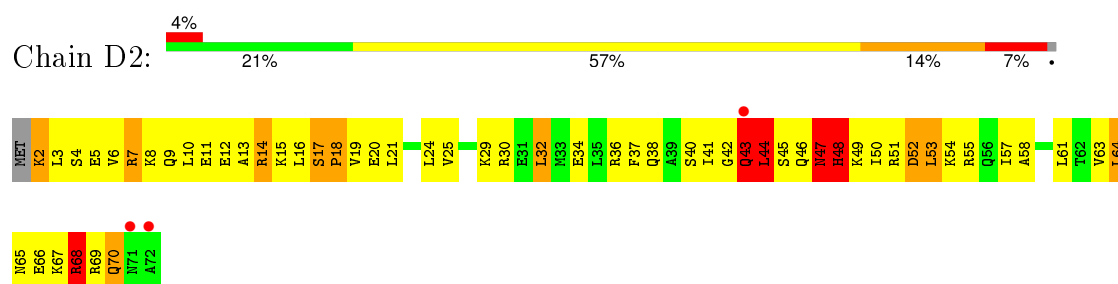
• Molecule 48: 50S ribosomal protein L28



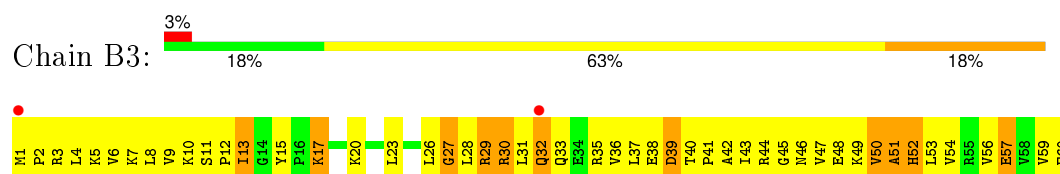
• Molecule 49: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L29

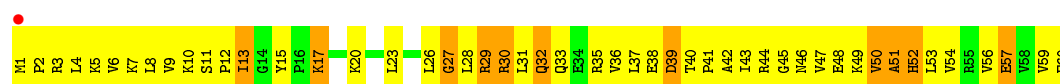


• Molecule 50: 50S ribosomal protein L30

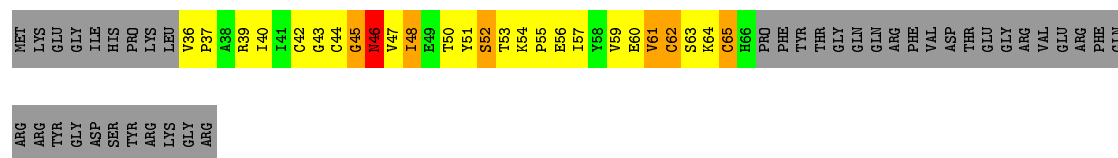
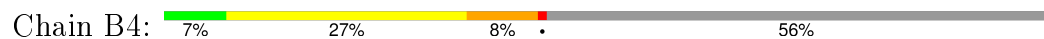


• Molecule 50: 50S ribosomal protein L30

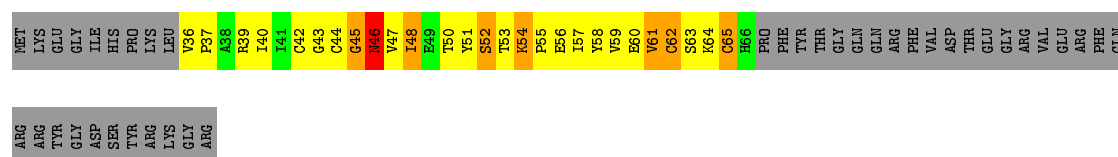
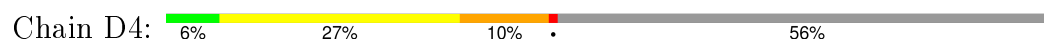




- Molecule 51: 50S ribosomal protein L31



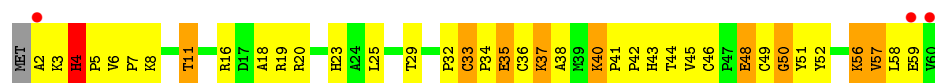
- Molecule 51: 50S ribosomal protein L31



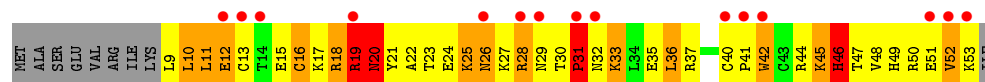
- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



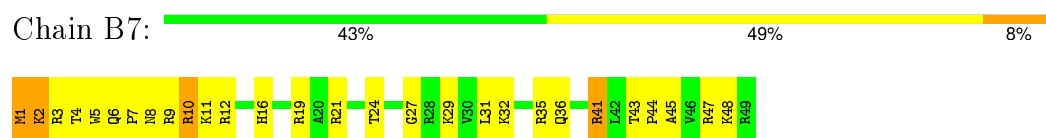
- Molecule 53: 50S ribosomal protein L33



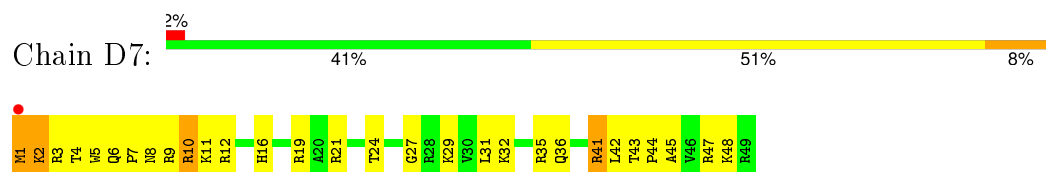
- Molecule 53: 50S ribosomal protein L33



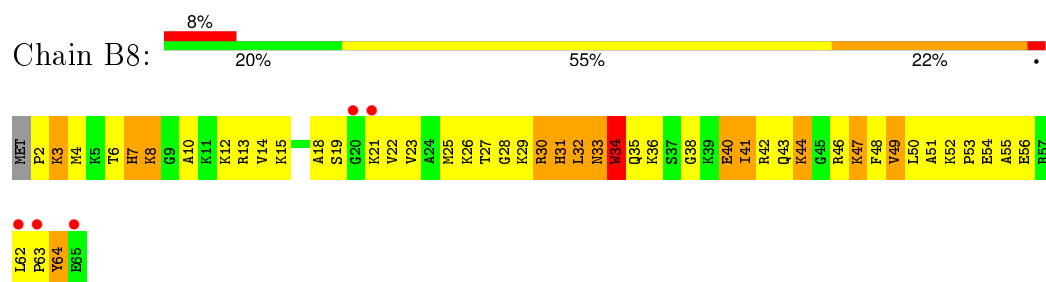
- Molecule 54: 50S ribosomal protein L34



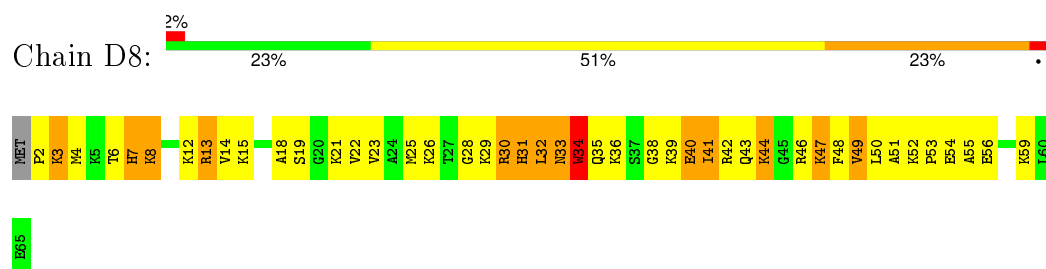
- Molecule 54: 50S ribosomal protein L34



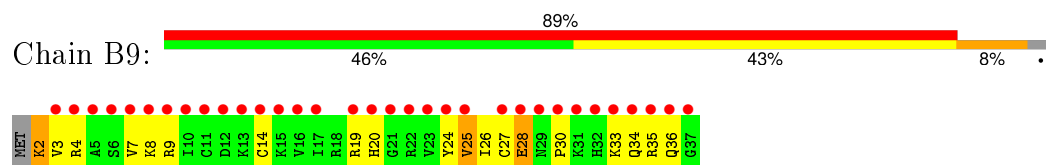
- Molecule 55: 50S ribosomal protein L35



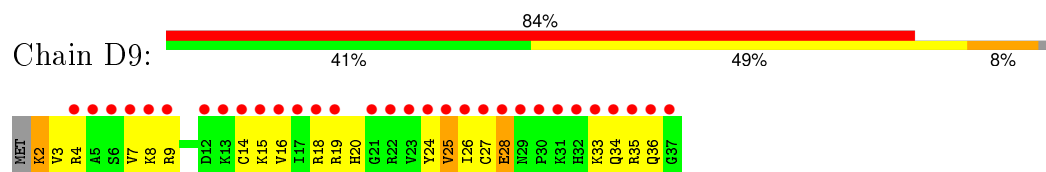
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.20Å 446.16Å 620.95Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.90 34.93 – 4.00 | Depositor EDS |
| % Data completeness (in resolution range) | 94.3 (50.00-3.90) 95.2 (34.93-4.00) | Depositor EDS |
| R_{merge} | 0.35 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.17 (at 3.99Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.1_1168) | Depositor |
| R, R_{free} | 0.242 , 0.269 0.252 , 0.277 | Depositor DCC |
| R_{free} test set | 20475 reflections (4.61%) | DCC |
| Wilson B-factor (Å ²) | 115.4 | Xtriage |
| Anisotropy | 0.219 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.25 , 38.4 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$ | Xtriage |
| Outliers | 0 of 464342 reflections | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 292667 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.53 | 1/36186 (0.0%) | 1.07 | 56/56479 (0.1%) |
| 1 | CA | 0.57 | 0/36161 | 1.11 | 53/56440 (0.1%) |
| 2 | AB | 0.36 | 0/1936 | 0.63 | 0/2611 |
| 2 | CB | 0.35 | 0/1936 | 0.62 | 0/2611 |
| 3 | AC | 0.35 | 0/1637 | 0.60 | 0/2207 |
| 3 | CC | 0.35 | 0/1637 | 0.59 | 0/2207 |
| 4 | AD | 0.39 | 0/1733 | 0.66 | 0/2318 |
| 4 | CD | 0.38 | 0/1733 | 0.65 | 0/2318 |
| 5 | AE | 0.41 | 0/1163 | 0.66 | 0/1566 |
| 5 | CE | 0.41 | 0/1163 | 0.66 | 0/1566 |
| 6 | AF | 0.35 | 0/856 | 0.63 | 0/1154 |
| 6 | CF | 0.36 | 0/856 | 0.65 | 0/1154 |
| 7 | AG | 0.34 | 0/1276 | 0.57 | 0/1709 |
| 7 | CG | 0.34 | 0/1276 | 0.57 | 0/1709 |
| 8 | AH | 0.34 | 0/1136 | 0.65 | 0/1527 |
| 8 | CH | 0.34 | 0/1136 | 0.64 | 0/1527 |
| 9 | AI | 0.35 | 0/1029 | 0.62 | 0/1379 |
| 9 | CI | 0.35 | 0/1029 | 0.63 | 0/1379 |
| 10 | AJ | 0.38 | 0/808 | 0.65 | 0/1087 |
| 10 | CJ | 0.38 | 0/808 | 0.64 | 0/1087 |
| 11 | AK | 0.36 | 0/900 | 0.66 | 0/1213 |
| 11 | CK | 0.36 | 0/900 | 0.66 | 0/1213 |
| 12 | AL | 0.45 | 0/987 | 0.78 | 1/1322 (0.1%) |
| 12 | CL | 0.43 | 0/987 | 0.78 | 0/1322 |
| 13 | AM | 0.40 | 0/999 | 0.72 | 0/1338 |
| 13 | CM | 0.34 | 0/999 | 0.68 | 1/1338 (0.1%) |
| 14 | AN | 0.37 | 0/501 | 0.63 | 0/664 |
| 14 | CN | 0.37 | 0/501 | 0.63 | 0/664 |
| 15 | AO | 0.36 | 0/745 | 0.58 | 0/992 |
| 15 | CO | 0.35 | 0/745 | 0.58 | 0/992 |
| 16 | AP | 0.39 | 0/717 | 0.65 | 0/965 |
| 16 | CP | 0.38 | 0/717 | 0.63 | 0/965 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.40 | 0/837 | 0.65 | 0/1119 |
| 17 | CQ | 0.36 | 0/837 | 0.61 | 0/1119 |
| 18 | AR | 0.39 | 0/579 | 0.71 | 0/768 |
| 18 | CR | 0.40 | 0/579 | 0.70 | 0/768 |
| 19 | AS | 0.38 | 0/643 | 0.68 | 0/867 |
| 19 | CS | 0.37 | 0/643 | 0.62 | 0/867 |
| 20 | AT | 0.36 | 0/765 | 0.66 | 0/1007 |
| 20 | CT | 0.34 | 0/765 | 0.66 | 0/1007 |
| 21 | AU | 0.71 | 0/213 | 0.84 | 0/279 |
| 21 | CU | 0.75 | 0/213 | 0.78 | 0/279 |
| 22 | AW | 0.51 | 0/1809 | 1.00 | 3/2819 (0.1%) |
| 22 | AY | 0.74 | 0/408 | 1.23 | 0/634 |
| 22 | CW | 0.53 | 0/1809 | 0.99 | 6/2819 (0.2%) |
| 22 | CY | 0.85 | 0/408 | 1.39 | 3/634 (0.5%) |
| 23 | AV | 0.80 | 0/1836 | 1.30 | 11/2859 (0.4%) |
| 23 | CV | 0.81 | 0/1836 | 1.29 | 9/2859 (0.3%) |
| 24 | AX | 0.78 | 0/188 | 1.33 | 2/290 (0.7%) |
| 24 | CX | 0.97 | 0/235 | 1.28 | 2/364 (0.5%) |
| 25 | BA | 0.52 | 1/67620 (0.0%) | 0.74 | 24/105555 (0.0%) |
| 25 | DA | 0.52 | 2/67620 (0.0%) | 0.74 | 23/105555 (0.0%) |
| 26 | BB | 0.41 | 0/2853 | 0.71 | 1/4451 (0.0%) |
| 26 | DB | 0.42 | 0/2853 | 0.72 | 1/4451 (0.0%) |
| 27 | BC | 0.37 | 0/1145 | 0.67 | 7/1556 (0.4%) |
| 27 | DC | 0.38 | 0/1145 | 0.67 | 7/1556 (0.4%) |
| 28 | BD | 0.52 | 0/2155 | 0.82 | 0/2907 |
| 28 | DD | 0.53 | 0/2155 | 0.83 | 0/2907 |
| 29 | BE | 0.44 | 0/1597 | 0.78 | 2/2155 (0.1%) |
| 29 | DE | 0.44 | 0/1597 | 0.77 | 1/2155 (0.0%) |
| 30 | BF | 0.45 | 0/1659 | 0.74 | 0/2246 |
| 30 | DF | 0.45 | 0/1659 | 0.73 | 0/2246 |
| 31 | BG | 0.41 | 0/1499 | 0.73 | 1/2016 (0.0%) |
| 31 | DG | 0.41 | 0/1499 | 0.74 | 1/2016 (0.0%) |
| 32 | BH | 0.37 | 0/1246 | 0.70 | 2/1684 (0.1%) |
| 32 | DH | 0.37 | 0/1246 | 0.70 | 2/1684 (0.1%) |
| 33 | BI | 0.35 | 0/1147 | 0.71 | 0/1553 |
| 33 | DI | 0.37 | 0/1147 | 0.71 | 0/1553 |
| 34 | BN | 0.40 | 0/1132 | 0.74 | 1/1527 (0.1%) |
| 34 | DN | 0.39 | 0/1132 | 0.75 | 1/1527 (0.1%) |
| 35 | BO | 0.66 | 0/943 | 0.68 | 0/1269 |
| 35 | DO | 0.82 | 0/943 | 0.71 | 0/1269 |
| 36 | BP | 0.47 | 0/1131 | 0.84 | 0/1504 |
| 36 | DP | 0.45 | 0/1131 | 0.82 | 1/1504 (0.1%) |
| 37 | BQ | 0.41 | 0/1143 | 0.69 | 0/1527 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | DQ | 0.40 | 0/1143 | 0.68 | 0/1527 |
| 38 | BR | 0.40 | 0/974 | 0.76 | 0/1302 |
| 38 | DR | 0.40 | 0/974 | 0.77 | 0/1302 |
| 39 | BS | 0.41 | 0/779 | 0.72 | 0/1038 |
| 39 | DS | 0.38 | 0/779 | 0.71 | 0/1038 |
| 40 | BT | 0.58 | 0/1156 | 0.68 | 0/1544 |
| 40 | DT | 0.65 | 0/1156 | 0.70 | 1/1544 (0.1%) |
| 41 | BU | 0.39 | 0/975 | 0.70 | 0/1297 |
| 41 | DU | 0.39 | 0/975 | 0.70 | 0/1297 |
| 42 | BV | 0.38 | 0/790 | 0.70 | 0/1057 |
| 42 | DV | 0.39 | 0/790 | 0.71 | 0/1057 |
| 43 | BW | 0.41 | 0/907 | 0.69 | 0/1216 |
| 43 | DW | 0.41 | 0/907 | 0.69 | 0/1216 |
| 44 | BX | 0.49 | 0/740 | 0.72 | 0/995 |
| 44 | DX | 0.49 | 0/740 | 0.72 | 0/995 |
| 45 | BY | 0.49 | 0/789 | 0.77 | 0/1053 |
| 45 | DY | 0.45 | 0/789 | 0.79 | 1/1053 (0.1%) |
| 46 | BZ | 0.38 | 0/1436 | 0.66 | 0/1951 |
| 46 | DZ | 0.37 | 0/1436 | 0.67 | 0/1951 |
| 47 | B0 | 0.39 | 0/671 | 0.67 | 0/892 |
| 47 | D0 | 0.39 | 0/671 | 0.67 | 0/892 |
| 48 | B1 | 0.46 | 0/739 | 0.84 | 1/983 (0.1%) |
| 48 | D1 | 0.45 | 0/739 | 0.84 | 1/983 (0.1%) |
| 49 | B2 | 0.43 | 0/600 | 0.69 | 0/793 |
| 49 | D2 | 0.44 | 0/600 | 0.71 | 0/793 |
| 50 | B3 | 0.38 | 0/473 | 0.67 | 0/636 |
| 50 | D3 | 0.38 | 0/473 | 0.67 | 0/636 |
| 51 | B4 | 0.44 | 0/229 | 0.66 | 0/311 |
| 51 | D4 | 0.45 | 0/229 | 0.66 | 0/311 |
| 52 | B5 | 0.38 | 0/473 | 0.68 | 0/639 |
| 52 | D5 | 0.38 | 0/473 | 0.68 | 0/639 |
| 53 | B6 | 0.47 | 0/388 | 0.65 | 0/520 |
| 53 | D6 | 0.48 | 0/388 | 0.65 | 0/520 |
| 54 | B7 | 0.56 | 0/427 | 0.75 | 0/563 |
| 54 | D7 | 0.56 | 0/427 | 0.75 | 0/563 |
| 55 | B8 | 0.51 | 0/516 | 0.85 | 0/681 |
| 55 | D8 | 0.52 | 0/516 | 0.85 | 0/681 |
| 56 | B9 | 0.31 | 0/302 | 0.58 | 0/397 |
| 56 | D9 | 0.31 | 0/302 | 0.58 | 0/397 |
| All | All | 0.50 | 4/317064 (0.0%) | 0.84 | 226/474017 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|------|-------------|----------|
| 1 | AA | 1480 | A | N9-C4 | 5.60 | 1.41 | 1.37 |
| 25 | DA | 2307 | G | O3'-P | 5.54 | 1.67 | 1.61 |
| 25 | BA | 271(U) | G | O3'-P | 5.17 | 1.67 | 1.61 |
| 25 | DA | 271(U) | G | O3'-P | 5.13 | 1.67 | 1.61 |

