



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 05:28 pm BST

PDB ID : 4V51
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with mRNA, tRNA and paromomycin
Authors : Selmer, M.; Dunham, C.M.; Murphy, F.V.; Weixlbaumer, A.; Petry, S.; Weir, J.R.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2006-07-31
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

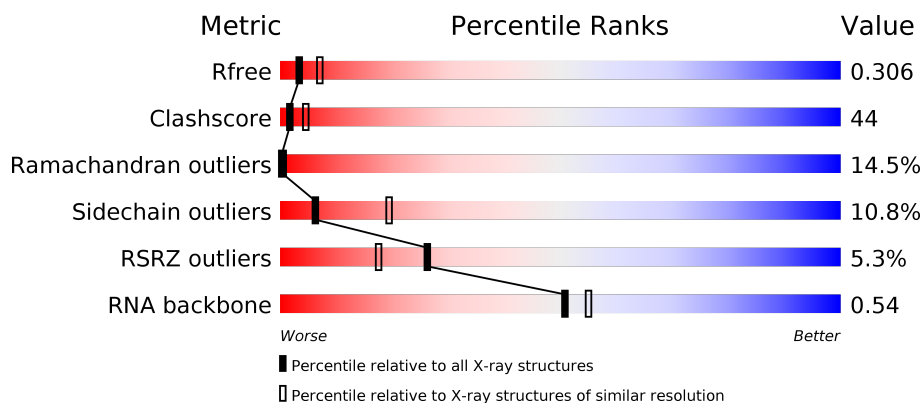
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 3140 (2.80-2.80) |
| Clashscore | 141614 | 3569 (2.80-2.80) |
| Ramachandran outliers | 138981 | 3498 (2.80-2.80) |
| Sidechain outliers | 138945 | 3500 (2.80-2.80) |
| RSRZ outliers | 127900 | 3078 (2.80-2.80) |
| RNA backbone | 3102 | 1227 (3.10-2.50) |

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 respectively. 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>2%</div> <div>24%</div> <div>62%</div> <div>11%</div> <div>..</div> </div> |
| 1 | CA | 1522 | <div> <div>2%</div> <div>23%</div> <div>64%</div> <div>11%</div> <div>..</div> </div> |
| 2 | AB | 256 | <div> <div>11%</div> <div>21%</div> <div>54%</div> <div>15%</div> <div>8%</div> </div> |
| 2 | CB | 256 | <div> <div>11%</div> <div>21%</div> <div>54%</div> <div>15%</div> <div>8%</div> </div> |

Continued on next page...

Continued from previous page...

| 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 | 135 | |
| 12 | CL | 135 | |
| 13 | AM | 126 | |
| 13 | CM | 126 | |
| 14 | AN | 61 | |
| 14 | CN | 61 | |
| 15 | AO | 89 | |

Continued on next page...

Continued from previous page...

| 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 | AV | 77 | |
| 22 | CV | 77 | |
| 23 | AW | 76 | |
| 23 | AY | 76 | |
| 23 | CW | 76 | |
| 23 | CY | 76 | |
| 24 | AX | 24 | |
| 24 | CX | 24 | |
| 25 | B0 | 85 | |
| 25 | D0 | 85 | |
| 26 | B1 | 98 | |
| 26 | D1 | 98 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27 | B2 | 72 | |
| 27 | D2 | 72 | |
| 28 | B3 | 60 | |
| 28 | D3 | 60 | |
| 29 | B4 | 71 | |
| 29 | D4 | 71 | |
| 30 | B5 | 60 | |
| 30 | D5 | 60 | |
| 31 | B6 | 54 | |
| 31 | D6 | 54 | |
| 32 | B7 | 49 | |
| 32 | D7 | 49 | |
| 33 | B8 | 65 | |
| 33 | D8 | 65 | |
| 34 | BA | 2787 | |
| 34 | DA | 2787 | |
| 35 | BB | 122 | |
| 35 | DB | 122 | |
| 36 | BC | 229 | |
| 36 | DC | 229 | |
| 37 | BD | 276 | |
| 37 | DD | 276 | |
| 38 | BE | 206 | |
| 38 | DE | 206 | |
| 39 | BF | 210 | |




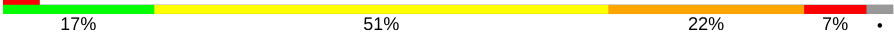
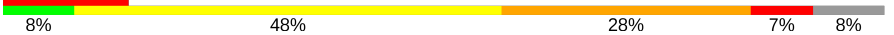
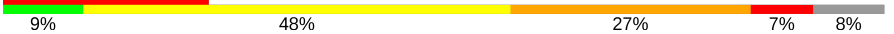
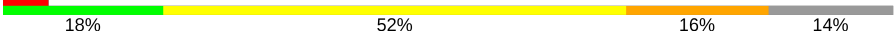
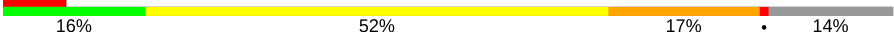
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39 | DF | 210 | |
| 40 | BG | 182 | |
| 40 | DG | 182 | |
| 41 | BH | 180 | |
| 41 | DH | 180 | |
| 42 | BI | 148 | |
| 42 | DI | 148 | |
| 43 | BN | 140 | |
| 43 | DN | 140 | |
| 44 | BO | 122 | |
| 44 | DO | 122 | |
| 45 | BP | 150 | |
| 45 | DP | 150 | |
| 46 | BQ | 141 | |
| 46 | DQ | 141 | |
| 47 | BR | 118 | |
| 47 | DR | 118 | |
| 48 | BS | 112 | |
| 48 | DS | 112 | |
| 49 | BT | 146 | |
| 49 | DT | 146 | |
| 50 | BU | 118 | |
| 50 | DU | 118 | |
| 51 | BV | 101 | |
| 51 | DV | 101 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 52 | BW | 113 |  |
| 52 | DW | 113 |  |
| 53 | BX | 96 |  |
| 53 | DX | 96 |  |
| 54 | BY | 110 |  |
| 54 | DY | 110 |  |
| 55 | BZ | 206 |  |
| 55 | DZ | 206 |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | AA | 1618 | - | - | - | X |
| 56 | MG | AA | 1633 | - | - | - | X |
| 56 | MG | AA | 1697 | - | - | - | X |
| 56 | MG | BA | 3004 | - | - | - | X |
| 56 | MG | BA | 3403 | - | - | - | X |
| 56 | MG | BA | 3413 | - | - | - | X |
| 56 | MG | BB | 201 | - | - | - | X |
| 56 | MG | BB | 213 | - | - | - | X |
| 56 | MG | CA | 1622 | - | - | - | X |
| 56 | MG | CA | 1637 | - | - | - | X |
| 56 | MG | CA | 1646 | - | - | - | X |
| 56 | MG | CA | 1685 | - | - | - | X |
| 56 | MG | CA | 1719 | - | - | - | X |
| 56 | MG | CA | 1729 | - | - | - | X |
| 56 | MG | CA | 1752 | - | - | - | X |
| 56 | MG | DA | 3004 | - | - | - | X |
| 56 | MG | DA | 3187 | - | - | - | X |
| 56 | MG | DA | 3219 | - | - | - | X |
| 56 | MG | DA | 3255 | - | - | - | X |
| 56 | MG | DA | 3261 | - | - | - | X |
| 56 | MG | DA | 3273 | - | - | - | X |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 291075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1504 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32329 | 14390 | 5992 | 10444 | 1503 | | | |
| 1 | CA | 1504 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32329 | 14390 | 5992 | 10444 | 1503 | | | |

- 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 | | | |
| 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 |
| | | | 1011 | 639 | 198 | 174 | | | |
| 9 | CI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1011 | 639 | 198 | 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 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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 | | | |
| 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 P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22 | AV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1645 | 733 | 297 | 538 | 77 | | | |
| 22 | CV | 77 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1645 | 733 | 297 | 538 | 77 | | | |

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23 | AW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1623 | 723 | 290 | 534 | 76 | | | |
| 23 | AY | 19 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 407 | 183 | 78 | 128 | 18 | | | |
| 23 | CW | 76 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 1623 | 723 | 290 | 534 | 76 | | | |
| 23 | CY | 19 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 407 | 183 | 78 | 128 | 18 | | | |

- Molecule 24 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 24 | AX | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 235 | 106 | 44 | 74 | 11 | | | |
| 24 | CX | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 235 | 106 | 44 | 74 | 11 | | | |

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | B0 | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 650 | 401 | 137 | 111 | 1 | | | |
| 25 | D0 | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 650 | 401 | 137 | 111 | 1 | | | |

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26 | B1 | 89 | Total | C | N | O | 0 | 0 | 1 |
| | | | 693 | 435 | 140 | 118 | | | |
| 26 | D1 | 89 | Total | C | N | O | 0 | 0 | 1 |
| | | | 693 | 435 | 140 | 118 | | | |

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | B2 | 51 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 421 | 263 | 85 | 72 | 1 | | | |
| 27 | D2 | 51 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 421 | 263 | 85 | 72 | 1 | | | |

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | B3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |
| 28 | D3 | 60 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 468 | 298 | 91 | 78 | 1 | | | |

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 29 | B4 | 50 | Total | C | N | O | 0 | 0 | 1 |
| | | | 242 | 143 | 50 | 49 | | | |
| 29 | D4 | 50 | Total | C | N | O | 0 | 0 | 1 |
| | | | 242 | 143 | 50 | 49 | | | |

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |
| 30 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | B6 | 45 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 381 | 235 | 78 | 64 | 4 | | | |
| 31 | D6 | 45 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 381 | 235 | 78 | 64 | 4 | | | |

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32 | B7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |
| 32 | D7 | 49 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 419 | 257 | 105 | 55 | 2 | | | |

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |
| 33 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 508 | 326 | 102 | 78 | 2 | | | |

- Molecule 34 is a RNA chain called 23S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 34 | BA | 2772 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59708 | 26573 | 11171 | 19193 | 2771 | | | |
| 34 | DA | 2772 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 59708 | 26573 | 11171 | 19193 | 2771 | | | |

- Molecule 35 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 35 | BB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |
| 35 | DB | 119 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2551 | 1136 | 471 | 826 | 118 | | | |

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36 | BC | 191 | Total | C | N | O | 0 | 0 | 1 |
| | | | 1142 | 691 | 221 | 230 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36 | DC | 191 | Total | C | N | O | 0 | 0 | 1 |
| | | | 1142 | 691 | 221 | 230 | | | |

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 37 | BD | 272 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2105 | 1329 | 417 | 356 | 3 | | | |
| 37 | DD | 272 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 2105 | 1329 | 417 | 356 | 3 | | | |

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BE | 205 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1564 | 988 | 300 | 270 | 6 | | | |
| 38 | DE | 205 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1564 | 988 | 300 | 270 | 6 | | | |

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39 | BF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |
| 39 | DF | 208 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1624 | 1035 | 304 | 282 | 3 | | | |

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |
| 40 | DG | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BH | 160 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1223 | 773 | 229 | 220 | 1 | | | |
| 41 | DH | 160 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1223 | 773 | 229 | 220 | 1 | | | |

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BI | 146 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1132 | 723 | 201 | 207 | 1 | | | |
| 42 | DI | 146 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1132 | 723 | 201 | 207 | 1 | | | |

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |
| 43 | DN | 139 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1105 | 712 | 207 | 182 | 4 | | | |

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |
| 44 | DO | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |
| 45 | DP | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1114 | 692 | 227 | 193 | 2 | | | |

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BQ | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1080 | 688 | 204 | 183 | 5 | | | |
| 46 | DQ | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1080 | 688 | 204 | 183 | 5 | | | |

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 47 | BR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |
| 47 | DR | 117 | Total | C | N | O | 0 | 0 | 0 |
| | | | 960 | 599 | 202 | 159 | | | |

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 48 | BS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |
| 48 | DS | 99 | Total | C | N | O | 0 | 0 | 1 |
| | | | 771 | 486 | 155 | 130 | | | |

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | BT | 138 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1142 | 710 | 235 | 196 | 1 | | | |
| 49 | DT | 138 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1142 | 710 | 235 | 196 | 1 | | | |

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | BU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 202 | 151 | 1 | | | |
| 50 | DU | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 202 | 151 | 1 | | | |

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 51 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 896 | 563 | 176 | 155 | 2 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | DW | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 896 | 563 | 176 | 155 | 2 | | | |

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 53 | BX | 93 | Total | C | N | O | | 0 | 0 | 1 |
| | | | 726 | 471 | 132 | 123 | | | | |
| 53 | DX | 93 | Total | C | N | O | | 0 | 0 | 1 |
| | | | 726 | 471 | 132 | 123 | | | | |

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54 | BY | 101 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 776 | 500 | 149 | 123 | 4 | | | |
| 54 | DY | 101 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 776 | 500 | 149 | 123 | 4 | | | |

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55 | BZ | 177 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1404 | 897 | 253 | 252 | 2 | | | |
| 55 | DZ | 177 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1404 | 897 | 253 | 252 | 2 | | | |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | BA | 454 | Total | Mg | 0 | 0 |
| | | | 454 | 454 | | |
| 56 | CA | 189 | Total | Mg | 0 | 0 |
| | | | 189 | 189 | | |
| 56 | DF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | CV | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | BE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AW | 22 | Total | Mg | 0 | 0 |
| | | | 22 | 22 | | |

Continued on next page...

Continued from previous page...

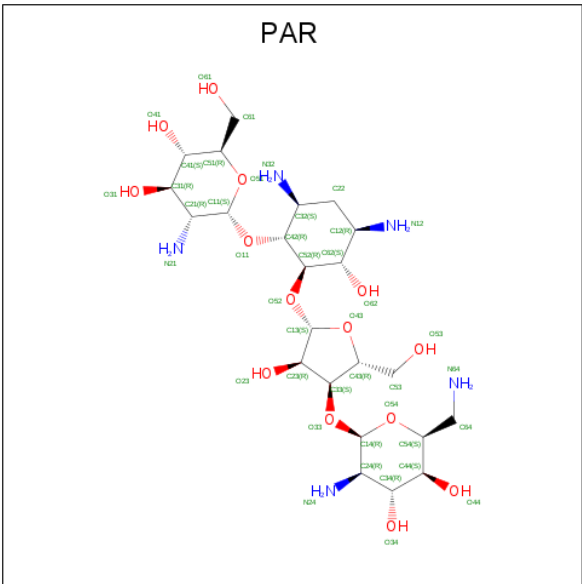
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | DU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AX | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | DD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | B5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | BB | 19 | Total 19 | Mg 19 | 0 | 0 |
| 56 | DO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | CU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BF | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | AV | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | BX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B2 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | AA | 215 | Total 215 | Mg 215 | 0 | 0 |
| 56 | CX | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | BN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DH | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DS | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | B3 | 1 | Total 1 | Mg 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | CJ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DA | 398 | Total | Mg | 0 | 0 |
| | | | 398 | 398 | | |
| 56 | B7 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | CF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | BV | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | CM | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | BO | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | CW | 13 | Total | Mg | 0 | 0 |
| | | | 13 | 13 | | |
| 56 | D5 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | DN | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AY | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DB | 12 | Total | Mg | 0 | 0 |
| | | | 12 | 12 | | |

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 57 | AA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |
| 57 | CA | 1 | Total | C | N | O | 0 | 0 |
| | | | 42 | 23 | 5 | 14 | | |

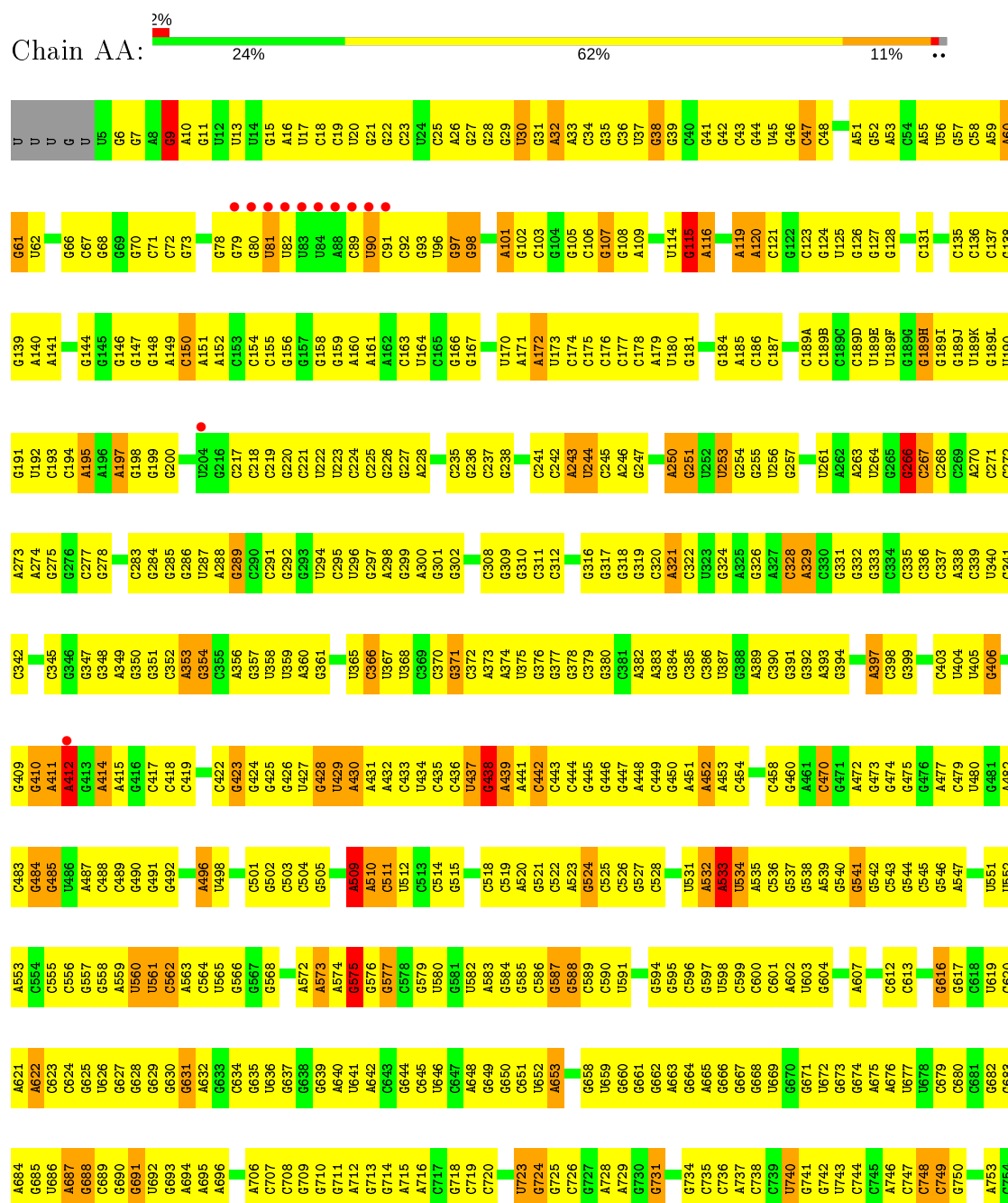
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

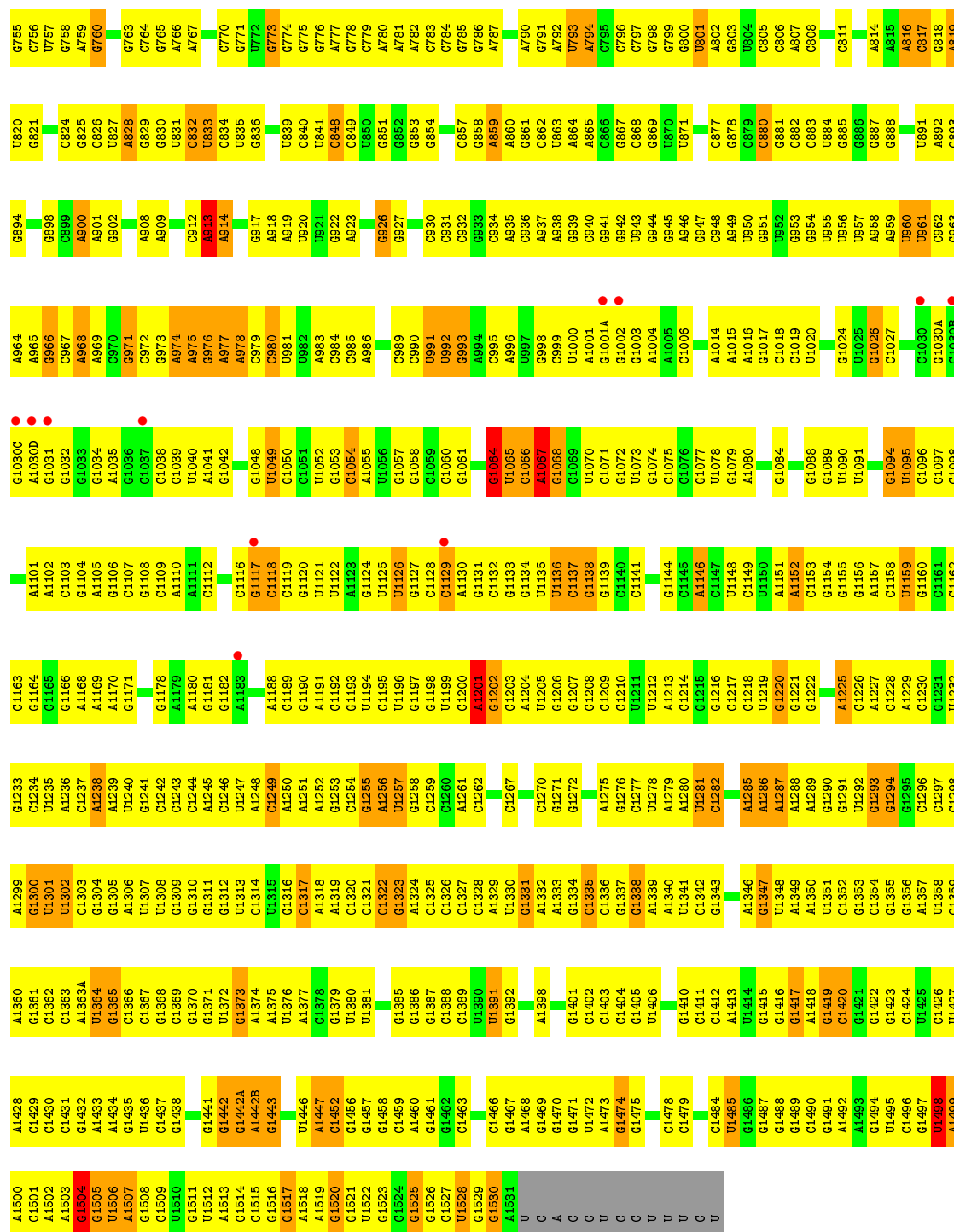
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58 | CN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | AD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | CD | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | AN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots [i](#)

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

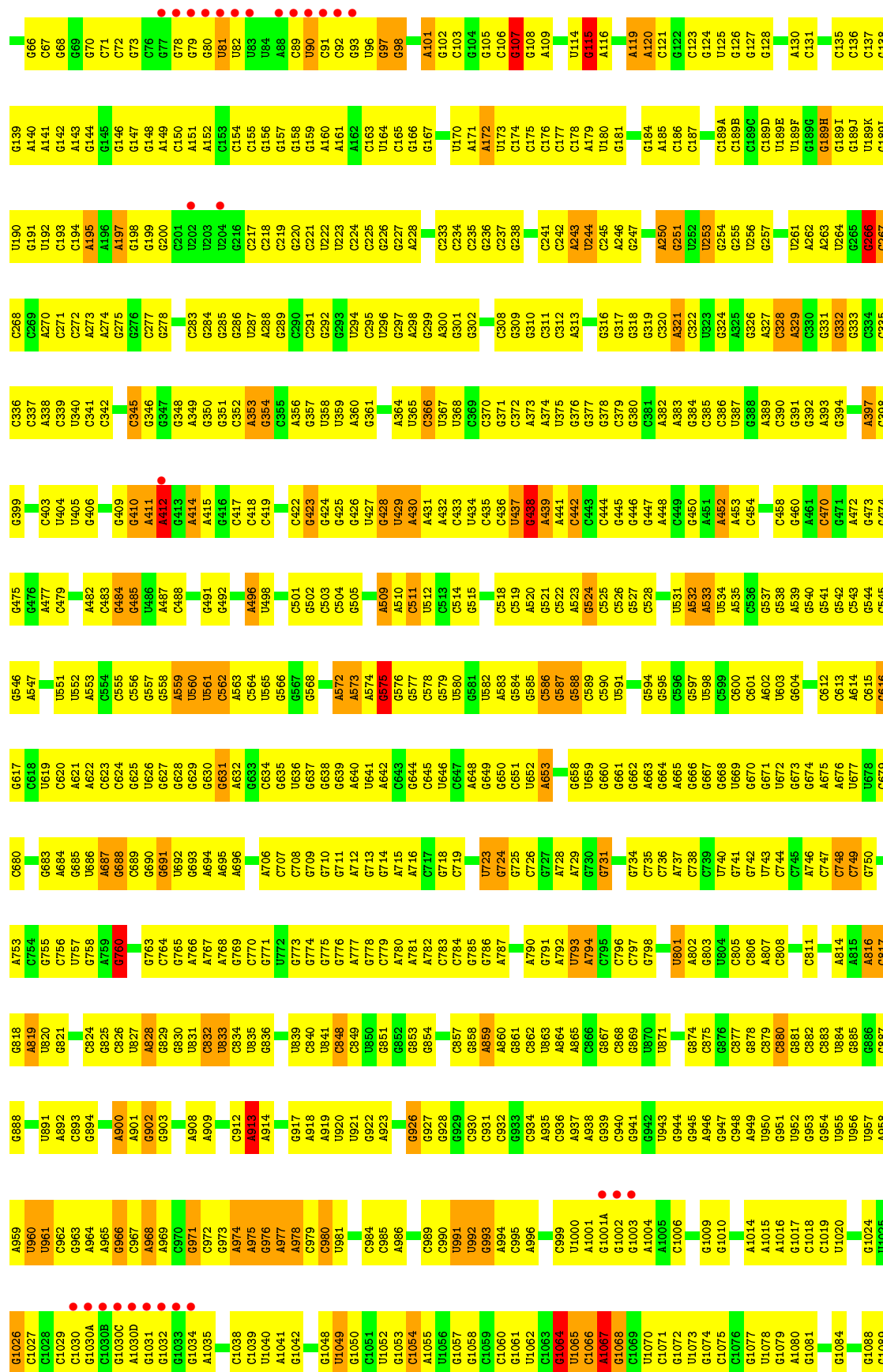
- Molecule 1: 16S ribosomal RNA

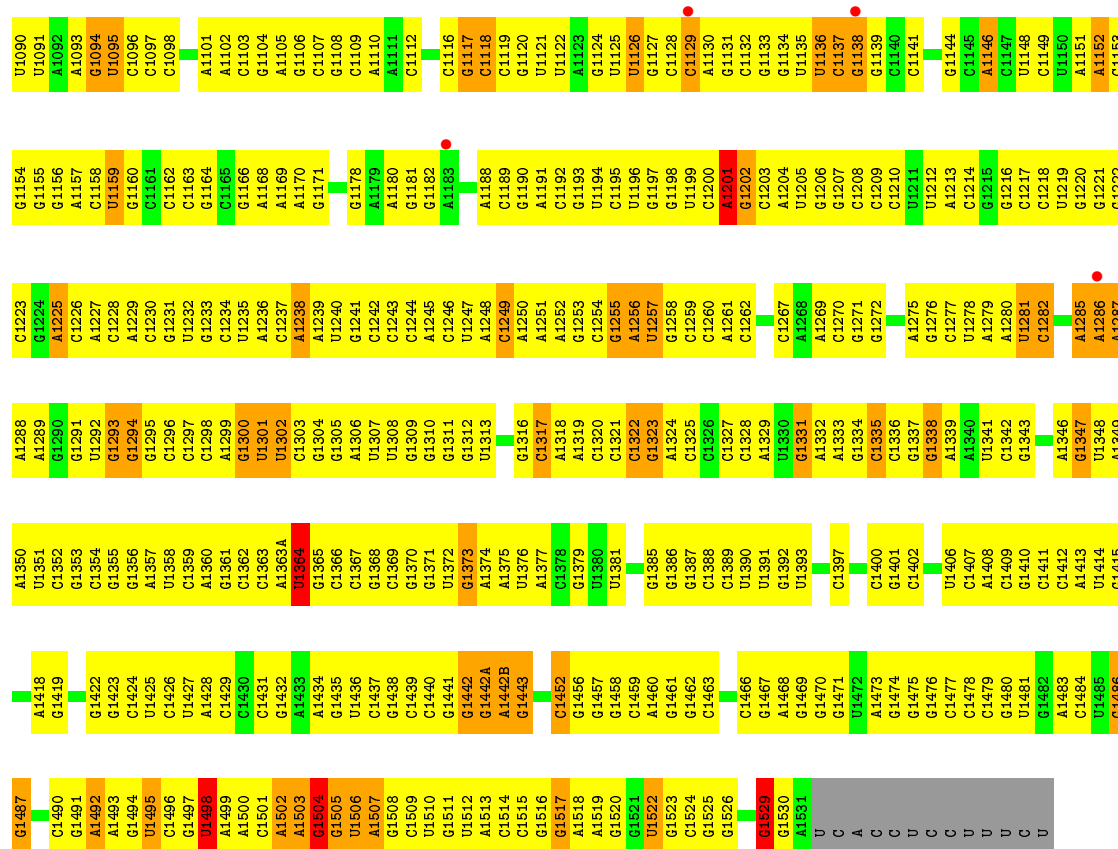




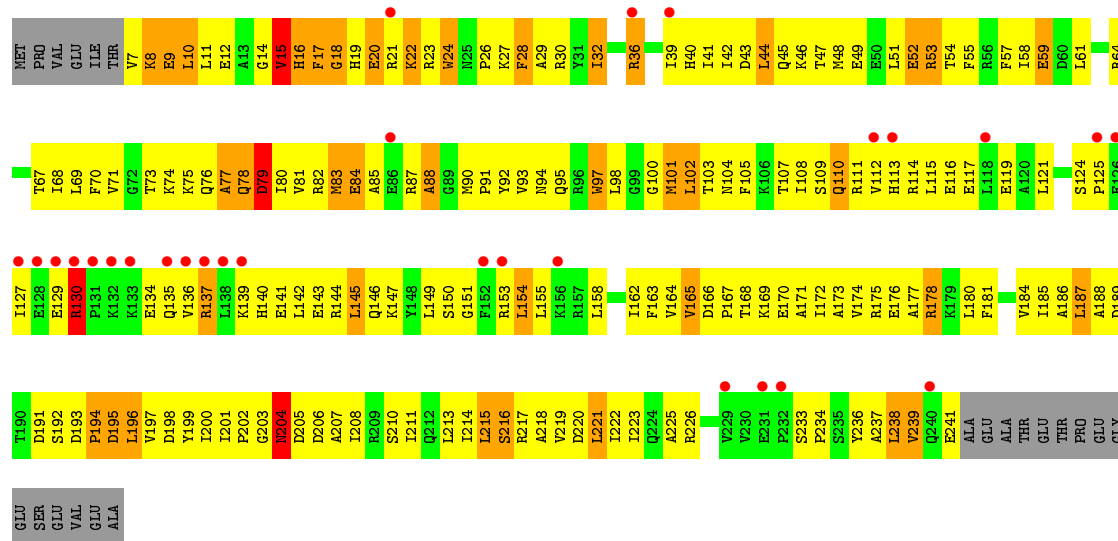
Chain CA:





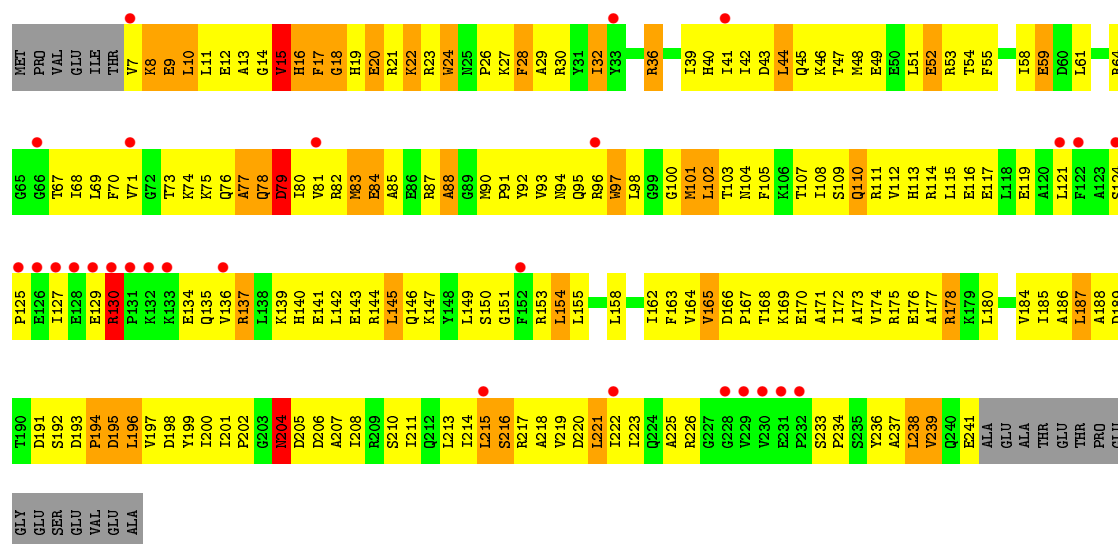


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

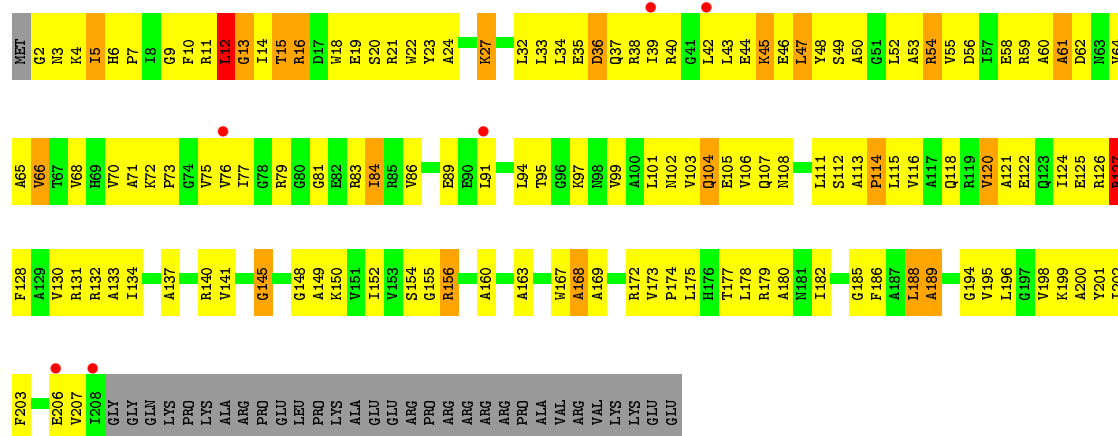


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

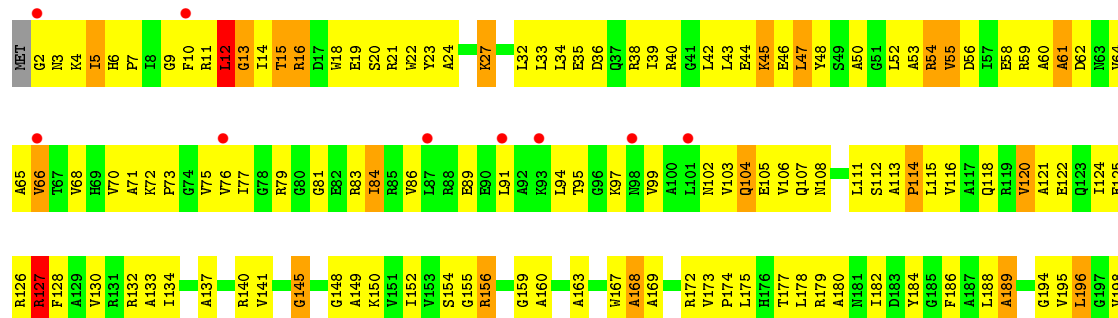


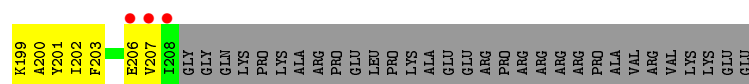


- Molecule 3: 30S RIBOSOMAL PROTEIN S3



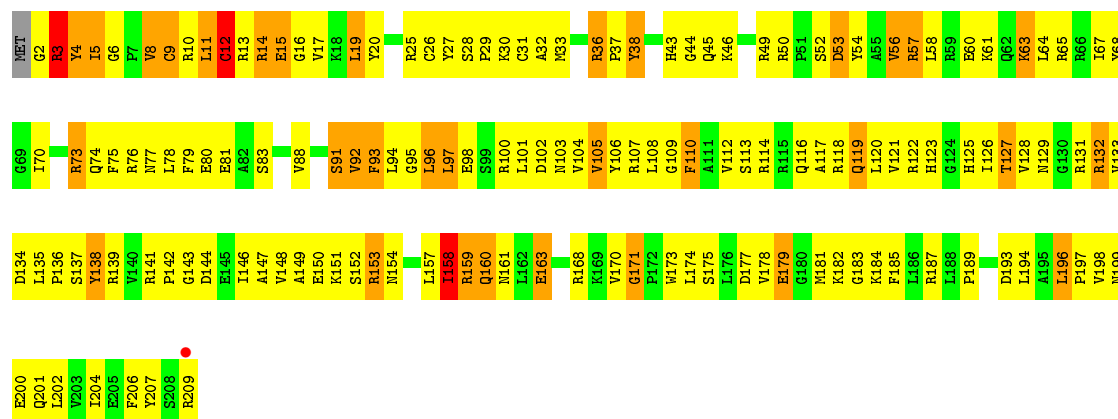
- Molecule 3: 30S RIBOSOMAL PROTEIN S3





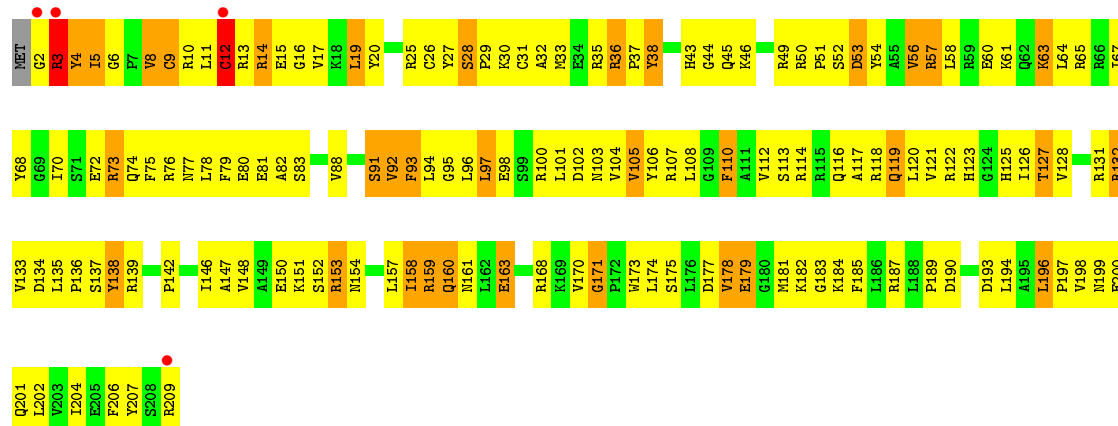
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 27% 56% 16%



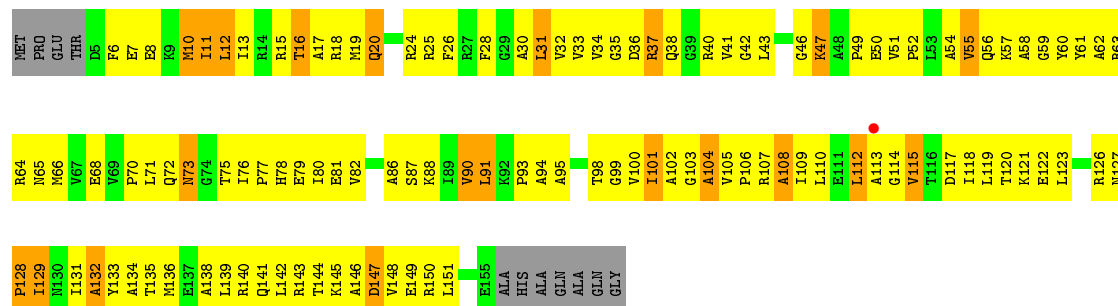
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD: 29% 27% 56% 16%

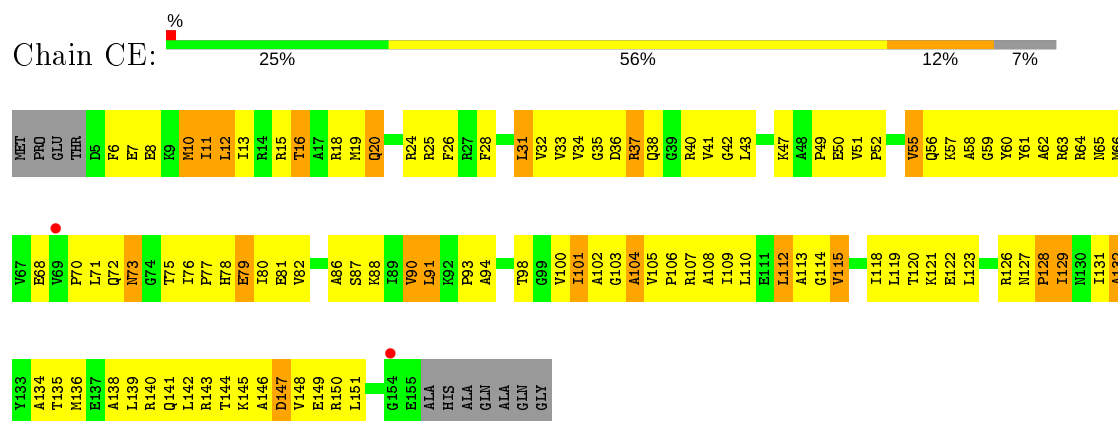


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

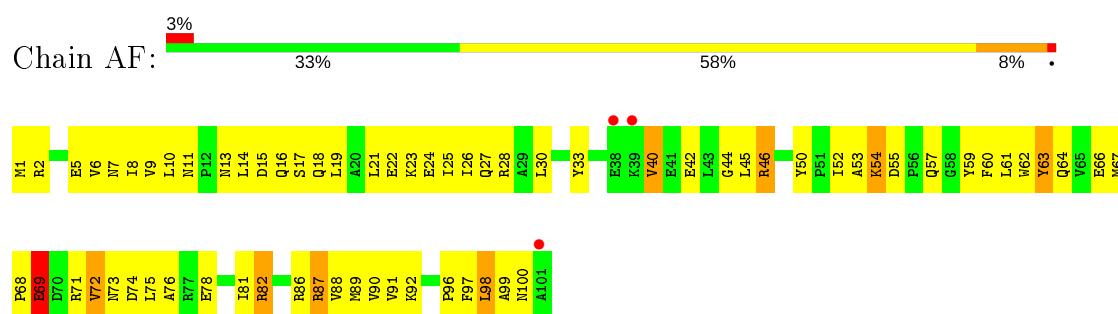
Chain AE: 20% 60% 13% 7%



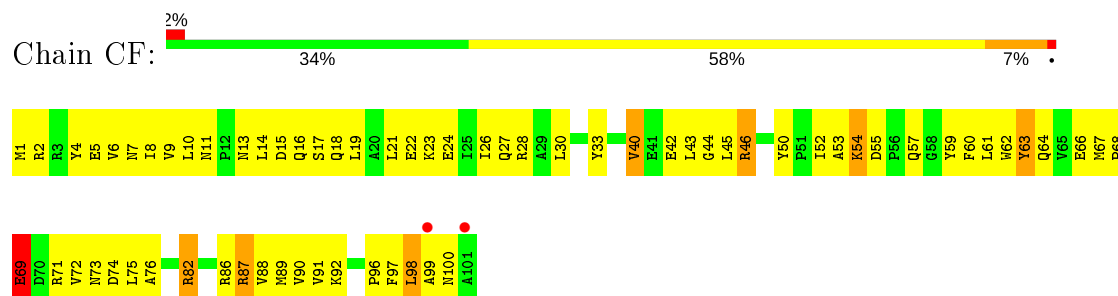
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



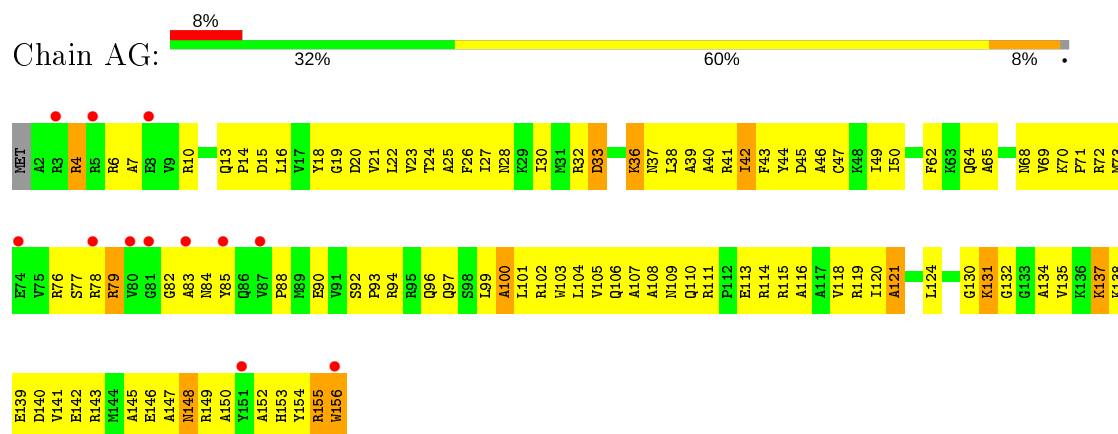
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



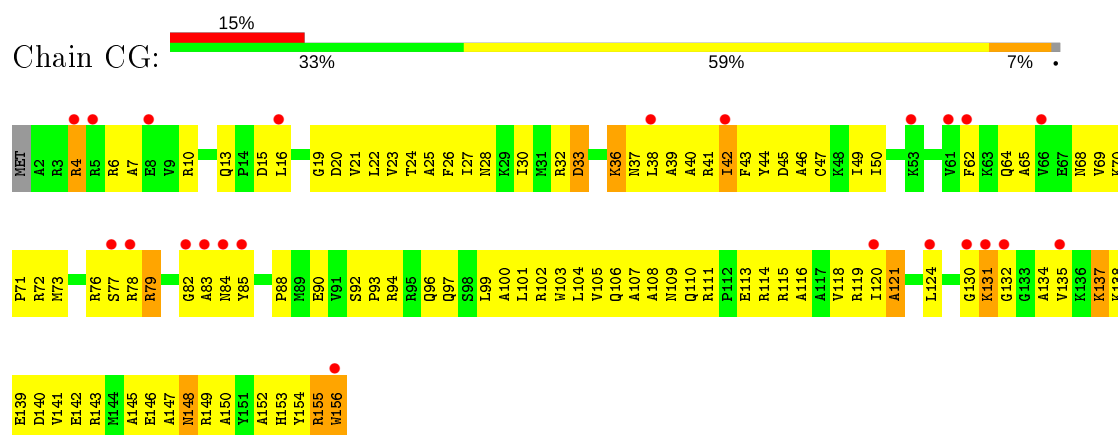
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



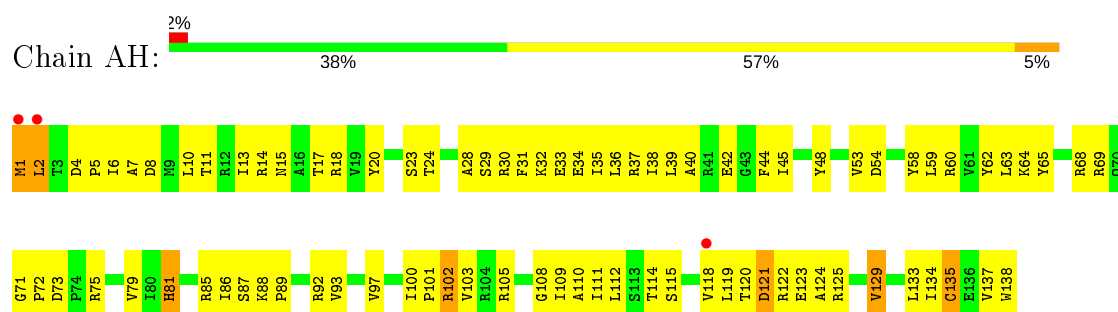
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



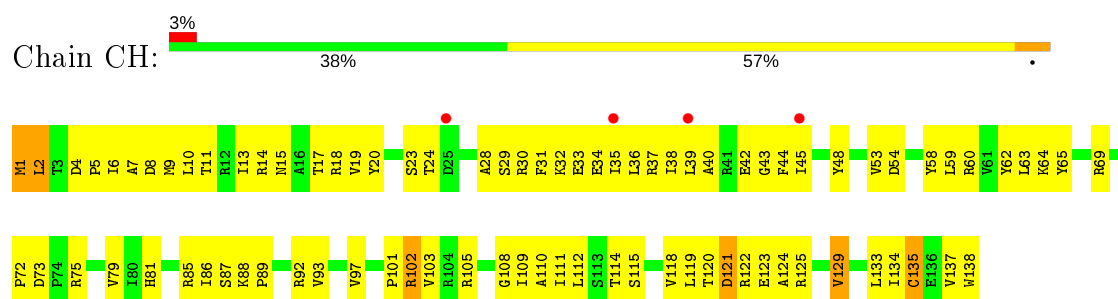
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



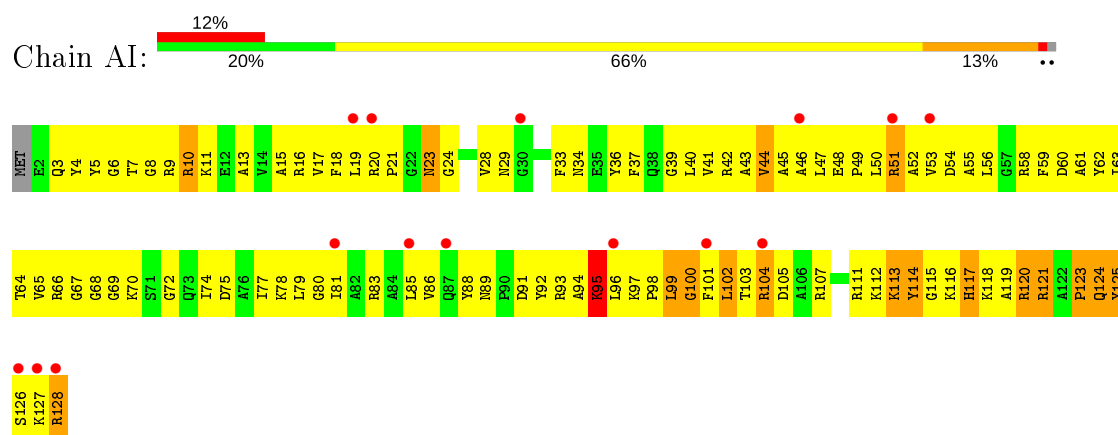
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



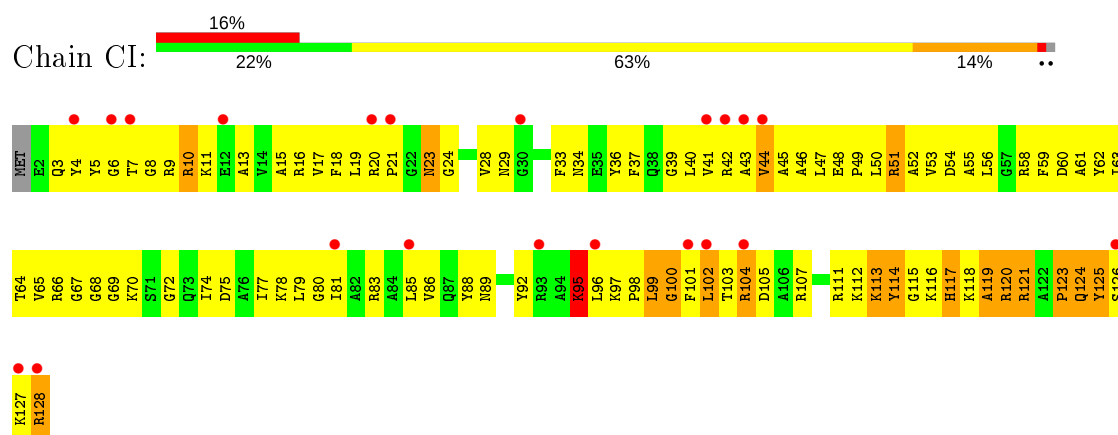
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



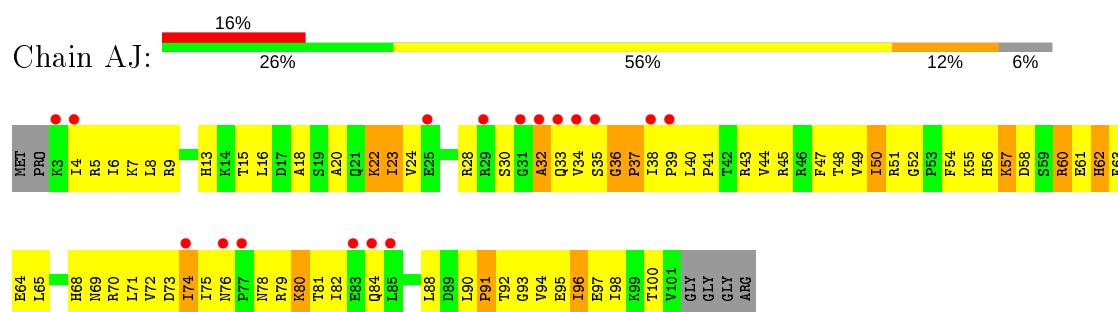
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



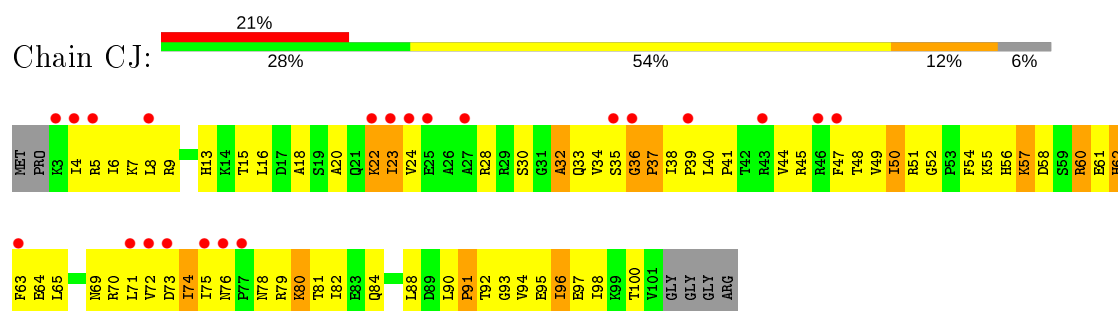
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



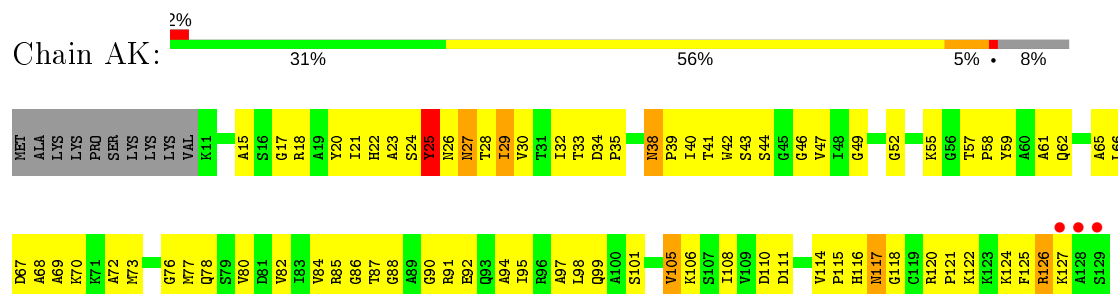
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

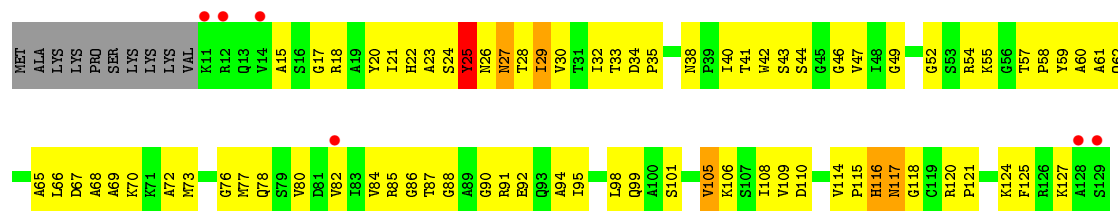


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

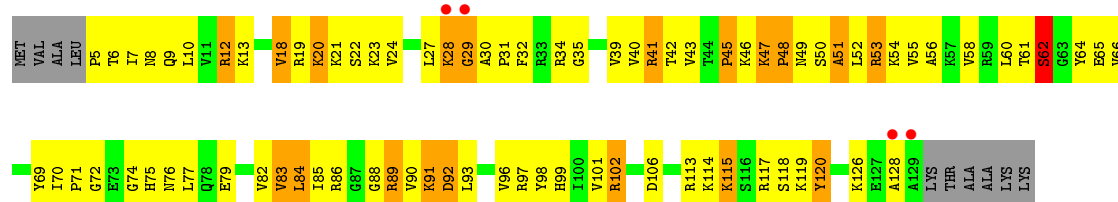


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

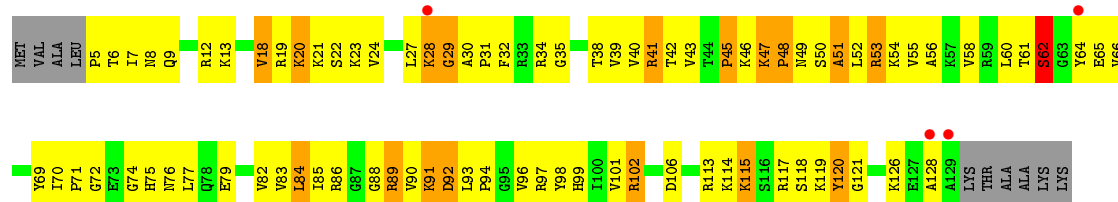




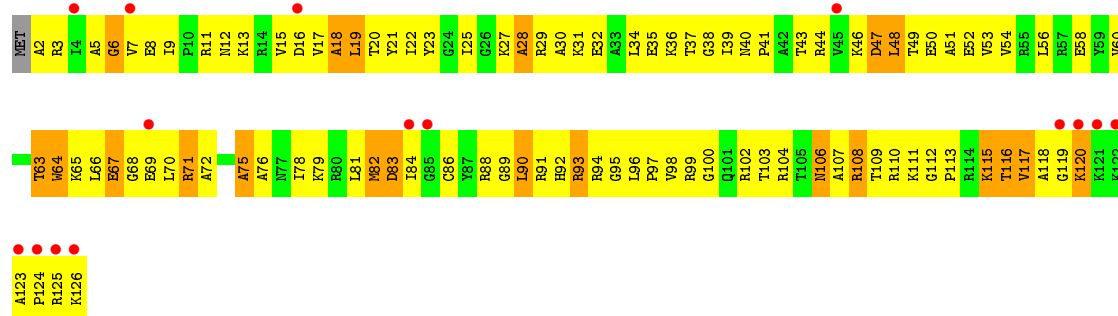
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



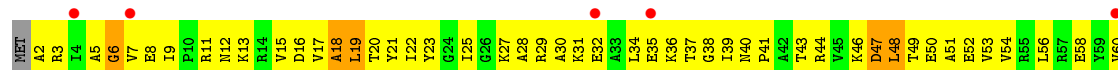
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

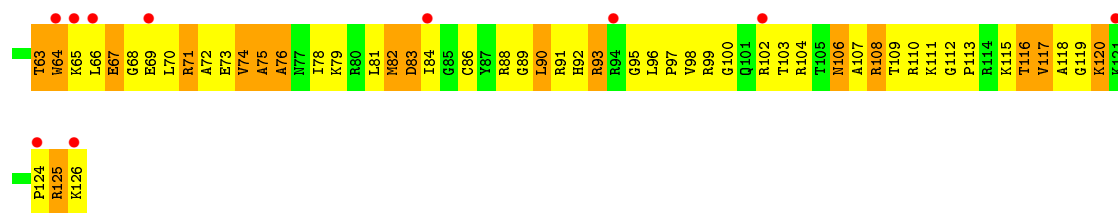


• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

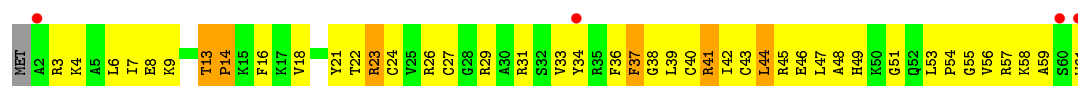




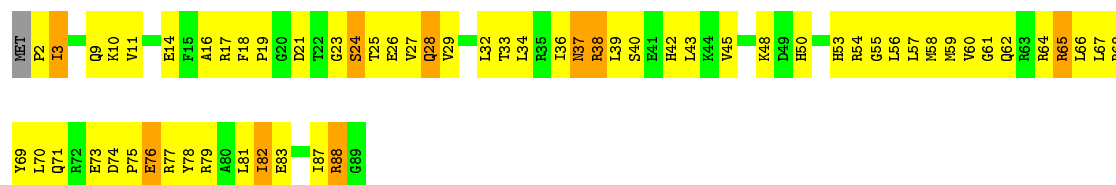
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



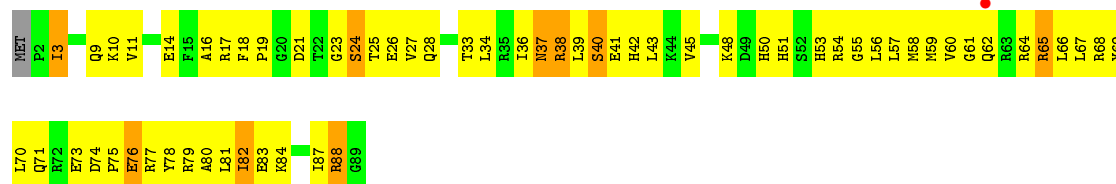
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



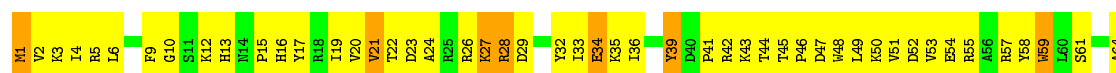
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

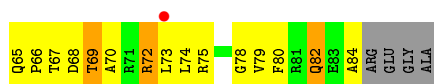


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

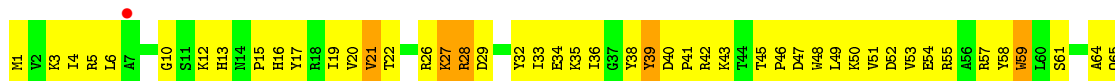


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

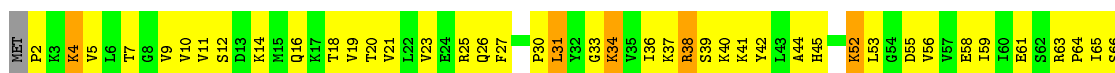




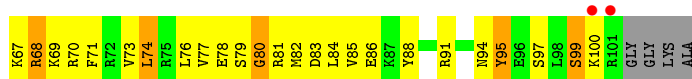
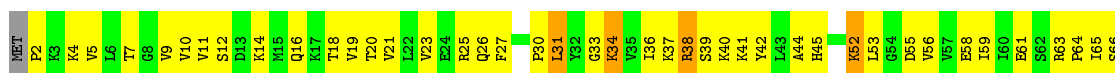
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



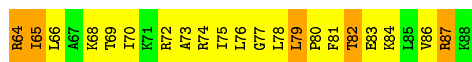
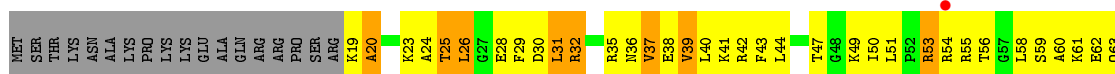
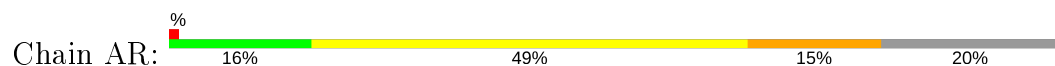
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



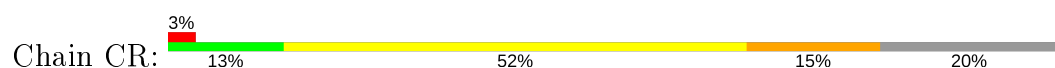
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

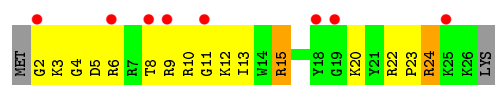


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

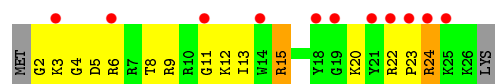
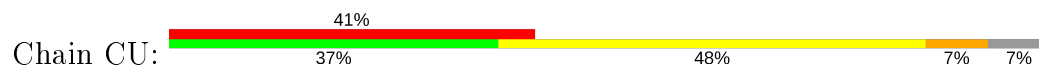


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

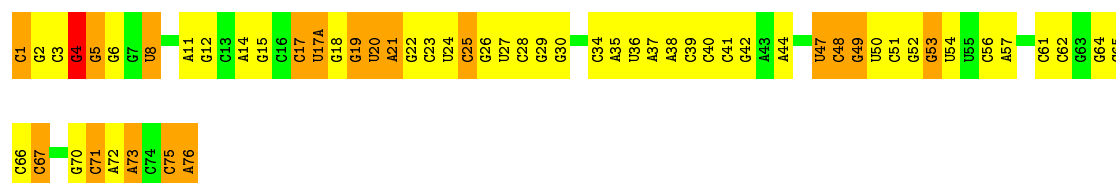




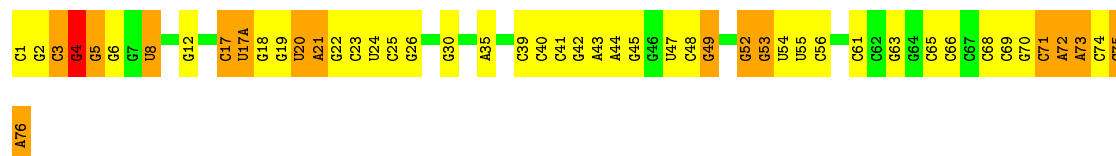
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



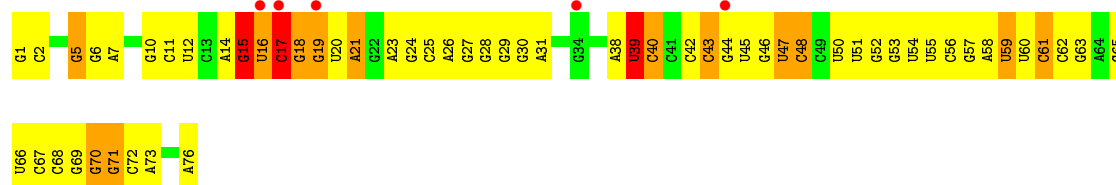
• Molecule 22: P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



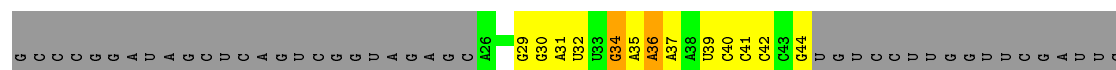
• Molecule 22: P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

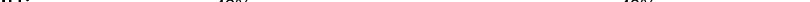


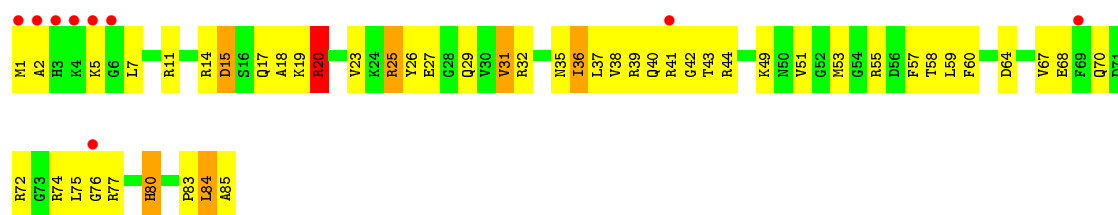
• Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)



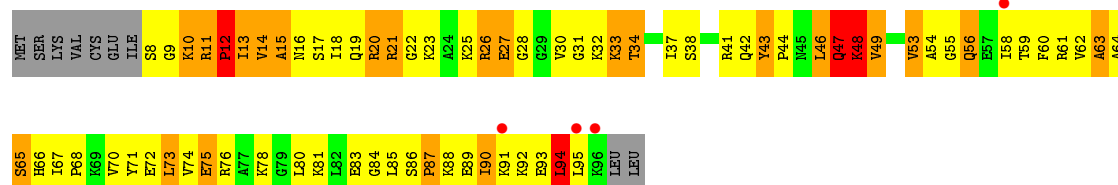
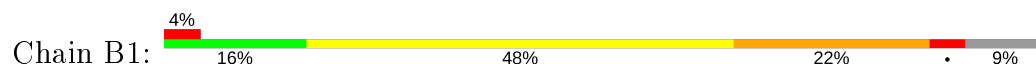
• Molecule 23: E-SITE TRNA PHE OR A-SITE TRNA PHE (UNMODIFIED BASES)



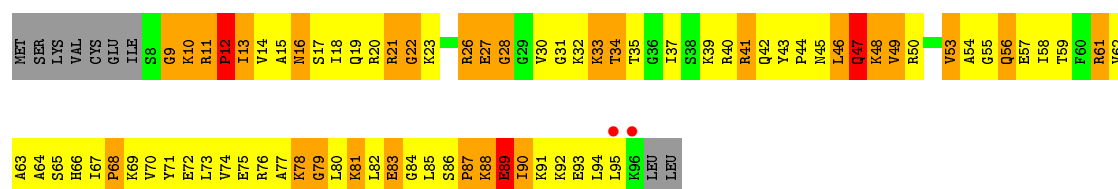
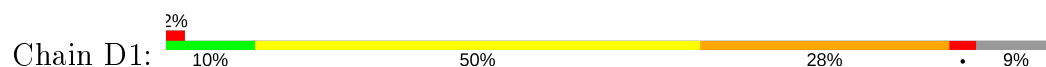
Chain D0: 



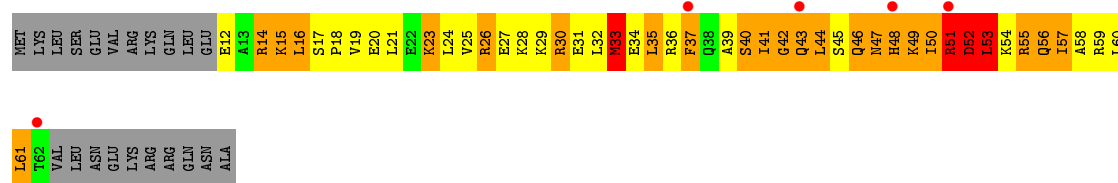
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



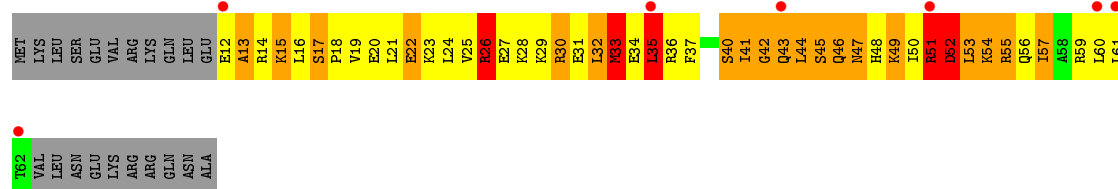
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



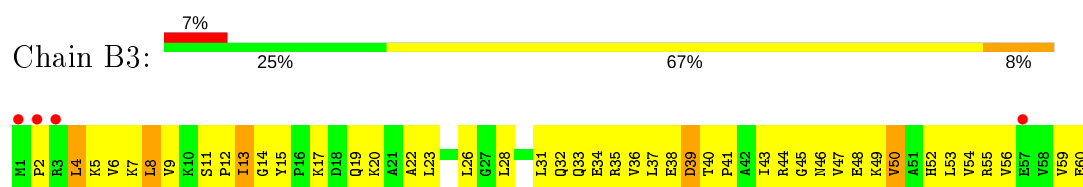
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



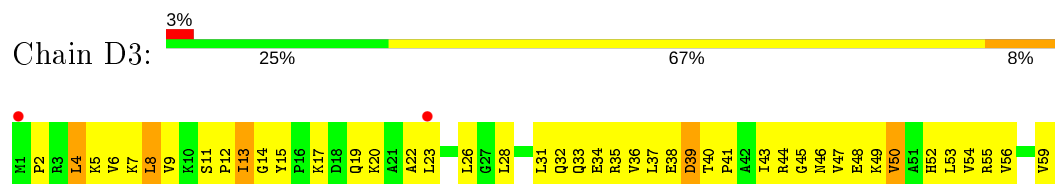
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



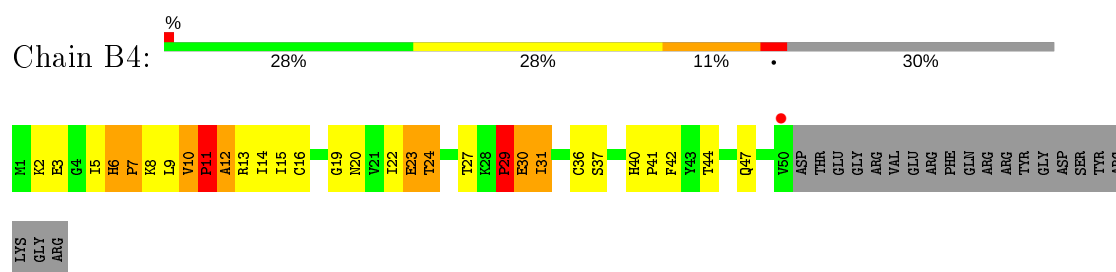
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



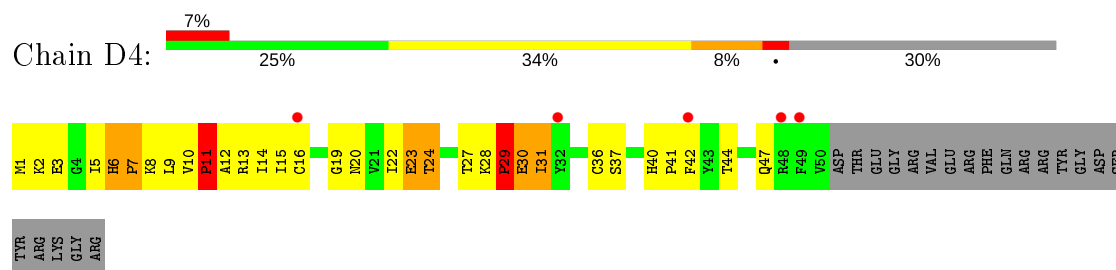
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



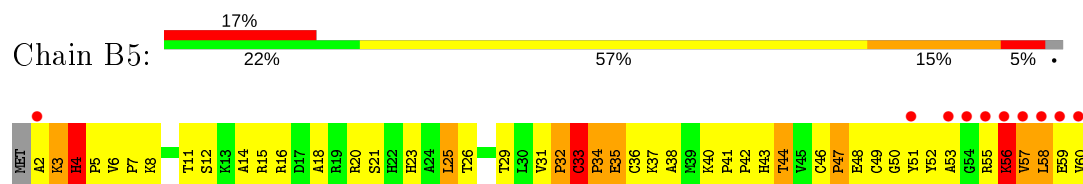
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



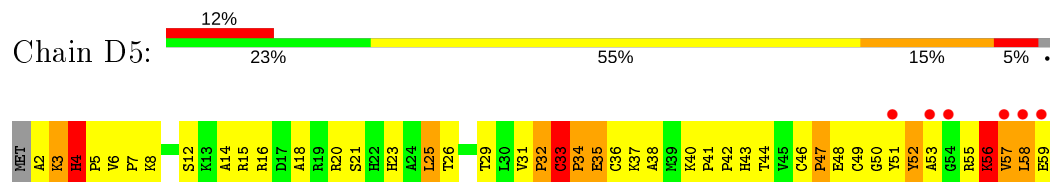
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



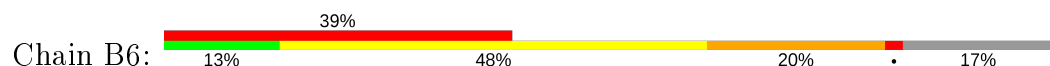
• Molecule 30: 50S RIBOSOMAL PROTEIN L32

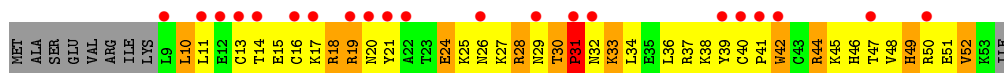


• Molecule 30: 50S RIBOSOMAL PROTEIN L32

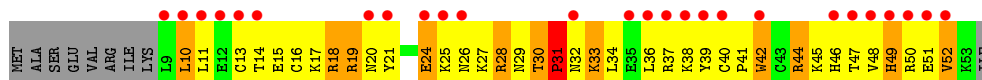
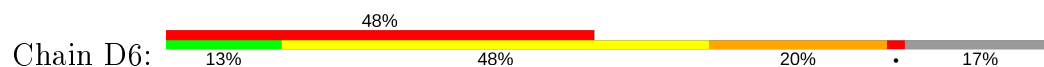


• Molecule 31: 50S RIBOSOMAL PROTEIN L33

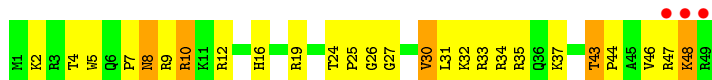




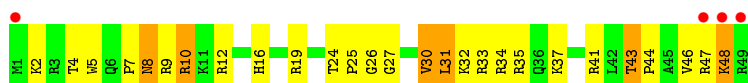
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