The worst 5 of 226 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 29 | BE | 52 | LEU | C-N-CD | -8.27 | 102.41 | 120.60 |
| 45 | DY | 55 | TYR | C-N-CD | -6.12 | 107.12 | 120.60 |
| 13 | CM | 112 | GLY | C-N-CD | -6.03 | 107.34 | 120.60 |
| 23 | CV | 72 | C | N3-C4-C5 | -6.00 | 119.50 | 121.90 |
| 1 | CA | 1164 | A | C8-N9-C4 | 5.99 | 108.19 | 105.80 |

There are no chirality outliers.

There are no planarity outliers.

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 | 32326 | 0 | 16316 | 985 | 0 |
| 1 | CA | 32304 | 0 | 16306 | 977 | 0 |
| 2 | AB | 1901 | 0 | 1951 | 288 | 0 |
| 2 | CB | 1901 | 0 | 1951 | 297 | 0 |
| 3 | AC | 1613 | 0 | 1677 | 215 | 0 |
| 3 | CC | 1613 | 0 | 1677 | 202 | 1 |
| 4 | AD | 1703 | 0 | 1765 | 202 | 0 |
| 4 | CD | 1703 | 0 | 1764 | 152 | 4 |
| 5 | AE | 1147 | 0 | 1207 | 147 | 0 |
| 5 | CE | 1147 | 0 | 1207 | 156 | 0 |
| 6 | AF | 843 | 0 | 857 | 81 | 0 |
| 6 | CF | 843 | 0 | 856 | 108 | 0 |
| 7 | AG | 1257 | 0 | 1296 | 137 | 0 |
| 7 | CG | 1257 | 0 | 1296 | 142 | 0 |
| 8 | AH | 1116 | 0 | 1177 | 148 | 0 |
| 8 | CH | 1116 | 0 | 1177 | 169 | 0 |
| 9 | AI | 1010 | 0 | 1037 | 169 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | CI | 1010 | 0 | 1037 | 135 | 0 |
| 10 | AJ | 795 | 0 | 840 | 143 | 0 |
| 10 | CJ | 795 | 0 | 840 | 137 | 0 |
| 11 | AK | 885 | 0 | 904 | 104 | 1 |
| 11 | CK | 885 | 0 | 904 | 120 | 0 |
| 12 | AL | 971 | 0 | 1057 | 129 | 0 |
| 12 | CL | 971 | 0 | 1057 | 134 | 0 |
| 13 | AM | 988 | 0 | 1059 | 197 | 0 |
| 13 | CM | 988 | 0 | 1059 | 203 | 0 |
| 14 | AN | 492 | 0 | 531 | 88 | 0 |
| 14 | CN | 492 | 0 | 532 | 92 | 0 |
| 15 | AO | 734 | 0 | 771 | 70 | 0 |
| 15 | CO | 734 | 0 | 771 | 71 | 0 |
| 16 | AP | 701 | 0 | 720 | 56 | 0 |
| 16 | CP | 701 | 0 | 720 | 58 | 0 |
| 17 | AQ | 824 | 0 | 891 | 77 | 0 |
| 17 | CQ | 824 | 0 | 891 | 74 | 0 |
| 18 | AR | 574 | 0 | 644 | 61 | 0 |
| 18 | CR | 574 | 0 | 644 | 63 | 0 |
| 19 | AS | 630 | 0 | 652 | 102 | 0 |
| 19 | CS | 630 | 0 | 652 | 119 | 0 |
| 20 | AT | 763 | 0 | 861 | 114 | 0 |
| 20 | CT | 763 | 0 | 861 | 153 | 0 |
| 21 | AU | 209 | 0 | 221 | 10 | 0 |
| 21 | CU | 209 | 0 | 221 | 20 | 0 |
| 22 | AW | 1619 | 0 | 822 | 155 | 0 |
| 22 | AY | 365 | 0 | 185 | 55 | 0 |
| 22 | CW | 1619 | 0 | 822 | 203 | 0 |
| 22 | CY | 365 | 0 | 185 | 45 | 0 |
| 23 | AV | 1644 | 0 | 836 | 169 | 0 |
| 23 | CV | 1644 | 0 | 836 | 173 | 0 |
| 24 | AX | 169 | 0 | 86 | 17 | 0 |
| 24 | CX | 210 | 0 | 109 | 24 | 0 |
| 25 | BA | 60378 | 0 | 30440 | 2704 | 3 |
| 25 | DA | 60378 | 0 | 30441 | 2817 | 12 |
| 26 | BB | 2551 | 0 | 1295 | 140 | 1 |
| 26 | DB | 2551 | 0 | 1295 | 193 | 1 |
| 27 | BC | 1142 | 0 | 865 | 103 | 0 |
| 27 | DC | 1142 | 0 | 865 | 135 | 0 |
| 28 | BD | 2105 | 0 | 2182 | 296 | 4 |
| 28 | DD | 2105 | 0 | 2182 | 328 | 0 |
| 29 | BE | 1564 | 0 | 1629 | 269 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29 | DE | 1564 | 0 | 1629 | 280 | 0 |
| 30 | BF | 1624 | 0 | 1677 | 241 | 0 |
| 30 | DF | 1624 | 0 | 1677 | 234 | 0 |
| 31 | BG | 1474 | 0 | 1535 | 318 | 0 |
| 31 | DG | 1474 | 0 | 1535 | 292 | 0 |
| 32 | BH | 1223 | 0 | 1282 | 198 | 0 |
| 32 | DH | 1223 | 0 | 1282 | 236 | 2 |
| 33 | BI | 1132 | 0 | 1218 | 217 | 0 |
| 33 | DI | 1132 | 0 | 1218 | 214 | 0 |
| 34 | BN | 1105 | 0 | 1180 | 169 | 0 |
| 34 | DN | 1105 | 0 | 1180 | 170 | 0 |
| 35 | BO | 933 | 0 | 995 | 88 | 0 |
| 35 | DO | 933 | 0 | 996 | 78 | 0 |
| 36 | BP | 1114 | 0 | 1187 | 318 | 0 |
| 36 | DP | 1114 | 0 | 1187 | 299 | 8 |
| 37 | BQ | 1122 | 0 | 1179 | 154 | 0 |
| 37 | DQ | 1122 | 0 | 1179 | 184 | 0 |
| 38 | BR | 960 | 0 | 1021 | 143 | 0 |
| 38 | DR | 960 | 0 | 1021 | 144 | 0 |
| 39 | BS | 771 | 0 | 832 | 194 | 0 |
| 39 | DS | 771 | 0 | 832 | 196 | 0 |
| 40 | BT | 1142 | 0 | 1202 | 149 | 0 |
| 40 | DT | 1142 | 0 | 1202 | 225 | 0 |
| 41 | BU | 958 | 0 | 1015 | 170 | 0 |
| 41 | DU | 958 | 0 | 1015 | 173 | 0 |
| 42 | BV | 779 | 0 | 852 | 169 | 0 |
| 42 | DV | 779 | 0 | 852 | 174 | 3 |
| 43 | BW | 896 | 0 | 953 | 107 | 1 |
| 43 | DW | 896 | 0 | 953 | 112 | 0 |
| 44 | BX | 726 | 0 | 778 | 72 | 0 |
| 44 | DX | 726 | 0 | 778 | 74 | 0 |
| 45 | BY | 776 | 0 | 870 | 158 | 11 |
| 45 | DY | 776 | 0 | 870 | 184 | 2 |
| 46 | BZ | 1404 | 0 | 1432 | 219 | 0 |
| 46 | DZ | 1404 | 0 | 1432 | 230 | 0 |
| 47 | B0 | 662 | 0 | 688 | 79 | 0 |
| 47 | D0 | 662 | 0 | 688 | 77 | 0 |
| 48 | B1 | 732 | 0 | 808 | 98 | 0 |
| 48 | D1 | 732 | 0 | 808 | 91 | 0 |
| 49 | B2 | 598 | 0 | 653 | 71 | 0 |
| 49 | D2 | 598 | 0 | 653 | 86 | 1 |
| 50 | B3 | 468 | 0 | 523 | 67 | 8 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 50 | D3 | 468 | 0 | 523 | 73 | 0 |
| 51 | B4 | 226 | 0 | 229 | 46 | 0 |
| 51 | D4 | 226 | 0 | 229 | 37 | 0 |
| 52 | B5 | 459 | 0 | 480 | 64 | 0 |
| 52 | D5 | 459 | 0 | 480 | 60 | 3 |
| 53 | B6 | 381 | 0 | 391 | 74 | 0 |
| 53 | D6 | 381 | 0 | 391 | 75 | 0 |
| 54 | B7 | 419 | 0 | 467 | 42 | 0 |
| 54 | D7 | 419 | 0 | 467 | 45 | 0 |
| 55 | B8 | 508 | 0 | 576 | 109 | 0 |
| 55 | D8 | 508 | 0 | 576 | 104 | 0 |
| 56 | B9 | 299 | 0 | 326 | 24 | 0 |
| 56 | D9 | 299 | 0 | 326 | 21 | 0 |
| 57 | AA | 93 | 0 | 0 | 0 | 0 |
| 57 | AX | 2 | 0 | 0 | 0 | 0 |
| 57 | B1 | 1 | 0 | 0 | 0 | 0 |
| 57 | B3 | 1 | 0 | 0 | 0 | 0 |
| 57 | B5 | 2 | 0 | 0 | 0 | 0 |
| 57 | BA | 261 | 0 | 0 | 7 | 0 |
| 57 | BB | 4 | 0 | 0 | 0 | 0 |
| 57 | BE | 1 | 0 | 0 | 0 | 0 |
| 57 | BF | 2 | 0 | 0 | 0 | 0 |
| 57 | BO | 1 | 0 | 0 | 0 | 0 |
| 57 | BU | 1 | 0 | 0 | 0 | 0 |
| 57 | CA | 94 | 0 | 0 | 0 | 0 |
| 57 | CV | 2 | 0 | 0 | 0 | 0 |
| 57 | D0 | 1 | 0 | 0 | 0 | 0 |
| 57 | D5 | 2 | 0 | 0 | 0 | 0 |
| 57 | DA | 268 | 0 | 0 | 0 | 0 |
| 57 | DB | 2 | 0 | 0 | 0 | 0 |
| 57 | DD | 1 | 0 | 0 | 0 | 0 |
| 57 | DE | 1 | 0 | 0 | 0 | 0 |
| 58 | AA | 42 | 0 | 45 | 3 | 0 |
| 58 | CA | 42 | 0 | 45 | 1 | 0 |
| 59 | AD | 1 | 0 | 0 | 1 | 0 |
| 59 | AN | 1 | 0 | 0 | 2 | 0 |
| 59 | CD | 1 | 0 | 0 | 0 | 0 |
| 59 | CN | 1 | 0 | 0 | 0 | 0 |
| All | All | 292667 | 0 | 198350 | 20561 | 33 |

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 42.