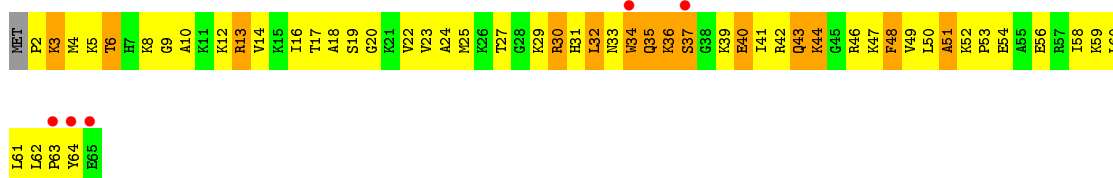
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



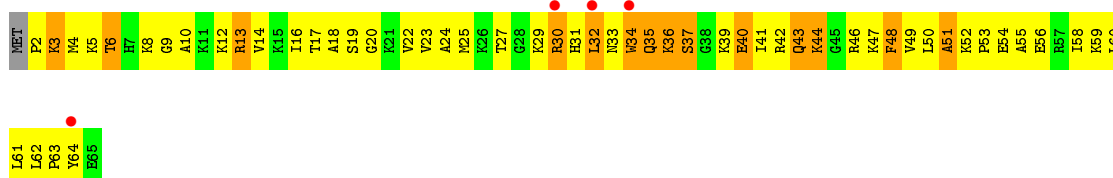
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 33: 50S RIBOSOMAL PROTEIN L35

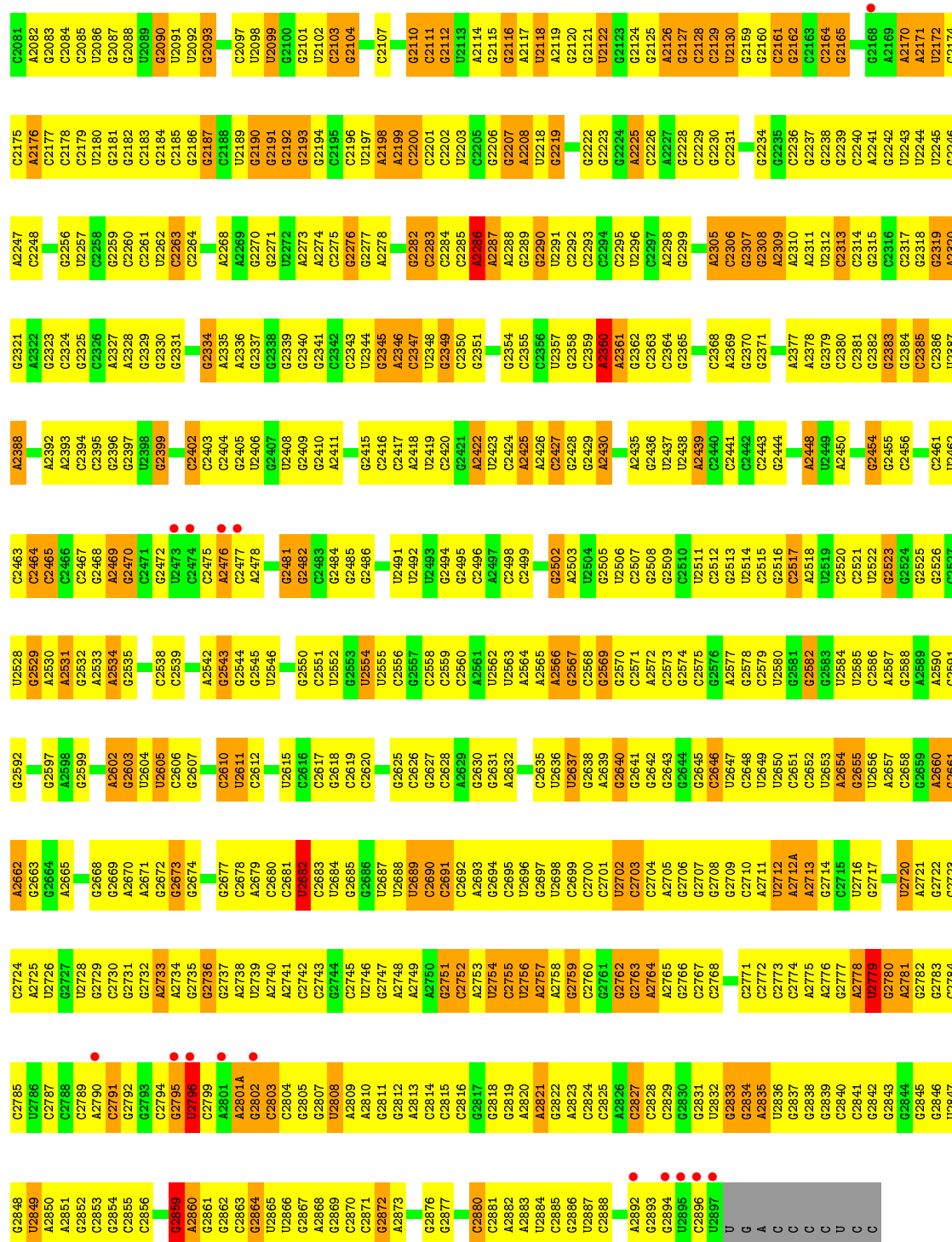


• Molecule 34: 23S RIBOSOMAL RNA



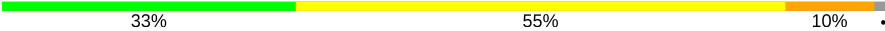
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|-------|-------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C961 | C962 | C963 | C964 | C965 | G968 | G969 | C970 | C971 | C972 | C973 | C974 | C975 | G977 | G978 | G979 | A980 | A981 | C982 | A983 | A984 | G985 | G986 | G987 | A988 | A989 | C990 | C991 | C992 | C993 | C994 | C995 | C996 | C997 | C998 | C999 | A1000 | A1001 | G1002 | G1003 | G1004 | G1005 | G1006 | C1007 | A1010 | G1011 | G1012 | C1013 | C1014 | C1018 | A1019 | A1020 | A1021 | G1022 | C1023 | G1024 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U895 | A896 | C897 | C898 | A899 | A900 | A901 | C902 | C903 | U907 | C908 | A909 | C910 | C911 | C912 | U913 | C914 | C915 | A916 | A917 | A918 | A919 | C920 | C921 | C922 | C923 | C924 | C925 | C926 | C927 | C928 | C929 | C930 | C931 | C932 | C933 | C934 | C935 | C936 | C937 | C938 | C939 | C940 | C941 | C942 | C943 | C944 | C945 | C946 | C947 | C948 | C949 | C950 | C951 | C952 | C953 | C954 | C955 | C956 | C957 | C958 | C959 | C960 | C961 | C962 | C963 | C964 | C965 | C966 | C967 | C968 | C969 | C970 | C971 | C972 | C973 | C974 | C975 | C976 | C977 | C978 | C979 | C980 | C981 | C982 | C983 | C984 | C985 | C986 | C987 | C988 | C989 | C990 | C991 | C992 | C993 | C994 | C995 | C996 | C997 | C998 | C999 | A1000 | A1001 | G1002 | G1003 | G1004 | G1005 | G1006 | C1007 | A1010 | G1011 | G1012 | C1013 | C1014 | C1018 | A1019 | A1020 | A1021 | G1022 | C1023 | G1024 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C814 | C815 | C816 | C817 | C818 | A819 | C820 | C821 | C822 | C823 | C824 | C825 | C826 | C827 | C828 | C829 | C830 | C831 | C832 | C833 | C834 | C835 | C836 | C837 | C838 | C839 | C840 | C841 | C842 | C843 | C844 | C845 | C846 | C847 | C848 | C849 | C850 | C851 | C852 | C853 | C854 | C855 | C856 | C857 | C858 | C859 | C860 | C861 | C862 | C863 | C864 | C865 | C866 | C867 | C868 | C869 | C870 | C871 | C872 | C873 | C874 | C875 | C876 | C877 | C878 | C879 | C880 | C881 | C882 | C883 | C884 | C885 | C886 | C887 | C888 | C889 | C890 | C891 | C892 | C893 | C894 | C895 | C896 | C897 | C898 | C899 | C900 | C901 | C902 | C903 | C904 | C905 | C906 | C907 | C908 | C909 | C910 | C911 | C912 | C913 | C914 | C915 | C916 | C917 | C918 | C919 | C920 | C921 | C922 | C923 | C924 | C925 | C926 | C927 | C928 | C929 | C930 | C931 | C932 | C933 | C934 | C935 | C936 | C937 | C938 | C939 | C940 | C941 | C942 | C943 | C944 | C945 | C946 | C947 | C948 | C949 | C950 | C951 | C952 | C953 | C954 | C955 | C956 | C957 | C958 | C959 | C960 | C961 | C962 | C963 | C964 | C965 | C966 | C967 | C968 | C969 | C970 | C971 | C972 | C973 | C974 | C975 | C976 | C977 | C978 | C979 | C980 | C981 | C982 | C983 | C984 | C985 | C986 | C987 | C988 | C989 | C990 | C991 | C992 | C993 | C994 | C995 | C996 | C997 | C998 | C999 | A1000 | A1001 | G1002 | G1003 | G1004 | G1005 | G1006 | C1007 | A1010 | G1011 | G1012 | C1013 | C1014 | C1018 | A1019 | A1020 | A1021 | G1022 | C1023 | G1024 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A746 | U747 | A751 | A752 | A753 | A754 | C755 | C756 | C757 | C758 | C759 | C760 | A761 | G765 | G766 | C767 | C768 | C769 | A774 | C775 | C776 | A777 | G780 | A781 | A782 | A783 | A784 | A785 | C786 | U787 | A788 | C789 | C790 | C791 | C792 | A793 | C794 | C795 | C796 | C797 | C798 | C799 | A800 | G801 | A802 | U803 | A804 | C805 | C806 | C807 | C808 | C809 | U810 | U811 | C812 | C813 | C814 | C815 | C816 | C817 | C818 | C819 | C820 | C821 | C822 | C823 | C824 | C825 | C826 | C827 | C828 | C829 | C830 | C831 | C832 | C833 | C834 | C835 | C836 | C837 | C838 | C839 | C840 | C841 | C842 | C843 | C844 | C845 | C846 | C847 | C848 | C849 | C850 | C851 | C852 | C853 | C854 | C855 | C856 | C857 | C858 | C859 | C860 | C861 | C862 | C863 | C864 | C865 | C866 | C867 | C868 | C869 | C870 | C871 | C872 | C873 | C874 | C875 | C876 | C877 | C878 | C879 | C880 | C881 | C882 | C883 | C884 | C885 | C886 | C887 | C888 | C889 | C890 | C891 | C892 | C893 | C894 | C895 | C896 | C897 | C898 | C899 | C900 | C901 | C902 | C903 | C904 | C905 | C906 | C907 | C908 | C909 | C910 | C911 | C912 | C913 | C914 | C915 | C916 | C917 | C918 | C919 | C920 | C921 | C922 | C923 | C924 | C925 | C926 | C927 | C928 | C929 | C930 | C931 | C932 | C933 | C934 | C935 | C936 | C937 | C938 | C939 | C940 | C941 | C942 | C943 | C944 | C945 | C946 | C947 | C948 | C949 | C950 | C951 | C952 | C953 | C954 | C955 | C956 | C957 | C958 | C959 | C960 | C961 | C962 | C963 | C964 | C965 | C966 | C967 | C968 | C969 | C970 | C971 | C972 | C973 | C974 | C975 | C976 | C977 | C978 | C979 | C980 | C981 | C982 | C983 | C984 | C985 | C986 | C987 | C988 | C989 | C990 | C991 | C992 | C993 | C994 | C995 | C996 | C997 | C998 | C999 | A1000 | A1001 | G1002 | G1003 | G1004 | G1005 | G1006 | C1007 | A1010 | G1011 | G1012 | C1013 | C1014 | C1018 | A1019 | A1020 | A1021 | G1022 | C1023 | G1024 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C671 | C672 | C673 | C674 | A675 | A676 | G680 | G681 | G684 | A685 | A686 | C687 | U688 | G689 | G690 | C691 | C692 | C693 | A699 | C699 | U703 | G704 | A705 | A706 | C707 | C708 | C709 | C710 | C711 | C717 | C718 | C719 | C720 | C721 | C722 | C723 | C724 | C725 | C726 | C729 | C730 | C731 | C732 | C733 | A734 | C737 | C738 | C739 | C740 | C741 | C742 | C743 | C744 | C745 | C746 | C747 | C748 | C749 | C750 | C751 | C752 | C753 | C754 | C755 | C756 | C757 | C758 | C759 | C760 | C761 | C762 | C763 | C764 | C765 | C766 | C767 | C768 | C769 | C770 | C771 | C772 | C773 | C774 | C775 | C776 | C777 | C778 | C779 | C780 | C781 | C782 | C783 | C784 | C785 | C786 | C787 | C788 | C789 | C790 | C791 | C792 | C793 | C794 | C795 | C796 | C797 | C798 | C799 | A800 | G801 | A802 | U803 | A804 | C805 | C806 | C807 | C808 | C809 | U810 | U811 | C812 | C813 | C814 | C815 | C816 | C817 | C818 | C819 | C820 | C821 | C822 | C823 | C824 | C825 | C826 | C827 | C828 | C829 | C830 | C831 | C832 | C833 | C834 | C835 | C836 | C837 | C838 | C839 | C840 | C841 | C842 | C843 | C844 | C845 | C846 | C847 | C848 | C849 | C850 | C851 | C852 | C853 | C854 | C855 | C856 | C857 | C858 | C859 | C860 | C861 | C862 | C863 | C864 | C865 | C866 | C867 | C868 | C869 | C870 | C871 | C872 | C873 | C874 | C875 | C876 | C877 | C878 | C879 | C880 | C881 | C882 | C883 | C884 | C885 | C886 | C887 | C888 | C889 | C890 | C891 | C892 | C893 | C894 | C895 | C896 | C897 | C898 | C899 | C900 | C901 | C902 | C903 | C904 | C905 | C906 | C907 | C908 | C909 | C910 | C911 | C912 | C913 | C914 | C915 | C916 | C917 | C918 | C919 | C920 | C921 | C922 | C923 | C924 | C925 | C926 | C927 | C928 | C929 | C930 | C931 | C932 | C933 | C934 | C935 | C936 | C937 | C938 | C939 | C940 | C941 | C942 | C943 | C944 | C945 | C946 | C947 | C948 | C949 | C950 | C951 | C952 | C953 | C954 | C955 | C956 | C957 | C958 | C959 | C960 | C961 | C962 | C963 | C964 | C965 | C966 | C967 | C968 | C969 | C970 | C971 | C972 | C973 | C974 | C975 | C976 | C977 | C978 | C979 | C980 | C981 | C982 | C983 | C984 | C985 | C986 | C987 | C988 | C989 | C990 | C991 | C992 | C993 | C994 | C995 | C996 | C997 | C998 | C999 | A1000 | A1001 | G1002 | G1003 | G1004 | G1005 | G1006 | C1007 | A1010 | G1011 | G1012 | C1013 | C1014 | C1018 | A1019 | A1020 | A1021 | G1022 | C1023 | G1024 |
| U606 | U607 | A608 | A609 | G610 | G611 | C612 | G613 | U614 | U614A | G614B | A614C | G616 | C618 | G619 | G620 | A621 | G622 | G623 | C624 | G625 | G626 | A627 | G628 | G629 | G630 | A631 | G632 | A633 | C634 | A635 | A636 | A637 | A638 | U639 | C640 | A643 | A644 | C645 | A646 | G647 | G648 | G649 | C650 | C651 | C652 | C653 | C654 | C655 | C656 | C657 | C658 | C659 | C660 | C661 | C662 | U667 | G668 | G669 | A670 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C537 | G538 | G539 | C540 | C541 | C542 | C543 | A547 | A548 | G549 | G550 | G551 | U554 | U555 | G556 | U557 | G558 | C559 | C560 | G561 | C562 | C563 | C564 | C565 | G570 | A571 | A572 | C573 | A574 | C575 | A576 | C577 | A578 | C579 | C580 | C581 | C582 | G583 | C584 | G585 | A586 | C587 | U588 | C589 | A590 | C591 | C592 | C593 | U594 | C595 | C596 | C597 | C598 | C599 | C600 | C601 | C602 | A603 | C604 | C605 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G468 | C469 | A470 | U471 | C472 | C473 | C474 | C475 | C476 | U477 | A478 | A479 | A480 | A481 | A482 | A483 | A484 | A485 | A486 | A487 | A488 | A489 | A490 | A491 | A492 | A493 | A494 | A495 | A496 | U497 | A498 | A499 | A500 | A501 | A502 | A503 | A504 | A505 | A506 | A507 | A508 | C509 | C510 | U511 | G512 | A513 | C517 | C518 | U519 | G520 | C521 | C522 | C523 | U524 | C527 | A528 | C529 | C530 | C531 | A532 | C533 | U534 | A535 | A536 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G400 | A401 | A402 | U403 | C404 | U405 | G406 | A407 | G408 | C409 | G410 | G411 | A412 | C413 | A414 | A415 | G418 | C419 | C420 | U421 | A422 | A423 | G424 | C426 | U427 | A428 | A429 | G430 | U431 | A432 | C433 | G438 | G440 | U441 | C442 | A443 | C444 | C445 | C446 | A447 | U448 | C451 | G452 | C453 | A456 | A457 | G458 | U459 | A460 | C461 | C462 | C463 | U464 | G465 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A320 | G321 | C322 | G323 | G329 | A330 | A331 | A332 | G333 | C334 | C335 | C336 | A340 | A341 | G342 | G343 | G344 | A345 | G348 | G349 | U350 | G351 | G352 | G353 | G354 | G355 | A359 | C360 | G361 | U362 | U363E | A363F | C364 | C365 | C366 | G372 | U373 | A374 | C378 | G379 | G386 | U387 | G388 | C389 | A390 | G391 | C392 | G396 | C397 | G398 | G399 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U271L | G271M | C271N | C271O | C271P | C271Q | C271R | C271S | C271T | C271U | C271V | C271W | C271X | C271Y | C271Z | C272 | C272B | C272C | C272D | C272H | C274 | C275 | C276 | C277 | C278 | C279 | C280 | C281 | C282 | A283 | U284 | C285 | C286 | C287 | C290 | C291 | C292 | G295 | C296 | C297 | C298 | A299 | U303 | G304 | U305 | C306 | G307 | C308 | C309 | A310 | A311 | C312 | C313 | A314 | C315 | C318 | C319 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G220 | A221 | A222 | A223 | G224 | A225 | C226 | A227 | A228 | C229 | U230 | C231 | C232 | U235 | C236 | C237 | C238 | U239 | C240 | A241 | C242 | U243 | A244 | C245 | C246 | G247 | C248 | C249 | G250 | A251 | C252 | C253 | G254 | A255 | A256 | A257 | C258 | G259 | C260 | C261 | A262 | A265 | G266 | C267 | A270 | A271 | A271A | C271B | C271C | U271E | C271F | C271G | C271H | C271J | C271K | U271L | U271M | C271N | C271O | C271P | C271Q | C271R | C271S | C271T | C271U | C271V | C271W | C271X | C271Y | C271Z | C272 | C272B | C272C | C272D | C272H | C274 | C275 | C276 | C277 | C278 | C279 | C280 | C281 | C282 | A283 | U284 | C285 | C286 | C287 | C290 | C291 | C292 | G295 | C296 | C297 | C298 | A299 | U303 | G304 | U305 | C306 | G307 | C308 | C309 | A310 | A311 | C312 | C313 | A314 | C315 | C318 | C319 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G140 | A141 | C142 | C142A | G143 | C143A | C144 | G145 | G146 | U147 | C148 | A149 | C150 | C151 | G152 | C153 | G154 | C154A | U157 | U158 | G171 | C172 | G173 | C174 | C184 | U185 | G188 | C189 | A190 | A191 | U192 | U193 | G194 | A195 | A196 | A197 | C198 | A199 | U200 | C201 | U202 | C203 | A204 | G205 | U206 | A207 | C208 | C209 | C210 | A211 | G212 | A213 | C214 | G215 | A216 | C217 | U218 | C219 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A74 | G75 | C76 | C77 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

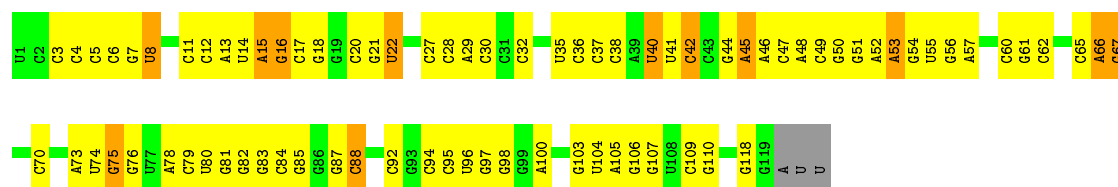
| | | | | | | | | | | | | |
|-------|-------|-------|-------|--------|-------|-------|--------|-------|-------|--------|--------|-------|
| A2013 | G1929 | C1843 | U1775 | G1695 | U1621 | C1547 | U1405 | G1337 | A1268 | U1205 | U1142 | G1025 |
| A2014 | G1776 | C1844 | G1776 | G1696 | G1622 | C1548 | U1406 | G1338 | A1269 | G1206 | A1142A | U1026 |
| A2015 | U1777 | G1845 | U1777 | G1697 | G1623 | C1549 | C1407 | G1339 | A1270 | C1207 | A1143 | A1027 |
| U2016 | G1932 | G1846 | U1778 | G1698 | G1624 | C1550 | C1408 | G1340 | G1271 | C1208 | G1144 | A1028 |
| U2017 | G1933 | A1847 | U1779 | G1699 | G1625 | C1551 | C1409 | U1341 | G1272 | G1209 | C1145 | A1029 |
| G2018 | G1935 | A1848 | U1780 | A1700 | G1626 | C1554 | G1410 | G1344 | U1273 | A1210 | C1146 | G1030 |
| A2019 | A1936 | G1849 | A1780 | A1701 | G1627 | A1554 | C1411 | G1345 | A1274 | U1211 | C1147 | G1031 |
| A2020 | A1937 | G1850 | A1783 | G1702 | U1629 | A1558 | A1412 | C1346 | A1275 | G1215 | A1148 | U1032 |
| C2021 | A1938 | U1851 | A1784 | G1703 | G1635 | A1559 | G1413 | G1347 | A1276 | G1216 | A1149 | U1033 |
| U2022 | U1939 | G1852 | A1785 | G1704 | G1636 | G1559 | A1414 | G1348 | G1277 | G1150 | C1150 | U1035 |
| G2023 | U1940 | A1853 | A1786 | G1705 | G1637 | A1560 | U1415 | A1349 | G1278 | G1151 | G1036 | U1036 |
| G2024 | U1946 | G1854 | A1789 | G1706 | U1639 | A1562 | G1416 | A1349 | G1279 | C1220 | G1152 | G1037 |
| C2025 | C1947 | G1855 | G1790 | U1709 | G1640 | C1564 | C1417 | A1350 | G1280 | C1221A | G1153 | G1038 |
| G2027 | G1948 | G1858 | A1791 | G1710 | A1641 | G1568 | A1418 | C1351 | G1281 | G1222 | G1154 | C1039 |
| U2028 | U1949 | A1859 | U1796 | G1711 | G1642 | A1569 | A1419 | U1352 | A1284 | G1223 | A1155 | G1040 |
| G2029 | G1950 | G1860 | U1797 | G1712 | G1643 | A1570 | A1420 | A1353 | G1285 | G1224 | A1156 | C1041 |
| A2030 | U1951 | G1861 | C1797 | U1713 | G1644 | A1571 | G1426 | G1355 | A1286 | G1225 | G1157 | G1042 |
| A2031 | A1952 | G1862 | U1798 | G1714 | G1647 | A1572 | G1425 | G1356 | A1287 | A1226 | U1159 | C1043 |
| G2032 | A1953 | G1863 | G1799 | G1717 | G1648 | A1573 | G1424 | U1357 | U1288 | G1227 | G1160 | G1044 |
| A2033 | G1954 | U1864 | C1800 | G1718 | G1649 | C1574 | A1427 | G1358 | C1289 | G1228 | C1161 | A1045 |
| G2034 | U1955 | G1865 | A1803 | G1719 | G1652 | U1577 | C1428 | A1359 | C1290 | G1229 | G1162 | U1046 |
| G2035 | G1956 | C1866 | G1804 | U1720 | G1653 | A1578 | G1429 | A1360 | G1291 | G1230 | G1163 | G1047 |
| G2036 | U1962 | A1876 | U1805 | G1721 | A1654 | U1579 | C1430 | G1361 | U1292 | G1231 | G1164 | A1048 |
| G2037 | G1963 | G1877 | U1806 | A1722 | A1655 | A1578 | U1431 | G1362 | U1293 | G1232 | U1165 | A1049 |
| G1964 | G1964 | G1878 | G1806 | U1739 | G1656 | A1579 | G1432 | C1363 | U1294 | G1233 | C1166 | A1050 |
| C2039 | C1967 | C1879 | U1807 | G1740 | C1657 | C1582 | U1433 | G1364 | C1295 | U1234 | U1167 | G1051 |
| C2040 | U1808 | G1880 | U1808 | A1741 | C1658 | A1583 | G1434 | A1365 | G1298 | G1235 | G1168 | C1052 |
| U2041 | A1809 | G1881 | A1809 | G1742 | C1659 | A1584 | G1435 | A1366 | C1299 | A1236 | G1169 | C1053 |
| A2042 | G1882 | C1882 | A1810 | C1743 | C1660 | C1585 | G1436 | A1367 | G1299 | G1237 | G1170 | A1106 |
| G2043 | G1883 | G1883 | G1811 | G1744 | G1661 | A1586 | U1437 | G1368 | U1300 | G1238 | G1171 | G1107 |
| A1971 | A1971 | A1884 | A1812 | C1745 | C1662 | C1587 | C1438 | G1369 | A1301 | G1239 | G1173 | U1108 |
| C2050 | A1972 | A1885 | G1813 | G1746 | C1663 | C1588 | U1439 | C1370 | A1302 | U1240 | A1174 | U1109 |
| A2051 | A2051 | C1886 | G1814 | G1747 | A1664 | C1589 | A1440 | C1371 | G1309 | A1241 | U1175 | G1110 |
| G2052 | G1980 | C1887 | A1815 | U1590 | G1665 | U1590 | G1441 | G1372 | G1310 | A1242 | G1176 | G1111 |
| C2055 | C1982 | G1888 | G1816 | G1747A | G1666 | A1591 | G1442 | A1378 | G1311 | A1243 | A1177 | G1112 |
| G2056 | C1983 | A1889 | G1817 | G1748 | G1667 | A1592 | G1443 | A1379 | U1312 | G1244 | G1178 | U1113 |
| A2059 | G1984 | U1898 | U1819 | A1749 | A1668 | G1593 | U1444 | C1380 | U1313 | G1245 | C1179 | G1114 |
| A2060 | G1985 | G1899 | U1820 | G1750 | C1670 | G1594 | A1445 | G1381 | U1314 | A1246 | C1180 | G1115 |
| G2061 | A1986 | A1900 | A1821 | C1751 | G1671 | G1595 | A1446A | G1382 | C1315 | G1247 | C1181 | G1116 |
| A2062 | G1987 | G1902 | G1823 | G1752 | G1672 | A1596 | C1446A | G1383 | C1316 | G1248 | A1182 | G1117 |
| C2063 | C1988 | C1903 | G1824 | C1754 | G1673 | C1597 | G1447 | C1384 | U1317 | U1249 | G1183 | C1118 |
| G2064 | G1989 | G1825 | G1824 | A1755 | C1675 | C1598 | G1448 | G1385 | A1317 | G1250 | G1184 | G1119 |
| C2065 | C1990 | G1826 | G1825 | G1756 | G1678 | U1602 | A1449 | C1386 | C1318 | C1251 | C1185 | G1120 |
| C2066 | U1991 | G1906 | G1826 | U1757 | U1679 | A1603 | G1450 | C1387 | G1322 | G1252 | G1186 | G1121 |
| G2067 | G1992 | G1907 | C1827 | G1758 | U1680 | G1596 | U1453 | G1388 | A1253 | A1253 | G1187 | G1122 |
| U2068 | U1993 | C1908 | G1828 | G1759 | U1681 | G1597 | G1454 | G1389 | U1254 | U1255 | U1188 | C1123 |
| G2069 | G1997 | G1909 | A1829 | A1762 | G1682 | A1608 | G1455 | G1390 | G1324 | G1256 | G1190 | G1124 |
| G2070 | G1998 | G1910 | G1830 | G1763 | G1683 | A1609 | G1456 | U1394 | G1325 | C1257 | G1191 | G1125 |
| A2071 | G2004 | A1912 | G1831 | G1764 | C1684 | A1610 | A1457 | A1395 | U1326 | G1258 | G1192 | A1129 |
| G2072 | A2005 | G1832 | U1833 | G1765 | C1685 | G1611 | C1458 | A1396 | C1327 | G1259 | G1193 | U1130 |
| C2073 | U2074 | C1914 | U1834 | U1766 | U1688 | A1614 | G1459 | U1397 | G1328 | G1260 | A1194 | G1131 |
| U2074 | C2006 | U1915 | G1835 | U1767 | A1689 | C1615 | A1460 | C1398 | U1329 | C1261 | A1195 | A1132 |
| U2075 | G2009 | C1924 | G1839 | U1768 | A1690 | A1616 | G1461 | G1400 | C1330 | A1263 | C1196 | U1135 |
| C2078 | U2010 | C1925 | G1840 | C1771 | C1691 | C1617 | C1464 | G1401 | G1332 | G1264 | C1201 | G1136 |
| U2079 | U2011 | U1926 | U1841 | A1772 | U1692 | A1618 | G1465 | C1402 | U1335 | A1265 | C1202 | C1140 |
| G2080 | G2012 | G1842 | G1842 | C1774 | U1693 | A1619 | G1466 | C1403 | U1336 | G1266 | A1204 | U1141 |



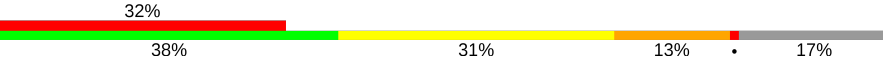
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C1043 | C1044 | G1045 | A1046 | A1047 | A1048 | C1049 | A1050 | G1051 | C1052 | C1053 | A1054 | A1107 | U1108 | C1109 | G1110 | A1111 | G1112 | U1113 | G1114 | G1115 | C1116 | G1117 | C1118 | C1119 | G1120 | C1121 | C1122 | C1123 | G1124 | G1125 | A1129 | U1130 | G1131 | A1132 | U1133 | C1135 | G1136 | C1140 | U1141 | U1142 | A1142A | A1143 | C1144 | C1145 | C1146 | C1147 | A1148 | G1149 | C1150 | G1151 | C1152 | G1153 | C1154 | A1155 | A1156 | C1158 | C1043 | C1044 | G1045 | A1046 | A1047 | A1048 | C1049 | A1050 | G1051 | C1052 | C1053 | A1054 | A1107 | U1108 | C1109 | G1110 | A1111 | G1112 | U1113 | G1114 | G1115 | C1116 | G1117 | C1118 | C1119 | G1120 | C1121 | C1122 | C1123 | G1124 | G1125 | A1129 | U1130 | G1131 | A1132 | U1133 | C1135 | G1136 | C1140 | U1141 | U1142 | A1142A | A1143 | C1144 | C1145 | C1146 | C1147 | A1148 | G1149 | C1150 | G1151 | C1152 | G1153 | C1154 | A1155 | A1156 | C1158 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G877 | G878 | G879 | A880 | A881 | G882 | A883 | A884 | G885 | G886 | G887 | G888 | G889 | G890 | G891 | G892 | G893 | G894 | G895 | G896 | G897 | G898 | G899 | G900 | G901 | G902 | G903 | G904 | G905 | G906 | G907 | G908 | G909 | G910 | G911 | G912 | G913 | G914 | G915 | G916 | G917 | G918 | G919 | G920 | G921 | G922 | G923 | G924 | G925 | G926 | G927 | G928 | G929 | G930 | G931 | G932 | G933 | G934 | G935 | G936 | G937 | G938 | G939 | G940 | G941 | G942 | G943 | G944 | G945 | G946 | G947 | G948 | G949 | G950 | G951 | G952 | G953 | G954 | G955 | G956 | G957 | G958 | G959 | G960 | G961 | G962 | G963 | G964 | G965 | G966 | G967 | G968 | G969 | G970 | G971 | G972 | G973 | G974 | G975 | G976 | G977 | G978 | G979 | G980 | G981 | G982 | G983 | G984 | G985 | G986 | G987 | G988 | G989 | G990 | G991 | G992 | G993 | G994 | G995 | G996 | G997 | G998 | G999 | G1000 | G1001 | G1002 | G1003 | G1004 | C1005 | C1006 | A1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | G877 | G878 | G879 | A880 | A881 | G882 | A883 | A884 | G885 | G886 | G887 | G888 | G889 | G890 | G891 | G892 | G893 | G894 | G895 | G896 | G897 | G898 | G899 | G900 | G901 | G902 | G903 | G904 | G905 | G906 | G907 | G908 | G909 | G910 | G911 | G912 | G913 | G914 | G915 | G916 | G917 | G918 | G919 | G920 | G921 | G922 | G923 | G924 | G925 | G926 | G927 | G928 | G929 | G930 | G931 | G932 | G933 | G934 | G935 | G936 | G937 | G938 | G939 | G940 | G941 | G942 | G943 | G944 | G945 | G946 | G947 | G948 | G949 | G950 | G951 | G952 | G953 | G954 | G955 | G956 | G957 | G958 | G959 | G960 | G961 | G962 | G963 | G964 | G965 | G966 | G967 | G968 | G969 | G970 | G971 | G972 | G973 | G974 | G975 | G976 | G977 | G978 | G979 | G980 | G981 | G982 | G983 | G984 | G985 | G986 | G987 | G988 | G989 | G990 | G991 | G992 | G993 | G994 | G995 | G996 | G997 | G998 | G999 | G1000 | G1001 | G1002 | G1003 | G1004 | C1005 | C1006 | A1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 |
| U907 | C908 | A909 | G910 | G911 | G912 | G913 | G914 | G915 | G916 | G917 | G918 | G919 | G920 | G921 | G922 | G923 | G924 | G925 | G926 | G927 | G928 | G929 | G930 | G931 | G932 | G933 | G934 | G935 | G936 | G937 | G938 | G939 | G940 | G941 | G942 | G943 | G944 | G945 | G946 | G947 | G948 | G949 | G950 | G951 | G952 | G953 | G954 | G955 | G956 | G957 | G958 | G959 | G960 | G961 | G962 | G963 | G964 | G965 | G966 | G967 | G968 | G969 | G970 | G971 | G972 | G973 | G974 | G975 | G976 | G977 | G978 | G979 | G980 | G981 | G982 | G983 | G984 | G985 | G986 | G987 | G988 | G989 | G990 | G991 | G992 | G993 | G994 | G995 | G996 | G997 | G998 | G999 | G1000 | G1001 | G1002 | G1003 | G1004 | C1005 | C1006 | A1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | U907 | C908 | A909 | G910 | G911 | G912 | G913 | G914 | G915 | G916 | G917 | G918 | G919 | G920 | G921 | G922 | G923 | G924 | G925 | G926 | G927 | G928 | G929 | G930 | G931 | G932 | G933 | G934 | G935 | G936 | G937 | G938 | G939 | G940 | G941 | G942 | G943 | G944 | G945 | G946 | G947 | G948 | G949 | G950 | G951 | G952 | G953 | G954 | G955 | G956 | G957 | G958 | G959 | G960 | G961 | G962 | G963 | G964 | G965 | G966 | G967 | G968 | G969 | G970 | G971 | G972 | G973 | G974 | G975 | G976 | G977 | G978 | G979 | G980 | G981 | G982 | G983 | G984 | G985 | G986 | G987 | G988 | G989 | G990 | G991 | G992 | G993 | G994 | G995 | G996 | G997 | G998 | G999 | G1000 | G1001 | G1002 | G1003 | G1004 | C1005 | C1006 | A1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U827 | U828 | A829 | G830 | G831 | G832 | U833 | C834 | A835 | G836 | C837 | C838 | U839 | U840 | U841 | U842 | U843 | U844 | U845 | U846 | U847 | U848 | U849 | U850 | U851 | U852 | U853 | U854 | U855 | U856 | U857 | U858 | U859 | U860 | U861 | U862 | U863 | U864 | U865 | U866 | U867 | U868 | U869 | U870 | U871 | U872 | U873 | U874 | U875 | U876 | U877 | U878 | U879 | U880 | U881 | U882 | U883 | U884 | U885 | U886 | U887 | U888 | U889 | U890 | U891 | U892 | U893 | U894 | U895 | U896 | U897 | U898 | U899 | U900 | U901 | U902 | U903 | U904 | U905 | U906 | U907 | U908 | U909 | U910 | U911 | U912 | U913 | U914 | U915 | U916 | U917 | U918 | U919 | U920 | U921 | U922 | U923 | U924 | U925 | U926 | U927 | U928 | U929 | U930 | U931 | U932 | U933 | U934 | U935 | U936 | U937 | U938 | U939 | U940 | U941 | U942 | U943 | U944 | U945 | U946 | U947 | U948 | U949 | U950 | U951 | U952 | U953 | U954 | U955 | U956 | U957 | U958 | U959 | U960 | U961 | U962 | U963 | U964 | U965 | U966 | U967 | U968 | U969 | U970 | U971 | U972 | U973 | U974 | U975 | U976 | U977 | U978 | U979 | U980 | U981 | U982 | U983 | U984 | U985 | U986 | U987 | U988 | U989 | U990 | U991 | U992 | U993 | U994 | U995 | U996 | U997 | U998 | U999 | G1000 | G1001 | G1002 | G1003 | G1004 | C1005 | C1006 | A1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C754 | C755 | C756 | C757 | C758 | C759 | C760 | C761 | C762 | C763 | C764 | C765 | C766 | C767 | C768 | C769 | C770 | C771 | C772 | C773 | C774 | C775 | C776 | C777 | C778 | C779 | C780 | C781 | C782 | C783 | C784 | C785 | C786 | C787 | C788 | C789 | C790 | C791 | C792 | C793 | C794 | C795 | C796 | C797 | C798 | C799 | C800 | C801 | C802 | C803 | C804 | C805 | C806 | C807 | C808 | C809 | C810 | C811 | C812 | C813 | C814 | C815 | C816 | C817 | C818 | C819 | C820 | C821 | C822 | C823 | C824 | C825 | C826 | C827 | C828 | C829 | C830 | C831 | C832 | C833 | C834 | C835 | C836 | C837 | C838 | C839 | C840 | C841 | C842 | C843 | C844 | C845 | C846 | C847 | C848 | C849 | C850 | C851 | C852 | C853 | C854 | C855 | C856 | C857 | C858 | C859 | C860 | C861 | C862 | C863 | C864 | C865 | C866 | C867 | C868 | C869 | C870 | C871 | C872 | C873 | C874 | C875 | C876 | C877 | C878 | C879 | C880 | C881 | C882 | C883 | C884 | C885 | C886 | C887 | C888 | C889 | C890 | C891 | C892 | C893 | C894 | C895 | C896 | C897 | C898 | C899 | C900 | C901 | C902 | C903 | C904 | C905 | C906 | C907 | C908 | C909 | C910 | C911 | C912 | C913 | C914 | C915 | C916 | C917 | C918 | C919 | C920 | C921 | C922 | C923 | C924 | C925 | C926 | C927 | C928 | C929 | C930 | C931 | C932 | C933 | C934 | C935 | C936 | C937 | C938 | C939 | C940 | C941 | C942 | C943 | C944 | C945 | C946 | C947 | C948 | C949 | C950 | C951 | C952 | C953 | C954 | C955 | C956 | C957 | C958 | C959 | C960 | C961 | C962 | C963 | C964 | C965 | C966 | C967 | C968 | C969 | C970 | C971 | C972 | C973 | C974 | C975 | C976 | C977 | C978 | C979 | C980 | C981 | C982 | C983 | C984 | C985 | C986 | C987 | C988 | C989 | C990 | C991 | C992 | C993 | C994 | C995 | C996 | C997 | C998 | C999 | G1000 | G1001 | G1002 | G1003 | G1004 | C1005 | C1006 | A1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| U271K | U271L | U271M | U271N | U271O | U271P | U271Q | U271R | U271S | U271T | U271U | U271V | U271W | U271X | U271Y | U271Z | U272A | U272B | U272C | U272D | U272E | U272F | U272G | U272H | U272I | U272J | U272K | U272L | U272M | U272N | U272O | U272P | U272Q | U272R | U272S | U272T | U272U | U272V | U272W | U272X | U272Y | U272Z | U273A | U273B | U273C | U273D | U273E | U273F | U273G | U273H | U273I | U273J | U273K | U273L | U273M | U273N | U273O | U273P | U273Q | U273R | U273S | U273T | U273U | U273V | U273W | U273X | U273Y | U273Z | U274A | U274B | U274C | U274D | U274E | U274F | U274G | U274H | U274I | U274J | U274K | U274L | U274M | U274N | U274O | U274P | U274Q | U274R | U274S | U274T | U274U | U274V | U274W | U274X | U274Y | U274Z | U275A | U275B | U275C | U275D | U275E | U275F | U275G | U275H | U275I | U275J | U275K | U275L | U275M | U275N | U275O | U275P | U275Q | U275R | U275S | U275T | U275U | U275V | U275W | U275X | U275Y | U275Z | U276A | U276B | U276C | U276D | U276E | U276F | U276G | U276H | U276I | U276J | U276K | U276L | U276M | U276N | U276O | U276P | U276Q | U276R | U276S | U276T | U276U | U276V | U276W | U276X | U276Y | U276Z | U277A | U277B | U277C | U277D | U277E | U277F | U277G | U277H | U277I | U277J | U277K | U277L | U277M | U277N | U277O | U277P | U277Q | U277R | U277S | U277T | U277U | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