The worst 5 of 20561 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) |
|------------------|-------------------|--------------------------|-------------------|
| 13:CM:93:ARG:CD | 25:DA:888:C:H5' | 1.15 | 1.61 |
| 4:AD:167:GLY:CA | 28:DD:135:PHE:CE2 | 1.85 | 1.56 |
| 25:BA:2584:U:C2' | 25:BA:2585:U:H5'' | 1.38 | 1.54 |
| 25:DA:2584:U:C2' | 25:DA:2585:U:H5'' | 1.38 | 1.54 |
| 4:AD:167:GLY:HA3 | 28:DD:135:PHE:CE2 | 1.43 | 1.50 |

The worst 5 of 33 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) |
|------------------|-------------------------|--------------------------|-------------------|
| 45:BY:55:TYR:CZ | 25:DA:355:G:O2'[3_555] | 0.78 | 1.42 |
| 45:BY:55:TYR:OH | 25:DA:355:G:C2'[3_555] | 1.05 | 1.15 |
| 50:B3:1:MET:CB | 36:DP:122:PRO:CG[3_455] | 1.20 | 1.00 |
| 50:B3:1:MET:CG | 36:DP:122:PRO:CB[3_455] | 1.33 | 0.87 |
| 45:BY:55:TYR:CE2 | 25:DA:355:G:O2'[3_555] | 1.37 | 0.83 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AB | 233/256 (91%) | 148 (64%) | 65 (28%) | 20 (9%) | 1 | 17 |
| 2 | CB | 233/256 (91%) | 148 (64%) | 65 (28%) | 20 (9%) | 1 | 17 |
| 3 | AC | 205/239 (86%) | 136 (66%) | 45 (22%) | 24 (12%) | 0 | 9 |
| 3 | CC | 205/239 (86%) | 137 (67%) | 43 (21%) | 25 (12%) | 0 | 8 |
| 4 | AD | 206/209 (99%) | 145 (70%) | 40 (19%) | 21 (10%) | 1 | 13 |
| 4 | CD | 206/209 (99%) | 144 (70%) | 40 (19%) | 22 (11%) | 0 | 11 |
| 5 | AE | 149/162 (92%) | 114 (76%) | 19 (13%) | 16 (11%) | 0 | 11 |
| 5 | CE | 149/162 (92%) | 114 (76%) | 19 (13%) | 16 (11%) | 0 | 11 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 6 | AF | 99/101 (98%) | 82 (83%) | 13 (13%) | 4 (4%) | 4 | 37 |
| 6 | CF | 99/101 (98%) | 81 (82%) | 15 (15%) | 3 (3%) | 5 | 44 |
| 7 | AG | 153/156 (98%) | 107 (70%) | 32 (21%) | 14 (9%) | 1 | 16 |
| 7 | CG | 153/156 (98%) | 107 (70%) | 32 (21%) | 14 (9%) | 1 | 16 |
| 8 | AH | 136/138 (99%) | 102 (75%) | 26 (19%) | 8 (6%) | 2 | 28 |
| 8 | CH | 136/138 (99%) | 100 (74%) | 28 (21%) | 8 (6%) | 2 | 28 |
| 9 | AI | 125/128 (98%) | 92 (74%) | 21 (17%) | 12 (10%) | 1 | 14 |
| 9 | CI | 125/128 (98%) | 93 (74%) | 22 (18%) | 10 (8%) | 1 | 19 |
| 10 | AJ | 97/105 (92%) | 66 (68%) | 22 (23%) | 9 (9%) | 1 | 16 |
| 10 | CJ | 97/105 (92%) | 67 (69%) | 21 (22%) | 9 (9%) | 1 | 16 |
| 11 | AK | 117/129 (91%) | 94 (80%) | 18 (15%) | 5 (4%) | 3 | 35 |
| 11 | CK | 117/129 (91%) | 92 (79%) | 20 (17%) | 5 (4%) | 3 | 35 |
| 12 | AL | 123/132 (93%) | 86 (70%) | 24 (20%) | 13 (11%) | 0 | 11 |
| 12 | CL | 123/132 (93%) | 85 (69%) | 25 (20%) | 13 (11%) | 0 | 11 |
| 13 | AM | 123/126 (98%) | 79 (64%) | 26 (21%) | 18 (15%) | 0 | 5 |
| 13 | CM | 123/126 (98%) | 84 (68%) | 23 (19%) | 16 (13%) | 0 | 7 |
| 14 | AN | 58/61 (95%) | 37 (64%) | 9 (16%) | 12 (21%) | 0 | 2 |
| 14 | CN | 58/61 (95%) | 37 (64%) | 9 (16%) | 12 (21%) | 0 | 2 |
| 15 | AO | 86/89 (97%) | 62 (72%) | 19 (22%) | 5 (6%) | 2 | 28 |
| 15 | CO | 86/89 (97%) | 63 (73%) | 18 (21%) | 5 (6%) | 2 | 28 |
| 16 | AP | 82/88 (93%) | 57 (70%) | 22 (27%) | 3 (4%) | 4 | 39 |
| 16 | CP | 82/88 (93%) | 58 (71%) | 21 (26%) | 3 (4%) | 4 | 39 |
| 17 | AQ | 98/105 (93%) | 77 (79%) | 14 (14%) | 7 (7%) | 1 | 23 |
| 17 | CQ | 98/105 (93%) | 77 (79%) | 13 (13%) | 8 (8%) | 1 | 18 |
| 18 | AR | 68/88 (77%) | 48 (71%) | 15 (22%) | 5 (7%) | 1 | 21 |
| 18 | CR | 68/88 (77%) | 45 (66%) | 17 (25%) | 6 (9%) | 1 | 17 |
| 19 | AS | 77/93 (83%) | 55 (71%) | 11 (14%) | 11 (14%) | 0 | 5 |
| 19 | CS | 77/93 (83%) | 55 (71%) | 12 (16%) | 10 (13%) | 0 | 7 |
| 20 | AT | 97/106 (92%) | 72 (74%) | 14 (14%) | 11 (11%) | 0 | 9 |
| 20 | CT | 97/106 (92%) | 72 (74%) | 15 (16%) | 10 (10%) | 1 | 12 |
| 21 | AU | 23/27 (85%) | 15 (65%) | 4 (17%) | 4 (17%) | 0 | 3 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 21 | CU | 23/27 (85%) | 18 (78%) | 3 (13%) | 2 (9%) | 1 | 17 |
| 27 | BC | 183/229 (80%) | 84 (46%) | 45 (25%) | 54 (30%) | 0 | 0 |
| 27 | DC | 183/229 (80%) | 84 (46%) | 44 (24%) | 55 (30%) | 0 | 0 |
| 28 | BD | 270/276 (98%) | 212 (78%) | 33 (12%) | 25 (9%) | 1 | 16 |
| 28 | DD | 270/276 (98%) | 209 (77%) | 36 (13%) | 25 (9%) | 1 | 16 |
| 29 | BE | 203/206 (98%) | 130 (64%) | 35 (17%) | 38 (19%) | 0 | 3 |
| 29 | DE | 203/206 (98%) | 129 (64%) | 36 (18%) | 38 (19%) | 0 | 3 |
| 30 | BF | 206/210 (98%) | 129 (63%) | 54 (26%) | 23 (11%) | 0 | 10 |
| 30 | DF | 206/210 (98%) | 128 (62%) | 55 (27%) | 23 (11%) | 0 | 10 |
| 31 | BG | 179/182 (98%) | 115 (64%) | 39 (22%) | 25 (14%) | 0 | 6 |
| 31 | DG | 179/182 (98%) | 114 (64%) | 39 (22%) | 26 (14%) | 0 | 5 |
| 32 | BH | 158/180 (88%) | 93 (59%) | 31 (20%) | 34 (22%) | 0 | 2 |
| 32 | DH | 158/180 (88%) | 95 (60%) | 31 (20%) | 32 (20%) | 0 | 2 |
| 33 | BI | 144/148 (97%) | 89 (62%) | 28 (19%) | 27 (19%) | 0 | 3 |
| 33 | DI | 144/148 (97%) | 87 (60%) | 30 (21%) | 27 (19%) | 0 | 3 |
| 34 | BN | 137/140 (98%) | 84 (61%) | 33 (24%) | 20 (15%) | 0 | 5 |
| 34 | DN | 137/140 (98%) | 84 (61%) | 33 (24%) | 20 (15%) | 0 | 5 |
| 35 | BO | 120/122 (98%) | 88 (73%) | 25 (21%) | 7 (6%) | 2 | 28 |
| 35 | DO | 120/122 (98%) | 94 (78%) | 16 (13%) | 10 (8%) | 1 | 18 |
| 36 | BP | 144/150 (96%) | 83 (58%) | 32 (22%) | 29 (20%) | 0 | 2 |
| 36 | DP | 144/150 (96%) | 81 (56%) | 33 (23%) | 30 (21%) | 0 | 2 |
| 37 | BQ | 139/141 (99%) | 104 (75%) | 19 (14%) | 16 (12%) | 0 | 9 |
| 37 | DQ | 139/141 (99%) | 104 (75%) | 17 (12%) | 18 (13%) | 0 | 7 |
| 38 | BR | 115/118 (98%) | 83 (72%) | 22 (19%) | 10 (9%) | 1 | 17 |
| 38 | DR | 115/118 (98%) | 83 (72%) | 21 (18%) | 11 (10%) | 1 | 14 |
| 39 | BS | 97/112 (87%) | 38 (39%) | 27 (28%) | 32 (33%) | 0 | 0 |
| 39 | DS | 97/112 (87%) | 38 (39%) | 27 (28%) | 32 (33%) | 0 | 0 |
| 40 | BT | 136/146 (93%) | 82 (60%) | 31 (23%) | 23 (17%) | 0 | 4 |
| 40 | DT | 136/146 (93%) | 88 (65%) | 33 (24%) | 15 (11%) | 0 | 10 |
| 41 | BU | 115/118 (98%) | 70 (61%) | 34 (30%) | 11 (10%) | 1 | 14 |
| 41 | DU | 115/118 (98%) | 70 (61%) | 34 (30%) | 11 (10%) | 1 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 42 | BV | 99/101 (98%) | 63 (64%) | 19 (19%) | 17 (17%) | 0 | 4 |
| 42 | DV | 99/101 (98%) | 64 (65%) | 19 (19%) | 16 (16%) | 0 | 5 |
| 43 | BW | 111/113 (98%) | 75 (68%) | 24 (22%) | 12 (11%) | 0 | 11 |
| 43 | DW | 111/113 (98%) | 75 (68%) | 24 (22%) | 12 (11%) | 0 | 11 |
| 44 | BX | 91/96 (95%) | 66 (72%) | 20 (22%) | 5 (6%) | 2 | 30 |
| 44 | DX | 91/96 (95%) | 66 (72%) | 20 (22%) | 5 (6%) | 2 | 30 |
| 45 | BY | 99/110 (90%) | 54 (54%) | 18 (18%) | 27 (27%) | 0 | 0 |
| 45 | DY | 99/110 (90%) | 53 (54%) | 16 (16%) | 30 (30%) | 0 | 0 |
| 46 | BZ | 175/206 (85%) | 103 (59%) | 35 (20%) | 37 (21%) | 0 | 2 |
| 46 | DZ | 175/206 (85%) | 103 (59%) | 35 (20%) | 37 (21%) | 0 | 2 |
| 47 | B0 | 82/85 (96%) | 63 (77%) | 12 (15%) | 7 (8%) | 1 | 17 |
| 47 | D0 | 82/85 (96%) | 63 (77%) | 12 (15%) | 7 (8%) | 1 | 17 |
| 48 | B1 | 92/98 (94%) | 64 (70%) | 19 (21%) | 9 (10%) | 1 | 14 |
| 48 | D1 | 92/98 (94%) | 64 (70%) | 19 (21%) | 9 (10%) | 1 | 14 |
| 49 | B2 | 69/72 (96%) | 47 (68%) | 13 (19%) | 9 (13%) | 0 | 7 |
| 49 | D2 | 69/72 (96%) | 51 (74%) | 9 (13%) | 9 (13%) | 0 | 7 |
| 50 | B3 | 58/60 (97%) | 41 (71%) | 7 (12%) | 10 (17%) | 0 | 4 |
| 50 | D3 | 58/60 (97%) | 41 (71%) | 7 (12%) | 10 (17%) | 0 | 4 |
| 51 | B4 | 29/71 (41%) | 15 (52%) | 7 (24%) | 7 (24%) | 0 | 1 |
| 51 | D4 | 29/71 (41%) | 15 (52%) | 7 (24%) | 7 (24%) | 0 | 1 |
| 52 | B5 | 57/60 (95%) | 42 (74%) | 8 (14%) | 7 (12%) | 0 | 8 |
| 52 | D5 | 57/60 (95%) | 42 (74%) | 8 (14%) | 7 (12%) | 0 | 8 |
| 53 | B6 | 43/54 (80%) | 20 (46%) | 12 (28%) | 11 (26%) | 0 | 1 |
| 53 | D6 | 43/54 (80%) | 20 (46%) | 12 (28%) | 11 (26%) | 0 | 1 |
| 54 | B7 | 47/49 (96%) | 44 (94%) | 2 (4%) | 1 (2%) | 9 | 51 |
| 54 | D7 | 47/49 (96%) | 44 (94%) | 2 (4%) | 1 (2%) | 9 | 51 |
| 55 | B8 | 62/65 (95%) | 40 (64%) | 13 (21%) | 9 (14%) | 0 | 5 |
| 55 | D8 | 62/65 (95%) | 39 (63%) | 14 (23%) | 9 (14%) | 0 | 5 |
| 56 | B9 | 34/37 (92%) | 27 (79%) | 6 (18%) | 1 (3%) | 6 | 45 |
| 56 | D9 | 34/37 (92%) | 27 (79%) | 6 (18%) | 1 (3%) | 6 | 45 |
| All | All | 11698/12586 (93%) | 7854 (67%) | 2318 (20%) | 1526 (13%) | 0 | 7 |