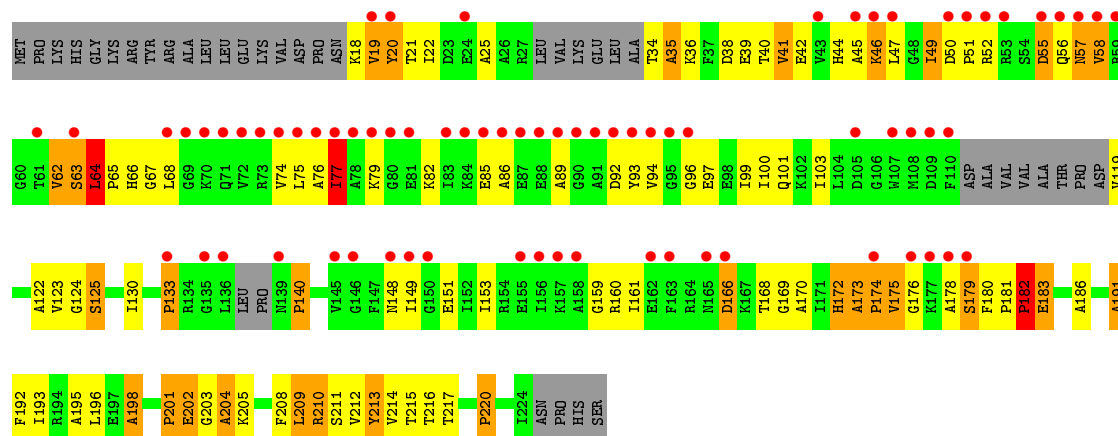
| | | | | | | | | | | | | |
|-------|-------|-------|-------|--------|-------|--------|--------|--------|-------|-------|-------|--------|
| C2027 | G1950 | G1862 | C1797 | G1714 | G1574 | A1495 | G1496 | G1426 | G1356 | A1287 | A1296 | U1159 |
| U2028 | U1951 | G1863 | U1798 | G1717 | G1651 | A1496 | A1497 | A1427 | U1357 | U1288 | G1227 | G1160 |
| A2029 | A1952 | U1864 | A1852 | G1718 | A1852 | U1497 | U1498 | A1428 | G1358 | C1289 | G1228 | C1161 |
| U2099 | A1953 | G1865 | C1800 | G1719 | G1653 | G1799 | G1429 | G1429 | A1359 | C1290 | G1229 | G1162 |
| A2031 | G1954 | G1866 | A1803 | U1720 | A1654 | C1499 | U1430 | U1430 | A1360 | C1291 | G1230 | G1163 |
| G2032 | U1955 | A1876 | G1804 | G1721 | A1655 | G1500 | U1431 | U1431 | G1361 | U1292 | G1231 | G1164 |
| A2033 | G1959 | A1877 | U1805 | A1722 | C1656 | C1501 | C1432 | C1432 | C1362 | G1293 | G1232 | U1165 |
| U2034 | G1959 | G1878 | U1806 | U1739 | C1657 | C1502 | U1433 | U1433 | G1363 | C1298 | G1233 | U1166 |
| G2035 | G1959 | G1879 | U1806 | U1740 | C1658 | U1503 | G1434 | G1434 | G1364 | U1294 | G1234 | U1167 |
| U2036 | U1962 | C1880 | G1807 | A1741 | C1584 | U1504 | G1435 | G1435 | G1365 | G1299 | G1235 | G1168 |
| G2037 | U1963 | C1881 | U1808 | G1742 | A1887 | C1505 | G1436 | G1436 | A1366 | U1300 | G1236 | G1169 |
| G2038 | G1964 | A1809 | G1809 | G1743 | G1882 | C1506 | U1437 | U1437 | A1367 | A1301 | G1237 | G1170 |
| C2039 | G1964 | G1882 | A1810 | G1744 | C1663 | A1507 | U1438 | U1438 | G1368 | A1302 | G1238 | G1171 |
| C2040 | G1967 | A1884 | G1811 | C1745 | A1684 | A1508 | A1439 | A1439 | G1369 | C1305 | G1239 | G1172 |
| U2041 | U1968 | A1885 | A1812 | G1745A | A1685 | C1509 | G1440 | G1440 | C1376 | U1175 | U1240 | G1173 |
| G2042 | A1969 | G1886 | A1813 | G1746 | G1666 | A1509A | G1441 | G1441 | C1377 | C1306 | A1241 | U1174 |
| C2043 | A1970 | C1887 | G1814 | G1747 | G1667 | U1509B | G1442 | G1442 | G1378 | G1176 | A1242 | G1176 |
| A2114 | A1971 | G1888 | A1815 | G1747A | G1668 | G1523 | G1443 | G1443 | A1379 | G1309 | G1243 | A1177 |
| G2115 | A1972 | A1889 | G1816 | G1748 | A1669 | U1524 | G1444 | G1444 | A1379 | G1310 | G1244 | C1178 |
| A2051 | A1972 | A1889 | G1817 | G1749 | A1670 | G1525 | A1445 | A1445 | G1380 | G1311 | G1245 | C1179 |
| A2052 | A1972 | A1889 | G1817 | G1749 | A1670 | G1525 | A1445 | A1445 | G1380 | G1311 | G1245 | C1179 |
| A2053 | A1981 | G1899 | U1818 | G1750 | A1671 | U1518 | G1445A | G1445A | A1384 | U1312 | G1246 | C1180 |
| G2054 | C1982 | A1901 | A1819 | C1751 | A1672 | G1519 | C1446 | C1446 | A1385 | U1313 | G1247 | C1181 |
| A2054 | C1982 | A1901 | A1819 | C1751 | A1672 | G1519 | C1446 | C1446 | A1385 | U1313 | G1247 | C1181 |
| C2055 | C1983 | G1902 | A1821 | G1753 | A1673 | U1520 | G1447 | G1447 | A1386 | C1314 | G1248 | A1182 |
| G2056 | G1984 | G1903 | G1822 | G1754 | A1677 | G1524 | G1448 | G1448 | G1387 | C1317 | U1249 | G1183 |
| A2056 | G1985 | G1904 | G1823 | A1755 | A1677 | U1525 | G1450 | G1450 | G1388 | C1318 | G1251 | C1185 |
| A2059 | A1986 | C1905 | G1824 | G1756 | C1677 | G1526 | U1453 | U1453 | G1389 | G1319 | G1252 | G1186 |
| A2060 | G1987 | G1906 | A1825 | U1757 | A1678 | G1527 | G1454 | G1454 | A1389 | G1387 | U1253 | G1187 |
| G2061 | C1988 | G1907 | A1826 | G1758 | U1679 | A1528A | G1455 | G1455 | U1394 | A1322 | A1254 | A1188 |
| A2062 | G1989 | G1908 | G1826 | G1759 | U1680 | G1529 | G1456 | G1456 | A1395 | G1323 | U1255 | A1189 |
| C2063 | C1990 | G1909 | G1828 | G1762 | C1611 | U1530 | A1457 | A1457 | U1396 | G1324 | G1256 | G1190 |
| C2064 | U1991 | G1910 | G1828 | G1763 | C1683 | C1531 | G1458 | G1458 | U1397 | G1325 | G1257 | G1191 |
| C2065 | G1992 | U1911 | G1831 | G1764 | C1684 | U1532 | G1459 | G1459 | C1398 | U1326 | G1258 | G1192 |
| C2066 | U1993 | A1912 | C1832 | G1765 | C1685 | G1533 | A1460 | A1460 | C1399 | G1327 | G1259 | G1193 |
| G2067 | G1993 | A1913 | U1833 | U1766 | C1685 | G1533 | G1461 | G1461 | G1400 | G1328 | G1260 | A1194 |
| U2068 | G1997 | G1914 | U1834 | C1767 | C1685 | C1543 | G1464 | G1464 | G1400 | U1329 | G1261 | G1195 |
| G2069 | G1998 | U1915 | G1835 | U1768 | U1688 | A1544 | G1465 | G1465 | C1402 | G1330 | U1262 | C1196 |
| C2070 | G2004 | U1923 | G1839 | C1771 | A1689 | A1545 | G1465 | G1465 | C1402 | A1331 | U1263 | C1201 |
| A2071 | A2005 | C1924 | G1840 | G1772 | C1691 | C1546 | G1466 | G1466 | C1403 | G1332 | G1264 | C1202 |
| C2072 | C2006 | C1925 | U1841 | A1773 | U1692 | C1547 | C1467 | C1467 | C1404 | U1335 | A1265 | G1203 |
| U2074 | G2009 | U1926 | G1842 | U1774 | C1693 | C1548 | A1471 | A1471 | U1406 | A1336 | U1266 | A1204 |
| U2075 | G2010 | G1929 | C1843 | U1775 | G1695 | C1549 | G1474 | G1474 | U1407 | G1337 | U1267 | U1205 |
| C2078 | U2011 | G1930 | C1844 | U1776 | G1696 | C1551 | G1475 | G1475 | C1408 | G1338 | A1268 | U1206 |
| U2079 | G2012 | U1931 | G1845 | U1777 | G1697 | A1554 | C1476 | C1476 | C1409 | U1339 | G1270 | G1207 |
| G2080 | A2013 | A1932 | G1846 | U1778 | A1698 | U1554 | A1477 | A1477 | C1410 | G1271 | G1271 | C1208 |
| C2081 | A2014 | G1933 | A1847 | U1779 | G1699 | A1558 | G1478 | G1478 | C1411 | U1340 | A1272 | G1209 |
| A2082 | A2015 | C1934 | G1848 | A1780 | U1701 | G1559 | G1478 | G1478 | A1412 | U1341 | U1273 | A1210 |
| C2083 | U2016 | G1935 | G1850 | A1781 | G1702 | G1559 | U1481 | U1481 | G1413 | G1344 | A1274 | U1211 |
| C2084 | U2017 | A1936 | U1851 | A1783 | G1703 | A1562 | G1482 | G1482 | G1414 | G1345 | A1275 | G1215 |
| G2085 | G2018 | A1937 | U1852 | A1784 | G1704 | G1563 | G1483 | G1483 | U1415 | G1346 | A1276 | G1216 |
| G2086 | A2019 | A1938 | A1853 | A1785 | U1699 | C1564 | G1485 | G1485 | C1416 | G1347 | G1277 | G1217 |
| G2087 | U2088 | U1939 | A1854 | A1786 | G1707 | A1568 | A1486 | A1486 | C1417 | G1348 | U1278 | A1220 |
| G2088 | C2021 | U1940 | G1855 | A1789 | U1708 | G1569 | A1486 | A1486 | U1418 | A1349 | G1279 | C1221 |
| U2089 | U2022 | U1940 | G1855 | A1790 | U1709 | A1570 | A1486 | A1486 | A1420 | C1350 | G1280 | C1221A |
| G2090 | G2023 | U1946 | G1858 | A1791 | C1710 | A1571 | A1486 | A1486 | G1421 | C1351 | G1281 | C1222 |
| U2091 | G2024 | C1947 | A1859 | G1792 | C1711 | A1572 | G1492 | G1492 | G1421 | A1353 | A1284 | G1223 |
| G2092 | C2025 | G1948 | A1859 | G1792 | C1712 | A1572 | G1492 | G1492 | G1421 | A1354 | A1284 | G1224 |
| G2093 | C2026 | G1949 | G1861 | U1796 | U1713 | G1573 | A1494 | A1494 | G1425 | G1355 | A1286 | G1225 |

Chain DB: 

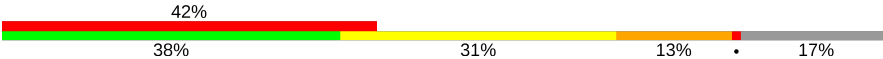


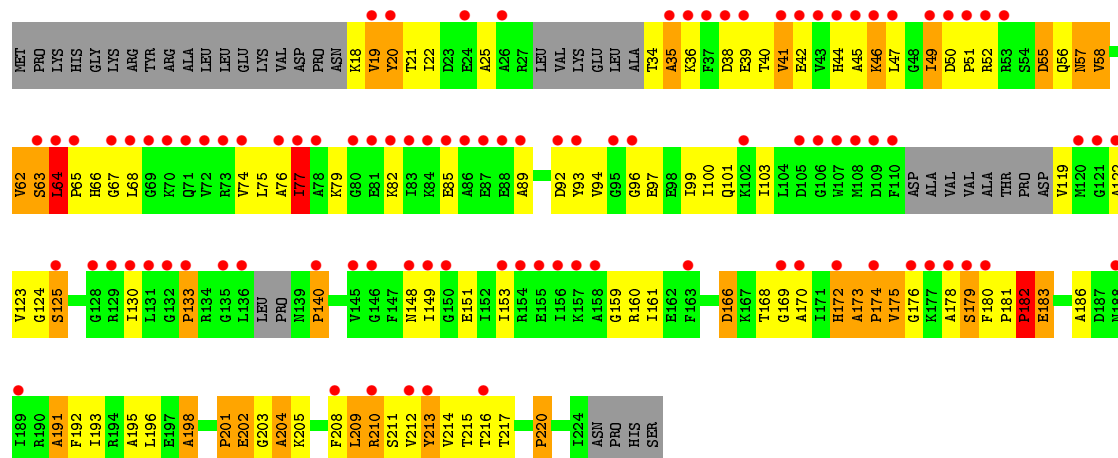
• Molecule 36: 50S RIBOSOMAL PROTEIN L1

Chain BC: 



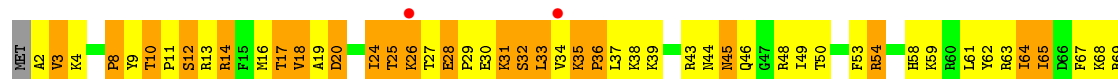
• Molecule 36: 50S RIBOSOMAL PROTEIN L1

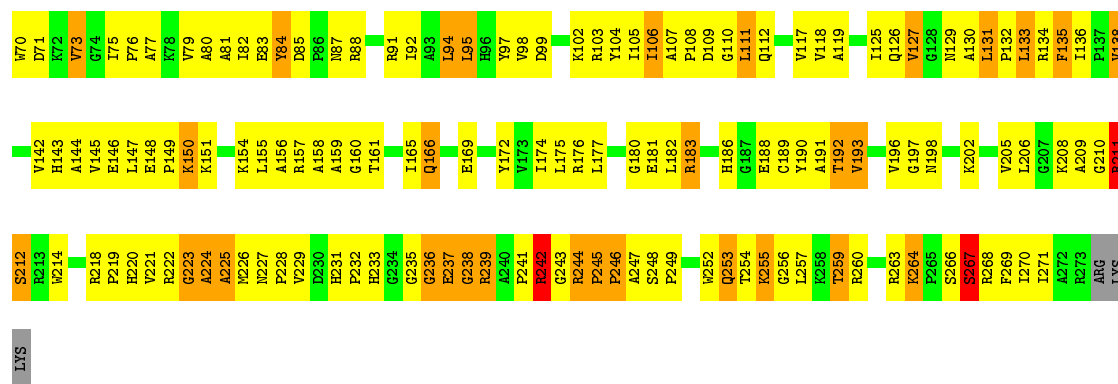
Chain DC: 



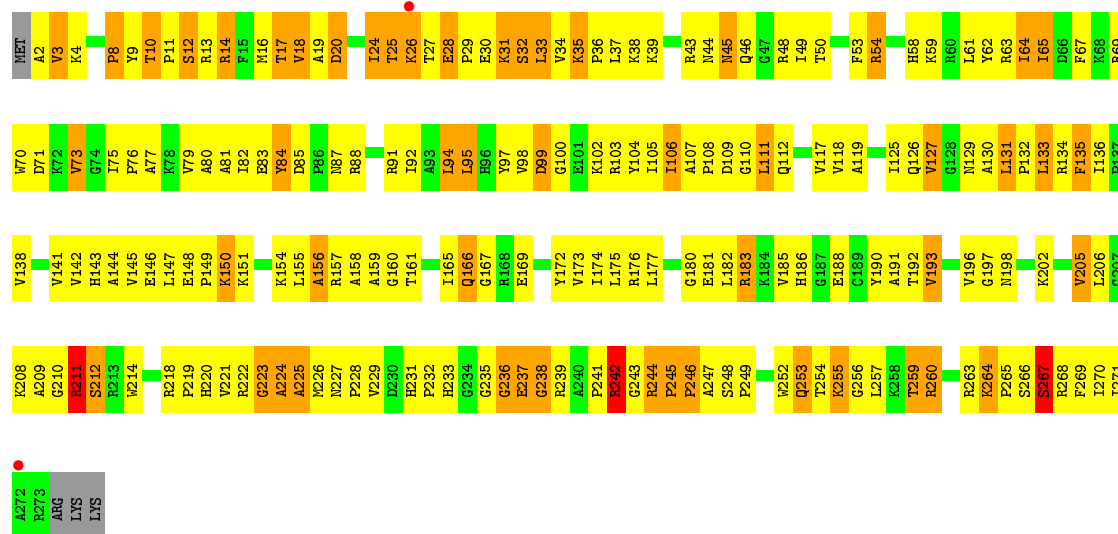
• Molecule 37: 50S RIBOSOMAL PROTEIN L2

Chain BD: 

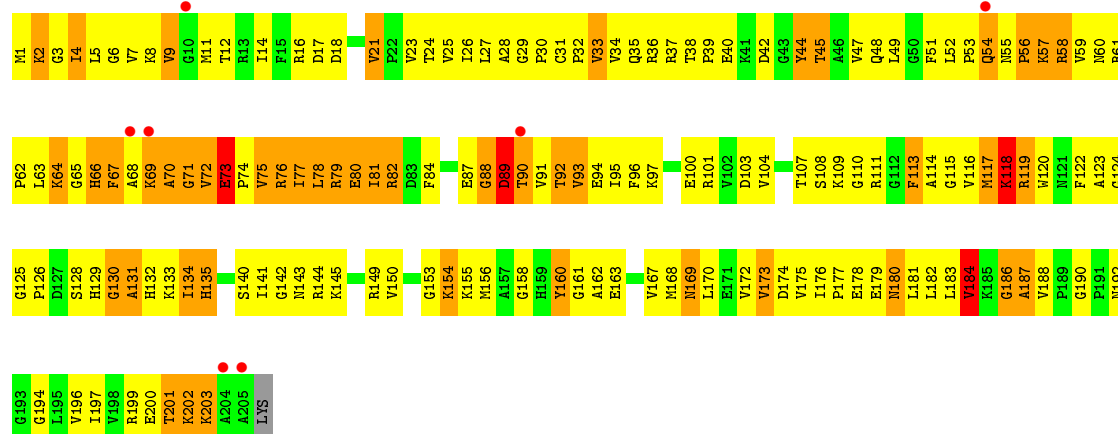




• Molecule 37: 50S RIBOSOMAL PROTEIN L2

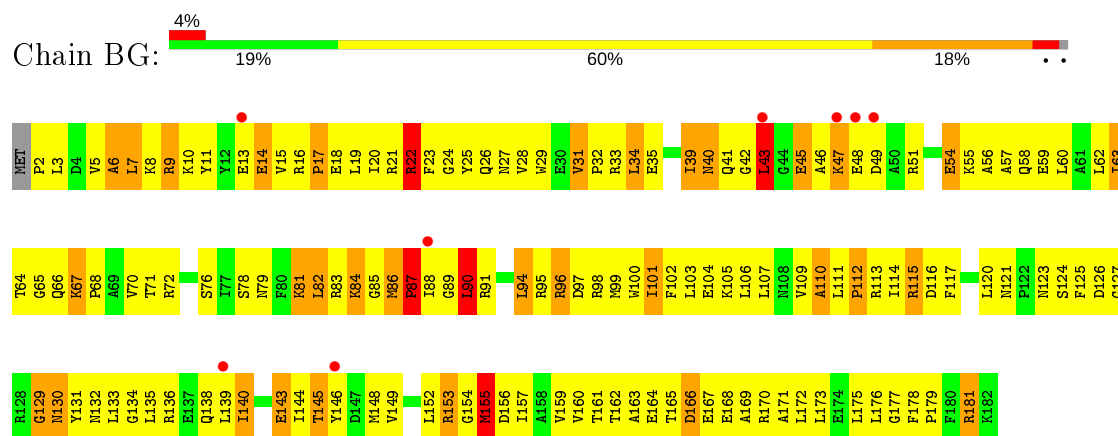


• Molecule 38: 50S RIBOSOMAL PROTEIN L3

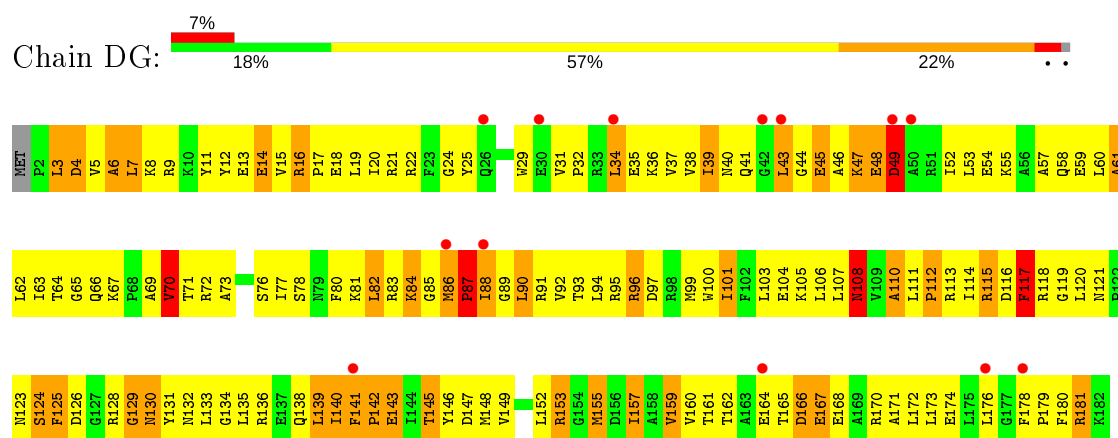


• Molecule 38: 50S RIBOSOMAL PROTEIN L3

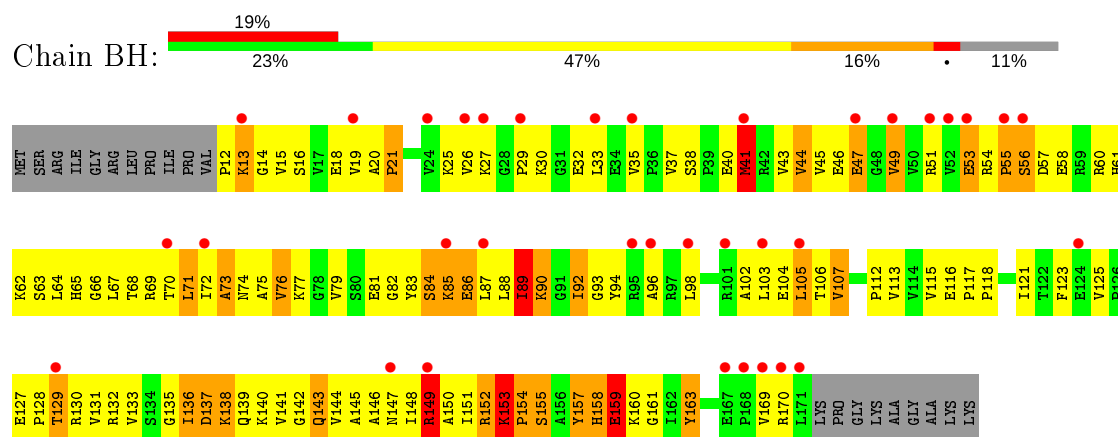
• Molecule 40: 50S RIBOSOMAL PROTEIN L5



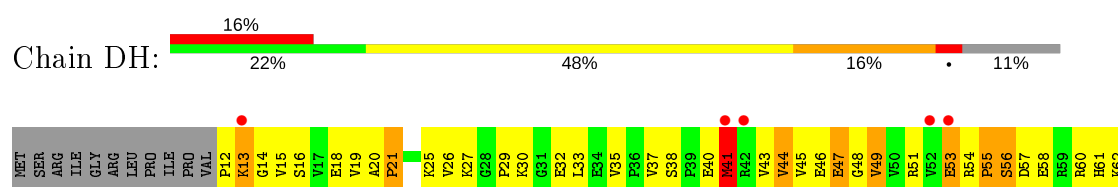
• Molecule 40: 50S RIBOSOMAL PROTEIN L5

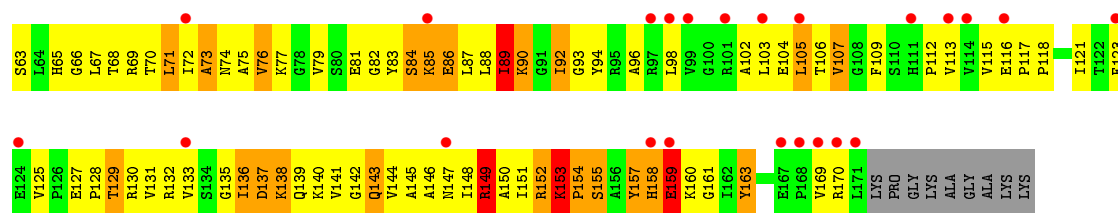


• Molecule 41: 50S RIBOSOMAL PROTEIN L6

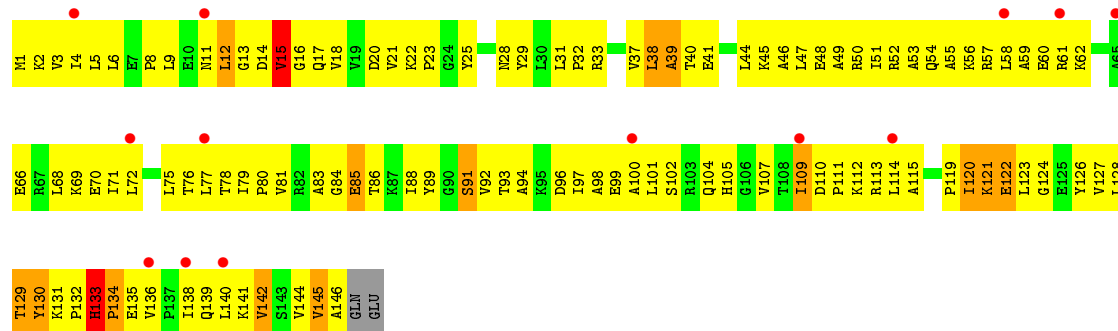


• Molecule 41: 50S RIBOSOMAL PROTEIN L6

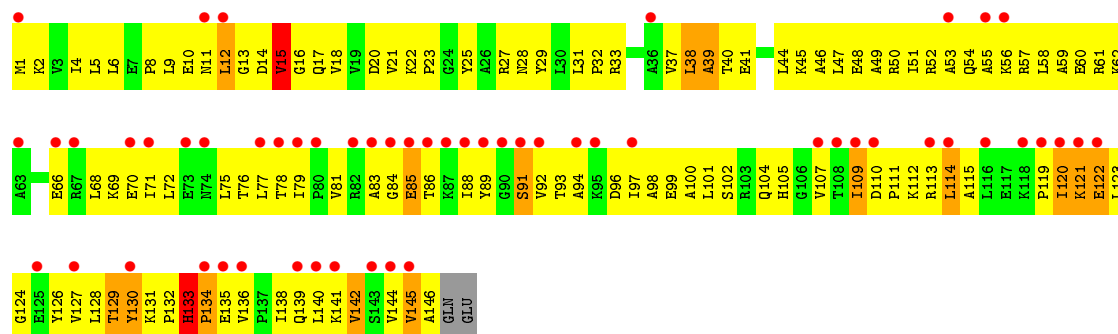




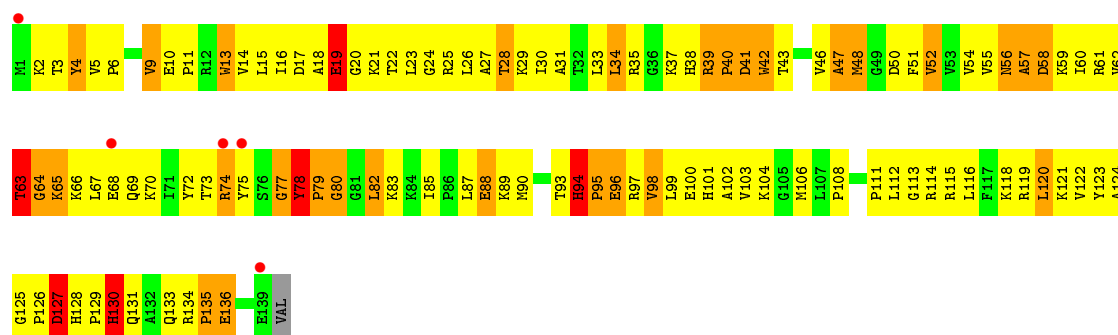
● Molecule 42: 50S RIBOSOMAL PROTEIN L9



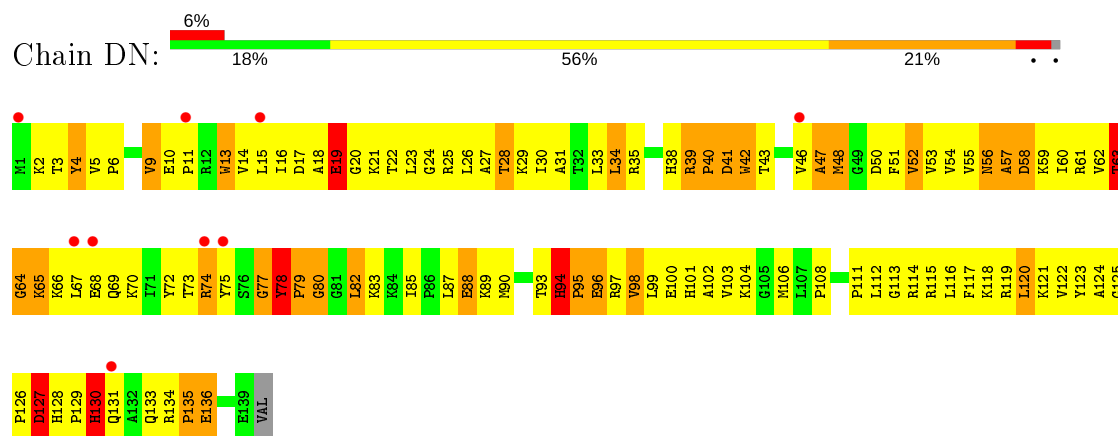
● Molecule 42: 50S RIBOSOMAL PROTEIN L9



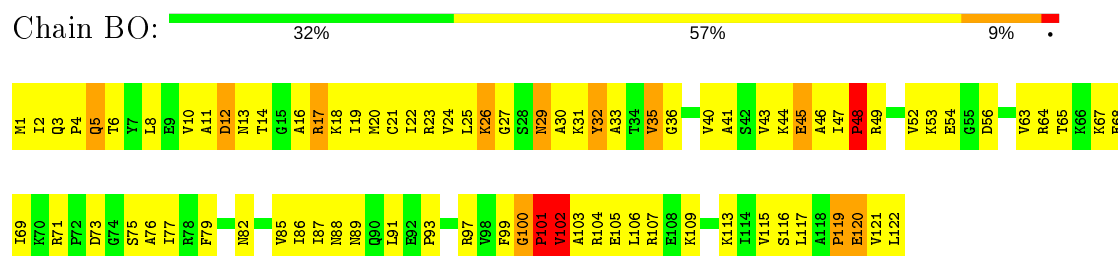
● Molecule 43: 50S RIBOSOMAL PROTEIN L13



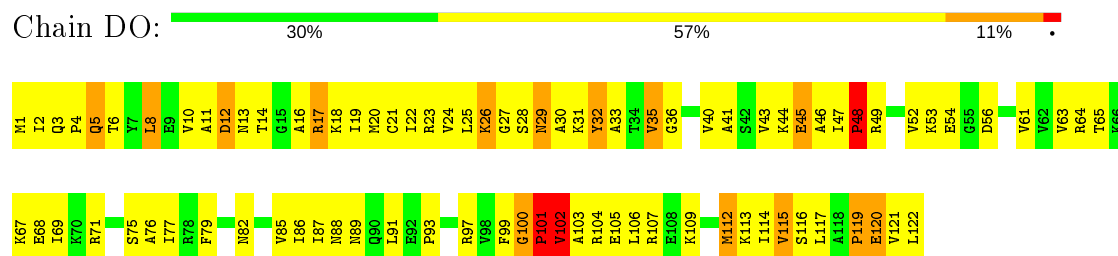
- Molecule 43: 50S RIBOSOMAL PROTEIN L13



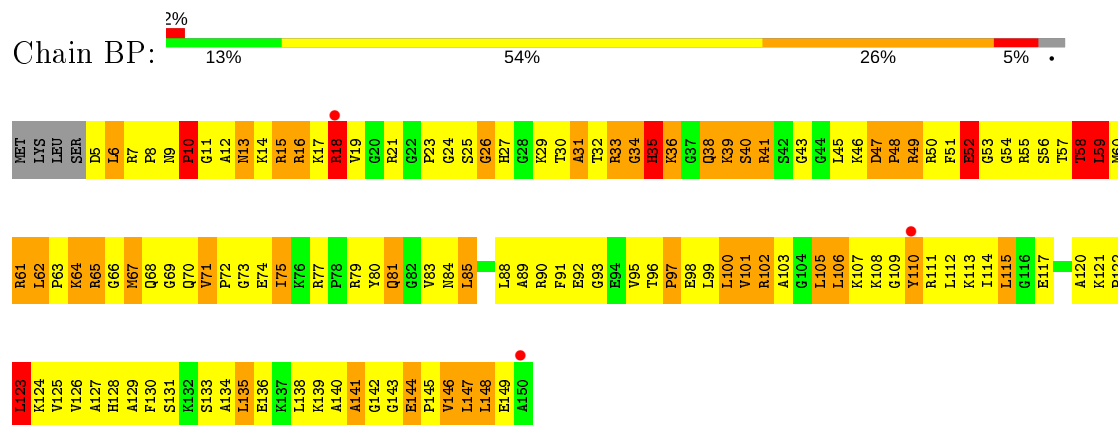
- Molecule 44: 50S RIBOSOMAL PROTEIN L14



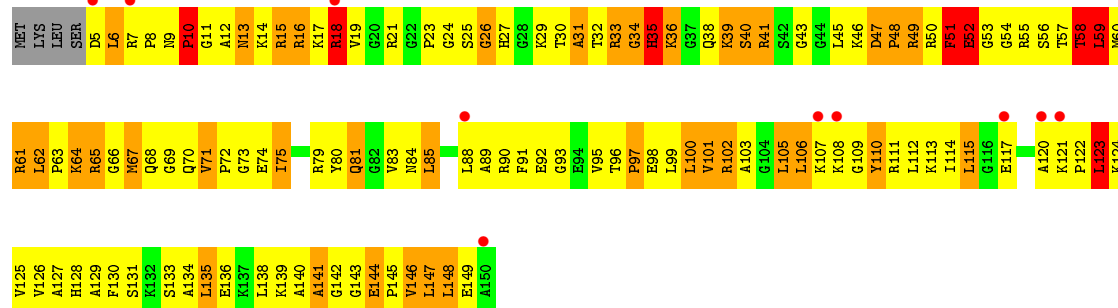
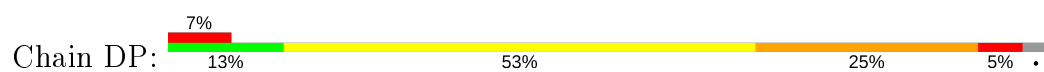
- Molecule 44: 50S RIBOSOMAL PROTEIN L14



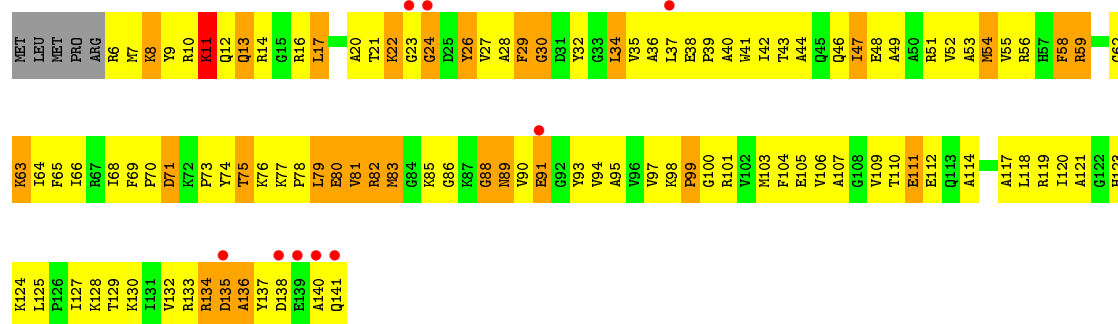
- Molecule 45: 50S RIBOSOMAL PROTEIN L15



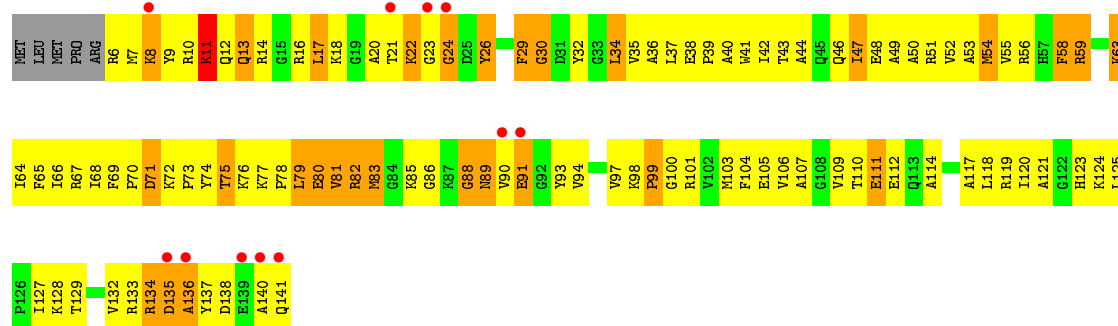
- Molecule 45: 50S RIBOSOMAL PROTEIN L15



● Molecule 46: 50S RIBOSOMAL PROTEIN L16

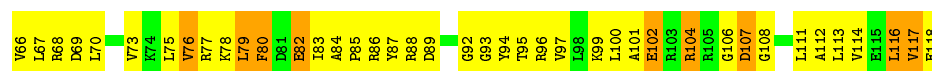


● Molecule 46: 50S RIBOSOMAL PROTEIN L16



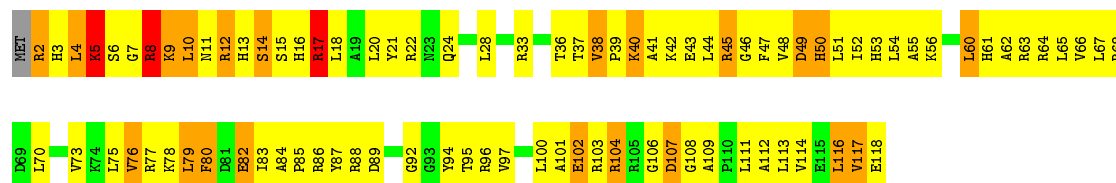
● Molecule 47: 50S RIBOSOMAL PROTEIN L17





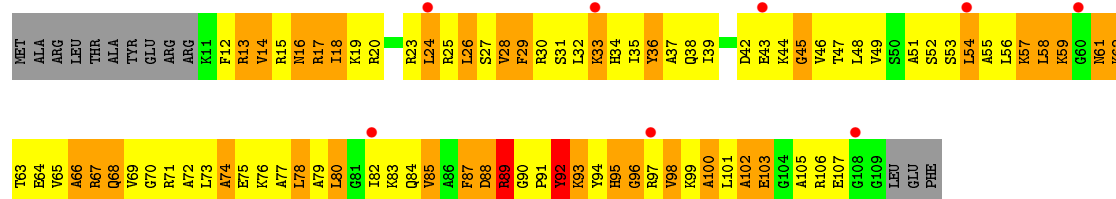
• Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain DR: 23% 56% 18%



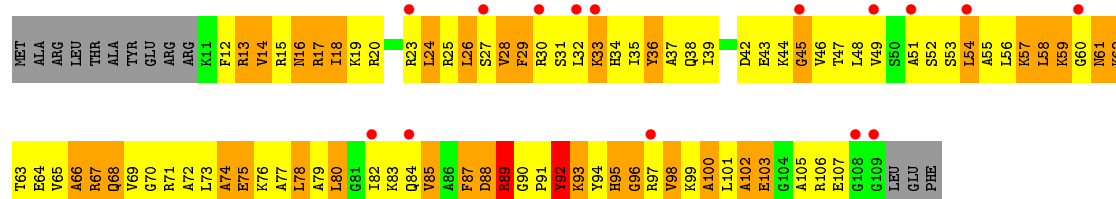
• Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain BS: 7% 11% 46% 30% 12%



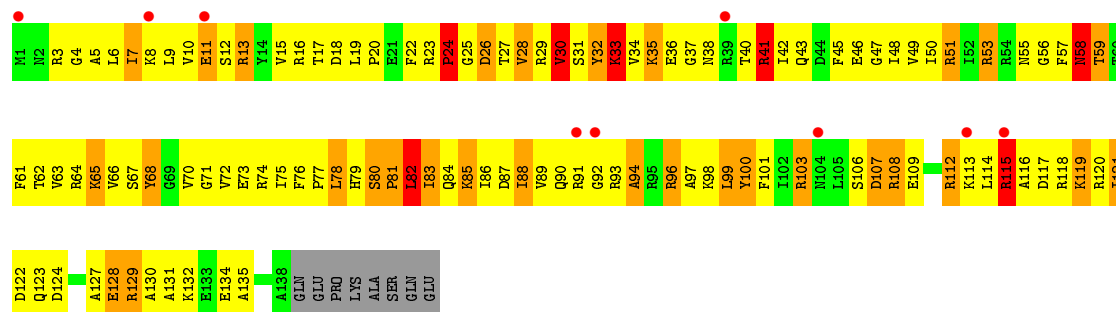
• Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain DS: 13% 10% 46% 31% 12%

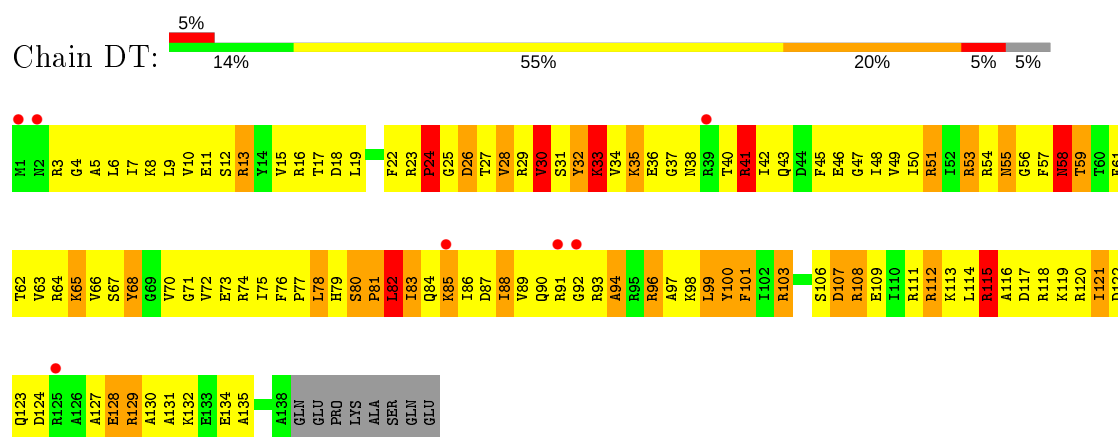


• Molecule 49: 50S RIBOSOMAL PROTEIN L19

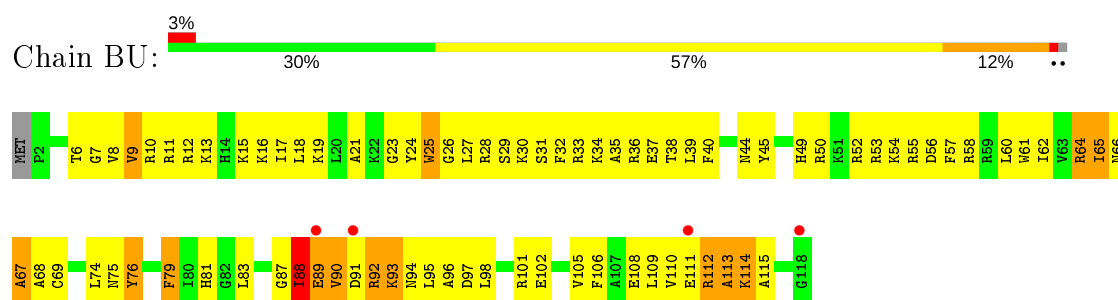
Chain BT: 6% 15% 54% 21% 5% 5%



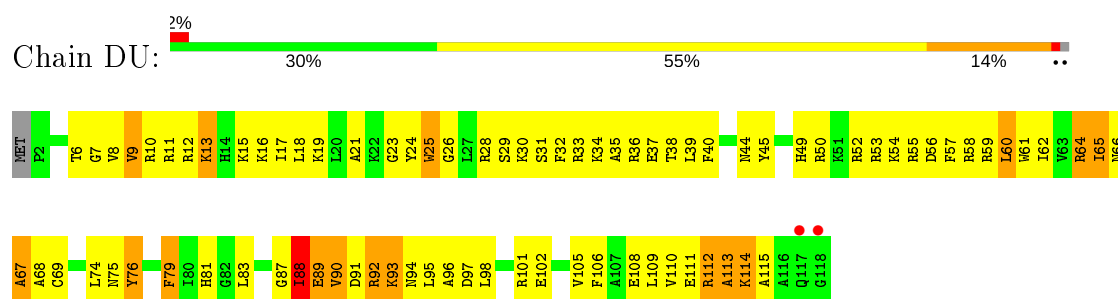
• Molecule 49: 50S RIBOSOMAL PROTEIN L19



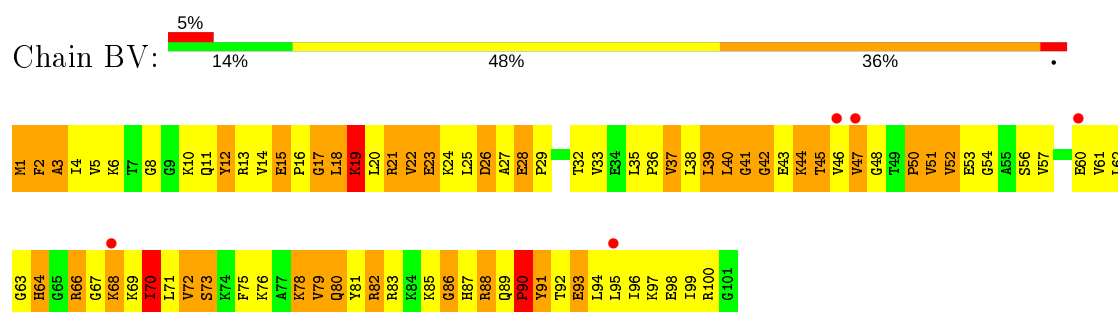
- Molecule 50: 50S RIBOSOMAL PROTEIN L20



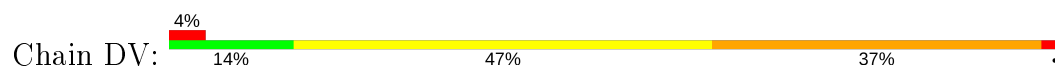
- Molecule 50: 50S RIBOSOMAL PROTEIN L20

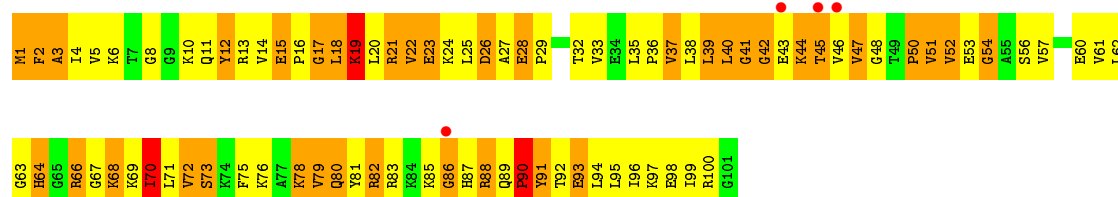


- Molecule 51: 50S RIBOSOMAL PROTEIN L21



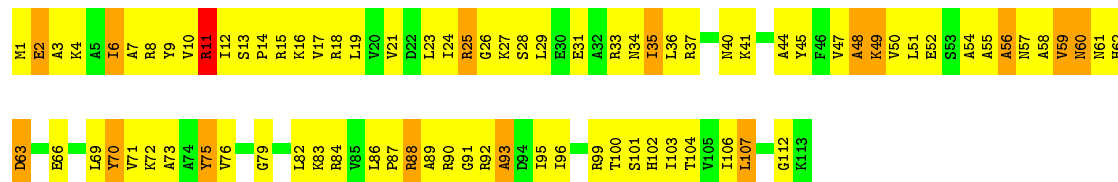
- Molecule 51: 50S RIBOSOMAL PROTEIN L21





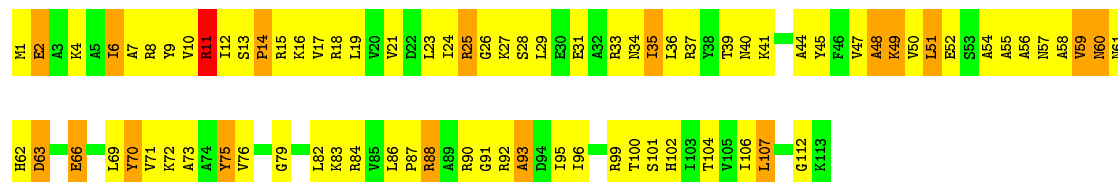
• Molecule 52: 50S RIBOSOMAL PROTEIN L22

Chain BW: 27% 59% 13%



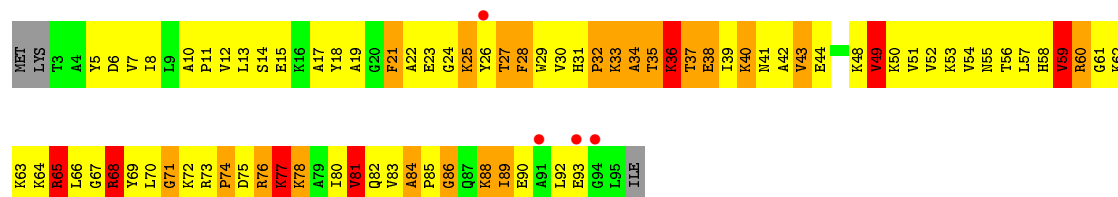
• Molecule 52: 50S RIBOSOMAL PROTEIN L22

Chain DW: 28% 56% 15%



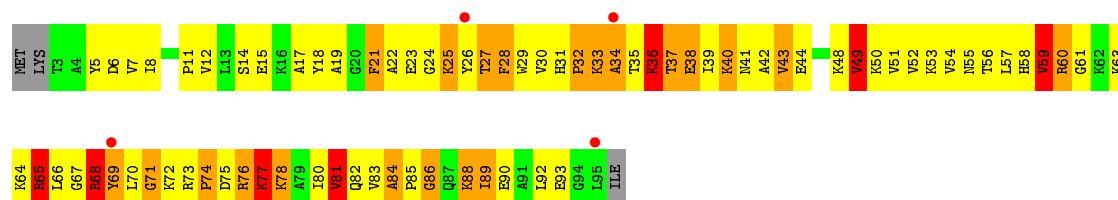
• Molecule 53: 50S RIBOSOMAL PROTEIN L23

Chain BX: 4% 14% 54% 22% 7%

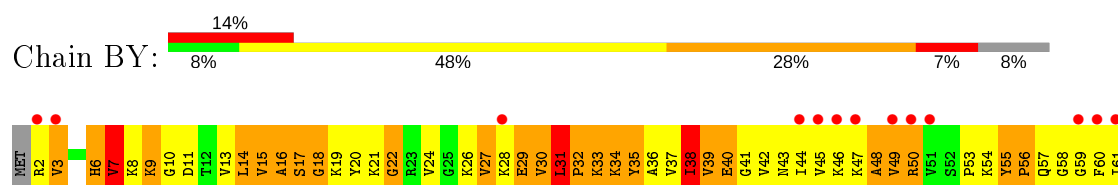


• Molecule 53: 50S RIBOSOMAL PROTEIN L23

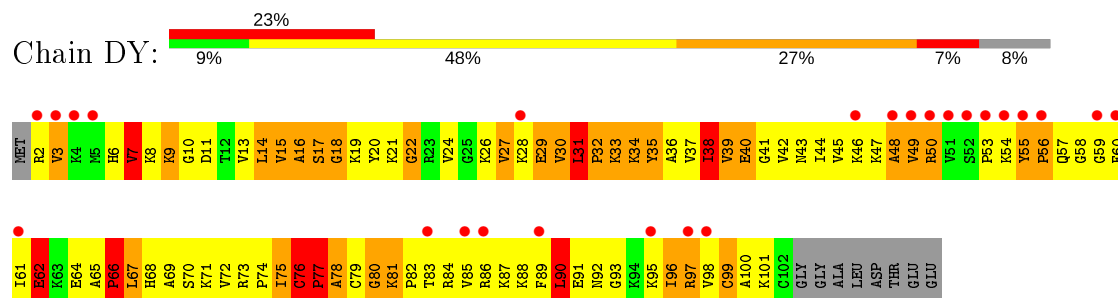
Chain DX: 4% 17% 51% 22% 7%



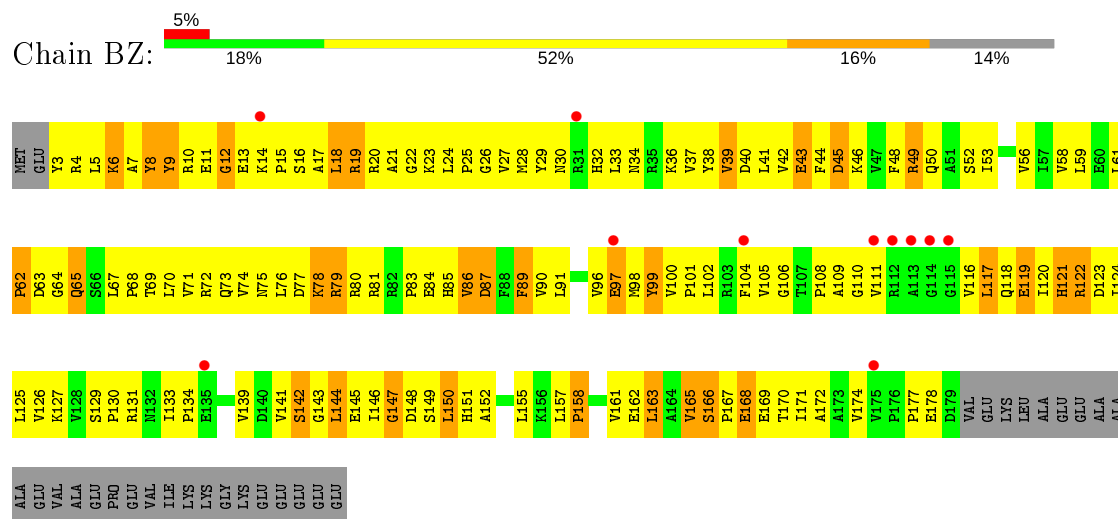
• Molecule 54: 50S RIBOSOMAL PROTEIN L24



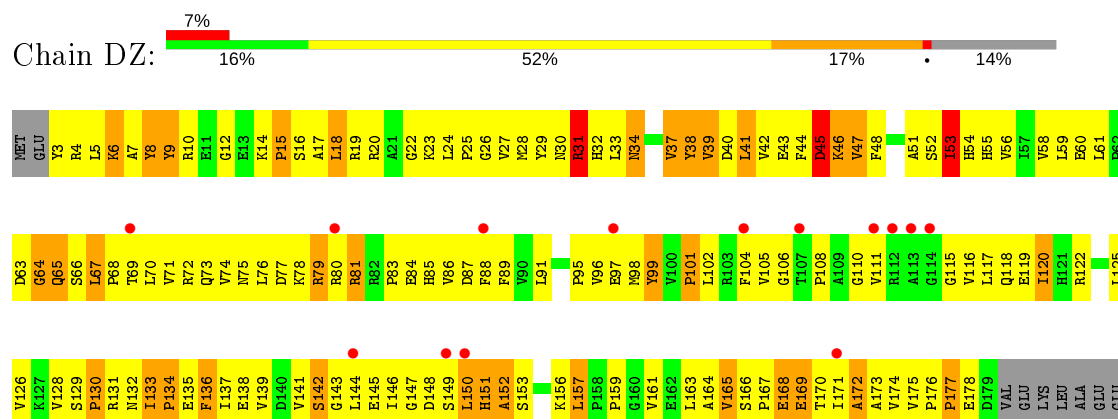
• Molecule 54: 50S RIBOSOMAL PROTEIN L24



• Molecule 55: 50S RIBOSOMAL PROTEIN L25



• Molecule 55: 50S RIBOSOMAL PROTEIN L25



ALA
ALA
ALA
GLU
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU
GLU

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 213.32Å 452.95Å 631.36Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 2.80 49.96 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 90.7 (50.00-2.80) 90.7 (49.96-2.80) | Depositor EDS |
| R_{merge} | 0.28 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.84 (at 2.81Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.272 , 0.313 0.266 , 0.306 | Depositor DCC |
| R_{free} test set | 64102 reflections (4.77%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 36.9 | Xtriage |
| Anisotropy | 0.160 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.19 , 81.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.17$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 291075 | wwPDB-VP |
| Average B, all atoms (Å ²) | 58.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 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 | 0.50 | 0/36190 | 0.71 | 20/56486 (0.0%) |
| 1 | CA | 0.47 | 0/36190 | 0.71 | 24/56486 (0.0%) |
| 2 | AB | 0.33 | 0/1936 | 0.59 | 0/2611 |
| 2 | CB | 0.33 | 0/1936 | 0.59 | 0/2611 |
| 3 | AC | 0.35 | 0/1637 | 0.58 | 0/2207 |
| 3 | CC | 0.34 | 0/1637 | 0.58 | 0/2207 |
| 4 | AD | 0.42 | 0/1733 | 0.67 | 0/2318 |
| 4 | CD | 0.41 | 0/1733 | 0.66 | 0/2318 |
| 5 | AE | 0.41 | 0/1163 | 0.66 | 0/1566 |
| 5 | CE | 0.39 | 0/1163 | 0.65 | 0/1566 |
| 6 | AF | 0.37 | 0/856 | 0.64 | 0/1154 |
| 6 | CF | 0.38 | 0/856 | 0.65 | 0/1154 |
| 7 | AG | 0.34 | 0/1276 | 0.54 | 0/1709 |
| 7 | CG | 0.33 | 0/1276 | 0.54 | 0/1709 |
| 8 | AH | 0.35 | 0/1136 | 0.62 | 0/1527 |
| 8 | CH | 0.34 | 0/1136 | 0.62 | 0/1527 |
| 9 | AI | 0.32 | 0/1027 | 0.55 | 0/1372 |
| 9 | CI | 0.32 | 0/1027 | 0.55 | 0/1372 |
| 10 | AJ | 0.36 | 0/808 | 0.62 | 0/1087 |
| 10 | CJ | 0.34 | 0/808 | 0.62 | 0/1087 |
| 11 | AK | 0.38 | 0/900 | 0.64 | 0/1213 |
| 11 | CK | 0.35 | 0/900 | 0.63 | 0/1213 |
| 12 | AL | 0.42 | 0/987 | 0.71 | 0/1322 |
| 12 | CL | 0.43 | 0/987 | 0.73 | 0/1322 |
| 13 | AM | 0.34 | 0/994 | 0.62 | 0/1322 |
| 13 | CM | 0.32 | 0/994 | 0.61 | 0/1322 |
| 14 | AN | 0.39 | 0/501 | 0.66 | 0/664 |
| 14 | CN | 0.38 | 0/501 | 0.64 | 0/664 |
| 15 | AO | 0.38 | 0/745 | 0.63 | 0/992 |
| 15 | CO | 0.36 | 0/745 | 0.61 | 0/992 |
| 16 | AP | 0.43 | 0/717 | 0.69 | 0/965 |
| 16 | CP | 0.42 | 0/717 | 0.68 | 0/965 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.41 | 0/837 | 0.67 | 0/1119 |
| 17 | CQ | 0.38 | 0/837 | 0.66 | 0/1119 |
| 18 | AR | 0.39 | 0/579 | 0.70 | 0/768 |
| 18 | CR | 0.38 | 0/579 | 0.70 | 0/768 |
| 19 | AS | 0.37 | 0/643 | 0.61 | 0/867 |
| 19 | CS | 0.36 | 0/643 | 0.60 | 0/867 |
| 20 | AT | 0.33 | 0/765 | 0.59 | 0/1007 |
| 20 | CT | 0.32 | 0/765 | 0.59 | 0/1007 |
| 21 | AU | 0.45 | 0/213 | 0.56 | 0/279 |
| 21 | CU | 0.44 | 0/213 | 0.55 | 0/279 |
| 22 | AV | 0.51 | 1/1814 (0.1%) | 0.72 | 0/2825 |
| 22 | CV | 0.50 | 1/1814 (0.1%) | 0.72 | 0/2825 |
| 23 | AW | 0.43 | 1/1813 (0.1%) | 0.77 | 6/2823 (0.2%) |
| 23 | AY | 0.36 | 0/456 | 0.72 | 0/710 |
| 23 | CW | 0.45 | 1/1813 (0.1%) | 0.76 | 2/2823 (0.1%) |
| 23 | CY | 0.35 | 0/456 | 0.68 | 0/710 |
| 24 | AX | 0.58 | 0/263 | 0.84 | 0/407 |
| 24 | CX | 0.58 | 0/263 | 0.81 | 1/407 (0.2%) |
| 25 | B0 | 0.38 | 0/658 | 0.65 | 0/878 |
| 25 | D0 | 0.39 | 0/658 | 0.65 | 0/878 |
| 26 | B1 | 0.61 | 0/700 | 1.04 | 1/931 (0.1%) |
| 26 | D1 | 0.52 | 0/700 | 0.99 | 1/931 (0.1%) |
| 27 | B2 | 0.45 | 0/423 | 0.99 | 3/560 (0.5%) |
| 27 | D2 | 0.45 | 0/423 | 0.89 | 2/560 (0.4%) |
| 28 | B3 | 0.37 | 0/473 | 0.61 | 0/636 |
| 28 | D3 | 0.39 | 0/473 | 0.61 | 0/636 |
| 29 | B4 | 0.47 | 0/241 | 0.88 | 4/334 (1.2%) |
| 29 | D4 | 0.44 | 0/241 | 0.88 | 4/334 (1.2%) |
| 30 | B5 | 0.42 | 0/473 | 0.74 | 0/639 |
| 30 | D5 | 0.40 | 0/473 | 0.73 | 0/639 |
| 31 | B6 | 0.39 | 0/387 | 0.62 | 0/517 |
| 31 | D6 | 0.39 | 0/387 | 0.62 | 0/517 |
| 32 | B7 | 0.51 | 0/427 | 0.73 | 0/563 |
| 32 | D7 | 0.53 | 0/427 | 0.70 | 0/563 |
| 33 | B8 | 0.50 | 0/516 | 0.81 | 0/681 |
| 33 | D8 | 0.48 | 0/516 | 0.80 | 0/681 |
| 34 | BA | 0.62 | 4/66876 (0.0%) | 0.77 | 56/104407 (0.1%) |
| 34 | DA | 0.62 | 5/66876 (0.0%) | 0.77 | 53/104407 (0.1%) |
| 35 | BB | 0.39 | 0/2853 | 0.70 | 0/4451 |
| 35 | DB | 0.38 | 0/2853 | 0.70 | 0/4451 |
| 36 | BC | 0.38 | 0/1145 | 0.68 | 7/1556 (0.4%) |
| 36 | DC | 0.40 | 0/1145 | 0.68 | 7/1556 (0.4%) |
| 37 | BD | 0.52 | 0/2155 | 0.87 | 3/2907 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | DD | 0.51 | 0/2155 | 0.86 | 3/2907 (0.1%) |
| 38 | BE | 0.43 | 0/1597 | 0.76 | 0/2155 |
| 38 | DE | 0.45 | 0/1597 | 0.77 | 0/2155 |
| 39 | BF | 0.45 | 0/1659 | 0.70 | 0/2246 |
| 39 | DF | 0.44 | 0/1659 | 0.69 | 0/2246 |
| 40 | BG | 0.39 | 0/1498 | 0.72 | 1/2013 (0.0%) |
| 40 | DG | 0.35 | 0/1498 | 0.73 | 0/2013 |
| 41 | BH | 0.33 | 0/1246 | 0.69 | 0/1684 |
| 41 | DH | 0.35 | 0/1246 | 0.69 | 0/1684 |
| 42 | BI | 0.35 | 0/1147 | 0.66 | 0/1553 |
| 42 | DI | 0.34 | 0/1147 | 0.66 | 0/1553 |
| 43 | BN | 0.40 | 0/1132 | 0.78 | 0/1527 |
| 43 | DN | 0.45 | 0/1132 | 0.79 | 0/1527 |
| 44 | BO | 0.48 | 0/943 | 0.74 | 0/1269 |
| 44 | DO | 0.49 | 0/943 | 0.75 | 0/1269 |
| 45 | BP | 0.42 | 0/1131 | 1.00 | 6/1504 (0.4%) |
| 45 | DP | 0.41 | 0/1131 | 1.00 | 7/1504 (0.5%) |
| 46 | BQ | 0.37 | 0/1100 | 0.72 | 1/1470 (0.1%) |
| 46 | DQ | 0.37 | 0/1100 | 0.72 | 1/1470 (0.1%) |
| 47 | BR | 0.40 | 0/974 | 0.74 | 1/1302 (0.1%) |
| 47 | DR | 0.38 | 0/974 | 0.74 | 1/1302 (0.1%) |
| 48 | BS | 0.40 | 0/779 | 0.73 | 0/1038 |
| 48 | DS | 0.39 | 0/779 | 0.73 | 0/1038 |
| 49 | BT | 0.42 | 0/1156 | 0.77 | 2/1544 (0.1%) |
| 49 | DT | 0.42 | 0/1156 | 0.77 | 1/1544 (0.1%) |
| 50 | BU | 0.37 | 0/975 | 0.68 | 0/1297 |
| 50 | DU | 0.40 | 0/975 | 0.69 | 0/1297 |
| 51 | BV | 0.38 | 0/789 | 0.73 | 0/1054 |
| 51 | DV | 0.40 | 0/789 | 0.73 | 0/1054 |
| 52 | BW | 0.43 | 0/907 | 0.72 | 0/1216 |
| 52 | DW | 0.45 | 0/907 | 0.72 | 0/1216 |
| 53 | BX | 0.53 | 0/740 | 0.89 | 3/995 (0.3%) |
| 53 | DX | 0.50 | 0/740 | 0.89 | 3/995 (0.3%) |
| 54 | BY | 0.41 | 0/789 | 0.78 | 0/1053 |
| 54 | DY | 0.43 | 0/789 | 0.78 | 0/1053 |
| 55 | BZ | 0.35 | 0/1436 | 0.64 | 0/1951 |
| 55 | DZ | 0.36 | 0/1436 | 0.62 | 0/1951 |
| All | All | 0.52 | 13/314628 (0.0%) | 0.74 | 224/470502 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 2 | 37 |
| 1 | CA | 2 | 29 |
| 22 | AV | 0 | 2 |
| 22 | CV | 0 | 2 |
| 23 | AW | 3 | 1 |
| 23 | CW | 2 | 0 |
| 24 | CX | 0 | 1 |
| 26 | B1 | 0 | 1 |
| 34 | BA | 30 | 81 |
| 34 | DA | 28 | 79 |
| All | All | 67 | 233 |

The worst 5 of 13 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23 | CW | 1 | G | OP3-P | -7.25 | 1.52 | 1.61 |
| 23 | AW | 1 | G | OP3-P | -7.19 | 1.52 | 1.61 |
| 22 | CV | 1 | C | OP3-P | -7.12 | 1.52 | 1.61 |
| 22 | AV | 1 | C | OP3-P | -6.95 | 1.52 | 1.61 |
| 34 | BA | 783 | A | C5-C6 | -6.34 | 1.35 | 1.41 |

The worst 5 of 224 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 23 | CW | 17 | C | N1-C1'-C2' | 10.99 | 128.28 | 114.00 |
| 34 | DA | 1962 | C | N1-C1'-C2' | 10.90 | 128.18 | 114.00 |
| 34 | BA | 1962 | C | N1-C1'-C2' | 10.48 | 127.62 | 114.00 |
| 34 | BA | 669 | G | N9-C1'-C2' | 10.36 | 127.47 | 114.00 |
| 34 | DA | 669 | G | N9-C1'-C2' | 10.24 | 127.32 | 114.00 |

5 of 67 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | AA | 410 | G | C3' |
| 1 | AA | 412 | A | C1' |
| 23 | AW | 17 | C | C1' |
| 23 | AW | 47 | U | C1' |
| 23 | AW | 70 | G | C3' |

5 of 233 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 107 | G | Sidechain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 253 | U | Sidechain |
| 1 | AA | 371 | G | Sidechain |
| 1 | AA | 38 | G | Sidechain |
| 1 | AA | 9 | G | Sidechain |

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 | 32329 | 0 | 16314 | 1350 | 0 |
| 1 | CA | 32329 | 0 | 16316 | 1333 | 0 |
| 2 | AB | 1901 | 0 | 1951 | 258 | 0 |
| 2 | CB | 1901 | 0 | 1951 | 256 | 0 |
| 3 | AC | 1613 | 0 | 1677 | 209 | 0 |
| 3 | CC | 1613 | 0 | 1677 | 203 | 0 |
| 4 | AD | 1703 | 0 | 1764 | 192 | 0 |
| 4 | CD | 1703 | 0 | 1766 | 191 | 0 |
| 5 | AE | 1147 | 0 | 1207 | 161 | 0 |
| 5 | CE | 1147 | 0 | 1206 | 159 | 0 |
| 6 | AF | 843 | 0 | 857 | 98 | 0 |
| 6 | CF | 843 | 0 | 857 | 101 | 0 |
| 7 | AG | 1257 | 0 | 1296 | 125 | 0 |
| 7 | CG | 1257 | 0 | 1296 | 122 | 0 |
| 8 | AH | 1116 | 0 | 1177 | 128 | 0 |
| 8 | CH | 1116 | 0 | 1177 | 130 | 0 |
| 9 | AI | 1011 | 0 | 1041 | 140 | 0 |
| 9 | CI | 1011 | 0 | 1041 | 140 | 0 |
| 10 | AJ | 795 | 0 | 840 | 147 | 0 |
| 10 | CJ | 795 | 0 | 840 | 144 | 0 |
| 11 | AK | 885 | 0 | 904 | 104 | 0 |
| 11 | CK | 885 | 0 | 904 | 96 | 0 |
| 12 | AL | 971 | 0 | 1057 | 122 | 0 |
| 12 | CL | 971 | 0 | 1057 | 120 | 0 |
| 13 | AM | 988 | 0 | 1055 | 156 | 0 |
| 13 | CM | 988 | 0 | 1055 | 151 | 0 |
| 14 | AN | 492 | 0 | 530 | 62 | 0 |
| 14 | CN | 492 | 0 | 529 | 61 | 0 |
| 15 | AO | 734 | 0 | 771 | 70 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15 | CO | 734 | 0 | 771 | 76 | 0 |
| 16 | AP | 701 | 0 | 720 | 83 | 0 |
| 16 | CP | 701 | 0 | 720 | 75 | 0 |
| 17 | AQ | 824 | 0 | 891 | 91 | 0 |
| 17 | CQ | 824 | 0 | 891 | 90 | 0 |
| 18 | AR | 574 | 0 | 644 | 97 | 0 |
| 18 | CR | 574 | 0 | 644 | 94 | 0 |
| 19 | AS | 630 | 0 | 652 | 106 | 0 |
| 19 | CS | 630 | 0 | 652 | 106 | 0 |
| 20 | AT | 763 | 0 | 861 | 106 | 0 |
| 20 | CT | 763 | 0 | 861 | 102 | 0 |
| 21 | AU | 209 | 0 | 221 | 23 | 0 |
| 21 | CU | 209 | 0 | 221 | 22 | 0 |
| 22 | AV | 1645 | 0 | 838 | 61 | 0 |
| 22 | CV | 1645 | 0 | 838 | 51 | 0 |
| 23 | AW | 1623 | 0 | 821 | 83 | 0 |
| 23 | AY | 407 | 0 | 208 | 16 | 0 |
| 23 | CW | 1623 | 0 | 821 | 81 | 0 |
| 23 | CY | 407 | 0 | 208 | 13 | 0 |
| 24 | AX | 235 | 0 | 119 | 6 | 0 |
| 24 | CX | 235 | 0 | 119 | 5 | 0 |
| 25 | B0 | 650 | 0 | 654 | 72 | 0 |
| 25 | D0 | 650 | 0 | 654 | 78 | 0 |
| 26 | B1 | 693 | 0 | 764 | 182 | 0 |
| 26 | D1 | 693 | 0 | 764 | 197 | 0 |
| 27 | B2 | 421 | 0 | 460 | 124 | 0 |
| 27 | D2 | 421 | 0 | 461 | 125 | 0 |
| 28 | B3 | 468 | 0 | 523 | 53 | 0 |
| 28 | D3 | 468 | 0 | 523 | 52 | 0 |
| 29 | B4 | 242 | 0 | 103 | 22 | 0 |
| 29 | D4 | 242 | 0 | 103 | 23 | 0 |
| 30 | B5 | 459 | 0 | 480 | 75 | 0 |
| 30 | D5 | 459 | 0 | 480 | 70 | 0 |
| 31 | B6 | 381 | 0 | 390 | 59 | 0 |
| 31 | D6 | 381 | 0 | 390 | 56 | 0 |
| 32 | B7 | 419 | 0 | 467 | 35 | 0 |
| 32 | D7 | 419 | 0 | 467 | 35 | 0 |
| 33 | B8 | 508 | 0 | 576 | 110 | 0 |
| 33 | D8 | 508 | 0 | 576 | 114 | 0 |
| 34 | BA | 59708 | 0 | 30096 | 2501 | 0 |
| 34 | DA | 59708 | 0 | 30096 | 2505 | 0 |
| 35 | BB | 2551 | 0 | 1294 | 106 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35 | DB | 2551 | 0 | 1294 | 100 | 0 |
| 36 | BC | 1142 | 0 | 865 | 109 | 0 |
| 36 | DC | 1142 | 0 | 865 | 106 | 0 |
| 37 | BD | 2105 | 0 | 2182 | 357 | 0 |
| 37 | DD | 2105 | 0 | 2182 | 362 | 0 |
| 38 | BE | 1564 | 0 | 1629 | 325 | 0 |
| 38 | DE | 1564 | 0 | 1629 | 323 | 0 |
| 39 | BF | 1624 | 0 | 1677 | 237 | 0 |
| 39 | DF | 1624 | 0 | 1677 | 235 | 0 |
| 40 | BG | 1474 | 0 | 1534 | 237 | 0 |
| 40 | DG | 1474 | 0 | 1534 | 242 | 0 |
| 41 | BH | 1223 | 0 | 1282 | 199 | 0 |
| 41 | DH | 1223 | 0 | 1282 | 211 | 0 |
| 42 | BI | 1132 | 0 | 1218 | 198 | 0 |
| 42 | DI | 1132 | 0 | 1218 | 200 | 0 |
| 43 | BN | 1105 | 0 | 1180 | 209 | 0 |
| 43 | DN | 1105 | 0 | 1180 | 215 | 0 |
| 44 | BO | 933 | 0 | 996 | 139 | 0 |
| 44 | DO | 933 | 0 | 996 | 139 | 0 |
| 45 | BP | 1114 | 0 | 1187 | 322 | 0 |
| 45 | DP | 1114 | 0 | 1187 | 322 | 0 |
| 46 | BQ | 1080 | 0 | 1127 | 224 | 0 |
| 46 | DQ | 1080 | 0 | 1127 | 214 | 0 |
| 47 | BR | 960 | 0 | 1021 | 171 | 0 |
| 47 | DR | 960 | 0 | 1021 | 170 | 0 |
| 48 | BS | 771 | 0 | 832 | 182 | 0 |
| 48 | DS | 771 | 0 | 831 | 186 | 0 |
| 49 | BT | 1142 | 0 | 1202 | 219 | 0 |
| 49 | DT | 1142 | 0 | 1202 | 231 | 0 |
| 50 | BU | 958 | 0 | 1015 | 183 | 0 |
| 50 | DU | 958 | 0 | 1014 | 186 | 0 |
| 51 | BV | 779 | 0 | 851 | 212 | 0 |
| 51 | DV | 779 | 0 | 851 | 216 | 0 |
| 52 | BW | 896 | 0 | 953 | 111 | 0 |
| 52 | DW | 896 | 0 | 953 | 110 | 0 |
| 53 | BX | 726 | 0 | 778 | 203 | 0 |
| 53 | DX | 726 | 0 | 778 | 200 | 0 |
| 54 | BY | 776 | 0 | 870 | 220 | 0 |
| 54 | DY | 776 | 0 | 870 | 216 | 0 |
| 55 | BZ | 1404 | 0 | 1432 | 219 | 0 |
| 55 | DZ | 1404 | 0 | 1432 | 241 | 0 |
| 56 | AA | 215 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | AE | 1 | 0 | 0 | 0 | 0 |
| 56 | AV | 7 | 0 | 0 | 0 | 0 |
| 56 | AW | 22 | 0 | 0 | 0 | 0 |
| 56 | AX | 4 | 0 | 0 | 0 | 0 |
| 56 | AY | 1 | 0 | 0 | 0 | 0 |
| 56 | B1 | 1 | 0 | 0 | 0 | 0 |
| 56 | B2 | 5 | 0 | 0 | 0 | 0 |
| 56 | B3 | 1 | 0 | 0 | 0 | 0 |
| 56 | B5 | 2 | 0 | 0 | 0 | 0 |
| 56 | B7 | 2 | 0 | 0 | 0 | 0 |
| 56 | BA | 454 | 0 | 0 | 0 | 0 |
| 56 | BB | 19 | 0 | 0 | 0 | 0 |
| 56 | BE | 1 | 0 | 0 | 0 | 0 |
| 56 | BF | 2 | 0 | 0 | 0 | 0 |
| 56 | BN | 1 | 0 | 0 | 0 | 0 |
| 56 | BO | 1 | 0 | 0 | 0 | 0 |
| 56 | BV | 1 | 0 | 0 | 0 | 0 |
| 56 | BX | 1 | 0 | 0 | 0 | 0 |
| 56 | CA | 189 | 0 | 0 | 0 | 0 |
| 56 | CF | 1 | 0 | 0 | 0 | 0 |
| 56 | CJ | 1 | 0 | 0 | 0 | 0 |
| 56 | CM | 1 | 0 | 0 | 0 | 0 |
| 56 | CU | 1 | 0 | 0 | 0 | 0 |
| 56 | CV | 4 | 0 | 0 | 0 | 0 |
| 56 | CW | 13 | 0 | 0 | 0 | 0 |
| 56 | CX | 6 | 0 | 0 | 0 | 0 |
| 56 | D5 | 2 | 0 | 0 | 0 | 0 |
| 56 | DA | 398 | 0 | 0 | 0 | 0 |
| 56 | DB | 12 | 0 | 0 | 0 | 0 |
| 56 | DD | 2 | 0 | 0 | 0 | 0 |
| 56 | DE | 1 | 0 | 0 | 0 | 0 |
| 56 | DF | 1 | 0 | 0 | 0 | 0 |
| 56 | DH | 1 | 0 | 0 | 0 | 0 |
| 56 | DN | 1 | 0 | 0 | 0 | 0 |
| 56 | DO | 1 | 0 | 0 | 0 | 0 |
| 56 | DS | 1 | 0 | 0 | 0 | 0 |
| 56 | DU | 1 | 0 | 0 | 0 | 0 |
| 56 | DZ | 1 | 0 | 0 | 0 | 0 |
| 57 | AA | 42 | 0 | 45 | 3 | 0 |
| 57 | CA | 42 | 0 | 45 | 0 | 0 |
| 58 | AD | 1 | 0 | 0 | 0 | 0 |
| 58 | AN | 1 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58 | CD | 1 | 0 | 0 | 0 | 0 |
| 58 | CN | 1 | 0 | 0 | 0 | 0 |
| All | All | 291075 | 0 | 196199 | 21274 | 0 |

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 44.