5 of 1526 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 9 | GLU |
| 2 | AB | 15 | VAL |
| 2 | AB | 20 | GLU |
| 2 | AB | 88 | ALA |
| 2 | AB | 195 | ASP |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AB | 202/220 (92%) | 177 (88%) | 25 (12%) | 6 | 32 |
| 2 | CB | 202/220 (92%) | 179 (89%) | 23 (11%) | 7 | 36 |
| 3 | AC | 160/188 (85%) | 149 (93%) | 11 (7%) | 19 | 59 |
| 3 | CC | 160/188 (85%) | 149 (93%) | 11 (7%) | 19 | 59 |
| 4 | AD | 180/181 (99%) | 161 (89%) | 19 (11%) | 8 | 39 |
| 4 | CD | 180/181 (99%) | 161 (89%) | 19 (11%) | 8 | 39 |
| 5 | AE | 115/123 (94%) | 101 (88%) | 14 (12%) | 6 | 33 |
| 5 | CE | 115/123 (94%) | 101 (88%) | 14 (12%) | 6 | 33 |
| 6 | AF | 90/90 (100%) | 83 (92%) | 7 (8%) | 16 | 54 |
| 6 | CF | 90/90 (100%) | 85 (94%) | 5 (6%) | 26 | 65 |
| 7 | AG | 126/127 (99%) | 117 (93%) | 9 (7%) | 18 | 58 |
| 7 | CG | 126/127 (99%) | 117 (93%) | 9 (7%) | 18 | 58 |
| 8 | AH | 119/119 (100%) | 112 (94%) | 7 (6%) | 24 | 64 |
| 8 | CH | 119/119 (100%) | 110 (92%) | 9 (8%) | 16 | 55 |
| 9 | AI | 98/99 (99%) | 86 (88%) | 12 (12%) | 6 | 33 |
| 9 | CI | 98/99 (99%) | 83 (85%) | 15 (15%) | 3 | 24 |
| 10 | AJ | 88/92 (96%) | 76 (86%) | 12 (14%) | 5 | 29 |
| 10 | CJ | 88/92 (96%) | 77 (88%) | 11 (12%) | 6 | 32 |
| 11 | AK | 90/99 (91%) | 82 (91%) | 8 (9%) | 12 | 48 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 11 | CK | 90/99 (91%) | 82 (91%) | 8 (9%) | 12 | 48 |
| 12 | AL | 104/109 (95%) | 94 (90%) | 10 (10%) | 10 | 44 |
| 12 | CL | 104/109 (95%) | 92 (88%) | 12 (12%) | 7 | 36 |
| 13 | AM | 99/101 (98%) | 81 (82%) | 18 (18%) | 2 | 16 |
| 13 | CM | 99/101 (98%) | 83 (84%) | 16 (16%) | 3 | 22 |
| 14 | AN | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 16 |
| 14 | CN | 49/50 (98%) | 42 (86%) | 7 (14%) | 4 | 28 |
| 15 | AO | 79/80 (99%) | 73 (92%) | 6 (8%) | 16 | 55 |
| 15 | CO | 79/80 (99%) | 73 (92%) | 6 (8%) | 16 | 55 |
| 16 | AP | 72/74 (97%) | 64 (89%) | 8 (11%) | 8 | 38 |
| 16 | CP | 72/74 (97%) | 66 (92%) | 6 (8%) | 14 | 51 |
| 17 | AQ | 94/97 (97%) | 85 (90%) | 9 (10%) | 10 | 44 |
| 17 | CQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 17 | 56 |
| 18 | AR | 61/77 (79%) | 57 (93%) | 4 (7%) | 21 | 60 |
| 18 | CR | 61/77 (79%) | 57 (93%) | 4 (7%) | 21 | 60 |
| 19 | AS | 69/80 (86%) | 58 (84%) | 11 (16%) | 3 | 23 |
| 19 | CS | 69/80 (86%) | 58 (84%) | 11 (16%) | 3 | 23 |
| 20 | AT | 76/82 (93%) | 71 (93%) | 5 (7%) | 21 | 60 |
| 20 | CT | 76/82 (93%) | 69 (91%) | 7 (9%) | 11 | 46 |
| 21 | AU | 19/22 (86%) | 18 (95%) | 1 (5%) | 28 | 67 |
| 21 | CU | 19/22 (86%) | 14 (74%) | 5 (26%) | 0 | 6 |
| 27 | BC | 61/181 (34%) | 56 (92%) | 5 (8%) | 14 | 52 |
| 27 | DC | 61/181 (34%) | 56 (92%) | 5 (8%) | 14 | 52 |
| 28 | BD | 213/218 (98%) | 179 (84%) | 34 (16%) | 3 | 23 |
| 28 | DD | 213/218 (98%) | 180 (84%) | 33 (16%) | 3 | 24 |
| 29 | BE | 165/166 (99%) | 140 (85%) | 25 (15%) | 3 | 25 |
| 29 | DE | 165/166 (99%) | 139 (84%) | 26 (16%) | 3 | 23 |
| 30 | BF | 165/166 (99%) | 146 (88%) | 19 (12%) | 7 | 36 |
| 30 | DF | 165/166 (99%) | 146 (88%) | 19 (12%) | 7 | 36 |
| 31 | BG | 155/156 (99%) | 138 (89%) | 17 (11%) | 8 | 38 |
| 31 | DG | 155/156 (99%) | 138 (89%) | 17 (11%) | 8 | 38 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 32 | BH | 132/148 (89%) | 119 (90%) | 13 (10%) | 10 | 43 |
| 32 | DH | 132/148 (89%) | 119 (90%) | 13 (10%) | 10 | 43 |
| 33 | BI | 122/124 (98%) | 102 (84%) | 20 (16%) | 3 | 21 |
| 33 | DI | 122/124 (98%) | 107 (88%) | 15 (12%) | 6 | 32 |
| 34 | BN | 117/119 (98%) | 96 (82%) | 21 (18%) | 2 | 17 |
| 34 | DN | 117/119 (98%) | 96 (82%) | 21 (18%) | 2 | 17 |
| 35 | BO | 100/100 (100%) | 92 (92%) | 8 (8%) | 15 | 53 |
| 35 | DO | 100/100 (100%) | 83 (83%) | 17 (17%) | 2 | 20 |
| 36 | BP | 112/116 (97%) | 86 (77%) | 26 (23%) | 1 | 8 |
| 36 | DP | 112/116 (97%) | 89 (80%) | 23 (20%) | 1 | 12 |
| 37 | BQ | 111/111 (100%) | 96 (86%) | 15 (14%) | 5 | 30 |
| 37 | DQ | 111/111 (100%) | 94 (85%) | 17 (15%) | 3 | 24 |
| 38 | BR | 100/101 (99%) | 87 (87%) | 13 (13%) | 5 | 31 |
| 38 | DR | 100/101 (99%) | 87 (87%) | 13 (13%) | 5 | 31 |
| 39 | BS | 77/88 (88%) | 66 (86%) | 11 (14%) | 4 | 28 |
| 39 | DS | 77/88 (88%) | 67 (87%) | 10 (13%) | 5 | 31 |
| 40 | BT | 120/127 (94%) | 90 (75%) | 30 (25%) | 1 | 7 |
| 40 | DT | 120/127 (94%) | 85 (71%) | 35 (29%) | 0 | 4 |
| 41 | BU | 92/94 (98%) | 85 (92%) | 7 (8%) | 16 | 55 |
| 41 | DU | 92/94 (98%) | 85 (92%) | 7 (8%) | 16 | 55 |
| 42 | BV | 82/82 (100%) | 72 (88%) | 10 (12%) | 6 | 33 |
| 42 | DV | 82/82 (100%) | 72 (88%) | 10 (12%) | 6 | 33 |
| 43 | BW | 91/92 (99%) | 82 (90%) | 9 (10%) | 10 | 42 |
| 43 | DW | 91/92 (99%) | 81 (89%) | 10 (11%) | 8 | 38 |
| 44 | BX | 74/78 (95%) | 67 (90%) | 7 (10%) | 11 | 44 |
| 44 | DX | 74/78 (95%) | 67 (90%) | 7 (10%) | 11 | 44 |
| 45 | BY | 84/91 (92%) | 72 (86%) | 12 (14%) | 4 | 28 |
| 45 | DY | 84/91 (92%) | 70 (83%) | 14 (17%) | 3 | 21 |
| 46 | BZ | 155/179 (87%) | 138 (89%) | 17 (11%) | 8 | 38 |
| 46 | DZ | 155/179 (87%) | 137 (88%) | 18 (12%) | 7 | 36 |
| 47 | B0 | 66/67 (98%) | 58 (88%) | 8 (12%) | 6 | 33 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 47 | D0 | 66/67 (98%) | 58 (88%) | 8 (12%) | 6 | 33 |
| 48 | B1 | 78/83 (94%) | 67 (86%) | 11 (14%) | 4 | 28 |
| 48 | D1 | 78/83 (94%) | 67 (86%) | 11 (14%) | 4 | 28 |
| 49 | B2 | 66/67 (98%) | 55 (83%) | 11 (17%) | 3 | 21 |
| 49 | D2 | 66/67 (98%) | 55 (83%) | 11 (17%) | 3 | 21 |
| 50 | B3 | 51/52 (98%) | 49 (96%) | 2 (4%) | 39 | 74 |
| 50 | D3 | 51/52 (98%) | 49 (96%) | 2 (4%) | 39 | 74 |
| 51 | B4 | 27/63 (43%) | 24 (89%) | 3 (11%) | 8 | 38 |
| 51 | D4 | 27/63 (43%) | 24 (89%) | 3 (11%) | 8 | 38 |
| 52 | B5 | 51/52 (98%) | 45 (88%) | 6 (12%) | 6 | 35 |
| 52 | D5 | 51/52 (98%) | 45 (88%) | 6 (12%) | 6 | 35 |
| 53 | B6 | 43/52 (83%) | 32 (74%) | 11 (26%) | 0 | 6 |
| 53 | D6 | 43/52 (83%) | 32 (74%) | 11 (26%) | 0 | 6 |
| 54 | B7 | 41/42 (98%) | 37 (90%) | 4 (10%) | 10 | 43 |
| 54 | D7 | 41/42 (98%) | 37 (90%) | 4 (10%) | 10 | 43 |
| 55 | B8 | 53/55 (96%) | 44 (83%) | 9 (17%) | 2 | 20 |
| 55 | D8 | 53/55 (96%) | 43 (81%) | 10 (19%) | 2 | 14 |
| 56 | B9 | 33/34 (97%) | 30 (91%) | 3 (9%) | 12 | 47 |
| 56 | D9 | 33/34 (97%) | 30 (91%) | 3 (9%) | 12 | 47 |
| All | All | 9654/10428 (93%) | 8458 (88%) | 1196 (12%) | 6 | 32 |

5 of 1196 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | B1 | 82 | LEU |
| 7 | CG | 88 | PRO |
| 45 | DY | 77 | PRO |
| 51 | B4 | 46 | ASN |
| 2 | CB | 155 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | B6 | 20 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CF | 100 | ASN |
| 47 | D0 | 29 | GLN |
| 53 | B6 | 26 | ASN |
| 2 | CB | 95 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1503/1522 (98%) | 291 (19%) | 27 (1%) |
| 1 | CA | 1502/1522 (98%) | 290 (19%) | 32 (2%) |
| 22 | AW | 75/76 (98%) | 22 (29%) | 0 |
| 22 | AY | 16/76 (21%) | 9 (56%) | 0 |
| 22 | CW | 75/76 (98%) | 26 (34%) | 0 |
| 22 | CY | 16/76 (21%) | 7 (43%) | 0 |
| 23 | AV | 76/77 (98%) | 37 (48%) | 5 (6%) |
| 23 | CV | 76/77 (98%) | 34 (44%) | 5 (6%) |
| 24 | AX | 7/24 (29%) | 2 (28%) | 0 |
| 24 | CX | 9/24 (37%) | 3 (33%) | 1 (11%) |
| 25 | BA | 2796/2916 (95%) | 557 (19%) | 53 (1%) |
| 25 | DA | 2796/2916 (95%) | 564 (20%) | 58 (2%) |
| 26 | BB | 118/122 (96%) | 18 (15%) | 1 (0%) |
| 26 | DB | 118/122 (96%) | 19 (16%) | 1 (0%) |
| All | All | 9183/9626 (95%) | 1879 (20%) | 183 (1%) |

5 of 1879 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |

5 of 183 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 25 | BA | 2763 | G |
| 1 | CA | 731 | C |
| 25 | DA | 2263 | C |
| 26 | BB | 66 | A |
| 1 | CA | 262 | C |

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 746 ligands modelled in this entry, 744 are monoatomic - leaving 2 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 | $\# Z > 2$ |
| 58 | PAR | AA | 1694 | - | 45,45,45 | 1.43 | 9 (20%) | 59,67,67 | 1.25 | 6 (10%) |
| 58 | PAR | CA | 1695 | - | 45,45,45 | 1.70 | 11 (24%) | 59,67,67 | 1.39 | 6 (10%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 58 | PAR | AA | 1694 | - | - | 0/18/94/94 | 0/4/4/4 |
| 58 | PAR | CA | 1695 | - | - | 0/18/94/94 | 0/4/4/4 |

The worst 5 of 20 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 58 | CA | 1695 | PAR | O52-C52 | 2.01 | 1.48 | 1.43 |
| 58 | AA | 1694 | PAR | O54-C54 | 2.01 | 1.49 | 1.44 |
| 58 | AA | 1694 | PAR | C31-C21 | 2.03 | 1.56 | 1.53 |
| 58 | CA | 1695 | PAR | O51-C11 | 2.06 | 1.47 | 1.41 |
| 58 | CA | 1695 | PAR | O11-C42 | 2.09 | 1.49 | 1.43 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|-------------|------|------------------------|---------------------|
| 58 | CA | 1695 | PAR | C11-O51-C51 | 2.42 | 118.44 | 113.75 |
| 58 | AA | 1694 | PAR | C11-O51-C51 | 2.47 | 118.55 | 113.75 |
| 58 | AA | 1694 | PAR | O11-C11-C21 | 3.08 | 113.66 | 107.96 |
| 58 | AA | 1694 | PAR | O52-C13-C23 | 3.26 | 114.53 | 107.75 |
| 58 | CA | 1695 | PAR | O33-C14-C24 | 3.32 | 114.11 | 107.96 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58 | AA | 1694 | PAR | 3 | 0 |
| 58 | CA | 1695 | PAR | 1 | 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 | 1504/1522 (98%) | 0.19 | 56 (3%) | 45 | 34 | 7, 49, 127, 206 | 0 |
| 1 | CA | 1503/1522 (98%) | 0.16 | 52 (3%) | 48 | 36 | 2, 41, 123, 215 | 0 |
| 2 | AB | 235/256 (91%) | 0.17 | 11 (4%) | 35 | 26 | 44, 88, 131, 174 | 0 |
| 2 | CB | 235/256 (91%) | 0.20 | 9 (3%) | 44 | 33 | 40, 81, 123, 166 | 0 |
| 3 | AC | 207/239 (86%) | 0.11 | 8 (3%) | 43 | 32 | 38, 71, 111, 143 | 0 |
| 3 | CC | 207/239 (86%) | 0.13 | 5 (2%) | 62 | 50 | 28, 62, 104, 145 | 0 |
| 4 | AD | 208/209 (99%) | -0.01 | 3 (1%) | 78 | 68 | 28, 59, 107, 141 | 0 |
| 4 | CD | 208/209 (99%) | 0.12 | 7 (3%) | 49 | 37 | 21, 52, 103, 125 | 0 |
| 5 | AE | 151/162 (93%) | 0.12 | 1 (0%) | 89 | 84 | 7, 52, 95, 111 | 0 |
| 5 | CE | 151/162 (93%) | 0.16 | 6 (3%) | 42 | 31 | 4, 46, 92, 114 | 0 |
| 6 | AF | 101/101 (100%) | -0.01 | 2 (1%) | 68 | 57 | 16, 53, 101, 141 | 0 |
| 6 | CF | 101/101 (100%) | 0.40 | 8 (7%) | 15 | 10 | 12, 55, 104, 131 | 0 |
| 7 | AG | 155/156 (99%) | 0.22 | 11 (7%) | 19 | 12 | 34, 66, 111, 154 | 0 |
| 7 | CG | 155/156 (99%) | 0.23 | 8 (5%) | 31 | 22 | 27, 64, 114, 148 | 0 |
| 8 | AH | 138/138 (100%) | 0.04 | 3 (2%) | 65 | 54 | 19, 59, 87, 125 | 0 |
| 8 | CH | 138/138 (100%) | -0.06 | 1 (0%) | 89 | 84 | 12, 49, 82, 122 | 0 |
| 9 | AI | 127/128 (99%) | 0.34 | 7 (5%) | 29 | 20 | 31, 75, 120, 153 | 0 |
| 9 | CI | 127/128 (99%) | 0.55 | 14 (11%) | 7 | 5 | 27, 75, 114, 148 | 0 |
| 10 | AJ | 99/105 (94%) | 0.79 | 15 (15%) | 3 | 3 | 41, 85, 128, 142 | 0 |
| 10 | CJ | 99/105 (94%) | 0.70 | 10 (10%) | 9 | 7 | 27, 77, 128, 143 | 0 |
| 11 | AK | 119/129 (92%) | 0.22 | 6 (5%) | 32 | 24 | 13, 49, 98, 129 | 0 |
| 11 | CK | 119/129 (92%) | 0.24 | 4 (3%) | 49 | 37 | 8, 46, 98, 121 | 0 |
| 12 | AL | 125/132 (94%) | 0.02 | 4 (3%) | 51 | 38 | 2, 39, 88, 141 | 0 |
| 12 | CL | 125/132 (94%) | 0.16 | 4 (3%) | 51 | 38 | 0, 27, 75, 143 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 13 | AM | 125/126 (99%) | 0.36 | 7 (5%) | 28 | 20 | 36, 76, 116, 147 | 0 |
| 13 | CM | 125/126 (99%) | 0.18 | 5 (4%) | 42 | 31 | 22, 61, 109, 136 | 0 |
| 14 | AN | 60/61 (98%) | 0.42 | 2 (3%) | 50 | 38 | 40, 67, 117, 132 | 0 |
| 14 | CN | 60/61 (98%) | 0.35 | 2 (3%) | 50 | 38 | 31, 50, 106, 121 | 0 |
| 15 | AO | 88/89 (98%) | 0.05 | 3 (3%) | 49 | 37 | 14, 48, 93, 116 | 0 |
| 15 | CO | 88/89 (98%) | -0.00 | 1 (1%) | 82 | 74 | 9, 45, 89, 132 | 0 |
| 16 | AP | 84/88 (95%) | 0.11 | 0 | 100 | 100 | 30, 51, 101, 137 | 0 |
| 16 | CP | 84/88 (95%) | 0.09 | 0 | 100 | 100 | 30, 52, 88, 106 | 0 |
| 17 | AQ | 100/105 (95%) | 0.18 | 5 (5%) | 32 | 24 | 24, 56, 103, 111 | 0 |
| 17 | CQ | 100/105 (95%) | 0.16 | 3 (3%) | 54 | 40 | 18, 53, 110, 121 | 0 |
| 18 | AR | 70/88 (79%) | 0.15 | 3 (4%) | 39 | 28 | 17, 54, 98, 118 | 0 |
| 18 | CR | 70/88 (79%) | 0.05 | 0 | 100 | 100 | 12, 47, 88, 116 | 0 |
| 19 | AS | 79/93 (84%) | 0.23 | 6 (7%) | 17 | 11 | 37, 76, 126, 161 | 0 |
| 19 | CS | 79/93 (84%) | 0.27 | 1 (1%) | 79 | 70 | 26, 55, 121, 146 | 0 |
| 20 | AT | 99/106 (93%) | 0.34 | 8 (8%) | 15 | 10 | 11, 59, 105, 121 | 0 |
| 20 | CT | 99/106 (93%) | 0.17 | 3 (3%) | 54 | 40 | 3, 58, 106, 125 | 0 |
| 21 | AU | 25/27 (92%) | 1.22 | 6 (24%) | 1 | 1 | 41, 69, 87, 97 | 0 |
| 21 | CU | 25/27 (92%) | 0.69 | 2 (8%) | 15 | 10 | 31, 55, 91, 125 | 0 |
| 22 | AW | 76/76 (100%) | 1.27 | 19 (25%) | 1 | 1 | 23, 129, 187, 208 | 0 |
| 22 | AY | 17/76 (22%) | 1.28 | 2 (11%) | 6 | 5 | 29, 51, 105, 123 | 0 |
| 22 | CW | 76/76 (100%) | 1.42 | 22 (28%) | 1 | 1 | 12, 118, 185, 207 | 0 |
| 22 | CY | 17/76 (22%) | 0.70 | 2 (11%) | 6 | 5 | 10, 37, 117, 125 | 0 |
| 23 | AV | 77/77 (100%) | 0.22 | 2 (2%) | 59 | 47 | 16, 67, 122, 137 | 0 |
| 23 | CV | 77/77 (100%) | 0.17 | 4 (5%) | 31 | 22 | 10, 55, 109, 155 | 0 |
| 24 | AX | 8/24 (33%) | 0.19 | 0 | 100 | 100 | 15, 33, 63, 66 | 0 |
| 24 | CX | 10/24 (41%) | 0.16 | 1 (10%) | 9 | 7 | 9, 26, 96, 134 | 0 |
| 25 | BA | 2803/2916 (96%) | 0.48 | 163 (5%) | 26 | 18 | 6, 38, 143, 240 | 0 |
| 25 | DA | 2803/2916 (96%) | 0.42 | 120 (4%) | 39 | 28 | 0, 20, 132, 232 | 0 |
| 26 | BB | 119/122 (97%) | 0.55 | 3 (2%) | 61 | 48 | 32, 70, 127, 179 | 0 |
| 26 | DB | 119/122 (97%) | 0.36 | 3 (2%) | 61 | 48 | 14, 44, 88, 118 | 0 |
| 27 | BC | 191/229 (83%) | 1.85 | 80 (41%) | 0 | 1 | 44, 115, 155, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27 | DC | 191/229 (83%) | 2.12 | 88 (46%) 0 1 | 33, 112, 151, 174 | 0 |
| 28 | BD | 272/276 (98%) | -0.04 | 0 100 100 | 6, 23, 70, 121 | 0 |
| 28 | DD | 272/276 (98%) | -0.17 | 2 (0%) 89 84 | 0, 11, 51, 96 | 0 |
| 29 | BE | 205/206 (99%) | 0.05 | 5 (2%) 62 50 | 13, 50, 111, 161 | 0 |
| 29 | DE | 205/206 (99%) | 0.14 | 6 (2%) 55 42 | 1, 29, 96, 158 | 0 |
| 30 | BF | 208/210 (99%) | 0.06 | 8 (3%) 44 33 | 10, 43, 115, 172 | 0 |
| 30 | DF | 208/210 (99%) | -0.11 | 3 (1%) 78 68 | 0, 23, 106, 154 | 0 |
| 31 | BG | 181/182 (99%) | 0.03 | 7 (3%) 43 32 | 9, 63, 118, 169 | 0 |
| 31 | DG | 181/182 (99%) | 0.11 | 10 (5%) 29 20 | 4, 51, 107, 178 | 0 |
| 32 | BH | 160/180 (88%) | 1.39 | 46 (28%) 1 1 | 37, 115, 166, 197 | 0 |
| 32 | DH | 160/180 (88%) | 0.52 | 9 (5%) 28 20 | 3, 61, 115, 143 | 0 |
| 33 | BI | 146/148 (98%) | 0.47 | 14 (9%) 10 7 | 19, 68, 125, 152 | 0 |
| 33 | DI | 146/148 (98%) | 0.21 | 5 (3%) 49 37 | 6, 64, 119, 168 | 0 |
| 34 | BN | 139/140 (99%) | 0.10 | 2 (1%) 78 68 | 23, 58, 106, 176 | 0 |
| 34 | DN | 139/140 (99%) | -0.17 | 0 100 100 | 2, 29, 83, 139 | 0 |
| 35 | BO | 122/122 (100%) | -0.34 | 0 100 100 | 17, 42, 82, 99 | 0 |
| 35 | DO | 122/122 (100%) | -0.45 | 0 100 100 | 0, 22, 61, 74 | 0 |
| 36 | BP | 146/150 (97%) | 0.31 | 4 (2%) 58 46 | 8, 49, 108, 157 | 0 |
| 36 | DP | 146/150 (97%) | 0.21 | 5 (3%) 49 37 | 0, 43, 108, 167 | 0 |
| 37 | BQ | 141/141 (100%) | 0.30 | 8 (5%) 27 19 | 7, 50, 102, 180 | 0 |
| 37 | DQ | 141/141 (100%) | -0.06 | 2 (1%) 78 68 | 1, 25, 75, 167 | 0 |
| 38 | BR | 117/118 (99%) | -0.13 | 1 (0%) 85 79 | 18, 39, 91, 120 | 0 |
| 38 | DR | 117/118 (99%) | -0.16 | 1 (0%) 85 79 | 4, 22, 64, 109 | 0 |
| 39 | BS | 99/112 (88%) | 0.24 | 1 (1%) 84 77 | 15, 67, 116, 158 | 0 |
| 39 | DS | 99/112 (88%) | 0.11 | 2 (2%) 68 57 | 11, 41, 91, 147 | 0 |
| 40 | BT | 138/146 (94%) | -0.01 | 7 (5%) 32 23 | 24, 57, 109, 142 | 0 |
| 40 | DT | 138/146 (94%) | -0.17 | 3 (2%) 65 54 | 3, 39, 96, 120 | 0 |
| 41 | BU | 117/118 (99%) | 0.16 | 4 (3%) 49 37 | 14, 48, 114, 142 | 0 |
| 41 | DU | 117/118 (99%) | -0.19 | 0 100 100 | 2, 19, 65, 93 | 0 |
| 42 | BV | 101/101 (100%) | 0.35 | 4 (3%) 42 31 | 15, 72, 122, 175 | 0 |
| 42 | DV | 101/101 (100%) | 0.09 | 2 (1%) 68 57 | 1, 39, 86, 153 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 43 | BW | 113/113 (100%) | 0.23 | 7 (6%) 24 15 | 11, 32, 89, 159 | 0 |
| 43 | DW | 113/113 (100%) | -0.10 | 1 (0%) 85 79 | 2, 17, 64, 110 | 0 |
| 44 | BX | 93/96 (96%) | 0.00 | 0 100 100 | 15, 35, 72, 98 | 0 |
| 44 | DX | 93/96 (96%) | 0.05 | 1 (1%) 82 74 | 2, 20, 73, 84 | 0 |
| 45 | BY | 101/110 (91%) | 0.75 | 18 (17%) 2 2 | 20, 63, 128, 197 | 0 |
| 45 | DY | 101/110 (91%) | 0.46 | 9 (8%) 12 8 | 6, 54, 131, 226 | 0 |
| 46 | BZ | 177/206 (85%) | 0.77 | 18 (10%) 9 7 | 0, 83, 131, 156 | 0 |
| 46 | DZ | 177/206 (85%) | 0.53 | 17 (9%) 10 7 | 4, 66, 131, 155 | 0 |
| 47 | B0 | 84/85 (98%) | 0.71 | 11 (13%) 5 4 | 11, 44, 92, 147 | 0 |
| 47 | D0 | 84/85 (98%) | 0.34 | 7 (8%) 14 9 | 4, 23, 85, 144 | 0 |
| 48 | B1 | 94/98 (95%) | 0.47 | 4 (4%) 39 28 | 6, 33, 89, 106 | 0 |
| 48 | D1 | 94/98 (95%) | 0.07 | 0 100 100 | 2, 28, 85, 136 | 0 |
| 49 | B2 | 71/72 (98%) | -0.07 | 1 (1%) 78 68 | 18, 49, 104, 122 | 0 |
| 49 | D2 | 71/72 (98%) | 0.11 | 3 (4%) 40 29 | 2, 30, 96, 132 | 0 |
| 50 | B3 | 60/60 (100%) | 0.38 | 2 (3%) 50 38 | 20, 59, 111, 177 | 0 |
| 50 | D3 | 60/60 (100%) | 0.16 | 1 (1%) 73 62 | 2, 26, 90, 130 | 0 |
| 51 | B4 | 31/71 (43%) | -0.19 | 0 100 100 | 33, 76, 100, 107 | 0 |
| 51 | D4 | 31/71 (43%) | -0.05 | 0 100 100 | 8, 66, 113, 156 | 0 |
| 52 | B5 | 59/60 (98%) | 0.48 | 7 (11%) 6 5 | 1, 43, 128, 147 | 0 |
| 52 | D5 | 59/60 (98%) | 0.09 | 3 (5%) 32 23 | 0, 29, 112, 160 | 0 |
| 53 | B6 | 45/54 (83%) | 1.52 | 15 (33%) 0 1 | 26, 85, 131, 153 | 0 |
| 53 | D6 | 45/54 (83%) | 1.49 | 14 (31%) 1 1 | 15, 78, 124, 159 | 0 |
| 54 | B7 | 49/49 (100%) | 0.01 | 0 100 100 | 0, 18, 70, 86 | 0 |
| 54 | D7 | 49/49 (100%) | -0.09 | 1 (2%) 68 57 | 0, 3, 44, 108 | 0 |
| 55 | B8 | 64/65 (98%) | 0.43 | 5 (7%) 16 10 | 0, 39, 92, 121 | 0 |
| 55 | D8 | 64/65 (98%) | 0.06 | 1 (1%) 74 64 | 0, 21, 71, 121 | 0 |
| 56 | B9 | 36/37 (97%) | 4.11 | 33 (91%) 0 0 | 79, 117, 145, 155 | 0 |
| 56 | D9 | 36/37 (97%) | 4.10 | 31 (86%) 0 0 | 45, 105, 140, 163 | 0 |
| All | All | 21119/22212 (95%) | 0.31 | 1192 (5%) 28 20 | 0, 46, 126, 240 | 0 |