The worst 5 of 21274 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:DV:70:ILE:HB | 51:DV:90:PRO:HB2 | 1.21 | 1.18 |
| 42:BI:79:ILE:HG12 | 42:BI:140:LEU:HD11 | 1.21 | 1.17 |
| 3:CC:20:SER:HB2 | 3:CC:40:ARG:HH22 | 1.00 | 1.17 |
| 37:DD:35:LYS:HD3 | 37:DD:63:ARG:HB3 | 1.24 | 1.17 |
| 34:DA:2491:U:H5' | 34:DA:2570:G:H5'' | 1.26 | 1.16 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%) | 147 (63%) | 54 (23%) | 32 (14%) | 0 | 0 |
| 2 | CB | 233/256 (91%) | 149 (64%) | 52 (22%) | 32 (14%) | 0 | 0 |
| 3 | AC | 205/239 (86%) | 130 (63%) | 55 (27%) | 20 (10%) | 0 | 1 |
| 3 | CC | 205/239 (86%) | 130 (63%) | 57 (28%) | 18 (9%) | 1 | 1 |
| 4 | AD | 206/209 (99%) | 130 (63%) | 51 (25%) | 25 (12%) | 0 | 1 |
| 4 | CD | 206/209 (99%) | 128 (62%) | 54 (26%) | 24 (12%) | 0 | 1 |
| 5 | AE | 149/162 (92%) | 108 (72%) | 28 (19%) | 13 (9%) | 1 | 1 |
| 5 | CE | 149/162 (92%) | 107 (72%) | 30 (20%) | 12 (8%) | 1 | 2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 6 | AF | 99/101 (98%) | 72 (73%) | 21 (21%) | 6 (6%) | 1 | 4 |
| 6 | CF | 99/101 (98%) | 72 (73%) | 22 (22%) | 5 (5%) | 2 | 6 |
| 7 | AG | 153/156 (98%) | 100 (65%) | 41 (27%) | 12 (8%) | 1 | 2 |
| 7 | CG | 153/156 (98%) | 100 (65%) | 42 (28%) | 11 (7%) | 1 | 2 |
| 8 | AH | 136/138 (99%) | 103 (76%) | 28 (21%) | 5 (4%) | 3 | 11 |
| 8 | CH | 136/138 (99%) | 102 (75%) | 29 (21%) | 5 (4%) | 3 | 11 |
| 9 | AI | 121/128 (94%) | 80 (66%) | 30 (25%) | 11 (9%) | 1 | 1 |
| 9 | CI | 121/128 (94%) | 81 (67%) | 28 (23%) | 12 (10%) | 0 | 1 |
| 10 | AJ | 97/105 (92%) | 70 (72%) | 18 (19%) | 9 (9%) | 0 | 1 |
| 10 | CJ | 97/105 (92%) | 70 (72%) | 18 (19%) | 9 (9%) | 0 | 1 |
| 11 | AK | 117/129 (91%) | 87 (74%) | 25 (21%) | 5 (4%) | 2 | 8 |
| 11 | CK | 117/129 (91%) | 88 (75%) | 24 (20%) | 5 (4%) | 2 | 8 |
| 12 | AL | 123/135 (91%) | 83 (68%) | 22 (18%) | 18 (15%) | 0 | 0 |
| 12 | CL | 123/135 (91%) | 84 (68%) | 20 (16%) | 19 (15%) | 0 | 0 |
| 13 | AM | 113/126 (90%) | 68 (60%) | 26 (23%) | 19 (17%) | 0 | 0 |
| 13 | CM | 113/126 (90%) | 69 (61%) | 23 (20%) | 21 (19%) | 0 | 0 |
| 14 | AN | 58/61 (95%) | 35 (60%) | 17 (29%) | 6 (10%) | 0 | 1 |
| 14 | CN | 58/61 (95%) | 35 (60%) | 17 (29%) | 6 (10%) | 0 | 1 |
| 15 | AO | 86/89 (97%) | 48 (56%) | 34 (40%) | 4 (5%) | 2 | 7 |
| 15 | CO | 86/89 (97%) | 50 (58%) | 31 (36%) | 5 (6%) | 1 | 4 |
| 16 | AP | 82/88 (93%) | 53 (65%) | 24 (29%) | 5 (6%) | 1 | 4 |
| 16 | CP | 82/88 (93%) | 53 (65%) | 25 (30%) | 4 (5%) | 2 | 7 |
| 17 | AQ | 98/105 (93%) | 74 (76%) | 15 (15%) | 9 (9%) | 1 | 1 |
| 17 | CQ | 98/105 (93%) | 75 (76%) | 15 (15%) | 8 (8%) | 1 | 2 |
| 18 | AR | 68/88 (77%) | 38 (56%) | 21 (31%) | 9 (13%) | 0 | 0 |
| 18 | CR | 68/88 (77%) | 38 (56%) | 21 (31%) | 9 (13%) | 0 | 0 |
| 19 | AS | 77/93 (83%) | 52 (68%) | 14 (18%) | 11 (14%) | 0 | 0 |
| 19 | CS | 77/93 (83%) | 51 (66%) | 15 (20%) | 11 (14%) | 0 | 0 |
| 20 | AT | 97/106 (92%) | 54 (56%) | 29 (30%) | 14 (14%) | 0 | 0 |
| 20 | CT | 97/106 (92%) | 56 (58%) | 27 (28%) | 14 (14%) | 0 | 0 |
| 21 | AU | 23/27 (85%) | 18 (78%) | 4 (17%) | 1 (4%) | 2 | 8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 21 | CU | 23/27 (85%) | 18 (78%) | 4 (17%) | 1 (4%) | 2 | 8 |
| 25 | B0 | 83/85 (98%) | 62 (75%) | 16 (19%) | 5 (6%) | 1 | 4 |
| 25 | D0 | 83/85 (98%) | 63 (76%) | 15 (18%) | 5 (6%) | 1 | 4 |
| 26 | B1 | 87/98 (89%) | 43 (49%) | 25 (29%) | 19 (22%) | 0 | 0 |
| 26 | D1 | 87/98 (89%) | 42 (48%) | 21 (24%) | 24 (28%) | 0 | 0 |
| 27 | B2 | 49/72 (68%) | 16 (33%) | 16 (33%) | 17 (35%) | 0 | 0 |
| 27 | D2 | 49/72 (68%) | 15 (31%) | 15 (31%) | 19 (39%) | 0 | 0 |
| 28 | B3 | 58/60 (97%) | 42 (72%) | 12 (21%) | 4 (7%) | 1 | 3 |
| 28 | D3 | 58/60 (97%) | 42 (72%) | 12 (21%) | 4 (7%) | 1 | 3 |
| 29 | B4 | 48/71 (68%) | 14 (29%) | 11 (23%) | 23 (48%) | 0 | 0 |
| 29 | D4 | 48/71 (68%) | 14 (29%) | 11 (23%) | 23 (48%) | 0 | 0 |
| 30 | B5 | 57/60 (95%) | 37 (65%) | 13 (23%) | 7 (12%) | 0 | 1 |
| 30 | D5 | 57/60 (95%) | 38 (67%) | 12 (21%) | 7 (12%) | 0 | 1 |
| 31 | B6 | 41/54 (76%) | 18 (44%) | 16 (39%) | 7 (17%) | 0 | 0 |
| 31 | D6 | 41/54 (76%) | 18 (44%) | 16 (39%) | 7 (17%) | 0 | 0 |
| 32 | B7 | 47/49 (96%) | 36 (77%) | 10 (21%) | 1 (2%) | 7 | 23 |
| 32 | D7 | 47/49 (96%) | 37 (79%) | 8 (17%) | 2 (4%) | 2 | 8 |
| 33 | B8 | 62/65 (95%) | 38 (61%) | 13 (21%) | 11 (18%) | 0 | 0 |
| 33 | D8 | 62/65 (95%) | 37 (60%) | 14 (23%) | 11 (18%) | 0 | 0 |
| 36 | BC | 183/229 (80%) | 88 (48%) | 52 (28%) | 43 (24%) | 0 | 0 |
| 36 | DC | 183/229 (80%) | 87 (48%) | 53 (29%) | 43 (24%) | 0 | 0 |
| 37 | BD | 270/276 (98%) | 193 (72%) | 51 (19%) | 26 (10%) | 0 | 1 |
| 37 | DD | 270/276 (98%) | 194 (72%) | 50 (18%) | 26 (10%) | 0 | 1 |
| 38 | BE | 203/206 (98%) | 116 (57%) | 49 (24%) | 38 (19%) | 0 | 0 |
| 38 | DE | 203/206 (98%) | 116 (57%) | 49 (24%) | 38 (19%) | 0 | 0 |
| 39 | BF | 206/210 (98%) | 142 (69%) | 40 (19%) | 24 (12%) | 0 | 1 |
| 39 | DF | 206/210 (98%) | 142 (69%) | 41 (20%) | 23 (11%) | 0 | 1 |
| 40 | BG | 177/182 (97%) | 93 (52%) | 56 (32%) | 28 (16%) | 0 | 0 |
| 40 | DG | 177/182 (97%) | 101 (57%) | 45 (25%) | 31 (18%) | 0 | 0 |
| 41 | BH | 158/180 (88%) | 100 (63%) | 31 (20%) | 27 (17%) | 0 | 0 |
| 41 | DH | 158/180 (88%) | 100 (63%) | 31 (20%) | 27 (17%) | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|---|
| 42 | BI | 144/148 (97%) | 98 (68%) | 36 (25%) | 10 (7%) | 1 | 3 |
| 42 | DI | 144/148 (97%) | 97 (67%) | 36 (25%) | 11 (8%) | 1 | 2 |
| 43 | BN | 137/140 (98%) | 75 (55%) | 35 (26%) | 27 (20%) | 0 | 0 |
| 43 | DN | 137/140 (98%) | 77 (56%) | 33 (24%) | 27 (20%) | 0 | 0 |
| 44 | BO | 120/122 (98%) | 92 (77%) | 17 (14%) | 11 (9%) | 1 | 1 |
| 44 | DO | 120/122 (98%) | 90 (75%) | 18 (15%) | 12 (10%) | 0 | 1 |
| 45 | BP | 144/150 (96%) | 72 (50%) | 37 (26%) | 35 (24%) | 0 | 0 |
| 45 | DP | 144/150 (96%) | 72 (50%) | 38 (26%) | 34 (24%) | 0 | 0 |
| 46 | BQ | 134/141 (95%) | 81 (60%) | 34 (25%) | 19 (14%) | 0 | 0 |
| 46 | DQ | 134/141 (95%) | 79 (59%) | 35 (26%) | 20 (15%) | 0 | 0 |
| 47 | BR | 115/118 (98%) | 74 (64%) | 20 (17%) | 21 (18%) | 0 | 0 |
| 47 | DR | 115/118 (98%) | 72 (63%) | 23 (20%) | 20 (17%) | 0 | 0 |
| 48 | BS | 97/112 (87%) | 49 (50%) | 19 (20%) | 29 (30%) | 0 | 0 |
| 48 | DS | 97/112 (87%) | 49 (50%) | 18 (19%) | 30 (31%) | 0 | 0 |
| 49 | BT | 136/146 (93%) | 77 (57%) | 34 (25%) | 25 (18%) | 0 | 0 |
| 49 | DT | 136/146 (93%) | 79 (58%) | 33 (24%) | 24 (18%) | 0 | 0 |
| 50 | BU | 115/118 (98%) | 61 (53%) | 42 (36%) | 12 (10%) | 0 | 1 |
| 50 | DU | 115/118 (98%) | 61 (53%) | 40 (35%) | 14 (12%) | 0 | 1 |
| 51 | BV | 97/101 (96%) | 47 (48%) | 23 (24%) | 27 (28%) | 0 | 0 |
| 51 | DV | 97/101 (96%) | 47 (48%) | 23 (24%) | 27 (28%) | 0 | 0 |
| 52 | BW | 111/113 (98%) | 74 (67%) | 23 (21%) | 14 (13%) | 0 | 1 |
| 52 | DW | 111/113 (98%) | 77 (69%) | 19 (17%) | 15 (14%) | 0 | 0 |
| 53 | BX | 91/96 (95%) | 45 (50%) | 23 (25%) | 23 (25%) | 0 | 0 |
| 53 | DX | 91/96 (95%) | 45 (50%) | 23 (25%) | 23 (25%) | 0 | 0 |
| 54 | BY | 99/110 (90%) | 41 (41%) | 24 (24%) | 34 (34%) | 0 | 0 |
| 54 | DY | 99/110 (90%) | 41 (41%) | 24 (24%) | 34 (34%) | 0 | 0 |
| 55 | BZ | 175/206 (85%) | 99 (57%) | 48 (27%) | 28 (16%) | 0 | 0 |
| 55 | DZ | 175/206 (85%) | 109 (62%) | 33 (19%) | 33 (19%) | 0 | 0 |
| All | All | 11570/12518 (92%) | 7170 (62%) | 2726 (24%) | 1674 (14%) | 0 | 0 |

5 of 1674 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 15 | VAL |
| 2 | AB | 52 | GLU |
| 2 | AB | 77 | ALA |
| 2 | AB | 84 | GLU |
| 2 | AB | 154 | LEU |

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%) | 182 (90%) | 20 (10%) | 8 | 23 |
| 2 | CB | 202/220 (92%) | 182 (90%) | 20 (10%) | 8 | 23 |
| 3 | AC | 160/188 (85%) | 151 (94%) | 9 (6%) | 21 | 51 |
| 3 | CC | 160/188 (85%) | 150 (94%) | 10 (6%) | 18 | 46 |
| 4 | AD | 180/181 (99%) | 159 (88%) | 21 (12%) | 5 | 16 |
| 4 | CD | 180/181 (99%) | 161 (89%) | 19 (11%) | 6 | 20 |
| 5 | AE | 115/123 (94%) | 102 (89%) | 13 (11%) | 6 | 18 |
| 5 | CE | 115/123 (94%) | 103 (90%) | 12 (10%) | 7 | 21 |
| 6 | AF | 90/90 (100%) | 84 (93%) | 6 (7%) | 16 | 43 |
| 6 | CF | 90/90 (100%) | 84 (93%) | 6 (7%) | 16 | 43 |
| 7 | AG | 126/127 (99%) | 122 (97%) | 4 (3%) | 39 | 73 |
| 7 | CG | 126/127 (99%) | 122 (97%) | 4 (3%) | 39 | 73 |
| 8 | AH | 119/119 (100%) | 114 (96%) | 5 (4%) | 30 | 63 |
| 8 | CH | 119/119 (100%) | 114 (96%) | 5 (4%) | 30 | 63 |
| 9 | AI | 98/99 (99%) | 88 (90%) | 10 (10%) | 7 | 22 |
| 9 | CI | 98/99 (99%) | 88 (90%) | 10 (10%) | 7 | 22 |
| 10 | AJ | 88/92 (96%) | 82 (93%) | 6 (7%) | 16 | 42 |
| 10 | CJ | 88/92 (96%) | 82 (93%) | 6 (7%) | 16 | 42 |
| 11 | AK | 90/99 (91%) | 85 (94%) | 5 (6%) | 21 | 51 |
| 11 | CK | 90/99 (91%) | 86 (96%) | 4 (4%) | 28 | 61 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 12 | AL | 104/111 (94%) | 95 (91%) | 9 (9%) | 10 | 30 |
| 12 | CL | 104/111 (94%) | 96 (92%) | 8 (8%) | 13 | 35 |
| 13 | AM | 99/101 (98%) | 93 (94%) | 6 (6%) | 18 | 48 |
| 13 | CM | 99/101 (98%) | 93 (94%) | 6 (6%) | 18 | 48 |
| 14 | AN | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 64 |
| 14 | CN | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 64 |
| 15 | AO | 79/80 (99%) | 74 (94%) | 5 (6%) | 18 | 46 |
| 15 | CO | 79/80 (99%) | 74 (94%) | 5 (6%) | 18 | 46 |
| 16 | AP | 72/74 (97%) | 65 (90%) | 7 (10%) | 8 | 24 |
| 16 | CP | 72/74 (97%) | 65 (90%) | 7 (10%) | 8 | 24 |
| 17 | AQ | 94/97 (97%) | 92 (98%) | 2 (2%) | 53 | 84 |
| 17 | CQ | 94/97 (97%) | 92 (98%) | 2 (2%) | 53 | 84 |
| 18 | AR | 61/77 (79%) | 55 (90%) | 6 (10%) | 8 | 24 |
| 18 | CR | 61/77 (79%) | 55 (90%) | 6 (10%) | 8 | 24 |
| 19 | AS | 69/80 (86%) | 62 (90%) | 7 (10%) | 7 | 22 |
| 19 | CS | 69/80 (86%) | 62 (90%) | 7 (10%) | 7 | 22 |
| 20 | AT | 76/82 (93%) | 65 (86%) | 11 (14%) | 3 | 9 |
| 20 | CT | 76/82 (93%) | 65 (86%) | 11 (14%) | 3 | 9 |
| 21 | AU | 19/22 (86%) | 17 (90%) | 2 (10%) | 7 | 20 |
| 21 | CU | 19/22 (86%) | 17 (90%) | 2 (10%) | 7 | 20 |
| 25 | B0 | 61/67 (91%) | 54 (88%) | 7 (12%) | 5 | 17 |
| 25 | D0 | 61/67 (91%) | 54 (88%) | 7 (12%) | 5 | 17 |
| 26 | B1 | 73/83 (88%) | 62 (85%) | 11 (15%) | 3 | 9 |
| 26 | D1 | 73/83 (88%) | 63 (86%) | 10 (14%) | 3 | 11 |
| 27 | B2 | 46/67 (69%) | 35 (76%) | 11 (24%) | 0 | 2 |
| 27 | D2 | 46/67 (69%) | 35 (76%) | 11 (24%) | 0 | 2 |
| 28 | B3 | 51/52 (98%) | 49 (96%) | 2 (4%) | 32 | 66 |
| 28 | D3 | 51/52 (98%) | 49 (96%) | 2 (4%) | 32 | 66 |
| 30 | B5 | 51/52 (98%) | 41 (80%) | 10 (20%) | 1 | 4 |
| 30 | D5 | 51/52 (98%) | 41 (80%) | 10 (20%) | 1 | 4 |
| 31 | B6 | 43/52 (83%) | 36 (84%) | 7 (16%) | 2 | 7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 31 | D6 | 43/52 (83%) | 36 (84%) | 7 (16%) | 2 | 7 |
| 32 | B7 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 24 |
| 32 | D7 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 24 |
| 33 | B8 | 53/55 (96%) | 45 (85%) | 8 (15%) | 3 | 9 |
| 33 | D8 | 53/55 (96%) | 45 (85%) | 8 (15%) | 3 | 9 |
| 36 | BC | 61/181 (34%) | 54 (88%) | 7 (12%) | 5 | 17 |
| 36 | DC | 61/181 (34%) | 54 (88%) | 7 (12%) | 5 | 17 |
| 37 | BD | 213/218 (98%) | 179 (84%) | 34 (16%) | 2 | 7 |
| 37 | DD | 213/218 (98%) | 181 (85%) | 32 (15%) | 3 | 9 |
| 38 | BE | 165/166 (99%) | 145 (88%) | 20 (12%) | 5 | 15 |
| 38 | DE | 165/166 (99%) | 145 (88%) | 20 (12%) | 5 | 15 |
| 39 | BF | 165/166 (99%) | 153 (93%) | 12 (7%) | 14 | 38 |
| 39 | DF | 165/166 (99%) | 153 (93%) | 12 (7%) | 14 | 38 |
| 40 | BG | 155/156 (99%) | 135 (87%) | 20 (13%) | 4 | 13 |
| 40 | DG | 155/156 (99%) | 132 (85%) | 23 (15%) | 3 | 9 |
| 41 | BH | 132/148 (89%) | 117 (89%) | 15 (11%) | 5 | 18 |
| 41 | DH | 132/148 (89%) | 117 (89%) | 15 (11%) | 5 | 18 |
| 42 | BI | 122/124 (98%) | 113 (93%) | 9 (7%) | 13 | 37 |
| 42 | DI | 122/124 (98%) | 113 (93%) | 9 (7%) | 13 | 37 |
| 43 | BN | 117/119 (98%) | 98 (84%) | 19 (16%) | 2 | 7 |
| 43 | DN | 117/119 (98%) | 97 (83%) | 20 (17%) | 2 | 6 |
| 44 | BO | 100/100 (100%) | 92 (92%) | 8 (8%) | 12 | 34 |
| 44 | DO | 100/100 (100%) | 91 (91%) | 9 (9%) | 9 | 28 |
| 45 | BP | 112/116 (97%) | 92 (82%) | 20 (18%) | 2 | 5 |
| 45 | DP | 112/116 (97%) | 91 (81%) | 21 (19%) | 1 | 5 |
| 46 | BQ | 106/111 (96%) | 93 (88%) | 13 (12%) | 4 | 15 |
| 46 | DQ | 106/111 (96%) | 93 (88%) | 13 (12%) | 4 | 15 |
| 47 | BR | 100/101 (99%) | 91 (91%) | 9 (9%) | 9 | 28 |
| 47 | DR | 100/101 (99%) | 91 (91%) | 9 (9%) | 9 | 28 |
| 48 | BS | 77/88 (88%) | 65 (84%) | 12 (16%) | 2 | 8 |
| 48 | DS | 77/88 (88%) | 65 (84%) | 12 (16%) | 2 | 8 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 49 | BT | 120/127 (94%) | 99 (82%) | 21 (18%) | 2 | 6 |
| 49 | DT | 120/127 (94%) | 99 (82%) | 21 (18%) | 2 | 6 |
| 50 | BU | 92/94 (98%) | 85 (92%) | 7 (8%) | 13 | 36 |
| 50 | DU | 92/94 (98%) | 85 (92%) | 7 (8%) | 13 | 36 |
| 51 | BV | 82/82 (100%) | 64 (78%) | 18 (22%) | 1 | 2 |
| 51 | DV | 82/82 (100%) | 64 (78%) | 18 (22%) | 1 | 2 |
| 52 | BW | 91/92 (99%) | 85 (93%) | 6 (7%) | 16 | 44 |
| 52 | DW | 91/92 (99%) | 84 (92%) | 7 (8%) | 13 | 35 |
| 53 | BX | 74/78 (95%) | 59 (80%) | 15 (20%) | 1 | 4 |
| 53 | DX | 74/78 (95%) | 60 (81%) | 14 (19%) | 1 | 5 |
| 54 | BY | 84/91 (92%) | 67 (80%) | 17 (20%) | 1 | 4 |
| 54 | DY | 84/91 (92%) | 67 (80%) | 17 (20%) | 1 | 4 |
| 55 | BZ | 155/179 (87%) | 144 (93%) | 11 (7%) | 14 | 39 |
| 55 | DZ | 155/179 (87%) | 141 (91%) | 14 (9%) | 9 | 28 |
| All | All | 9464/10238 (92%) | 8444 (89%) | 1020 (11%) | 6 | 19 |

5 of 1020 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | BW | 25 | ARG |
| 6 | CF | 46 | ARG |
| 49 | DT | 128 | GLU |
| 53 | BX | 49 | VAL |
| 2 | CB | 59 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | BV | 89 | GLN |
| 6 | CF | 13 | ASN |
| 48 | DS | 84 | GLN |
| 52 | BW | 62 | HIS |
| 2 | CB | 78 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1503/1522 (98%) | 200 (13%) | 36 (2%) |
| 1 | CA | 1503/1522 (98%) | 204 (13%) | 36 (2%) |
| 22 | AV | 76/77 (98%) | 18 (23%) | 0 |
| 22 | CV | 76/77 (98%) | 20 (26%) | 0 |
| 23 | AW | 75/76 (98%) | 15 (20%) | 3 (4%) |
| 23 | AY | 18/76 (23%) | 2 (11%) | 0 |
| 23 | CW | 75/76 (98%) | 16 (21%) | 3 (4%) |
| 23 | CY | 18/76 (23%) | 3 (16%) | 0 |
| 24 | AX | 10/24 (41%) | 2 (20%) | 0 |
| 24 | CX | 10/24 (41%) | 2 (20%) | 0 |
| 34 | BA | 2771/2787 (99%) | 563 (20%) | 76 (2%) |
| 34 | DA | 2771/2787 (99%) | 560 (20%) | 76 (2%) |
| 35 | BB | 118/122 (96%) | 14 (11%) | 1 (0%) |
| 35 | DB | 118/122 (96%) | 14 (11%) | 1 (0%) |
| All | All | 9142/9368 (97%) | 1633 (17%) | 232 (2%) |

5 of 1633 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 1 | AA | 31 | G |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |

5 of 232 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 34 | BA | 2422 | A |
| 1 | CA | 429 | U |
| 34 | DA | 2031 | A |
| 34 | BA | 2662 | A |
| 1 | CA | 60 | A |

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 22 | 5MU | CV | 54 | 22 | 15,22,23 | 1.21 | 2 (13%) | 16,32,35 | 3.69 | 1 (6%) |
| 22 | 5MU | AV | 54 | 22 | 15,22,23 | 1.10 | 2 (13%) | 16,32,35 | 3.69 | 2 (12%) |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 22 | 5MU | CV | 54 | 22 | - | 0/5/25/26 | 0/2/2/2 |
| 22 | 5MU | AV | 54 | 22 | - | 0/5/25/26 | 0/2/2/2 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 22 | CV | 54 | 5MU | C4-N3 | 3.46 | 1.39 | 1.33 |
| 22 | AV | 54 | 5MU | C4-N3 | 3.19 | 1.38 | 1.33 |
| 22 | AV | 54 | 5MU | C6-C5 | -2.12 | 1.34 | 1.40 |
| 22 | CV | 54 | 5MU | C6-C5 | -2.08 | 1.34 | 1.40 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 22 | CV | 54 | 5MU | C4-N3-C2 | 14.39 | 127.29 | 115.14 |
| 22 | AV | 54 | 5MU | C4-N3-C2 | 14.37 | 127.27 | 115.14 |
| 22 | AV | 54 | 5MU | C5M-C5-C6 | 2.01 | 122.92 | 118.68 |

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 |
|-----|-------|-----|------|---------|--------------|
| 22 | CV | 54 | 5MU | 2 | 0 |
| 22 | AV | 54 | 5MU | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1385 ligands modelled in this entry, 1383 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$ |
| 57 | PAR | AA | 1816 | - | 45,45,45 | 1.59 | 8 (17%) | 64,67,67 | 1.20 | 4 (6%) |
| 57 | PAR | CA | 1790 | - | 45,45,45 | 1.56 | 10 (22%) | 64,67,67 | 1.30 | 7 (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 |
|-----|------|-------|------|------|---------|------------|---------|
| 57 | PAR | AA | 1816 | - | - | 5/18/94/94 | 0/4/4/4 |
| 57 | PAR | CA | 1790 | - | - | 4/18/94/94 | 0/4/4/4 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 57 | AA | 1816 | PAR | C64-C54 | 5.15 | 1.59 | 1.52 |
| 57 | CA | 1790 | PAR | C64-C54 | 4.38 | 1.58 | 1.52 |
| 57 | CA | 1790 | PAR | C34-C24 | 4.37 | 1.59 | 1.53 |
| 57 | AA | 1816 | PAR | C52-C42 | 3.08 | 1.58 | 1.52 |
| 57 | AA | 1816 | PAR | O54-C14 | 2.82 | 1.49 | 1.41 |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 57 | AA | 1816 | PAR | O33-C14-C24 | 4.79 | 116.47 | 108.22 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 57 | CA | 1790 | PAR | O33-C14-C24 | 4.44 | 115.86 | 108.22 |
| 57 | CA | 1790 | PAR | O54-C54-C64 | 3.85 | 113.18 | 106.01 |
| 57 | CA | 1790 | PAR | C14-O54-C54 | 3.51 | 120.57 | 113.69 |
| 57 | AA | 1816 | PAR | O52-C13-C23 | 3.34 | 114.89 | 107.96 |

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

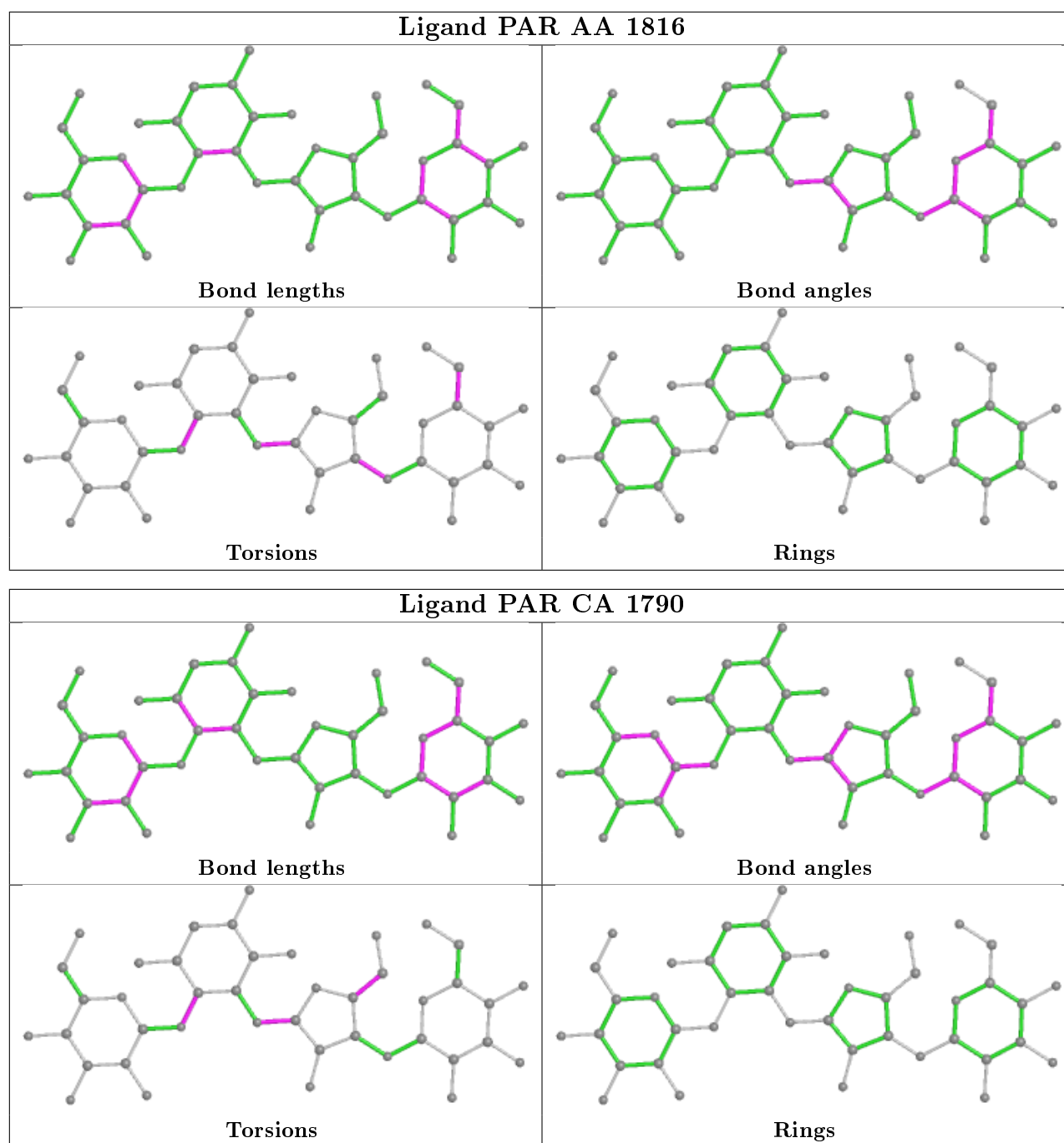
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 57 | CA | 1790 | PAR | O43-C43-C53-O53 |
| 57 | CA | 1790 | PAR | C33-C43-C53-O53 |
| 57 | AA | 1816 | PAR | O43-C13-O52-C52 |
| 57 | AA | 1816 | PAR | C23-C13-O52-C52 |
| 57 | AA | 1816 | PAR | O54-C54-C64-N64 |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57 | AA | 1816 | PAR | 3 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 13 | CM | 5 |
| 13 | AM | 5 |
| 9 | AI | 2 |
| 9 | CI | 2 |
| 51 | DV | 1 |
| 40 | DG | 1 |
| 40 | BG | 1 |
| 51 | BV | 1 |
| 31 | D6 | 1 |
| 31 | B6 | 1 |

The worst 5 of 20 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B6 | 46:HIS | C | 47:THR | N | 4.89 |
| 1 | D6 | 46:HIS | C | 47:THR | N | 4.87 |
| 1 | AM | 69:GLU | C | 70:LEU | N | 4.66 |
| 1 | CM | 69:GLU | C | 70:LEU | N | 4.66 |
| 1 | CI | 53:VAL | C | 54:ASP | N | 4.02 |