The worst 5 of 1192 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 25 | DA | 2802 | G | 13.5 |
| 11 | AK | 129 | SER | 13.3 |
| 25 | BA | 2802 | G | 13.2 |
| 56 | B9 | 14 | CYS | 12.5 |
| 27 | DC | 166 | ASP | 12.4 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | DA | 3141 | 1/1 | 0.94 | 0.85 | 65.99 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3033 | 1/1 | 0.92 | 1.67 | 64.44 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3020 | 1/1 | 0.40 | 1.03 | 60.57 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3003 | 1/1 | 0.78 | 1.18 | 60.39 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3072 | 1/1 | 0.88 | 1.41 | 57.64 | 1,1,1,1 | 0 |
| 57 | MG | CA | 1694 | 1/1 | 0.88 | 0.88 | 57.63 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3127 | 1/1 | 0.78 | 1.40 | 52.91 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3103 | 1/1 | 0.91 | 1.28 | 51.63 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3227 | 1/1 | 0.71 | 0.43 | 44.76 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3235 | 1/1 | 0.94 | 0.96 | 43.98 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3050 | 1/1 | 0.90 | 1.28 | 43.02 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3214 | 1/1 | 0.92 | 1.10 | 41.15 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3007 | 1/1 | 0.93 | 1.25 | 40.68 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3245 | 1/1 | 0.85 | 0.99 | 39.87 | 0,0,0,0 | 1 |
| 57 | MG | BA | 3035 | 1/1 | 0.95 | 1.46 | 39.68 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3056 | 1/1 | 0.87 | 0.83 | 39.40 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3091 | 1/1 | 0.88 | 0.99 | 37.07 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | AA | 1650 | 1/1 | 0.86 | 1.10 | 35.80 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3146 | 1/1 | 0.96 | 0.58 | 35.30 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1689 | 1/1 | 0.81 | 1.28 | 33.22 | 0,0,0,0 | 1 |
| 57 | MG | CA | 1670 | 1/1 | 0.67 | 0.83 | 32.91 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3048 | 1/1 | 0.96 | 0.58 | 32.27 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3093 | 1/1 | 0.90 | 1.04 | 31.80 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3128 | 1/1 | 0.74 | 1.46 | 31.54 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3051 | 1/1 | 0.90 | 0.67 | 31.47 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3173 | 1/1 | 0.87 | 0.80 | 31.09 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3087 | 1/1 | 0.94 | 1.10 | 30.53 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3023 | 1/1 | 0.96 | 1.12 | 29.97 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1635 | 1/1 | 0.89 | 1.26 | 29.47 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3104 | 1/1 | 0.81 | 0.93 | 28.08 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3177 | 1/1 | 0.70 | 0.81 | 27.20 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3251 | 1/1 | 0.46 | 0.69 | 27.10 | 0,0,0,0 | 1 |
| 57 | MG | DA | 3099 | 1/1 | 0.96 | 0.55 | 25.88 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3098 | 1/1 | 0.88 | 0.83 | 25.87 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3086 | 1/1 | 0.89 | 0.93 | 25.51 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3262 | 1/1 | 0.93 | 0.80 | 25.46 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3045 | 1/1 | 0.89 | 0.61 | 25.33 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3043 | 1/1 | 0.86 | 0.86 | 25.33 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3047 | 1/1 | 0.89 | 0.71 | 24.50 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3259 | 1/1 | 0.70 | 1.08 | 24.47 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3100 | 1/1 | 0.84 | 0.80 | 24.40 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1624 | 1/1 | 0.87 | 0.72 | 23.81 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3145 | 1/1 | 0.82 | 0.68 | 23.44 | 1,1,1,1 | 0 |
| 57 | MG | CA | 1690 | 1/1 | 0.98 | 0.34 | 22.92 | 3,3,3,3 | 0 |
| 57 | MG | DA | 3061 | 1/1 | 0.95 | 0.63 | 22.63 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3070 | 1/1 | 0.94 | 0.99 | 22.31 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3157 | 1/1 | 0.98 | 0.80 | 22.30 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3129 | 1/1 | 0.93 | 0.53 | 22.30 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3007 | 1/1 | 0.89 | 0.88 | 22.27 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3152 | 1/1 | 0.91 | 0.93 | 22.24 | 3,3,3,3 | 0 |
| 57 | MG | DA | 3004 | 1/1 | 0.88 | 1.03 | 22.08 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3005 | 1/1 | 0.92 | 0.71 | 21.78 | 0,0,0,0 | 0 |
| 57 | MG | BU | 201 | 1/1 | 0.27 | 0.94 | 21.66 | 8,8,8,8 | 0 |
| 57 | MG | BA | 3233 | 1/1 | 0.77 | 0.88 | 21.23 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1626 | 1/1 | 0.70 | 1.19 | 20.98 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3019 | 1/1 | 0.96 | 0.67 | 20.37 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1619 | 1/1 | 0.70 | 0.46 | 20.28 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3020 | 1/1 | 0.97 | 0.70 | 20.01 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | DA | 3055 | 1/1 | 0.92 | 0.34 | 19.93 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1617 | 1/1 | 0.88 | 0.69 | 19.44 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3201 | 1/1 | 0.75 | 1.25 | 19.16 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3073 | 1/1 | 0.90 | 0.53 | 18.57 | 0,0,0,0 | 0 |
| 57 | MG | D5 | 102 | 1/1 | 0.71 | 0.82 | 18.38 | 0,0,0,0 | 1 |
| 57 | MG | DA | 3161 | 1/1 | 0.79 | 0.64 | 17.80 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1691 | 1/1 | 0.96 | 0.80 | 17.47 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3183 | 1/1 | 0.96 | 0.50 | 17.45 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3103 | 1/1 | 0.91 | 0.65 | 17.04 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3257 | 1/1 | 0.98 | 0.59 | 16.63 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3194 | 1/1 | 0.90 | 0.58 | 16.16 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3009 | 1/1 | 0.89 | 1.03 | 16.07 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3112 | 1/1 | 0.71 | 0.81 | 16.06 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3048 | 1/1 | 0.95 | 0.53 | 15.23 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3088 | 1/1 | 0.82 | 0.74 | 15.05 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3125 | 1/1 | 0.93 | 0.67 | 14.66 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3044 | 1/1 | 0.87 | 0.60 | 14.61 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3169 | 1/1 | 0.84 | 0.82 | 14.60 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1664 | 1/1 | 0.78 | 0.39 | 14.38 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3197 | 1/1 | 0.16 | 0.97 | 14.24 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3063 | 1/1 | 0.72 | 0.94 | 14.17 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1620 | 1/1 | 0.70 | 1.01 | 13.89 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3018 | 1/1 | 0.95 | 0.76 | 13.72 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1613 | 1/1 | 0.92 | 0.75 | 13.64 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3138 | 1/1 | 0.95 | 0.81 | 13.57 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3046 | 1/1 | 0.87 | 0.59 | 13.53 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1609 | 1/1 | 0.95 | 0.86 | 13.49 | 3,3,3,3 | 0 |
| 57 | MG | BA | 3095 | 1/1 | 0.93 | 0.62 | 12.79 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3051 | 1/1 | 0.87 | 0.63 | 12.67 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3209 | 1/1 | 0.94 | 0.41 | 12.50 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3189 | 1/1 | 0.98 | 0.57 | 12.37 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3161 | 1/1 | 0.93 | 0.73 | 12.07 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3144 | 1/1 | 0.92 | 0.54 | 11.97 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3211 | 1/1 | 0.76 | 0.53 | 11.89 | 12,12,12,12 | 0 |
| 57 | MG | BA | 3055 | 1/1 | 0.97 | 0.41 | 11.75 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3019 | 1/1 | 0.84 | 0.47 | 11.46 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3251 | 1/1 | 0.79 | 0.55 | 11.16 | 8,8,8,8 | 0 |
| 57 | MG | DA | 3062 | 1/1 | 0.93 | 0.41 | 11.08 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3258 | 1/1 | 0.88 | 0.61 | 10.99 | 8,8,8,8 | 0 |
| 57 | MG | DA | 3228 | 1/1 | 0.84 | 0.40 | 10.64 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3238 | 1/1 | 0.79 | 0.42 | 10.26 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | BA | 3247 | 1/1 | 0.93 | 0.59 | 10.16 | 7,7,7,7 | 0 |
| 57 | MG | BA | 3036 | 1/1 | 0.87 | 0.73 | 10.12 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3075 | 1/1 | 0.92 | 0.73 | 9.63 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3141 | 1/1 | 0.90 | 0.59 | 9.60 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3084 | 1/1 | 0.87 | 0.46 | 9.58 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3053 | 1/1 | 0.95 | 0.37 | 9.36 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1616 | 1/1 | 0.91 | 0.73 | 9.27 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1644 | 1/1 | 0.90 | 0.51 | 9.26 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3158 | 1/1 | 0.97 | 0.41 | 9.04 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1602 | 1/1 | 0.98 | 0.29 | 8.97 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3191 | 1/1 | 0.77 | 0.39 | 8.94 | 13,13,13,13 | 0 |
| 57 | MG | DA | 3155 | 1/1 | 0.93 | 0.52 | 8.94 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3174 | 1/1 | 0.93 | 0.49 | 8.69 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1651 | 1/1 | 0.92 | 0.29 | 8.60 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3092 | 1/1 | 0.97 | 0.37 | 8.57 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1648 | 1/1 | 0.97 | 0.32 | 8.55 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3079 | 1/1 | 0.98 | 0.56 | 8.50 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3201 | 1/1 | 0.95 | 0.47 | 8.40 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3240 | 1/1 | 0.67 | 0.44 | 8.34 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1673 | 1/1 | 0.85 | 0.41 | 8.31 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3114 | 1/1 | 0.85 | 0.52 | 8.28 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3035 | 1/1 | 0.96 | 0.34 | 8.18 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3094 | 1/1 | 0.79 | 0.56 | 8.00 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3109 | 1/1 | 0.97 | 0.56 | 7.92 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3150 | 1/1 | 0.67 | 1.37 | 7.70 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1652 | 1/1 | 0.86 | 0.29 | 7.63 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3046 | 1/1 | 0.92 | 0.35 | 7.54 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3074 | 1/1 | 0.97 | 0.39 | 7.42 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3117 | 1/1 | 0.55 | 0.80 | 7.34 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3142 | 1/1 | 0.93 | 0.62 | 6.96 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3149 | 1/1 | 0.95 | 0.44 | 6.66 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3122 | 1/1 | 0.87 | 0.32 | 6.62 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1639 | 1/1 | 0.94 | 0.54 | 6.49 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3250 | 1/1 | 0.81 | 0.35 | 6.48 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3117 | 1/1 | 0.98 | 0.32 | 6.47 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3174 | 1/1 | 0.95 | 0.64 | 6.43 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1622 | 1/1 | 0.90 | 0.58 | 6.33 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3239 | 1/1 | 0.94 | 0.41 | 5.97 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3170 | 1/1 | 0.83 | 0.59 | 5.85 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1667 | 1/1 | 0.90 | 0.33 | 5.83 | 15,15,15,15 | 0 |
| 57 | MG | BA | 3081 | 1/1 | 0.88 | 0.36 | 5.78 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3067 | 1/1 | 0.72 | 0.67 | 5.77 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3119 | 1/1 | 0.97 | 0.48 | 5.76 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1640 | 1/1 | 0.73 | 0.62 | 5.71 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3135 | 1/1 | 0.94 | 0.28 | 5.68 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3173 | 1/1 | 0.68 | 0.43 | 5.66 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3047 | 1/1 | 0.97 | 0.32 | 5.46 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3225 | 1/1 | 0.98 | 0.73 | 5.37 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3080 | 1/1 | 0.98 | 0.40 | 5.25 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3123 | 1/1 | 0.96 | 0.43 | 5.01 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3082 | 1/1 | 0.98 | 0.33 | 4.99 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1666 | 1/1 | 0.96 | 0.57 | 4.93 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1611 | 1/1 | 0.96 | 0.41 | 4.78 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3248 | 1/1 | 0.70 | 0.42 | 4.76 | 0,0,0,0 | 1 |
| 57 | MG | DA | 3107 | 1/1 | 0.63 | 0.53 | 4.70 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1671 | 1/1 | 0.96 | 0.44 | 4.60 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1606 | 1/1 | 0.93 | 0.54 | 4.53 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3232 | 1/1 | 0.83 | 0.33 | 4.51 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3140 | 1/1 | 0.90 | 0.24 | 4.33 | 12,12,12,12 | 0 |
| 57 | MG | BA | 3151 | 1/1 | 0.97 | 0.33 | 4.28 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3146 | 1/1 | 0.89 | 0.24 | 4.25 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3064 | 1/1 | 0.72 | 0.50 | 4.24 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1653 | 1/1 | 0.94 | 0.50 | 4.23 | 1,1,1,1 | 0 |
| 57 | MG | AA | 1604 | 1/1 | 0.91 | 0.34 | 4.22 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3089 | 1/1 | 0.96 | 0.36 | 4.13 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3120 | 1/1 | 0.95 | 0.45 | 3.95 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3215 | 1/1 | 0.95 | 0.29 | 3.76 | 18,18,18,18 | 0 |
| 57 | MG | DA | 3205 | 1/1 | 0.98 | 0.40 | 3.76 | 0,0,0,0 | 0 |
| 58 | PAR | CA | 1695 | 42/42 | 0.90 | 0.34 | 3.72 | 36,39,47,50 | 0 |
| 57 | MG | BA | 3227 | 1/1 | 0.94 | 0.56 | 3.67 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3166 | 1/1 | 0.91 | 0.34 | 3.63 | 0,0,0,0 | 0 |
| 58 | PAR | AA | 1694 | 42/42 | 0.87 | 0.31 | 3.61 | 11,14,23,25 | 0 |
| 57 | MG | DA | 3114 | 1/1 | 0.96 | 0.27 | 3.57 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1629 | 1/1 | 0.98 | 0.26 | 3.57 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1603 | 1/1 | 0.95 | 0.34 | 3.42 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1615 | 1/1 | 0.88 | 0.37 | 3.33 | 1,1,1,1 | 0 |
| 57 | MG | AA | 1653 | 1/1 | 0.97 | 0.29 | 3.31 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3138 | 1/1 | 0.98 | 0.30 | 3.29 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3183 | 1/1 | 0.96 | 0.30 | 3.28 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3068 | 1/1 | 0.95 | 0.38 | 3.21 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3197 | 1/1 | 0.92 | 0.39 | 3.11 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1657 | 1/1 | 0.92 | 0.27 | 3.00 | 1,1,1,1 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 57 | MG | CA | 1663 | 1/1 | 0.91 | 0.27 | 2.99 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3059 | 1/1 | 0.87 | 0.28 | 2.98 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3194 | 1/1 | 0.65 | 0.33 | 2.92 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3182 | 1/1 | 0.82 | 0.37 | 2.92 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1615 | 1/1 | 0.96 | 0.31 | 2.78 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3196 | 1/1 | 0.74 | 0.25 | 2.77 | 3,3,3,3 | 0 |
| 57 | MG | BA | 3139 | 1/1 | 0.92 | 0.32 | 2.64 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3002 | 1/1 | 0.82 | 0.27 | 2.62 | 13,13,13,13 | 0 |
| 57 | MG | BA | 3113 | 1/1 | 0.93 | 0.30 | 2.49 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1692 | 1/1 | 0.96 | 0.26 | 2.22 | 2,2,2,2 | 0 |
| 57 | MG | DA | 3108 | 1/1 | 0.91 | 0.31 | 2.20 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1650 | 1/1 | 0.98 | 0.29 | 2.15 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3070 | 1/1 | 0.85 | 0.26 | 2.06 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3118 | 1/1 | 0.97 | 0.29 | 1.98 | 3,3,3,3 | 0 |
| 57 | MG | BA | 3033 | 1/1 | 0.94 | 0.32 | 1.85 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1657 | 1/1 | 0.81 | 0.21 | 1.82 | 0,0,0,0 | 0 |
| 57 | MG | D0 | 101 | 1/1 | 0.75 | 0.54 | 1.77 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3030 | 1/1 | 0.82 | 0.24 | 1.74 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3032 | 1/1 | 0.99 | 0.25 | 1.65 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1659 | 1/1 | 0.94 | 0.43 | 1.64 | 8,8,8,8 | 0 |
| 57 | MG | CA | 1623 | 1/1 | 0.92 | 0.38 | 1.49 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3078 | 1/1 | 0.59 | 0.22 | 1.48 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3206 | 1/1 | 0.95 | 0.28 | 1.44 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3243 | 1/1 | 0.91 | 0.27 | 1.29 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1688 | 1/1 | 0.96 | 0.28 | 1.23 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3041 | 1/1 | 0.94 | 0.24 | 1.07 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3090 | 1/1 | 0.94 | 0.28 | 1.03 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1614 | 1/1 | 0.95 | 0.20 | 1.01 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3005 | 1/1 | 0.98 | 0.26 | 0.95 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3037 | 1/1 | 0.83 | 0.24 | 0.89 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3140 | 1/1 | 0.95 | 0.28 | 0.86 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1655 | 1/1 | 0.88 | 0.24 | 0.81 | 21,21,21,21 | 0 |
| 57 | MG | AA | 1618 | 1/1 | 0.94 | 0.21 | 0.77 | 7,7,7,7 | 0 |
| 57 | MG | AA | 1655 | 1/1 | 0.97 | 0.20 | 0.66 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1659 | 1/1 | 0.90 | 0.22 | 0.53 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1637 | 1/1 | 0.83 | 0.33 | 0.48 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1648 | 1/1 | 0.88 | 0.18 | 0.47 | 1,1,1,1 | 0 |
| 57 | MG | DA | 3030 | 1/1 | 0.88 | 0.20 | 0.35 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3213 | 1/1 | 0.89 | 0.19 | 0.15 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3198 | 1/1 | 0.84 | 0.19 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | BF | 302 | 1/1 | 0.84 | 0.34 | -0.02 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1658 | 1/1 | 0.94 | 0.18 | -0.17 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | BA | 3179 | 1/1 | 0.94 | 0.24 | -0.18 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3239 | 1/1 | 0.90 | 0.22 | -0.19 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3223 | 1/1 | 0.98 | 0.24 | -0.19 | 0,0,0,0 | 0 |
| 57 | MG | CA | 1649 | 1/1 | 0.96 | 0.18 | -0.22 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1656 | 1/1 | 0.89 | 0.24 | -0.22 | 9,9,9,9 | 0 |
| 57 | MG | DA | 3190 | 1/1 | 0.91 | 0.22 | -0.32 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1665 | 1/1 | 0.96 | 0.18 | -0.36 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3153 | 1/1 | 0.93 | 0.21 | -0.42 | 0,0,0,0 | 0 |
| 59 | ZN | CD | 801 | 1/1 | 0.86 | 0.30 | -0.43 | 8,8,8,8 | 0 |
| 57 | MG | AA | 1668 | 1/1 | 0.93 | 0.18 | -0.46 | 36,36,36,36 | 0 |
| 57 | MG | CA | 1691 | 1/1 | 0.98 | 0.12 | -0.86 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3027 | 1/1 | 0.95 | 0.13 | -0.87 | 0,0,0,0 | 1 |
| 57 | MG | DA | 3115 | 1/1 | 0.97 | 0.19 | -0.87 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3057 | 1/1 | 0.98 | 0.21 | -0.89 | 0,0,0,0 | 0 |
| 57 | MG | DA | 3052 | 1/1 | 0.94 | 0.21 | -0.97 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1663 | 1/1 | 0.93 | 0.16 | -0.98 | 4,4,4,4 | 0 |
| 57 | MG | AA | 1693 | 1/1 | 0.90 | 0.12 | -1.17 | 5,5,5,5 | 0 |
| 59 | ZN | CN | 101 | 1/1 | 0.91 | 0.15 | -1.20 | 125,125,125,125 | 0 |
| 57 | MG | BA | 3107 | 1/1 | 0.94 | 0.17 | -1.21 | 12,12,12,12 | 0 |
| 57 | MG | AA | 1658 | 1/1 | 0.85 | 0.14 | -1.27 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3224 | 1/1 | 0.95 | 0.23 | -1.28 | 0,0,0,0 | 0 |
| 59 | ZN | AD | 801 | 1/1 | 0.95 | 0.26 | -1.32 | 9,9,9,9 | 0 |
| 59 | ZN | AN | 101 | 1/1 | 0.95 | 0.10 | -1.32 | 76,76,76,76 | 0 |
| 57 | MG | DA | 3217 | 1/1 | 0.97 | 0.06 | -1.42 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3207 | 1/1 | 0.88 | 0.19 | -1.45 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3034 | 1/1 | 0.95 | 0.16 | -1.51 | 2,2,2,2 | 0 |
| 57 | MG | BA | 3224 | 1/1 | 0.96 | 0.14 | -1.57 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3052 | 1/1 | 0.90 | 0.16 | -1.64 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3164 | 1/1 | 0.96 | 0.15 | -1.67 | 54,54,54,54 | 0 |
| 57 | MG | CA | 1612 | 1/1 | 0.94 | 0.15 | -1.70 | 8,8,8,8 | 0 |
| 57 | MG | CV | 101 | 1/1 | 0.97 | 0.12 | -1.73 | 1,1,1,1 | 0 |
| 57 | MG | BA | 3032 | 1/1 | 0.91 | 0.15 | -1.76 | 0,0,0,0 | 0 |
| 57 | MG | AA | 1602 | 1/1 | 0.97 | 0.18 | -1.76 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3171 | 1/1 | 0.89 | 0.12 | -1.89 | 6,6,6,6 | 0 |
| 57 | MG | DB | 202 | 1/1 | 0.95 | 0.13 | -2.05 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3088 | 1/1 | 0.82 | 0.17 | -2.05 | 2,2,2,2 | 0 |
| 57 | MG | BA | 3182 | 1/1 | 0.94 | 0.15 | -2.16 | 17,17,17,17 | 0 |
| 57 | MG | BA | 3008 | 1/1 | 0.90 | 0.15 | -2.24 | 0,0,0,0 | 0 |
| 57 | MG | BA | 3246 | 1/1 | 0.83 | 0.09 | -2.27 | 21,21,21,21 | 0 |
| 57 | MG | BB | 204 | 1/1 | 0.81 | 0.13 | -2.62 | 0,0,0,0 | 1 |
| 57 | MG | DB | 201 | 1/1 | 0.91 | 0.15 | -2.70 | 0,0,0,0 | 1 |
| 57 | MG | CA | 1631 | 1/1 | 0.97 | 0.07 | -3.32 | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 57 | MG | BA | 3060 | 1/1 | 0.96 | 0.08 | -3.39 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3137 | 1/1 | 0.94 | 0.11 | -3.74 | 108,108,108,108 | 0 |
| 57 | MG | AA | 1642 | 1/1 | 0.90 | 0.10 | -3.94 | 46,46,46,46 | 0 |
| 57 | MG | AA | 1661 | 1/1 | 0.97 | 0.08 | -4.96 | 1,1,1,1 | 0 |
| 57 | MG | CA | 1621 | 1/1 | 0.95 | 0.10 | -5.07 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3022 | 1/1 | 0.94 | 0.14 | - | 8,8,8,8 | 0 |
| 57 | MG | DA | 3008 | 1/1 | 0.89 | 0.67 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1687 | 1/1 | 0.65 | 0.64 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1644 | 1/1 | 0.93 | 0.48 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3120 | 1/1 | 0.70 | 0.84 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3222 | 1/1 | 0.97 | 0.21 | - | 4,4,4,4 | 0 |
| 57 | MG | CA | 1647 | 1/1 | 0.85 | 0.84 | - | 0,0,0,0 | 1 |
| 57 | MG | CA | 1635 | 1/1 | 0.67 | 0.89 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3217 | 1/1 | 0.78 | 0.49 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3247 | 1/1 | 0.63 | 0.54 | - | 0,0,0,0 | 1 |
| 57 | MG | BA | 3163 | 1/1 | 0.70 | 1.33 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3001 | 1/1 | 0.67 | 1.59 | - | 17,17,17,17 | 0 |
| 57 | MG | DA | 3253 | 1/1 | 0.99 | 0.41 | - | 5,5,5,5 | 0 |
| 57 | MG | BA | 3043 | 1/1 | 0.89 | 0.14 | - | 0,0,0,0 | 1 |
| 57 | MG | CA | 1669 | 1/1 | 0.71 | 0.71 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3131 | 1/1 | 0.92 | 0.32 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3093 | 1/1 | 0.97 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3187 | 1/1 | 0.80 | 0.43 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3097 | 1/1 | 0.98 | 0.45 | - | 1,1,1,1 | 0 |
| 57 | MG | CA | 1608 | 1/1 | 0.83 | 0.39 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1654 | 1/1 | 0.84 | 0.56 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1679 | 1/1 | 0.77 | 0.61 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3162 | 1/1 | 0.80 | 0.71 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1614 | 1/1 | 0.96 | 0.65 | - | 2,2,2,2 | 0 |
| 57 | MG | DA | 3029 | 1/1 | 0.89 | 0.30 | - | 0,0,0,0 | 0 |
| 57 | MG | BE | 301 | 1/1 | 0.90 | 0.52 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1613 | 1/1 | 0.96 | 0.39 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3044 | 1/1 | 0.82 | 0.96 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1664 | 1/1 | 0.84 | 0.31 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3170 | 1/1 | 0.96 | 0.32 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3106 | 1/1 | 0.96 | 0.29 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3242 | 1/1 | 0.55 | 0.63 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3156 | 1/1 | 0.96 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3229 | 1/1 | 0.97 | 0.55 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3065 | 1/1 | 0.68 | 0.73 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3159 | 1/1 | 0.96 | 0.46 | - | 7,7,7,7 | 0 |
| 57 | MG | CA | 1684 | 1/1 | 0.90 | 0.67 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3125 | 1/1 | 0.99 | 0.13 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3235 | 1/1 | 0.91 | 0.22 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3258 | 1/1 | 0.89 | 0.13 | - | 23,23,23,23 | 0 |
| 57 | MG | DA | 3002 | 1/1 | 0.81 | 1.16 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3092 | 1/1 | 0.94 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3021 | 1/1 | 0.80 | 0.35 | - | 18,18,18,18 | 0 |
| 57 | MG | AA | 1647 | 1/1 | 0.77 | 0.27 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1684 | 1/1 | 0.82 | 0.36 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3260 | 1/1 | 0.93 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1605 | 1/1 | 0.93 | 0.12 | - | 26,26,26,26 | 0 |
| 57 | MG | BA | 3230 | 1/1 | 0.84 | 0.84 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3186 | 1/1 | 0.91 | 1.17 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3135 | 1/1 | 0.76 | 0.84 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3029 | 1/1 | 0.90 | 0.30 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3096 | 1/1 | 0.90 | 0.30 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1622 | 1/1 | 0.90 | 0.22 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1619 | 1/1 | 0.89 | 0.44 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3072 | 1/1 | 0.96 | 0.63 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3056 | 1/1 | 0.93 | 1.18 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3108 | 1/1 | 0.88 | 1.13 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3062 | 1/1 | 0.97 | 0.06 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3238 | 1/1 | 0.94 | 0.27 | - | 2,2,2,2 | 1 |
| 57 | MG | AA | 1652 | 1/1 | 0.42 | 1.74 | - | 0,0,0,0 | 1 |
| 57 | MG | BA | 3124 | 1/1 | 0.56 | 1.21 | - | 2,2,2,2 | 1 |
| 57 | MG | DA | 3012 | 1/1 | 0.85 | 0.28 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3200 | 1/1 | 0.98 | 0.06 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3184 | 1/1 | 0.92 | 0.56 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3221 | 1/1 | 0.65 | 0.80 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3049 | 1/1 | 0.94 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3068 | 1/1 | 0.96 | 0.94 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1660 | 1/1 | 0.95 | 0.11 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1632 | 1/1 | 0.90 | 1.28 | - | 0,0,0,0 | 0 |
| 57 | MG | DD | 301 | 1/1 | 0.71 | 0.35 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3016 | 1/1 | 0.94 | 0.52 | - | 1,1,1,1 | 0 |
| 57 | MG | B1 | 101 | 1/1 | 0.87 | 0.20 | - | 59,59,59,59 | 1 |
| 57 | MG | DA | 3207 | 1/1 | 0.94 | 0.51 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3204 | 1/1 | 0.75 | 0.37 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3079 | 1/1 | 0.96 | 0.58 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3249 | 1/1 | 0.69 | 1.44 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3178 | 1/1 | 0.90 | 0.72 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3034 | 1/1 | 0.90 | 0.36 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3249 | 1/1 | 0.82 | 0.17 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | CA | 1681 | 1/1 | 0.98 | 0.29 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3076 | 1/1 | 0.87 | 0.24 | - | 34,34,34,34 | 0 |
| 57 | MG | AA | 1643 | 1/1 | 0.93 | 0.14 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3134 | 1/1 | 0.73 | 1.42 | - | 0,0,0,0 | 1 |
| 57 | MG | CA | 1609 | 1/1 | 0.70 | 1.56 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1674 | 1/1 | 0.93 | 0.54 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3248 | 1/1 | 0.61 | 0.62 | - | 7,7,7,7 | 0 |
| 57 | MG | CA | 1679 | 1/1 | 0.81 | 0.18 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1645 | 1/1 | 0.75 | 0.81 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3240 | 1/1 | 0.81 | 0.43 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3144 | 1/1 | 0.86 | 0.37 | - | 1,1,1,1 | 0 |
| 57 | MG | AA | 1685 | 1/1 | 0.84 | 1.01 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3169 | 1/1 | 0.88 | 1.21 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3069 | 1/1 | 0.88 | 0.08 | - | 24,24,24,24 | 0 |
| 57 | MG | BA | 3160 | 1/1 | 0.64 | 0.65 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3097 | 1/1 | 0.76 | 0.46 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3223 | 1/1 | 0.59 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1678 | 1/1 | 0.94 | 0.51 | - | 2,2,2,2 | 0 |
| 57 | MG | BA | 3216 | 1/1 | 0.89 | 0.24 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3017 | 1/1 | 0.93 | 0.42 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3220 | 1/1 | 0.97 | 0.11 | - | 16,16,16,16 | 0 |
| 57 | MG | BA | 3165 | 1/1 | 0.96 | 0.33 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3094 | 1/1 | 0.55 | 0.92 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3132 | 1/1 | 0.81 | 0.96 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1682 | 1/1 | 0.96 | 0.14 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3154 | 1/1 | 0.93 | 0.21 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3121 | 1/1 | 0.93 | 0.50 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3010 | 1/1 | 0.95 | 0.61 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3004 | 1/1 | 0.88 | 1.38 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3015 | 1/1 | 0.89 | 0.24 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3178 | 1/1 | 0.95 | 0.41 | - | 0,0,0,0 | 1 |
| 57 | MG | BA | 3129 | 1/1 | 0.93 | 0.22 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3267 | 1/1 | 0.96 | 0.11 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3105 | 1/1 | 0.66 | 1.18 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3028 | 1/1 | 0.71 | 0.56 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3042 | 1/1 | 0.89 | 0.50 | - | 0,0,0,0 | 0 |
| 57 | MG | AX | 102 | 1/1 | 0.96 | 0.17 | - | 29,29,29,29 | 0 |
| 57 | MG | BA | 3122 | 1/1 | 0.98 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3040 | 1/1 | 0.96 | 0.85 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1641 | 1/1 | 0.84 | 1.80 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3212 | 1/1 | 0.69 | 1.32 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3060 | 1/1 | 0.52 | 0.72 | - | 11,11,11,11 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | CA | 1686 | 1/1 | 0.97 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3127 | 1/1 | 0.91 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3172 | 1/1 | 0.96 | 0.18 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3045 | 1/1 | 0.83 | 0.67 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1626 | 1/1 | 0.87 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3142 | 1/1 | 0.93 | 0.60 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3087 | 1/1 | 0.64 | 0.48 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3187 | 1/1 | 0.65 | 0.72 | - | 5,5,5,5 | 0 |
| 57 | MG | DA | 3026 | 1/1 | 0.78 | 0.35 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3252 | 1/1 | 0.86 | 0.27 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3168 | 1/1 | 0.98 | 0.47 | - | 37,37,37,37 | 1 |
| 57 | MG | BB | 201 | 1/1 | 0.88 | 0.41 | - | 0,0,0,0 | 1 |
| 57 | MG | CA | 1675 | 1/1 | 0.96 | 0.39 | - | 0,0,0,0 | 0 |
| 57 | MG | BO | 201 | 1/1 | 0.78 | 0.30 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3126 | 1/1 | 0.91 | 0.38 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3099 | 1/1 | 0.84 | 0.68 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3226 | 1/1 | 0.98 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3054 | 1/1 | 0.91 | 0.76 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3192 | 1/1 | 0.70 | 0.90 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3049 | 1/1 | 0.92 | 0.50 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3147 | 1/1 | 0.93 | 0.14 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3080 | 1/1 | 0.95 | 0.24 | - | 13,13,13,13 | 0 |
| 57 | MG | BA | 3037 | 1/1 | 0.64 | 0.72 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3102 | 1/1 | 0.92 | 0.71 | - | 0,0,0,0 | 0 |
| 57 | MG | BB | 202 | 1/1 | 0.95 | 0.08 | - | 29,29,29,29 | 0 |
| 57 | MG | CA | 1661 | 1/1 | 0.85 | 0.47 | - | 1,1,1,1 | 0 |
| 57 | MG | AA | 1629 | 1/1 | 0.88 | 0.14 | - | 29,29,29,29 | 0 |
| 57 | MG | CA | 1642 | 1/1 | 0.91 | 1.07 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3261 | 1/1 | 0.94 | 0.16 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3109 | 1/1 | 0.93 | 0.27 | - | 2,2,2,2 | 0 |
| 57 | MG | DA | 3053 | 1/1 | 0.98 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3036 | 1/1 | 0.88 | 0.71 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3116 | 1/1 | 0.87 | 0.30 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3025 | 1/1 | 0.88 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3244 | 1/1 | 0.83 | 0.64 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3066 | 1/1 | 0.86 | 0.13 | - | 86,86,86,86 | 0 |
| 57 | MG | BA | 3231 | 1/1 | 0.50 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3133 | 1/1 | 0.98 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3027 | 1/1 | 0.59 | 0.22 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3213 | 1/1 | 0.86 | 0.45 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3181 | 1/1 | 0.72 | 0.72 | - | 15,15,15,15 | 0 |
| 57 | MG | B3 | 101 | 1/1 | 0.89 | 0.67 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1601 | 1/1 | 0.80 | 1.05 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3265 | 1/1 | 0.71 | 0.70 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1654 | 1/1 | 0.77 | 0.57 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3195 | 1/1 | 0.65 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3134 | 1/1 | 0.87 | 0.57 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3176 | 1/1 | 0.95 | 0.19 | - | 24,24,24,24 | 0 |
| 57 | MG | BA | 3071 | 1/1 | 0.92 | 0.44 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3256 | 1/1 | 0.88 | 0.87 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3110 | 1/1 | 0.49 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1627 | 1/1 | 0.94 | 0.24 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3219 | 1/1 | 0.85 | 0.10 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1669 | 1/1 | 0.82 | 0.93 | - | 3,3,3,3 | 1 |
| 57 | MG | CA | 1624 | 1/1 | 0.82 | 0.27 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3057 | 1/1 | 0.94 | 0.08 | - | 29,29,29,29 | 0 |
| 57 | MG | AA | 1673 | 1/1 | 0.95 | 1.30 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3003 | 1/1 | 0.84 | 0.48 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3189 | 1/1 | 0.95 | 0.63 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3175 | 1/1 | 0.95 | 0.82 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3038 | 1/1 | 0.78 | 0.54 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3071 | 1/1 | 0.81 | 1.22 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3124 | 1/1 | 0.80 | 0.51 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3067 | 1/1 | 0.92 | 1.37 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3148 | 1/1 | 0.98 | 0.19 | - | 0,0,0,0 | 0 |
| 57 | MG | AX | 101 | 1/1 | 0.95 | 0.10 | - | 3,3,3,3 | 0 |
| 57 | MG | CA | 1611 | 1/1 | 0.90 | 0.58 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3196 | 1/1 | 0.98 | 0.26 | - | 0,0,0,0 | 1 |
| 57 | MG | AA | 1634 | 1/1 | 0.51 | 1.89 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3220 | 1/1 | 0.83 | 0.75 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3200 | 1/1 | 0.89 | 0.84 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3017 | 1/1 | 0.87 | 0.32 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1639 | 1/1 | 0.97 | 0.47 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3202 | 1/1 | 0.72 | 0.35 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3254 | 1/1 | 0.71 | 2.39 | - | 0,0,0,0 | 1 |
| 57 | MG | CA | 1685 | 1/1 | 0.68 | 0.34 | - | 11,11,11,11 | 0 |
| 57 | MG | AA | 1608 | 1/1 | 0.98 | 0.28 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3081 | 1/1 | 0.91 | 0.28 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1677 | 1/1 | 0.76 | 0.37 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3111 | 1/1 | 0.94 | 0.71 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3233 | 1/1 | 0.84 | 1.20 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1688 | 1/1 | 0.72 | 1.02 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3210 | 1/1 | 0.44 | 0.38 | - | 15,15,15,15 | 0 |
| 57 | MG | DA | 3153 | 1/1 | 0.78 | 0.39 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3050 | 1/1 | 0.91 | 0.18 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1616 | 1/1 | 0.95 | 0.25 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1604 | 1/1 | 0.68 | 0.38 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3230 | 1/1 | 0.71 | 0.54 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3149 | 1/1 | 0.93 | 0.18 | - | 10,10,10,10 | 0 |
| 57 | MG | BA | 3154 | 1/1 | 0.76 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3024 | 1/1 | 0.83 | 0.52 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1618 | 1/1 | 0.95 | 0.13 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1677 | 1/1 | 0.94 | 0.43 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1632 | 1/1 | 0.90 | 0.16 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3102 | 1/1 | 0.91 | 0.33 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3116 | 1/1 | 0.93 | 0.33 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3237 | 1/1 | 0.28 | 1.25 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3228 | 1/1 | 0.78 | 0.29 | - | 1,1,1,1 | 0 |