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%) | -0.41 | 23 (1%) 73 68 | 2, 42, 165, 200 | 0 |
| 1 | CA | 1504/1522 (98%) | -0.33 | 32 (2%) 63 54 | 3, 50, 172, 200 | 0 |
| 2 | AB | 235/256 (91%) | 0.26 | 28 (11%) 4 2 | 17, 94, 183, 200 | 0 |
| 2 | CB | 235/256 (91%) | 0.38 | 28 (11%) 4 2 | 17, 104, 187, 200 | 0 |
| 3 | AC | 207/239 (86%) | -0.15 | 6 (2%) 51 41 | 17, 70, 156, 200 | 0 |
| 3 | CC | 207/239 (86%) | 0.14 | 12 (5%) 23 15 | 19, 84, 149, 190 | 0 |
| 4 | AD | 208/209 (99%) | -0.32 | 1 (0%) 91 88 | 1, 43, 127, 198 | 0 |
| 4 | CD | 208/209 (99%) | -0.25 | 4 (1%) 66 59 | 4, 51, 133, 182 | 0 |
| 5 | AE | 151/162 (93%) | -0.32 | 1 (0%) 87 84 | 4, 51, 128, 177 | 0 |
| 5 | CE | 151/162 (93%) | -0.09 | 2 (1%) 77 72 | 3, 56, 140, 185 | 0 |
| 6 | AF | 101/101 (100%) | -0.36 | 3 (2%) 50 40 | 5, 48, 131, 156 | 0 |
| 6 | CF | 101/101 (100%) | -0.37 | 2 (1%) 65 56 | 2, 54, 130, 151 | 0 |
| 7 | AG | 155/156 (99%) | 0.07 | 12 (7%) 13 7 | 8, 68, 151, 184 | 0 |
| 7 | CG | 155/156 (99%) | 0.61 | 23 (14%) 2 1 | 15, 87, 155, 190 | 0 |
| 8 | AH | 138/138 (100%) | -0.24 | 3 (2%) 62 52 | 3, 52, 120, 173 | 0 |
| 8 | CH | 138/138 (100%) | -0.14 | 4 (2%) 51 41 | 16, 58, 138, 152 | 0 |
| 9 | AI | 127/128 (99%) | 0.66 | 15 (11%) 4 2 | 26, 97, 171, 200 | 0 |
| 9 | CI | 127/128 (99%) | 0.66 | 21 (16%) 1 1 | 28, 111, 175, 200 | 0 |
| 10 | AJ | 99/105 (94%) | 0.75 | 17 (17%) 1 1 | 17, 105, 178, 200 | 0 |
| 10 | CJ | 99/105 (94%) | 1.11 | 22 (22%) 0 0 | 34, 123, 176, 197 | 0 |
| 11 | AK | 119/129 (92%) | -0.29 | 3 (2%) 57 47 | 8, 46, 151, 192 | 0 |
| 11 | CK | 119/129 (92%) | 0.06 | 6 (5%) 28 19 | 16, 61, 147, 200 | 0 |
| 12 | AL | 125/135 (92%) | -0.12 | 4 (3%) 47 37 | 5, 38, 133, 200 | 0 |
| 12 | CL | 125/135 (92%) | -0.08 | 4 (3%) 47 37 | 1, 38, 132, 200 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 13 | AM | 125/126 (99%) | 0.37 | 15 (12%) 4 2 | 13, 74, 159, 196 | 0 |
| 13 | CM | 125/126 (99%) | 0.43 | 15 (12%) 4 2 | 19, 91, 160, 191 | 0 |
| 14 | AN | 60/61 (98%) | 0.47 | 6 (10%) 7 4 | 14, 66, 161, 184 | 0 |
| 14 | CN | 60/61 (98%) | 0.20 | 4 (6%) 17 10 | 19, 73, 143, 182 | 0 |
| 15 | AO | 88/89 (98%) | -0.54 | 0 100 100 | 2, 42, 129, 141 | 0 |
| 15 | CO | 88/89 (98%) | -0.36 | 1 (1%) 80 75 | 2, 56, 124, 167 | 0 |
| 16 | AP | 84/88 (95%) | -0.21 | 1 (1%) 79 73 | 6, 36, 104, 190 | 0 |
| 16 | CP | 84/88 (95%) | -0.06 | 1 (1%) 79 73 | 6, 49, 121, 199 | 0 |
| 17 | AQ | 100/105 (95%) | -0.33 | 2 (2%) 65 56 | 1, 45, 110, 193 | 0 |
| 17 | CQ | 100/105 (95%) | 0.17 | 2 (2%) 65 56 | 18, 60, 105, 194 | 0 |
| 18 | AR | 70/88 (79%) | -0.13 | 1 (1%) 75 70 | 10, 50, 140, 172 | 0 |
| 18 | CR | 70/88 (79%) | 0.19 | 3 (4%) 35 25 | 7, 56, 144, 179 | 0 |
| 19 | AS | 79/93 (84%) | 0.26 | 8 (10%) 7 4 | 22, 79, 186, 200 | 0 |
| 19 | CS | 79/93 (84%) | 0.68 | 11 (13%) 2 1 | 25, 83, 175, 197 | 0 |
| 20 | AT | 99/106 (93%) | 0.30 | 9 (9%) 9 5 | 5, 60, 152, 180 | 0 |
| 20 | CT | 99/106 (93%) | 0.21 | 6 (6%) 21 13 | 17, 77, 141, 183 | 0 |
| 21 | AU | 25/27 (92%) | 1.42 | 8 (32%) 0 0 | 27, 72, 128, 141 | 0 |
| 21 | CU | 25/27 (92%) | 2.31 | 11 (44%) 0 0 | 40, 74, 127, 139 | 0 |
| 22 | AV | 76/77 (98%) | -0.64 | 0 100 100 | 14, 53, 143, 194 | 0 |
| 22 | CV | 76/77 (98%) | -0.53 | 0 100 100 | 21, 55, 146, 198 | 0 |
| 23 | AW | 76/76 (100%) | -0.23 | 5 (6%) 18 11 | 30, 103, 164, 199 | 0 |
| 23 | AY | 19/76 (25%) | -0.27 | 0 100 100 | 23, 72, 190, 196 | 0 |
| 23 | CW | 76/76 (100%) | -0.03 | 5 (6%) 18 11 | 35, 116, 165, 196 | 0 |
| 23 | CY | 19/76 (25%) | -0.28 | 0 100 100 | 26, 76, 186, 196 | 0 |
| 24 | AX | 11/24 (45%) | -0.11 | 1 (9%) 9 5 | 12, 33, 170, 190 | 0 |
| 24 | CX | 11/24 (45%) | 0.28 | 2 (18%) 1 1 | 14, 39, 167, 197 | 0 |
| 25 | B0 | 85/85 (100%) | 0.44 | 7 (8%) 11 6 | 8, 43, 138, 196 | 0 |
| 25 | D0 | 85/85 (100%) | 0.54 | 9 (10%) 6 3 | 18, 57, 137, 179 | 0 |
| 26 | B1 | 89/98 (90%) | 0.05 | 4 (4%) 33 23 | 1, 35, 143, 157 | 0 |
| 26 | D1 | 89/98 (90%) | -0.06 | 2 (2%) 62 52 | 1, 44, 145, 200 | 0 |
| 27 | B2 | 51/72 (70%) | 0.03 | 5 (9%) 7 4 | 5, 66, 145, 200 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 27 | D2 | 51/72 (70%) | 0.53 | 7 (13%) 3 1 | 13, 79, 154, 200 | 0 |
| 28 | B3 | 60/60 (100%) | 0.24 | 4 (6%) 17 10 | 5, 57, 140, 190 | 0 |
| 28 | D3 | 60/60 (100%) | 0.28 | 2 (3%) 46 36 | 5, 58, 146, 198 | 0 |
| 29 | B4 | 50/71 (70%) | -0.49 | 1 (2%) 65 56 | 38, 90, 158, 173 | 0 |
| 29 | D4 | 50/71 (70%) | 0.07 | 5 (10%) 7 4 | 54, 117, 160, 198 | 0 |
| 30 | B5 | 59/60 (98%) | 0.59 | 10 (16%) 1 1 | 5, 51, 192, 200 | 0 |
| 30 | D5 | 59/60 (98%) | 0.38 | 7 (11%) 4 2 | 1, 65, 179, 200 | 0 |
| 31 | B6 | 45/54 (83%) | 1.92 | 21 (46%) 0 0 | 54, 103, 171, 180 | 0 |
| 31 | D6 | 45/54 (83%) | 2.77 | 26 (57%) 0 0 | 64, 139, 171, 189 | 0 |
| 32 | B7 | 49/49 (100%) | -0.15 | 3 (6%) 21 13 | 1, 19, 115, 165 | 0 |
| 32 | D7 | 49/49 (100%) | -0.16 | 4 (8%) 11 6 | 1, 19, 88, 174 | 0 |
| 33 | B8 | 64/65 (98%) | 0.37 | 5 (7%) 13 7 | 4, 44, 140, 195 | 0 |
| 33 | D8 | 64/65 (98%) | 0.28 | 4 (6%) 20 12 | 5, 52, 155, 192 | 0 |
| 34 | BA | 2772/2787 (99%) | -0.52 | 33 (1%) 79 73 | 1, 29, 145, 200 | 0 |
| 34 | DA | 2772/2787 (99%) | -0.49 | 25 (0%) 84 80 | 1, 30, 152, 200 | 0 |
| 35 | BB | 119/122 (97%) | -0.54 | 0 100 100 | 22, 64, 108, 197 | 0 |
| 35 | DB | 119/122 (97%) | -0.38 | 0 100 100 | 34, 76, 127, 188 | 0 |
| 36 | BC | 191/229 (83%) | 1.99 | 73 (38%) 0 0 | 51, 144, 186, 200 | 0 |
| 36 | DC | 191/229 (83%) | 2.54 | 97 (50%) 0 0 | 61, 146, 186, 200 | 0 |
| 37 | BD | 272/276 (98%) | -0.52 | 2 (0%) 87 84 | 1, 19, 89, 196 | 0 |
| 37 | DD | 272/276 (98%) | -0.49 | 2 (0%) 87 84 | 1, 21, 89, 200 | 0 |
| 38 | BE | 205/206 (99%) | 0.04 | 7 (3%) 45 35 | 1, 46, 141, 193 | 0 |
| 38 | DE | 205/206 (99%) | -0.15 | 7 (3%) 45 35 | 1, 43, 144, 199 | 0 |
| 39 | BF | 208/210 (99%) | -0.26 | 9 (4%) 35 25 | 1, 44, 155, 200 | 0 |
| 39 | DF | 208/210 (99%) | 0.07 | 13 (6%) 20 12 | 1, 44, 160, 200 | 0 |
| 40 | BG | 181/182 (99%) | -0.09 | 8 (4%) 34 24 | 8, 65, 142, 188 | 0 |
| 40 | DG | 181/182 (99%) | 0.15 | 13 (7%) 15 8 | 10, 82, 149, 195 | 0 |
| 41 | BH | 160/180 (88%) | 1.07 | 35 (21%) 0 0 | 51, 124, 175, 200 | 0 |
| 41 | DH | 160/180 (88%) | 0.80 | 28 (17%) 1 1 | 10, 102, 174, 194 | 0 |
| 42 | BI | 146/148 (98%) | 0.25 | 13 (8%) 9 5 | 5, 78, 148, 187 | 0 |
| 42 | DI | 146/148 (98%) | 2.60 | 56 (38%) 0 0 | 9, 124, 184, 200 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 43 | BN | 139/140 (99%) | -0.04 | 5 (3%) 42 32 | 10, 68, 144, 163 | 0 |
| 43 | DN | 139/140 (99%) | 0.11 | 9 (6%) 18 11 | 15, 63, 141, 165 | 0 |
| 44 | BO | 122/122 (100%) | -0.44 | 0 100 100 | 3, 32, 103, 177 | 0 |
| 44 | DO | 122/122 (100%) | -0.49 | 0 100 100 | 1, 33, 102, 126 | 0 |
| 45 | BP | 146/150 (97%) | 0.12 | 3 (2%) 63 54 | 1, 61, 159, 193 | 0 |
| 45 | DP | 146/150 (97%) | 0.25 | 10 (6%) 17 10 | 2, 71, 165, 198 | 0 |
| 46 | BQ | 136/141 (96%) | 0.46 | 9 (6%) 18 11 | 7, 58, 171, 200 | 0 |
| 46 | DQ | 136/141 (96%) | 0.16 | 11 (8%) 12 6 | 7, 54, 164, 200 | 0 |
| 47 | BR | 117/118 (99%) | -0.20 | 1 (0%) 84 80 | 3, 32, 132, 146 | 0 |
| 47 | DR | 117/118 (99%) | -0.11 | 0 100 100 | 3, 42, 126, 166 | 0 |
| 48 | BS | 99/112 (88%) | 0.33 | 8 (8%) 12 6 | 21, 76, 134, 173 | 0 |
| 48 | DS | 99/112 (88%) | 0.81 | 15 (15%) 2 1 | 24, 89, 143, 171 | 0 |
| 49 | BT | 138/146 (94%) | 0.02 | 9 (6%) 18 11 | 3, 67, 169, 190 | 0 |
| 49 | DT | 138/146 (94%) | -0.00 | 7 (5%) 28 19 | 7, 65, 171, 200 | 0 |
| 50 | BU | 117/118 (99%) | -0.04 | 4 (3%) 45 35 | 5, 50, 142, 200 | 0 |
| 50 | DU | 117/118 (99%) | -0.14 | 2 (1%) 70 63 | 1, 46, 145, 190 | 0 |
| 51 | BV | 101/101 (100%) | 0.25 | 5 (4%) 28 19 | 14, 96, 174, 192 | 0 |
| 51 | DV | 101/101 (100%) | 0.16 | 4 (3%) 38 28 | 11, 93, 172, 193 | 0 |
| 52 | BW | 113/113 (100%) | -0.46 | 0 100 100 | 1, 26, 121, 161 | 0 |
| 52 | DW | 113/113 (100%) | -0.37 | 0 100 100 | 3, 28, 126, 200 | 0 |
| 53 | BX | 93/96 (96%) | -0.22 | 4 (4%) 35 25 | 1, 46, 137, 168 | 0 |
| 53 | DX | 93/96 (96%) | -0.02 | 4 (4%) 35 25 | 8, 54, 138, 157 | 0 |
| 54 | BY | 101/110 (91%) | 0.95 | 15 (14%) 2 1 | 1, 79, 170, 195 | 0 |
| 54 | DY | 101/110 (91%) | 1.38 | 25 (24%) 0 0 | 1, 79, 177, 196 | 0 |
| 55 | BZ | 177/206 (85%) | 0.20 | 11 (6%) 20 13 | 19, 96, 177, 200 | 0 |
| 55 | DZ | 177/206 (85%) | 0.26 | 14 (7%) 12 7 | 18, 98, 178, 198 | 0 |
| All | All | 20972/21886 (95%) | -0.08 | 1115 (5%) 26 17 | 1, 51, 163, 200 | 0 |

The worst 5 of 1115 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 42 | DI | 84 | GLY | 32.2 |
| 46 | BQ | 140 | ALA | 23.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 42 | DI | 120 | ILE | 21.9 |
| 42 | DI | 88 | ILE | 21.5 |
| 17 | CQ | 101 | ARG | 20.9 |