| 57 | MG | CA | 1606 | 1/1 | 0.78 | 1.14 | - | 5,5,5,5 | 0 |
| 57 | MG | DA | 3006 | 1/1 | 0.73 | 0.56 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3061 | 1/1 | 0.91 | 0.22 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3151 | 1/1 | 0.87 | 0.26 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3058 | 1/1 | 0.84 | 0.30 | - | 4,4,4,4 | 0 |
| 57 | MG | BA | 3115 | 1/1 | 0.97 | 0.48 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3198 | 1/1 | 0.51 | 0.90 | - | 0,0,0,0 | 1 |
| 57 | MG | AA | 1674 | 1/1 | 0.83 | 1.25 | - | 16,16,16,16 | 0 |
| 57 | MG | AA | 1623 | 1/1 | 0.70 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3218 | 1/1 | 0.91 | 0.54 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3152 | 1/1 | 0.90 | 0.25 | - | 2,2,2,2 | 0 |
| 57 | MG | AA | 1633 | 1/1 | 0.92 | 1.06 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3100 | 1/1 | 0.97 | 0.10 | - | 73,73,73,73 | 0 |
| 57 | MG | AA | 1683 | 1/1 | 0.97 | 0.20 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3225 | 1/1 | 0.93 | 0.96 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1638 | 1/1 | 0.57 | 0.64 | - | 9,9,9,9 | 0 |
| 57 | MG | DA | 3001 | 1/1 | 0.88 | 0.55 | - | 0,0,0,0 | 0 |
| 57 | MG | BB | 203 | 1/1 | 0.65 | 0.75 | - | 0,0,0,0 | 1 |
| 57 | MG | BA | 3218 | 1/1 | 0.88 | 0.24 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1687 | 1/1 | 0.85 | 0.93 | - | 0,0,0,0 | 1 |
| 57 | MG | BA | 3064 | 1/1 | 0.91 | 0.18 | - | 51,51,51,51 | 0 |
| 57 | MG | AA | 1649 | 1/1 | 0.94 | 0.06 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3172 | 1/1 | 0.97 | 0.22 | - | 43,43,43,43 | 0 |
| 57 | MG | CA | 1682 | 1/1 | 0.77 | 0.72 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3105 | 1/1 | 0.84 | 0.60 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1617 | 1/1 | 0.84 | 0.82 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3074 | 1/1 | 0.95 | 0.25 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1651 | 1/1 | 0.97 | 0.36 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3215 | 1/1 | 0.86 | 0.31 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3162 | 1/1 | 0.95 | 0.22 | - | 6,6,6,6 | 0 |
| 57 | MG | BA | 3123 | 1/1 | 0.86 | 0.56 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3059 | 1/1 | 0.71 | 0.87 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3039 | 1/1 | 0.81 | 0.53 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3132 | 1/1 | 0.33 | 0.97 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3090 | 1/1 | 0.83 | 0.56 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3014 | 1/1 | 0.95 | 0.19 | - | 8,8,8,8 | 0 |
| 57 | MG | DA | 3266 | 1/1 | 0.82 | 0.53 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3253 | 1/1 | 0.83 | 1.01 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3237 | 1/1 | 0.73 | 1.39 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3014 | 1/1 | 0.97 | 0.21 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1692 | 1/1 | 0.98 | 0.08 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3255 | 1/1 | 0.91 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3255 | 1/1 | 0.93 | 0.09 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3180 | 1/1 | 0.89 | 0.52 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3082 | 1/1 | 0.85 | 0.28 | - | 88,88,88,88 | 0 |
| 57 | MG | BA | 3202 | 1/1 | 0.80 | 0.72 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1671 | 1/1 | 0.95 | 1.05 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3167 | 1/1 | 0.70 | 0.61 | - | 1,1,1,1 | 0 |
| 57 | MG | AA | 1631 | 1/1 | 0.50 | 1.27 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3143 | 1/1 | 0.91 | 0.57 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3175 | 1/1 | 0.95 | 0.19 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3181 | 1/1 | 0.94 | 1.45 | - | 8,8,8,8 | 0 |
| 57 | MG | DA | 3203 | 1/1 | 0.93 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3130 | 1/1 | 0.91 | 0.22 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1607 | 1/1 | 0.92 | 0.17 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1630 | 1/1 | 0.74 | 0.46 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3018 | 1/1 | 0.55 | 1.16 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3136 | 1/1 | 0.99 | 0.50 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3023 | 1/1 | 0.93 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3232 | 1/1 | 0.89 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3256 | 1/1 | 0.76 | 1.10 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1662 | 1/1 | 0.87 | 0.45 | - | 26,26,26,26 | 0 |
| 57 | MG | AA | 1603 | 1/1 | 0.97 | 0.08 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3063 | 1/1 | 0.90 | 0.19 | - | 32,32,32,32 | 0 |
| 57 | MG | BA | 3128 | 1/1 | 0.77 | 0.19 | - | 4,4,4,4 | 0 |
| 57 | MG | DA | 3268 | 1/1 | 0.28 | 0.84 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3118 | 1/1 | 0.93 | 0.98 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1681 | 1/1 | 0.83 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1640 | 1/1 | 0.82 | 0.45 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3101 | 1/1 | 0.92 | 0.08 | - | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3263 | 1/1 | 0.90 | 0.43 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3234 | 1/1 | 0.83 | 1.01 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3131 | 1/1 | 0.86 | 0.24 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1665 | 1/1 | 0.87 | 0.32 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1675 | 1/1 | 0.91 | 0.94 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3084 | 1/1 | 0.88 | 0.65 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3229 | 1/1 | 0.85 | 0.32 | - | 13,13,13,13 | 0 |
| 57 | MG | BA | 3042 | 1/1 | 0.95 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3095 | 1/1 | 0.94 | 0.95 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1689 | 1/1 | 0.93 | 0.53 | - | 0,0,0,0 | 0 |
| 57 | MG | B5 | 101 | 1/1 | 0.91 | 0.29 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3021 | 1/1 | 0.80 | 1.50 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3188 | 1/1 | 0.98 | 0.53 | - | 5,5,5,5 | 0 |
| 57 | MG | CA | 1672 | 1/1 | 0.89 | 0.54 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3101 | 1/1 | 0.96 | 0.60 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3158 | 1/1 | 0.91 | 0.96 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1625 | 1/1 | 0.47 | 1.28 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3259 | 1/1 | 0.85 | 0.87 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1676 | 1/1 | 0.95 | 0.19 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3066 | 1/1 | 0.93 | 0.61 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3206 | 1/1 | 0.79 | 0.32 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3010 | 1/1 | 0.70 | 0.57 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3241 | 1/1 | 0.26 | 1.00 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3159 | 1/1 | 0.93 | 0.65 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3160 | 1/1 | 0.82 | 1.12 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3028 | 1/1 | 0.82 | 0.17 | - | 83,83,83,83 | 0 |
| 57 | MG | CA | 1638 | 1/1 | 0.74 | 0.57 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1686 | 1/1 | 0.70 | 0.97 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3083 | 1/1 | 0.94 | 0.72 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3126 | 1/1 | 0.83 | 0.61 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3166 | 1/1 | 0.65 | 0.37 | - | 11,11,11,11 | 0 |
| 57 | MG | BA | 3012 | 1/1 | 0.95 | 0.17 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3195 | 1/1 | 0.54 | 0.59 | - | 32,32,32,32 | 0 |
| 57 | MG | DA | 3176 | 1/1 | 0.74 | 0.93 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3246 | 1/1 | 0.76 | 1.28 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3234 | 1/1 | 0.98 | 0.44 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3075 | 1/1 | 0.73 | 0.51 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3177 | 1/1 | 0.98 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1660 | 1/1 | 0.82 | 0.45 | - | 2,2,2,2 | 0 |
| 57 | MG | CA | 1683 | 1/1 | 0.74 | 1.04 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3065 | 1/1 | 0.95 | 0.12 | - | 16,16,16,16 | 0 |
| 57 | MG | BA | 3254 | 1/1 | 0.76 | 0.82 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3236 | 1/1 | 0.74 | 1.43 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3155 | 1/1 | 0.92 | 0.62 | - | 0,0,0,0 | 0 |
| 57 | MG | CV | 102 | 1/1 | 0.70 | 0.78 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1630 | 1/1 | 0.89 | 0.37 | - | 29,29,29,29 | 0 |
| 57 | MG | DA | 3016 | 1/1 | 0.83 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3024 | 1/1 | 0.88 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1668 | 1/1 | 0.82 | 1.06 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3199 | 1/1 | 0.26 | 0.49 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3191 | 1/1 | 0.85 | 0.89 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3209 | 1/1 | 0.81 | 1.44 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3077 | 1/1 | 0.95 | 0.44 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1610 | 1/1 | 0.66 | 1.51 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1680 | 1/1 | 0.88 | 1.77 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3165 | 1/1 | 0.61 | 1.07 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1667 | 1/1 | 0.65 | 0.62 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3031 | 1/1 | 0.95 | 0.34 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3185 | 1/1 | 0.75 | 0.30 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3219 | 1/1 | 0.94 | 0.63 | - | 0,0,0,0 | 0 |
| 57 | MG | DE | 301 | 1/1 | 0.78 | 0.26 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3193 | 1/1 | 0.69 | 0.75 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3083 | 1/1 | 0.94 | 0.47 | - | 1,1,1,1 | 0 |
| 57 | MG | B5 | 102 | 1/1 | 0.90 | 1.07 | - | 0,0,0,0 | 1 |
| 57 | MG | BA | 3203 | 1/1 | 0.81 | 0.56 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1678 | 1/1 | 0.73 | 0.47 | - | 0,0,0,0 | 1 |
| 57 | MG | D5 | 101 | 1/1 | 0.95 | 0.57 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3204 | 1/1 | 0.45 | 0.45 | - | 3,3,3,3 | 0 |
| 57 | MG | DA | 3104 | 1/1 | 0.94 | 0.73 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1636 | 1/1 | 0.77 | 0.79 | - | 4,4,4,4 | 0 |
| 57 | MG | BA | 3243 | 1/1 | 0.59 | 1.02 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3186 | 1/1 | 0.95 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1676 | 1/1 | 0.64 | 0.52 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3139 | 1/1 | 0.85 | 0.47 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3119 | 1/1 | 0.90 | 0.39 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3078 | 1/1 | 0.89 | 0.16 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3192 | 1/1 | 0.87 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3137 | 1/1 | 0.99 | 0.26 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3212 | 1/1 | 0.88 | 1.07 | - | 11,11,11,11 | 0 |
| 57 | MG | DA | 3054 | 1/1 | 0.96 | 0.85 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3264 | 1/1 | 0.68 | 0.71 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3193 | 1/1 | 0.95 | 0.65 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3091 | 1/1 | 0.93 | 0.68 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3069 | 1/1 | 0.96 | 0.56 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3184 | 1/1 | 0.76 | 0.71 | - | 0,0,0,0 | 1 |
| 57 | MG | AA | 1670 | 1/1 | 0.95 | 0.37 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3252 | 1/1 | 0.89 | 0.28 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3110 | 1/1 | 0.86 | 0.85 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3026 | 1/1 | 0.81 | 0.77 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3058 | 1/1 | 0.88 | 1.24 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1633 | 1/1 | 0.97 | 0.41 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3164 | 1/1 | 0.49 | 1.04 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3015 | 1/1 | 0.97 | 0.64 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1646 | 1/1 | 0.86 | 0.50 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3121 | 1/1 | 0.93 | 0.70 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3221 | 1/1 | 0.95 | 0.13 | - | 79,79,79,79 | 0 |
| 57 | MG | DA | 3244 | 1/1 | 0.66 | 1.32 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1672 | 1/1 | 0.97 | 0.69 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3167 | 1/1 | 0.75 | 0.82 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1607 | 1/1 | 0.90 | 1.17 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3009 | 1/1 | 0.77 | 0.46 | - | 0,0,0,0 | 0 |
| 57 | MG | BF | 301 | 1/1 | 0.92 | 0.25 | - | 27,27,27,27 | 1 |
| 57 | MG | CA | 1693 | 1/1 | 0.64 | 0.44 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3148 | 1/1 | 0.65 | 0.37 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1634 | 1/1 | 0.85 | 0.97 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3180 | 1/1 | 0.96 | 0.25 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3163 | 1/1 | 0.92 | 0.79 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3025 | 1/1 | 0.96 | 0.15 | - | 1,1,1,1 | 0 |
| 57 | MG | AA | 1625 | 1/1 | 0.94 | 0.07 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3260 | 1/1 | 0.87 | 0.19 | - | 13,13,13,13 | 0 |
| 57 | MG | DA | 3242 | 1/1 | 0.93 | 0.59 | - | 1,1,1,1 | 0 |
| 57 | MG | AA | 1646 | 1/1 | 0.86 | 0.85 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1636 | 1/1 | 0.77 | 0.48 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1680 | 1/1 | 0.79 | 0.52 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3199 | 1/1 | 0.53 | 0.60 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3011 | 1/1 | 0.98 | 0.12 | - | 10,10,10,10 | 0 |
| 57 | MG | DA | 3257 | 1/1 | 0.97 | 0.32 | - | 0,0,0,0 | 1 |
| 57 | MG | AA | 1628 | 1/1 | 0.63 | 1.07 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1610 | 1/1 | 0.94 | 0.48 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1627 | 1/1 | 0.91 | 0.25 | - | 3,3,3,3 | 0 |
| 57 | MG | BA | 3039 | 1/1 | 0.84 | 0.37 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3245 | 1/1 | 0.78 | 0.69 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3231 | 1/1 | 0.95 | 0.31 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3031 | 1/1 | 0.97 | 0.12 | - | 21,21,21,21 | 0 |
| 57 | MG | AA | 1690 | 1/1 | 0.94 | 0.20 | - | 23,23,23,23 | 0 |
| 57 | MG | BA | 3098 | 1/1 | 0.94 | 1.14 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3130 | 1/1 | 0.88 | 0.42 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1662 | 1/1 | 0.93 | 0.32 | - | 13,13,13,13 | 0 |
| 57 | MG | DA | 3150 | 1/1 | 0.95 | 0.35 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3086 | 1/1 | 0.93 | 0.17 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3188 | 1/1 | 0.94 | 0.75 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3236 | 1/1 | 0.69 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3106 | 1/1 | 0.92 | 0.21 | - | 7,7,7,7 | 0 |
| 57 | MG | BA | 3208 | 1/1 | 0.87 | 0.33 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3145 | 1/1 | 0.84 | 1.10 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3076 | 1/1 | 0.93 | 0.30 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3190 | 1/1 | 0.45 | 0.76 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3113 | 1/1 | 0.88 | 0.44 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3241 | 1/1 | 0.74 | 0.33 | - | 5,5,5,5 | 0 |
| 57 | MG | CA | 1601 | 1/1 | 0.91 | 0.43 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3222 | 1/1 | 0.86 | 1.32 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3040 | 1/1 | 0.84 | 0.66 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3208 | 1/1 | 0.90 | 0.21 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3133 | 1/1 | 0.92 | 0.33 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1620 | 1/1 | 0.84 | 0.34 | - | 1,1,1,1 | 0 |
| 57 | MG | CA | 1628 | 1/1 | 0.93 | 0.19 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3205 | 1/1 | 0.85 | 0.22 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3261 | 1/1 | 0.81 | 0.35 | - | 31,31,31,31 | 0 |
| 57 | MG | AA | 1612 | 1/1 | 0.59 | 1.05 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3089 | 1/1 | 0.96 | 0.45 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3013 | 1/1 | 0.93 | 0.18 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3038 | 1/1 | 0.86 | 0.50 | - | 28,28,28,28 | 0 |
| 57 | MG | DA | 3085 | 1/1 | 0.84 | 0.77 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3085 | 1/1 | 0.77 | 1.26 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3157 | 1/1 | 0.96 | 0.42 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3171 | 1/1 | 0.96 | 0.14 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3179 | 1/1 | 0.54 | 0.69 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3073 | 1/1 | 0.86 | 0.52 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1666 | 1/1 | 0.96 | 0.12 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3077 | 1/1 | 0.82 | 0.61 | - | 1,1,1,1 | 0 |
| 57 | MG | CA | 1645 | 1/1 | 0.72 | 1.94 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3147 | 1/1 | 0.94 | 0.18 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3168 | 1/1 | 0.88 | 0.13 | - | 11,11,11,11 | 0 |
| 57 | MG | BA | 3011 | 1/1 | 0.83 | 1.91 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1637 | 1/1 | 0.91 | 0.18 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3111 | 1/1 | 0.84 | 0.90 | - | 2,2,2,2 | 0 |
| 57 | MG | BA | 3185 | 1/1 | 0.94 | 0.30 | - | 13,13,13,13 | 1 |
| 57 | MG | BA | 3112 | 1/1 | 0.95 | 0.34 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3226 | 1/1 | 0.91 | 0.32 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3041 | 1/1 | 0.91 | 0.45 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3214 | 1/1 | 0.71 | 1.17 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1621 | 1/1 | 0.89 | 1.04 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3143 | 1/1 | 0.93 | 0.49 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3136 | 1/1 | 0.75 | 0.78 | - | 1,1,1,1 | 0 |
| 57 | MG | BA | 3210 | 1/1 | 0.93 | 0.23 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1643 | 1/1 | 0.97 | 0.32 | - | 0,0,0,0 | 0 |
| 57 | MG | AA | 1641 | 1/1 | 0.77 | 0.29 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3250 | 1/1 | 0.92 | 1.37 | - | 0,0,0,0 | 1 |
| 57 | MG | CA | 1656 | 1/1 | 0.74 | 1.31 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3006 | 1/1 | 0.84 | 0.77 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3096 | 1/1 | 0.95 | 0.40 | - | 0,0,0,0 | 0 |
| 57 | MG | CA | 1605 | 1/1 | 0.95 | 0.22 | - | 1,1,1,1 | 0 |
| 57 | MG | DA | 3156 | 1/1 | 0.96 | 0.29 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3216 | 1/1 | 0.94 | 0.59 | - | 0,0,0,0 | 0 |
| 57 | MG | BA | 3211 | 1/1 | 0.88 | 0.28 | - | 0,0,0,0 | 1 |
| 57 | MG | DA | 3022 | 1/1 | 0.94 | 0.73 | - | 0,0,0,0 | 0 |
| 57 | MG | DA | 3013 | 1/1 | 0.96 | 0.23 | - | 0,0,0,0 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.