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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 | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 22 | 5MU | AV | 54 | 21/22 | 0.92 | 0.14 | 75,83,108,108 | 0 |
| 22 | 5MU | CV | 54 | 21/22 | 0.93 | 0.12 | 64,75,79,79 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56 | MG | DA | 3261 | 1/1 | 0.23 | 0.80 | 94,94,94,94 | 0 |
| 56 | MG | BB | 213 | 1/1 | 0.27 | 0.60 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3187 | 1/1 | 0.41 | 0.41 | 86,86,86,86 | 0 |
| 56 | MG | CV | 103 | 1/1 | 0.46 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | CA | 1637 | 1/1 | 0.51 | 0.46 | 81,81,81,81 | 0 |
| 56 | MG | CW | 111 | 1/1 | 0.54 | 0.22 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3233 | 1/1 | 0.55 | 0.33 | 77,77,77,77 | 0 |
| 56 | MG | CA | 1685 | 1/1 | 0.56 | 0.47 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3255 | 1/1 | 0.57 | 0.47 | 92,92,92,92 | 0 |
| 56 | MG | CA | 1719 | 1/1 | 0.58 | 1.11 | 99,99,99,99 | 0 |
| 56 | MG | AA | 1633 | 1/1 | 0.58 | 0.44 | 90,90,90,90 | 0 |
| 56 | MG | CA | 1622 | 1/1 | 0.60 | 0.81 | 123,123,123,123 | 0 |
| 56 | MG | BA | 3043 | 1/1 | 0.61 | 0.33 | 82,82,82,82 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3403 | 1/1 | 0.62 | 0.48 | 78,78,78,78 | 0 |
| 56 | MG | CA | 1725 | 1/1 | 0.62 | 0.26 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3168 | 1/1 | 0.65 | 0.38 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3004 | 1/1 | 0.67 | 0.41 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3408 | 1/1 | 0.67 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | CA | 1646 | 1/1 | 0.68 | 0.42 | 62,62,62,62 | 0 |
| 56 | MG | BB | 201 | 1/1 | 0.69 | 0.42 | 54,54,54,54 | 1 |
| 56 | MG | DA | 3213 | 1/1 | 0.69 | 0.35 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3208 | 1/1 | 0.69 | 0.21 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3413 | 1/1 | 0.69 | 0.47 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3433 | 1/1 | 0.70 | 0.17 | 74,74,74,74 | 0 |
| 56 | MG | CA | 1729 | 1/1 | 0.70 | 0.51 | 71,71,71,71 | 0 |
| 56 | MG | CA | 1673 | 1/1 | 0.71 | 0.21 | 80,80,80,80 | 1 |
| 56 | MG | AA | 1697 | 1/1 | 0.72 | 0.45 | 88,88,88,88 | 0 |
| 56 | MG | BA | 3353 | 1/1 | 0.72 | 0.39 | 42,42,42,42 | 1 |
| 56 | MG | DA | 3231 | 1/1 | 0.72 | 0.40 | 72,72,72,72 | 0 |
| 56 | MG | DA | 3219 | 1/1 | 0.72 | 0.56 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3275 | 1/1 | 0.73 | 0.36 | 75,75,75,75 | 0 |
| 56 | MG | CA | 1706 | 1/1 | 0.73 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3217 | 1/1 | 0.73 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | CW | 107 | 1/1 | 0.73 | 0.27 | 63,63,63,63 | 1 |
| 56 | MG | DA | 3273 | 1/1 | 0.74 | 0.60 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3278 | 1/1 | 0.74 | 0.37 | 90,90,90,90 | 0 |
| 56 | MG | CA | 1752 | 1/1 | 0.74 | 0.51 | 83,83,83,83 | 0 |
| 56 | MG | DA | 3169 | 1/1 | 0.75 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3238 | 1/1 | 0.75 | 0.26 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3155 | 1/1 | 0.75 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3323 | 1/1 | 0.75 | 0.13 | 79,79,79,79 | 0 |
| 56 | MG | DA | 3002 | 1/1 | 0.76 | 0.28 | 38,38,38,38 | 0 |
| 56 | MG | CA | 1751 | 1/1 | 0.76 | 0.18 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3320 | 1/1 | 0.76 | 0.17 | 70,70,70,70 | 0 |
| 56 | MG | AA | 1618 | 1/1 | 0.76 | 0.41 | 66,66,66,66 | 0 |
| 56 | MG | AA | 1748 | 1/1 | 0.77 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1675 | 1/1 | 0.77 | 0.24 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3296 | 1/1 | 0.78 | 0.34 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3268 | 1/1 | 0.78 | 0.21 | 51,51,51,51 | 0 |
| 56 | MG | DA | 3004 | 1/1 | 0.78 | 0.41 | 90,90,90,90 | 0 |
| 56 | MG | DA | 3358 | 1/1 | 0.79 | 0.36 | 54,54,54,54 | 0 |
| 56 | MG | AA | 1651 | 1/1 | 0.79 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | CA | 1739 | 1/1 | 0.79 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3380 | 1/1 | 0.79 | 0.33 | 55,55,55,55 | 0 |
| 56 | MG | CA | 1722 | 1/1 | 0.79 | 0.31 | 70,70,70,70 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DH | 201 | 1/1 | 0.79 | 0.19 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3138 | 1/1 | 0.80 | 0.27 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1698 | 1/1 | 0.80 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | CA | 1695 | 1/1 | 0.80 | 0.14 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3250 | 1/1 | 0.80 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1733 | 1/1 | 0.80 | 0.40 | 63,63,63,63 | 0 |
| 56 | MG | AA | 1647 | 1/1 | 0.80 | 0.18 | 71,71,71,71 | 0 |
| 56 | MG | BA | 3212 | 1/1 | 0.80 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | CW | 109 | 1/1 | 0.81 | 0.11 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1661 | 1/1 | 0.81 | 0.30 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3342 | 1/1 | 0.81 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1716 | 1/1 | 0.81 | 0.31 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3376 | 1/1 | 0.81 | 0.20 | 47,47,47,47 | 0 |
| 56 | MG | AA | 1714 | 1/1 | 0.81 | 0.25 | 28,28,28,28 | 0 |
| 56 | MG | AY | 101 | 1/1 | 0.81 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1782 | 1/1 | 0.81 | 0.28 | 68,68,68,68 | 0 |
| 56 | MG | BA | 3285 | 1/1 | 0.81 | 0.51 | 74,74,74,74 | 0 |
| 56 | MG | DA | 3310 | 1/1 | 0.81 | 0.30 | 50,50,50,50 | 0 |
| 56 | MG | CA | 1691 | 1/1 | 0.82 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | CA | 1750 | 1/1 | 0.82 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1750 | 1/1 | 0.82 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3258 | 1/1 | 0.82 | 0.49 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3248 | 1/1 | 0.82 | 0.94 | 82,82,82,82 | 0 |
| 56 | MG | DB | 204 | 1/1 | 0.82 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | CA | 1745 | 1/1 | 0.82 | 0.42 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1677 | 1/1 | 0.82 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | AW | 110 | 1/1 | 0.82 | 0.26 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3277 | 1/1 | 0.82 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3262 | 1/1 | 0.82 | 0.33 | 72,72,72,72 | 0 |
| 56 | MG | BA | 3227 | 1/1 | 0.82 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | AA | 1660 | 1/1 | 0.82 | 0.30 | 61,61,61,61 | 0 |
| 56 | MG | DA | 3274 | 1/1 | 0.82 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | AW | 116 | 1/1 | 0.82 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3394 | 1/1 | 0.83 | 0.32 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3067 | 1/1 | 0.83 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | AA | 1794 | 1/1 | 0.83 | 0.28 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3391 | 1/1 | 0.83 | 0.21 | 62,62,62,62 | 1 |
| 56 | MG | CA | 1696 | 1/1 | 0.83 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3257 | 1/1 | 0.83 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1694 | 1/1 | 0.83 | 0.35 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3279 | 1/1 | 0.83 | 0.21 | 55,55,55,55 | 0 |
| 56 | MG | AW | 113 | 1/1 | 0.83 | 0.26 | 46,46,46,46 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AX | 102 | 1/1 | 0.83 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3312 | 1/1 | 0.83 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1647 | 1/1 | 0.83 | 0.39 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3036 | 1/1 | 0.83 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | CW | 112 | 1/1 | 0.83 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3152 | 1/1 | 0.84 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3147 | 1/1 | 0.84 | 0.20 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3109 | 1/1 | 0.84 | 0.28 | 34,34,34,34 | 0 |
| 56 | MG | CA | 1645 | 1/1 | 0.84 | 0.14 | 74,74,74,74 | 0 |
| 56 | MG | AA | 1693 | 1/1 | 0.84 | 0.42 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3216 | 1/1 | 0.84 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3319 | 1/1 | 0.84 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3381 | 1/1 | 0.84 | 0.23 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3016 | 1/1 | 0.84 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | AA | 1658 | 1/1 | 0.84 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | AW | 103 | 1/1 | 0.85 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3103 | 1/1 | 0.85 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | AA | 1716 | 1/1 | 0.85 | 0.39 | 73,73,73,73 | 0 |
| 56 | MG | D5 | 102 | 1/1 | 0.85 | 0.11 | 6,6,6,6 | 1 |
| 56 | MG | BA | 3375 | 1/1 | 0.85 | 0.26 | 42,42,42,42 | 1 |
| 56 | MG | CA | 1688 | 1/1 | 0.85 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3377 | 1/1 | 0.85 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3261 | 1/1 | 0.85 | 0.11 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3275 | 1/1 | 0.85 | 0.17 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1799 | 1/1 | 0.85 | 0.09 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1670 | 1/1 | 0.85 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3330 | 1/1 | 0.85 | 0.49 | 81,81,81,81 | 0 |
| 56 | MG | CA | 1615 | 1/1 | 0.85 | 0.34 | 61,61,61,61 | 0 |
| 56 | MG | BB | 205 | 1/1 | 0.85 | 0.36 | 35,35,35,35 | 1 |
| 56 | MG | AA | 1727 | 1/1 | 0.85 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3393 | 1/1 | 0.85 | 0.60 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3451 | 1/1 | 0.85 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3422 | 1/1 | 0.85 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3346 | 1/1 | 0.85 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3357 | 1/1 | 0.85 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3334 | 1/1 | 0.85 | 0.09 | 34,34,34,34 | 1 |
| 56 | MG | DA | 3024 | 1/1 | 0.85 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | CA | 1642 | 1/1 | 0.85 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3178 | 1/1 | 0.85 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | CA | 1767 | 1/1 | 0.85 | 0.27 | 67,67,67,67 | 0 |
| 56 | MG | BA | 3332 | 1/1 | 0.86 | 0.20 | 53,53,53,53 | 1 |
| 56 | MG | DO | 201 | 1/1 | 0.86 | 0.13 | 67,67,67,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3237 | 1/1 | 0.86 | 0.32 | 35,35,35,35 | 0 |
| 56 | MG | AA | 1730 | 1/1 | 0.86 | 0.36 | 82,82,82,82 | 0 |
| 56 | MG | BA | 3143 | 1/1 | 0.86 | 0.26 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1747 | 1/1 | 0.86 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | AE | 201 | 1/1 | 0.86 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3412 | 1/1 | 0.86 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | DA | 3353 | 1/1 | 0.86 | 0.35 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1753 | 1/1 | 0.86 | 0.23 | 33,33,33,33 | 0 |
| 56 | MG | CX | 102 | 1/1 | 0.86 | 0.40 | 75,75,75,75 | 0 |
| 56 | MG | BA | 3329 | 1/1 | 0.86 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | CA | 1742 | 1/1 | 0.86 | 0.15 | 76,76,76,76 | 0 |
| 56 | MG | CA | 1730 | 1/1 | 0.86 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1626 | 1/1 | 0.86 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3149 | 1/1 | 0.86 | 0.48 | 84,84,84,84 | 0 |
| 56 | MG | BA | 3425 | 1/1 | 0.86 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | CA | 1744 | 1/1 | 0.86 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3048 | 1/1 | 0.86 | 0.27 | 53,53,53,53 | 0 |
| 56 | MG | BB | 203 | 1/1 | 0.86 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3022 | 1/1 | 0.86 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3276 | 1/1 | 0.86 | 0.37 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1644 | 1/1 | 0.86 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3107 | 1/1 | 0.87 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3193 | 1/1 | 0.87 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3293 | 1/1 | 0.87 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1795 | 1/1 | 0.87 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | AW | 120 | 1/1 | 0.87 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3247 | 1/1 | 0.87 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3212 | 1/1 | 0.87 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | AA | 1802 | 1/1 | 0.87 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3160 | 1/1 | 0.87 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1657 | 1/1 | 0.87 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | B3 | 101 | 1/1 | 0.87 | 0.24 | 48,48,48,48 | 1 |
| 56 | MG | AA | 1663 | 1/1 | 0.87 | 0.13 | 24,24,24,24 | 0 |
| 56 | MG | CW | 104 | 1/1 | 0.87 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3329 | 1/1 | 0.87 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1763 | 1/1 | 0.87 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3372 | 1/1 | 0.87 | 0.11 | 43,43,43,43 | 1 |
| 56 | MG | DB | 202 | 1/1 | 0.87 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3283 | 1/1 | 0.87 | 0.20 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3342 | 1/1 | 0.87 | 0.35 | 52,52,52,52 | 1 |
| 56 | MG | BA | 3383 | 1/1 | 0.87 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | BB | 209 | 1/1 | 0.88 | 0.12 | 49,49,49,49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3249 | 1/1 | 0.88 | 0.47 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1697 | 1/1 | 0.88 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1619 | 1/1 | 0.88 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3258 | 1/1 | 0.88 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | BA | 3400 | 1/1 | 0.88 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3419 | 1/1 | 0.88 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1688 | 1/1 | 0.88 | 0.29 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3246 | 1/1 | 0.88 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3265 | 1/1 | 0.88 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1734 | 1/1 | 0.88 | 0.20 | 48,48,48,48 | 1 |
| 56 | MG | CA | 1714 | 1/1 | 0.88 | 0.16 | 81,81,81,81 | 0 |
| 56 | MG | CA | 1726 | 1/1 | 0.88 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3070 | 1/1 | 0.88 | 0.21 | 24,24,24,24 | 0 |
| 56 | MG | DB | 209 | 1/1 | 0.88 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3137 | 1/1 | 0.88 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | BA | 3374 | 1/1 | 0.88 | 0.26 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3414 | 1/1 | 0.88 | 0.32 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3222 | 1/1 | 0.88 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3181 | 1/1 | 0.88 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | CX | 103 | 1/1 | 0.88 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | CA | 1680 | 1/1 | 0.88 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3064 | 1/1 | 0.88 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3171 | 1/1 | 0.88 | 0.20 | 37,37,37,37 | 0 |
| 56 | MG | CA | 1618 | 1/1 | 0.88 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | CV | 102 | 1/1 | 0.88 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3153 | 1/1 | 0.89 | 0.31 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3379 | 1/1 | 0.89 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3124 | 1/1 | 0.89 | 0.19 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3206 | 1/1 | 0.89 | 0.19 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3018 | 1/1 | 0.89 | 0.24 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3278 | 1/1 | 0.89 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3254 | 1/1 | 0.89 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3282 | 1/1 | 0.89 | 0.31 | 49,49,49,49 | 0 |
| 56 | MG | BN | 201 | 1/1 | 0.89 | 0.31 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3008 | 1/1 | 0.89 | 0.17 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3159 | 1/1 | 0.89 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | CA | 1759 | 1/1 | 0.89 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | AA | 1665 | 1/1 | 0.89 | 0.21 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3166 | 1/1 | 0.89 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3001 | 1/1 | 0.89 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3415 | 1/1 | 0.89 | 0.32 | 38,38,38,38 | 0 |
| 56 | MG | CJ | 201 | 1/1 | 0.89 | 0.10 | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1789 | 1/1 | 0.89 | 0.18 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3272 | 1/1 | 0.89 | 0.41 | 47,47,47,47 | 0 |
| 56 | MG | CA | 1761 | 1/1 | 0.89 | 0.26 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3142 | 1/1 | 0.89 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3111 | 1/1 | 0.89 | 0.24 | 1,1,1,1 | 0 |
| 56 | MG | CA | 1786 | 1/1 | 0.89 | 0.23 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3009 | 1/1 | 0.89 | 0.23 | 20,20,20,20 | 0 |
| 56 | MG | CA | 1663 | 1/1 | 0.89 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1643 | 1/1 | 0.89 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3300 | 1/1 | 0.89 | 0.10 | 6,6,6,6 | 0 |
| 56 | MG | CV | 104 | 1/1 | 0.89 | 0.21 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3333 | 1/1 | 0.89 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | B2 | 102 | 1/1 | 0.89 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | DN | 201 | 1/1 | 0.89 | 0.09 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3173 | 1/1 | 0.89 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3368 | 1/1 | 0.90 | 0.67 | 71,71,71,71 | 0 |
| 56 | MG | AA | 1620 | 1/1 | 0.90 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3140 | 1/1 | 0.90 | 0.11 | 10,10,10,10 | 0 |
| 56 | MG | AA | 1708 | 1/1 | 0.90 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | CA | 1732 | 1/1 | 0.90 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | AW | 118 | 1/1 | 0.90 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3057 | 1/1 | 0.90 | 0.30 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3367 | 1/1 | 0.90 | 0.26 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1745 | 1/1 | 0.90 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3009 | 1/1 | 0.90 | 0.18 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3241 | 1/1 | 0.90 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | CX | 106 | 1/1 | 0.90 | 0.37 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3330 | 1/1 | 0.90 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3230 | 1/1 | 0.90 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | B2 | 103 | 1/1 | 0.90 | 0.29 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1768 | 1/1 | 0.90 | 0.15 | 14,14,14,14 | 1 |
| 56 | MG | DA | 3369 | 1/1 | 0.90 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3409 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | DA | 3132 | 1/1 | 0.90 | 0.09 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3165 | 1/1 | 0.90 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3154 | 1/1 | 0.90 | 0.14 | 28,28,28,28 | 1 |
| 56 | MG | DA | 3371 | 1/1 | 0.90 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | BB | 212 | 1/1 | 0.90 | 0.11 | 18,18,18,18 | 1 |
| 56 | MG | AA | 1810 | 1/1 | 0.90 | 0.26 | 47,47,47,47 | 0 |
| 56 | MG | AA | 1749 | 1/1 | 0.90 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3331 | 1/1 | 0.90 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3435 | 1/1 | 0.90 | 0.09 | 52,52,52,52 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3387 | 1/1 | 0.90 | 0.11 | 11,11,11,11 | 0 |
| 56 | MG | CA | 1627 | 1/1 | 0.90 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | CA | 1734 | 1/1 | 0.90 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | CA | 1723 | 1/1 | 0.90 | 0.34 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3429 | 1/1 | 0.90 | 0.16 | 41,41,41,41 | 0 |
| 56 | MG | CA | 1643 | 1/1 | 0.90 | 0.42 | 48,48,48,48 | 0 |
| 56 | MG | AA | 1763 | 1/1 | 0.90 | 0.43 | 58,58,58,58 | 1 |
| 56 | MG | AA | 1772 | 1/1 | 0.90 | 0.23 | 73,73,73,73 | 0 |
| 56 | MG | DA | 3240 | 1/1 | 0.90 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | AW | 121 | 1/1 | 0.90 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3446 | 1/1 | 0.90 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | AA | 1776 | 1/1 | 0.90 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | CW | 110 | 1/1 | 0.90 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3286 | 1/1 | 0.90 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3345 | 1/1 | 0.90 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3129 | 1/1 | 0.91 | 0.14 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3349 | 1/1 | 0.91 | 0.16 | 28,28,28,28 | 1 |
| 56 | MG | DA | 3389 | 1/1 | 0.91 | 0.11 | 22,22,22,22 | 0 |
| 56 | MG | AV | 107 | 1/1 | 0.91 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | AA | 1767 | 1/1 | 0.91 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | DZ | 301 | 1/1 | 0.91 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3219 | 1/1 | 0.91 | 0.06 | 45,45,45,45 | 0 |
| 56 | MG | CX | 104 | 1/1 | 0.91 | 0.17 | 31,31,31,31 | 1 |
| 56 | MG | BA | 3002 | 1/1 | 0.91 | 0.17 | 21,21,21,21 | 0 |
| 56 | MG | DA | 3133 | 1/1 | 0.91 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | BB | 204 | 1/1 | 0.91 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3344 | 1/1 | 0.91 | 0.31 | 32,32,32,32 | 0 |
| 56 | MG | DU | 201 | 1/1 | 0.91 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3245 | 1/1 | 0.91 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | AA | 1743 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3016 | 1/1 | 0.91 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1738 | 1/1 | 0.91 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3233 | 1/1 | 0.91 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1629 | 1/1 | 0.91 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | BB | 218 | 1/1 | 0.91 | 0.12 | 36,36,36,36 | 1 |
| 56 | MG | DA | 3197 | 1/1 | 0.91 | 0.16 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1729 | 1/1 | 0.91 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3111 | 1/1 | 0.91 | 0.16 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3167 | 1/1 | 0.91 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1796 | 1/1 | 0.91 | 0.10 | 10,10,10,10 | 1 |
| 56 | MG | CA | 1737 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | AV | 106 | 1/1 | 0.91 | 0.07 | 40,40,40,40 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1792 | 1/1 | 0.91 | 0.19 | 74,74,74,74 | 0 |
| 56 | MG | BA | 3231 | 1/1 | 0.91 | 0.42 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3160 | 1/1 | 0.91 | 0.12 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3448 | 1/1 | 0.91 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | BB | 214 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3358 | 1/1 | 0.91 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1780 | 1/1 | 0.91 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | AA | 1627 | 1/1 | 0.91 | 0.45 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3298 | 1/1 | 0.91 | 0.14 | 5,5,5,5 | 0 |
| 56 | MG | DA | 3069 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | BB | 206 | 1/1 | 0.91 | 0.38 | 78,78,78,78 | 0 |
| 56 | MG | BA | 3294 | 1/1 | 0.91 | 0.10 | 6,6,6,6 | 0 |
| 56 | MG | CA | 1711 | 1/1 | 0.91 | 0.29 | 63,63,63,63 | 0 |
| 56 | MG | CA | 1760 | 1/1 | 0.91 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1638 | 1/1 | 0.91 | 0.24 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3343 | 1/1 | 0.91 | 0.30 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3051 | 1/1 | 0.91 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | AA | 1808 | 1/1 | 0.91 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | CA | 1772 | 1/1 | 0.91 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3322 | 1/1 | 0.91 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3393 | 1/1 | 0.91 | 0.13 | 80,80,80,80 | 0 |
| 56 | MG | DF | 301 | 1/1 | 0.91 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3410 | 1/1 | 0.91 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | CA | 1633 | 1/1 | 0.91 | 0.27 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3201 | 1/1 | 0.91 | 0.18 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3392 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3388 | 1/1 | 0.92 | 0.22 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3277 | 1/1 | 0.92 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3308 | 1/1 | 0.92 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | CA | 1694 | 1/1 | 0.92 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | CA | 1661 | 1/1 | 0.92 | 0.17 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1601 | 1/1 | 0.92 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | B2 | 101 | 1/1 | 0.92 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3071 | 1/1 | 0.92 | 0.24 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1635 | 1/1 | 0.92 | 0.09 | 16,16,16,16 | 0 |
| 56 | MG | AA | 1809 | 1/1 | 0.92 | 0.17 | 40,40,40,40 | 1 |
| 56 | MG | CA | 1775 | 1/1 | 0.92 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3270 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3383 | 1/1 | 0.92 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3116 | 1/1 | 0.92 | 0.11 | 10,10,10,10 | 0 |
| 56 | MG | AA | 1640 | 1/1 | 0.92 | 0.29 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1615 | 1/1 | 0.92 | 0.12 | 33,33,33,33 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1731 | 1/1 | 0.92 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3157 | 1/1 | 0.92 | 0.28 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3431 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | AA | 1755 | 1/1 | 0.92 | 0.26 | 47,47,47,47 | 0 |
| 56 | MG | AA | 1632 | 1/1 | 0.92 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3350 | 1/1 | 0.92 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3040 | 1/1 | 0.92 | 0.04 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3267 | 1/1 | 0.92 | 0.13 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1686 | 1/1 | 0.92 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1700 | 1/1 | 0.92 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | CA | 1682 | 1/1 | 0.92 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3180 | 1/1 | 0.92 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1715 | 1/1 | 0.92 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3379 | 1/1 | 0.92 | 0.22 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3450 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3172 | 1/1 | 0.92 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3158 | 1/1 | 0.92 | 0.26 | 44,44,44,44 | 0 |
| 56 | MG | AA | 1783 | 1/1 | 0.92 | 0.37 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3228 | 1/1 | 0.92 | 0.15 | 19,19,19,19 | 0 |
| 56 | MG | BV | 201 | 1/1 | 0.92 | 0.12 | 23,23,23,23 | 0 |
| 56 | MG | CA | 1769 | 1/1 | 0.92 | 0.11 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3150 | 1/1 | 0.92 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3279 | 1/1 | 0.92 | 0.19 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3316 | 1/1 | 0.92 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3052 | 1/1 | 0.92 | 0.24 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3190 | 1/1 | 0.92 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | CA | 1788 | 1/1 | 0.92 | 0.21 | 42,42,42,42 | 1 |
| 56 | MG | AA | 1807 | 1/1 | 0.92 | 0.12 | 19,19,19,19 | 1 |
| 56 | MG | BA | 3318 | 1/1 | 0.92 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | CA | 1665 | 1/1 | 0.92 | 0.43 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3296 | 1/1 | 0.92 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | DA | 3333 | 1/1 | 0.92 | 0.23 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3188 | 1/1 | 0.92 | 0.32 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3250 | 1/1 | 0.92 | 0.19 | 22,22,22,22 | 1 |
| 56 | MG | CA | 1776 | 1/1 | 0.92 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3439 | 1/1 | 0.92 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3214 | 1/1 | 0.92 | 0.39 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1639 | 1/1 | 0.92 | 0.23 | 71,71,71,71 | 0 |
| 56 | MG | CV | 101 | 1/1 | 0.92 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1737 | 1/1 | 0.92 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | CA | 1758 | 1/1 | 0.92 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3061 | 1/1 | 0.92 | 0.16 | 0,0,0,0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3257 | 1/1 | 0.92 | 0.19 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3362 | 1/1 | 0.93 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | BA | 3370 | 1/1 | 0.93 | 0.28 | 28,28,28,28 | 1 |
| 56 | MG | BA | 3253 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | AA | 1791 | 1/1 | 0.93 | 0.45 | 22,22,22,22 | 1 |
| 56 | MG | CA | 1698 | 1/1 | 0.93 | 0.37 | 42,42,42,42 | 0 |
| 56 | MG | AW | 101 | 1/1 | 0.93 | 0.35 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3324 | 1/1 | 0.93 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | CA | 1721 | 1/1 | 0.93 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | AA | 1764 | 1/1 | 0.93 | 0.10 | 6,6,6,6 | 0 |
| 56 | MG | BA | 3215 | 1/1 | 0.93 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3269 | 1/1 | 0.93 | 0.32 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1674 | 1/1 | 0.93 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1811 | 1/1 | 0.93 | 0.12 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3325 | 1/1 | 0.93 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | CA | 1672 | 1/1 | 0.93 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1758 | 1/1 | 0.93 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | AA | 1678 | 1/1 | 0.93 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | BB | 210 | 1/1 | 0.93 | 0.10 | 33,33,33,33 | 1 |
| 56 | MG | CA | 1671 | 1/1 | 0.93 | 0.26 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1695 | 1/1 | 0.93 | 0.18 | 13,13,13,13 | 1 |
| 56 | MG | CW | 102 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | DA | 3230 | 1/1 | 0.93 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3120 | 1/1 | 0.93 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3318 | 1/1 | 0.93 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1611 | 1/1 | 0.93 | 0.27 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3313 | 1/1 | 0.93 | 0.12 | 35,35,35,35 | 1 |
| 56 | MG | DA | 3309 | 1/1 | 0.93 | 0.13 | 6,6,6,6 | 0 |
| 56 | MG | AA | 1648 | 1/1 | 0.93 | 0.19 | 86,86,86,86 | 0 |
| 56 | MG | AA | 1681 | 1/1 | 0.93 | 0.13 | 21,21,21,21 | 0 |
| 57 | PAR | AA | 1816 | 42/42 | 0.93 | 0.16 | 15,20,38,42 | 0 |
| 56 | MG | BA | 3155 | 1/1 | 0.93 | 0.44 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3339 | 1/1 | 0.93 | 0.07 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3299 | 1/1 | 0.93 | 0.19 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3106 | 1/1 | 0.93 | 0.15 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3228 | 1/1 | 0.93 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | DA | 3321 | 1/1 | 0.93 | 0.11 | 45,45,45,45 | 1 |
| 56 | MG | CA | 1741 | 1/1 | 0.93 | 0.31 | 40,40,40,40 | 0 |
| 56 | MG | CA | 1702 | 1/1 | 0.93 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1674 | 1/1 | 0.93 | 0.24 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1769 | 1/1 | 0.93 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | AA | 1785 | 1/1 | 0.93 | 0.15 | 32,32,32,32 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3341 | 1/1 | 0.93 | 0.11 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3268 | 1/1 | 0.93 | 0.14 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3140 | 1/1 | 0.93 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | CA | 1718 | 1/1 | 0.93 | 0.22 | 47,47,47,47 | 0 |
| 56 | MG | DA | 3148 | 1/1 | 0.93 | 0.14 | 5,5,5,5 | 0 |
| 56 | MG | DA | 3214 | 1/1 | 0.93 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3367 | 1/1 | 0.93 | 0.11 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3348 | 1/1 | 0.93 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | CA | 1787 | 1/1 | 0.93 | 0.29 | 39,39,39,39 | 1 |
| 56 | MG | DA | 3006 | 1/1 | 0.93 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | CA | 1762 | 1/1 | 0.93 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3168 | 1/1 | 0.93 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | CA | 1713 | 1/1 | 0.93 | 0.19 | 93,93,93,93 | 0 |
| 56 | MG | CA | 1738 | 1/1 | 0.93 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3428 | 1/1 | 0.93 | 0.49 | 72,72,72,72 | 1 |
| 56 | MG | DA | 3096 | 1/1 | 0.93 | 0.24 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3144 | 1/1 | 0.93 | 0.16 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3288 | 1/1 | 0.93 | 0.23 | 32,32,32,32 | 1 |
| 56 | MG | DB | 205 | 1/1 | 0.93 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | DB | 207 | 1/1 | 0.93 | 0.21 | 52,52,52,52 | 1 |
| 56 | MG | AA | 1786 | 1/1 | 0.93 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | AA | 1784 | 1/1 | 0.93 | 0.29 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3407 | 1/1 | 0.93 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1765 | 1/1 | 0.93 | 0.05 | 43,43,43,43 | 0 |
| 56 | MG | CA | 1670 | 1/1 | 0.93 | 0.13 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3058 | 1/1 | 0.93 | 0.20 | 6,6,6,6 | 0 |
| 56 | MG | AW | 111 | 1/1 | 0.93 | 0.25 | 32,32,32,32 | 1 |
| 56 | MG | BA | 3447 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3003 | 1/1 | 0.93 | 0.20 | 28,28,28,28 | 0 |
| 56 | MG | CA | 1708 | 1/1 | 0.93 | 0.30 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3442 | 1/1 | 0.93 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3360 | 1/1 | 0.93 | 0.34 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3216 | 1/1 | 0.93 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3454 | 1/1 | 0.93 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3263 | 1/1 | 0.93 | 0.07 | 4,4,4,4 | 0 |
| 56 | MG | CA | 1612 | 1/1 | 0.93 | 0.09 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3218 | 1/1 | 0.93 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | AA | 1654 | 1/1 | 0.93 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3390 | 1/1 | 0.93 | 0.11 | 20,20,20,20 | 1 |
| 56 | MG | BA | 3276 | 1/1 | 0.93 | 0.09 | 6,6,6,6 | 0 |
| 56 | MG | BA | 3259 | 1/1 | 0.93 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3375 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1735 | 1/1 | 0.93 | 0.18 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3053 | 1/1 | 0.93 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3351 | 1/1 | 0.93 | 0.18 | 16,16,16,16 | 0 |
| 56 | MG | AV | 103 | 1/1 | 0.93 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1803 | 1/1 | 0.93 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3126 | 1/1 | 0.93 | 0.09 | 1,1,1,1 | 0 |
| 57 | PAR | CA | 1790 | 42/42 | 0.93 | 0.17 | 7,11,29,33 | 0 |
| 56 | MG | BA | 3119 | 1/1 | 0.93 | 0.25 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3320 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3153 | 1/1 | 0.93 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3027 | 1/1 | 0.93 | 0.28 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3146 | 1/1 | 0.93 | 0.24 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3199 | 1/1 | 0.94 | 0.14 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3266 | 1/1 | 0.94 | 0.28 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3297 | 1/1 | 0.94 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3307 | 1/1 | 0.94 | 0.11 | 34,34,34,34 | 1 |
| 56 | MG | CA | 1601 | 1/1 | 0.94 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3144 | 1/1 | 0.94 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3030 | 1/1 | 0.94 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | DB | 208 | 1/1 | 0.94 | 0.17 | 9,9,9,9 | 0 |
| 56 | MG | AA | 1683 | 1/1 | 0.94 | 0.13 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3373 | 1/1 | 0.94 | 0.04 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1655 | 1/1 | 0.94 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1701 | 1/1 | 0.94 | 0.12 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3221 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3143 | 1/1 | 0.94 | 0.22 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1676 | 1/1 | 0.94 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3335 | 1/1 | 0.94 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | CA | 1649 | 1/1 | 0.94 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | CF | 201 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3088 | 1/1 | 0.94 | 0.30 | 35,35,35,35 | 0 |
| 56 | MG | CA | 1638 | 1/1 | 0.94 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | CA | 1720 | 1/1 | 0.94 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | AW | 102 | 1/1 | 0.94 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | DD | 302 | 1/1 | 0.94 | 0.09 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3354 | 1/1 | 0.94 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | CA | 1736 | 1/1 | 0.94 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | CA | 1650 | 1/1 | 0.94 | 0.24 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3180 | 1/1 | 0.94 | 0.26 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3366 | 1/1 | 0.94 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3086 | 1/1 | 0.94 | 0.21 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1617 | 1/1 | 0.94 | 0.09 | 25,25,25,25 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3314 | 1/1 | 0.94 | 0.45 | 47,47,47,47 | 1 |
| 56 | MG | DA | 3363 | 1/1 | 0.94 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | CA | 1779 | 1/1 | 0.94 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3217 | 1/1 | 0.94 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1609 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3256 | 1/1 | 0.94 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | AA | 1790 | 1/1 | 0.94 | 0.08 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3301 | 1/1 | 0.94 | 0.20 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3189 | 1/1 | 0.94 | 0.23 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3161 | 1/1 | 0.94 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3056 | 1/1 | 0.94 | 0.16 | 9,9,9,9 | 0 |
| 56 | MG | AA | 1616 | 1/1 | 0.94 | 0.14 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3396 | 1/1 | 0.94 | 0.16 | 27,27,27,27 | 1 |
| 56 | MG | BA | 3452 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | CA | 1654 | 1/1 | 0.94 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3384 | 1/1 | 0.94 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3102 | 1/1 | 0.94 | 0.11 | 15,15,15,15 | 0 |
| 56 | MG | AA | 1709 | 1/1 | 0.94 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3175 | 1/1 | 0.94 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3229 | 1/1 | 0.94 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | CA | 1676 | 1/1 | 0.94 | 0.36 | 46,46,46,46 | 0 |
| 56 | MG | B2 | 104 | 1/1 | 0.94 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3436 | 1/1 | 0.94 | 0.11 | 39,39,39,39 | 1 |
| 56 | MG | AA | 1604 | 1/1 | 0.94 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | CA | 1731 | 1/1 | 0.94 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | DA | 3152 | 1/1 | 0.94 | 0.10 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3088 | 1/1 | 0.94 | 0.20 | 4,4,4,4 | 0 |
| 56 | MG | DA | 3282 | 1/1 | 0.94 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | AW | 115 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3344 | 1/1 | 0.94 | 0.15 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3068 | 1/1 | 0.94 | 0.14 | 14,14,14,14 | 0 |
| 56 | MG | AA | 1619 | 1/1 | 0.94 | 0.33 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3028 | 1/1 | 0.94 | 0.30 | 36,36,36,36 | 0 |
| 56 | MG | BA | 3255 | 1/1 | 0.94 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | DB | 210 | 1/1 | 0.94 | 0.05 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3361 | 1/1 | 0.94 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3117 | 1/1 | 0.94 | 0.24 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3218 | 1/1 | 0.94 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3223 | 1/1 | 0.94 | 0.13 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3149 | 1/1 | 0.94 | 0.10 | 10,10,10,10 | 0 |
| 56 | MG | DA | 3232 | 1/1 | 0.94 | 0.12 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3141 | 1/1 | 0.94 | 0.10 | 20,20,20,20 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3203 | 1/1 | 0.94 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | DA | 3347 | 1/1 | 0.94 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | DA | 3204 | 1/1 | 0.94 | 0.12 | 8,8,8,8 | 0 |
| 56 | MG | CA | 1657 | 1/1 | 0.94 | 0.15 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3226 | 1/1 | 0.94 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3331 | 1/1 | 0.94 | 0.26 | 42,42,42,42 | 0 |
| 56 | MG | DA | 3122 | 1/1 | 0.94 | 0.18 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3304 | 1/1 | 0.94 | 0.06 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3135 | 1/1 | 0.94 | 0.13 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3010 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | B7 | 102 | 1/1 | 0.94 | 0.10 | 11,11,11,11 | 1 |
| 56 | MG | DA | 3074 | 1/1 | 0.94 | 0.22 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3012 | 1/1 | 0.94 | 0.16 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3243 | 1/1 | 0.94 | 0.13 | 18,18,18,18 | 0 |
| 56 | MG | CA | 1652 | 1/1 | 0.94 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | BA | 3174 | 1/1 | 0.94 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1757 | 1/1 | 0.94 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | BA | 3204 | 1/1 | 0.94 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3272 | 1/1 | 0.94 | 0.40 | 49,49,49,49 | 0 |
| 56 | MG | DA | 3151 | 1/1 | 0.94 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1653 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3170 | 1/1 | 0.94 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | DA | 3235 | 1/1 | 0.94 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | CA | 1768 | 1/1 | 0.94 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | CA | 1717 | 1/1 | 0.94 | 0.07 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3395 | 1/1 | 0.94 | 0.20 | 54,54,54,54 | 1 |
| 56 | MG | AA | 1690 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | AA | 1606 | 1/1 | 0.94 | 0.36 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1609 | 1/1 | 0.94 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1622 | 1/1 | 0.94 | 0.10 | 8,8,8,8 | 0 |
| 56 | MG | AA | 1630 | 1/1 | 0.94 | 0.10 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3130 | 1/1 | 0.94 | 0.15 | 14,14,14,14 | 0 |
| 56 | MG | CA | 1684 | 1/1 | 0.94 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1717 | 1/1 | 0.94 | 0.08 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1736 | 1/1 | 0.94 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3185 | 1/1 | 0.94 | 0.12 | 8,8,8,8 | 1 |
| 56 | MG | CA | 1724 | 1/1 | 0.94 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | DB | 211 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3309 | 1/1 | 0.95 | 0.15 | 14,14,14,14 | 0 |
| 56 | MG | AA | 1650 | 1/1 | 0.95 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | CA | 1667 | 1/1 | 0.95 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | CA | 1610 | 1/1 | 0.95 | 0.22 | 15,15,15,15 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AW | 105 | 1/1 | 0.95 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3380 | 1/1 | 0.95 | 0.33 | 77,77,77,77 | 0 |
| 56 | MG | BA | 3072 | 1/1 | 0.95 | 0.20 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3142 | 1/1 | 0.95 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | AA | 1773 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3406 | 1/1 | 0.95 | 0.16 | 18,18,18,18 | 0 |
| 56 | MG | CA | 1658 | 1/1 | 0.95 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3179 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3314 | 1/1 | 0.95 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | CA | 1620 | 1/1 | 0.95 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3069 | 1/1 | 0.95 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1673 | 1/1 | 0.95 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3317 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | CA | 1765 | 1/1 | 0.95 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3019 | 1/1 | 0.95 | 0.24 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1789 | 1/1 | 0.95 | 0.13 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3229 | 1/1 | 0.95 | 0.21 | 1,1,1,1 | 0 |
| 56 | MG | BA | 3148 | 1/1 | 0.95 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3082 | 1/1 | 0.95 | 0.18 | 10,10,10,10 | 0 |
| 56 | MG | CA | 1616 | 1/1 | 0.95 | 0.24 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3346 | 1/1 | 0.95 | 0.08 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3005 | 1/1 | 0.95 | 0.11 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3177 | 1/1 | 0.95 | 0.18 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3114 | 1/1 | 0.95 | 0.21 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1612 | 1/1 | 0.95 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | CA | 1626 | 1/1 | 0.95 | 0.14 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3162 | 1/1 | 0.95 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | BA | 3336 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3449 | 1/1 | 0.95 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3033 | 1/1 | 0.95 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1770 | 1/1 | 0.95 | 0.12 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3347 | 1/1 | 0.95 | 0.17 | 22,22,22,22 | 1 |
| 56 | MG | BA | 3287 | 1/1 | 0.95 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1725 | 1/1 | 0.95 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | CA | 1764 | 1/1 | 0.95 | 0.11 | 15,15,15,15 | 0 |
| 56 | MG | CA | 1781 | 1/1 | 0.95 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3361 | 1/1 | 0.95 | 0.27 | 5,5,5,5 | 0 |
| 56 | MG | BA | 3438 | 1/1 | 0.95 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3373 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3091 | 1/1 | 0.95 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3207 | 1/1 | 0.95 | 0.11 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3351 | 1/1 | 0.95 | 0.28 | 78,78,78,78 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3430 | 1/1 | 0.95 | 0.21 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3012 | 1/1 | 0.95 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1634 | 1/1 | 0.95 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | AA | 1668 | 1/1 | 0.95 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3405 | 1/1 | 0.95 | 0.09 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3252 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | AA | 1607 | 1/1 | 0.95 | 0.07 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3195 | 1/1 | 0.95 | 0.19 | 16,16,16,16 | 0 |
| 56 | MG | AX | 104 | 1/1 | 0.95 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | BA | 3392 | 1/1 | 0.95 | 0.11 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3075 | 1/1 | 0.95 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3145 | 1/1 | 0.95 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | CA | 1785 | 1/1 | 0.95 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3084 | 1/1 | 0.95 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | CA | 1636 | 1/1 | 0.95 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1726 | 1/1 | 0.95 | 0.11 | 12,12,12,12 | 0 |
| 56 | MG | AA | 1777 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | DA | 3037 | 1/1 | 0.95 | 0.12 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3441 | 1/1 | 0.95 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3402 | 1/1 | 0.95 | 0.18 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1684 | 1/1 | 0.95 | 0.13 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3207 | 1/1 | 0.95 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3328 | 1/1 | 0.95 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | AA | 1781 | 1/1 | 0.95 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3191 | 1/1 | 0.95 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3240 | 1/1 | 0.95 | 0.23 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3034 | 1/1 | 0.95 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3401 | 1/1 | 0.95 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3292 | 1/1 | 0.95 | 0.12 | 14,14,14,14 | 0 |
| 56 | MG | BF | 302 | 1/1 | 0.95 | 0.24 | 46,46,46,46 | 0 |
| 56 | MG | AA | 1706 | 1/1 | 0.95 | 0.09 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3416 | 1/1 | 0.95 | 0.15 | 16,16,16,16 | 0 |
| 56 | MG | DB | 203 | 1/1 | 0.95 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3186 | 1/1 | 0.95 | 0.24 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3241 | 1/1 | 0.95 | 0.10 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3211 | 1/1 | 0.95 | 0.10 | 1,1,1,1 | 0 |
| 56 | MG | AA | 1687 | 1/1 | 0.95 | 0.12 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3364 | 1/1 | 0.95 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3374 | 1/1 | 0.95 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3147 | 1/1 | 0.95 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3112 | 1/1 | 0.95 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3115 | 1/1 | 0.95 | 0.11 | 16,16,16,16 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3014 | 1/1 | 0.95 | 0.18 | 4,4,4,4 | 0 |
| 56 | MG | CA | 1625 | 1/1 | 0.95 | 0.20 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3364 | 1/1 | 0.95 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3426 | 1/1 | 0.95 | 0.09 | 3,3,3,3 | 0 |
| 56 | MG | CA | 1690 | 1/1 | 0.95 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3205 | 1/1 | 0.95 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3093 | 1/1 | 0.95 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | CA | 1602 | 1/1 | 0.95 | 0.12 | 14,14,14,14 | 0 |
| 56 | MG | BA | 3139 | 1/1 | 0.95 | 0.11 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3201 | 1/1 | 0.95 | 0.20 | 21,21,21,21 | 0 |
| 56 | MG | DA | 3001 | 1/1 | 0.95 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1804 | 1/1 | 0.95 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | CA | 1746 | 1/1 | 0.95 | 0.26 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1685 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3236 | 1/1 | 0.95 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | DE | 301 | 1/1 | 0.95 | 0.23 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1602 | 1/1 | 0.95 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3093 | 1/1 | 0.95 | 0.13 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3248 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 56 | MG | AW | 106 | 1/1 | 0.95 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3019 | 1/1 | 0.95 | 0.32 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3122 | 1/1 | 0.95 | 0.13 | 8,8,8,8 | 0 |
| 56 | MG | AA | 1721 | 1/1 | 0.95 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3146 | 1/1 | 0.95 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | AW | 112 | 1/1 | 0.95 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | BX | 101 | 1/1 | 0.95 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3197 | 1/1 | 0.95 | 0.12 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1631 | 1/1 | 0.95 | 0.28 | 21,21,21,21 | 0 |
| 56 | MG | DA | 3253 | 1/1 | 0.95 | 0.15 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3354 | 1/1 | 0.95 | 0.06 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3026 | 1/1 | 0.95 | 0.22 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3007 | 1/1 | 0.95 | 0.31 | 39,39,39,39 | 0 |
| 56 | MG | AA | 1812 | 1/1 | 0.95 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1814 | 1/1 | 0.95 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3399 | 1/1 | 0.95 | 0.19 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3061 | 1/1 | 0.95 | 0.25 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3035 | 1/1 | 0.95 | 0.28 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3311 | 1/1 | 0.95 | 0.08 | 2,2,2,2 | 0 |
| 56 | MG | AA | 1666 | 1/1 | 0.95 | 0.18 | 1,1,1,1 | 0 |
| 56 | MG | CA | 1683 | 1/1 | 0.95 | 0.10 | 2,2,2,2 | 0 |
| 56 | MG | DA | 3150 | 1/1 | 0.95 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | BB | 219 | 1/1 | 0.95 | 0.08 | 24,24,24,24 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1692 | 1/1 | 0.95 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1756 | 1/1 | 0.95 | 0.22 | 15,15,15,15 | 0 |
| 56 | MG | BB | 215 | 1/1 | 0.95 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | CA | 1727 | 1/1 | 0.95 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3183 | 1/1 | 0.95 | 0.07 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3384 | 1/1 | 0.95 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3285 | 1/1 | 0.95 | 0.20 | 15,15,15,15 | 0 |
| 56 | MG | CA | 1705 | 1/1 | 0.95 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3234 | 1/1 | 0.95 | 0.26 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3163 | 1/1 | 0.96 | 0.13 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3338 | 1/1 | 0.96 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | CU | 101 | 1/1 | 0.96 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | AW | 109 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 1 |
| 56 | MG | BA | 3242 | 1/1 | 0.96 | 0.08 | 4,4,4,4 | 0 |
| 56 | MG | DA | 3102 | 1/1 | 0.96 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1671 | 1/1 | 0.96 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3305 | 1/1 | 0.96 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3417 | 1/1 | 0.96 | 0.30 | 29,29,29,29 | 0 |
| 56 | MG | CA | 1766 | 1/1 | 0.96 | 0.23 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3324 | 1/1 | 0.96 | 0.15 | 18,18,18,18 | 1 |
| 56 | MG | BA | 3389 | 1/1 | 0.96 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1760 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | BA | 3065 | 1/1 | 0.96 | 0.09 | 1,1,1,1 | 0 |
| 56 | MG | DA | 3370 | 1/1 | 0.96 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3081 | 1/1 | 0.96 | 0.20 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3191 | 1/1 | 0.96 | 0.23 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3337 | 1/1 | 0.96 | 0.06 | 4,4,4,4 | 0 |
| 56 | MG | AA | 1669 | 1/1 | 0.96 | 0.40 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3071 | 1/1 | 0.96 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1667 | 1/1 | 0.96 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | AA | 1752 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | CA | 1656 | 1/1 | 0.96 | 0.08 | 14,14,14,14 | 0 |
| 56 | MG | BA | 3038 | 1/1 | 0.96 | 0.22 | 10,10,10,10 | 0 |
| 56 | MG | DA | 3018 | 1/1 | 0.96 | 0.09 | 3,3,3,3 | 0 |
| 56 | MG | DA | 3365 | 1/1 | 0.96 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3305 | 1/1 | 0.96 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | CA | 1693 | 1/1 | 0.96 | 0.15 | 18,18,18,18 | 1 |
| 56 | MG | BA | 3029 | 1/1 | 0.96 | 0.22 | 30,30,30,30 | 0 |
| 56 | MG | CA | 1756 | 1/1 | 0.96 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3234 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3100 | 1/1 | 0.96 | 0.22 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1617 | 1/1 | 0.96 | 0.28 | 24,24,24,24 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1815 | 1/1 | 0.96 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | CA | 1632 | 1/1 | 0.96 | 0.06 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3215 | 1/1 | 0.96 | 0.05 | 31,31,31,31 | 0 |
| 56 | MG | CA | 1780 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3022 | 1/1 | 0.96 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3271 | 1/1 | 0.96 | 0.32 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3280 | 1/1 | 0.96 | 0.12 | 10,10,10,10 | 0 |
| 56 | MG | CA | 1748 | 1/1 | 0.96 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3128 | 1/1 | 0.96 | 0.16 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1623 | 1/1 | 0.96 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1628 | 1/1 | 0.96 | 0.14 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3193 | 1/1 | 0.96 | 0.22 | 8,8,8,8 | 0 |
| 56 | MG | DA | 3011 | 1/1 | 0.96 | 0.20 | 11,11,11,11 | 0 |
| 56 | MG | CA | 1648 | 1/1 | 0.96 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3371 | 1/1 | 0.96 | 0.09 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3411 | 1/1 | 0.96 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | DA | 3052 | 1/1 | 0.96 | 0.16 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3192 | 1/1 | 0.96 | 0.13 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3311 | 1/1 | 0.96 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3315 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | BA | 3104 | 1/1 | 0.96 | 0.18 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3183 | 1/1 | 0.96 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3199 | 1/1 | 0.96 | 0.09 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3200 | 1/1 | 0.96 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | AV | 101 | 1/1 | 0.96 | 0.06 | 5,5,5,5 | 0 |
| 56 | MG | BA | 3049 | 1/1 | 0.96 | 0.28 | 36,36,36,36 | 0 |
| 56 | MG | B5 | 102 | 1/1 | 0.96 | 0.29 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3308 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3098 | 1/1 | 0.96 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3066 | 1/1 | 0.96 | 0.23 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3394 | 1/1 | 0.96 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | CA | 1641 | 1/1 | 0.96 | 0.16 | 13,13,13,13 | 0 |
| 56 | MG | CA | 1715 | 1/1 | 0.96 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | BA | 3156 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1793 | 1/1 | 0.96 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | DA | 3247 | 1/1 | 0.96 | 0.21 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1779 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | BA | 3165 | 1/1 | 0.96 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | BO | 201 | 1/1 | 0.96 | 0.18 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3243 | 1/1 | 0.96 | 0.08 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3015 | 1/1 | 0.96 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3162 | 1/1 | 0.96 | 0.19 | 12,12,12,12 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1747 | 1/1 | 0.96 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3167 | 1/1 | 0.96 | 0.11 | 101,101,101,101 | 0 |
| 56 | MG | DA | 3264 | 1/1 | 0.96 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | AA | 1788 | 1/1 | 0.96 | 0.09 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3113 | 1/1 | 0.96 | 0.09 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3377 | 1/1 | 0.96 | 0.10 | 6,6,6,6 | 1 |
| 56 | MG | DA | 3349 | 1/1 | 0.96 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | DA | 3291 | 1/1 | 0.96 | 0.10 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3423 | 1/1 | 0.96 | 0.16 | 21,21,21,21 | 0 |
| 56 | MG | DA | 3316 | 1/1 | 0.96 | 0.12 | 7,7,7,7 | 0 |
| 56 | MG | CA | 1735 | 1/1 | 0.96 | 0.16 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3293 | 1/1 | 0.96 | 0.10 | 2,2,2,2 | 0 |
| 56 | MG | DA | 3222 | 1/1 | 0.96 | 0.23 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3116 | 1/1 | 0.96 | 0.30 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3125 | 1/1 | 0.96 | 0.31 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3126 | 1/1 | 0.96 | 0.08 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3090 | 1/1 | 0.96 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | BB | 211 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 1 |
| 56 | MG | BA | 3396 | 1/1 | 0.96 | 0.18 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3021 | 1/1 | 0.96 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | CA | 1607 | 1/1 | 0.96 | 0.19 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3337 | 1/1 | 0.96 | 0.05 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3348 | 1/1 | 0.96 | 0.18 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3398 | 1/1 | 0.96 | 0.13 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3420 | 1/1 | 0.96 | 0.25 | 59,59,59,59 | 1 |
| 56 | MG | BA | 3326 | 1/1 | 0.96 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3339 | 1/1 | 0.96 | 0.10 | 0,0,0,0 | 1 |
| 56 | MG | DA | 3269 | 1/1 | 0.96 | 0.35 | 33,33,33,33 | 0 |
| 56 | MG | AA | 1611 | 1/1 | 0.96 | 0.15 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3300 | 1/1 | 0.96 | 0.14 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3120 | 1/1 | 0.96 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3280 | 1/1 | 0.96 | 0.06 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3186 | 1/1 | 0.96 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3251 | 1/1 | 0.96 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | CA | 1677 | 1/1 | 0.96 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1778 | 1/1 | 0.96 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | CW | 106 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 1 |
| 56 | MG | CA | 1605 | 1/1 | 0.96 | 0.07 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3381 | 1/1 | 0.96 | 0.10 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1689 | 1/1 | 0.96 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | DA | 3289 | 1/1 | 0.96 | 0.09 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3044 | 1/1 | 0.96 | 0.14 | 15,15,15,15 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1703 | 1/1 | 0.96 | 0.22 | 23,23,23,23 | 0 |
| 56 | MG | AW | 108 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3206 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3151 | 1/1 | 0.96 | 0.07 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3220 | 1/1 | 0.96 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | CA | 1668 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3101 | 1/1 | 0.96 | 0.12 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3017 | 1/1 | 0.96 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1680 | 1/1 | 0.96 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3184 | 1/1 | 0.96 | 0.09 | 10,10,10,10 | 0 |
| 56 | MG | DA | 3101 | 1/1 | 0.96 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | BA | 3184 | 1/1 | 0.96 | 0.16 | 1,1,1,1 | 0 |
| 56 | MG | BA | 3267 | 1/1 | 0.96 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3352 | 1/1 | 0.96 | 0.11 | 9,9,9,9 | 0 |
| 56 | MG | DA | 3112 | 1/1 | 0.96 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3453 | 1/1 | 0.96 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | BA | 3006 | 1/1 | 0.96 | 0.26 | 24,24,24,24 | 0 |
| 56 | MG | AA | 1742 | 1/1 | 0.96 | 0.40 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3236 | 1/1 | 0.96 | 0.10 | 3,3,3,3 | 0 |
| 56 | MG | CA | 1635 | 1/1 | 0.96 | 0.21 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3202 | 1/1 | 0.96 | 0.20 | 37,37,37,37 | 0 |
| 56 | MG | DA | 3109 | 1/1 | 0.96 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1775 | 1/1 | 0.96 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | AA | 1741 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | CA | 1681 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | BA | 3421 | 1/1 | 0.96 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | CA | 1728 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | BA | 3032 | 1/1 | 0.96 | 0.07 | 17,17,17,17 | 0 |
| 56 | MG | CA | 1608 | 1/1 | 0.96 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | DB | 212 | 1/1 | 0.96 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | BA | 3057 | 1/1 | 0.96 | 0.27 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3094 | 1/1 | 0.96 | 0.09 | 10,10,10,10 | 0 |
| 56 | MG | AA | 1787 | 1/1 | 0.96 | 0.09 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3376 | 1/1 | 0.96 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | CA | 1782 | 1/1 | 0.96 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3340 | 1/1 | 0.96 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3327 | 1/1 | 0.96 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3040 | 1/1 | 0.96 | 0.05 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3304 | 1/1 | 0.96 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3063 | 1/1 | 0.96 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3205 | 1/1 | 0.96 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3105 | 1/1 | 0.96 | 0.18 | 6,6,6,6 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3350 | 1/1 | 0.96 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3055 | 1/1 | 0.96 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3288 | 1/1 | 0.96 | 0.08 | 25,25,25,25 | 1 |
| 56 | MG | CA | 1704 | 1/1 | 0.96 | 0.10 | 5,5,5,5 | 0 |
| 56 | MG | CA | 1603 | 1/1 | 0.96 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3054 | 1/1 | 0.96 | 0.13 | 5,5,5,5 | 0 |
| 56 | MG | DA | 3359 | 1/1 | 0.97 | 0.25 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3110 | 1/1 | 0.97 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1603 | 1/1 | 0.97 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3264 | 1/1 | 0.97 | 0.24 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3023 | 1/1 | 0.97 | 0.28 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3302 | 1/1 | 0.97 | 0.09 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3246 | 1/1 | 0.97 | 0.14 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3287 | 1/1 | 0.97 | 0.25 | 17,17,17,17 | 0 |
| 56 | MG | AV | 104 | 1/1 | 0.97 | 0.17 | 27,27,27,27 | 0 |
| 56 | MG | AA | 1614 | 1/1 | 0.97 | 0.07 | 19,19,19,19 | 0 |
| 56 | MG | D5 | 101 | 1/1 | 0.97 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | AA | 1710 | 1/1 | 0.97 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | DA | 3099 | 1/1 | 0.97 | 0.12 | 10,10,10,10 | 0 |
| 56 | MG | DA | 3041 | 1/1 | 0.97 | 0.19 | 8,8,8,8 | 0 |
| 56 | MG | AA | 1644 | 1/1 | 0.97 | 0.16 | 17,17,17,17 | 0 |
| 56 | MG | AW | 114 | 1/1 | 0.97 | 0.10 | 25,25,25,25 | 1 |
| 56 | MG | BA | 3387 | 1/1 | 0.97 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | DA | 3260 | 1/1 | 0.97 | 0.37 | 44,44,44,44 | 0 |
| 56 | MG | DA | 3020 | 1/1 | 0.97 | 0.30 | 1,1,1,1 | 0 |
| 56 | MG | DA | 3157 | 1/1 | 0.97 | 0.25 | 34,34,34,34 | 0 |
| 56 | MG | BA | 3136 | 1/1 | 0.97 | 0.21 | 8,8,8,8 | 0 |
| 56 | MG | AA | 1801 | 1/1 | 0.97 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | AA | 1700 | 1/1 | 0.97 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3118 | 1/1 | 0.97 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1739 | 1/1 | 0.97 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | CA | 1655 | 1/1 | 0.97 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3073 | 1/1 | 0.97 | 0.08 | 4,4,4,4 | 0 |
| 56 | MG | DA | 3166 | 1/1 | 0.97 | 0.08 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3254 | 1/1 | 0.97 | 0.10 | 1,1,1,1 | 0 |
| 56 | MG | AA | 1754 | 1/1 | 0.97 | 0.12 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3139 | 1/1 | 0.97 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3283 | 1/1 | 0.97 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3033 | 1/1 | 0.97 | 0.20 | 17,17,17,17 | 1 |
| 56 | MG | DA | 3114 | 1/1 | 0.97 | 0.09 | 8,8,8,8 | 0 |
| 56 | MG | DA | 3194 | 1/1 | 0.97 | 0.10 | 0,0,0,0 | 1 |
| 56 | MG | DA | 3226 | 1/1 | 0.97 | 0.08 | 5,5,5,5 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3194 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | BA | 3208 | 1/1 | 0.97 | 0.11 | 8,8,8,8 | 0 |
| 56 | MG | DA | 3026 | 1/1 | 0.97 | 0.26 | 0,0,0,0 | 0 |
| 56 | MG | CW | 105 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | AX | 103 | 1/1 | 0.97 | 0.08 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3440 | 1/1 | 0.97 | 0.19 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3189 | 1/1 | 0.97 | 0.10 | 3,3,3,3 | 0 |
| 56 | MG | AW | 119 | 1/1 | 0.97 | 0.06 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3266 | 1/1 | 0.97 | 0.07 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3203 | 1/1 | 0.97 | 0.21 | 14,14,14,14 | 0 |
| 56 | MG | BA | 3164 | 1/1 | 0.97 | 0.06 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3008 | 1/1 | 0.97 | 0.38 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3220 | 1/1 | 0.97 | 0.10 | 3,3,3,3 | 0 |
| 56 | MG | BB | 208 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | CA | 1640 | 1/1 | 0.97 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3323 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3010 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | AA | 1645 | 1/1 | 0.97 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | AA | 1636 | 1/1 | 0.97 | 0.20 | 27,27,27,27 | 1 |
| 56 | MG | DA | 3388 | 1/1 | 0.97 | 0.16 | 15,15,15,15 | 0 |
| 56 | MG | CW | 103 | 1/1 | 0.97 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3080 | 1/1 | 0.97 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1660 | 1/1 | 0.97 | 0.23 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3042 | 1/1 | 0.97 | 0.56 | 58,58,58,58 | 0 |
| 56 | MG | AA | 1621 | 1/1 | 0.97 | 0.10 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3076 | 1/1 | 0.97 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1634 | 1/1 | 0.97 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3024 | 1/1 | 0.97 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3302 | 1/1 | 0.97 | 0.18 | 14,14,14,14 | 0 |
| 56 | MG | CA | 1712 | 1/1 | 0.97 | 0.16 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3301 | 1/1 | 0.97 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | BF | 301 | 1/1 | 0.97 | 0.16 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3087 | 1/1 | 0.97 | 0.20 | 16,16,16,16 | 0 |
| 56 | MG | AV | 102 | 1/1 | 0.97 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | BA | 3200 | 1/1 | 0.97 | 0.07 | 5,5,5,5 | 1 |
| 56 | MG | BA | 3271 | 1/1 | 0.97 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3209 | 1/1 | 0.97 | 0.31 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3172 | 1/1 | 0.97 | 0.16 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3103 | 1/1 | 0.97 | 0.13 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3211 | 1/1 | 0.97 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1608 | 1/1 | 0.97 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | BA | 3063 | 1/1 | 0.97 | 0.25 | 0,0,0,0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | CA | 1686 | 1/1 | 0.97 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | BA | 3235 | 1/1 | 0.97 | 0.06 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3195 | 1/1 | 0.97 | 0.14 | 0,0,0,0 | 1 |
| 56 | MG | DA | 3332 | 1/1 | 0.97 | 0.06 | 45,45,45,45 | 0 |
| 56 | MG | AA | 1664 | 1/1 | 0.97 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | CW | 108 | 1/1 | 0.97 | 0.04 | 10,10,10,10 | 1 |
| 56 | MG | BA | 3173 | 1/1 | 0.97 | 0.16 | 14,14,14,14 | 0 |
| 56 | MG | AA | 1766 | 1/1 | 0.97 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | CA | 1710 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | CA | 1755 | 1/1 | 0.97 | 0.16 | 26,26,26,26 | 1 |
| 56 | MG | DA | 3060 | 1/1 | 0.97 | 0.31 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3418 | 1/1 | 0.97 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | BA | 3138 | 1/1 | 0.97 | 0.17 | 12,12,12,12 | 0 |
| 56 | MG | CA | 1651 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3083 | 1/1 | 0.97 | 0.24 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1605 | 1/1 | 0.97 | 0.09 | 16,16,16,16 | 0 |
| 56 | MG | AW | 122 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3108 | 1/1 | 0.97 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1798 | 1/1 | 0.97 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3182 | 1/1 | 0.97 | 0.09 | 5,5,5,5 | 0 |
| 56 | MG | BA | 3260 | 1/1 | 0.97 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | DA | 3382 | 1/1 | 0.97 | 0.09 | 6,6,6,6 | 0 |
| 56 | MG | CA | 1749 | 1/1 | 0.97 | 0.08 | 7,7,7,7 | 0 |
| 56 | MG | CW | 113 | 1/1 | 0.97 | 0.05 | 24,24,24,24 | 0 |
| 56 | MG | BA | 3434 | 1/1 | 0.97 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | AA | 1720 | 1/1 | 0.97 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | BB | 217 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | CA | 1709 | 1/1 | 0.97 | 0.07 | 9,9,9,9 | 0 |
| 56 | MG | AA | 1691 | 1/1 | 0.97 | 0.07 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3136 | 1/1 | 0.97 | 0.21 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3432 | 1/1 | 0.97 | 0.07 | 15,15,15,15 | 0 |
| 56 | MG | AA | 1702 | 1/1 | 0.97 | 0.21 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3086 | 1/1 | 0.97 | 0.13 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3011 | 1/1 | 0.97 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3070 | 1/1 | 0.97 | 0.18 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3223 | 1/1 | 0.97 | 0.31 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3210 | 1/1 | 0.97 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3068 | 1/1 | 0.97 | 0.18 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3368 | 1/1 | 0.97 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | BA | 3298 | 1/1 | 0.97 | 0.31 | 25,25,25,25 | 0 |
| 56 | MG | AA | 1762 | 1/1 | 0.97 | 0.14 | 18,18,18,18 | 0 |
| 56 | MG | BA | 3363 | 1/1 | 0.97 | 0.09 | 8,8,8,8 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1682 | 1/1 | 0.97 | 0.19 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3118 | 1/1 | 0.97 | 0.09 | 6,6,6,6 | 0 |
| 56 | MG | DA | 3256 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | DA | 3164 | 1/1 | 0.97 | 0.07 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3245 | 1/1 | 0.97 | 0.11 | 9,9,9,9 | 0 |
| 56 | MG | DA | 3034 | 1/1 | 0.97 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3031 | 1/1 | 0.97 | 0.08 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3322 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | CA | 1662 | 1/1 | 0.97 | 0.09 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3290 | 1/1 | 0.97 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1723 | 1/1 | 0.97 | 0.07 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3171 | 1/1 | 0.97 | 0.10 | 0,0,0,0 | 1 |
| 56 | MG | DA | 3029 | 1/1 | 0.97 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | AA | 1753 | 1/1 | 0.97 | 0.11 | 26,26,26,26 | 0 |
| 56 | MG | CA | 1733 | 1/1 | 0.97 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3045 | 1/1 | 0.97 | 0.14 | 1,1,1,1 | 0 |
| 56 | MG | BA | 3185 | 1/1 | 0.97 | 0.04 | 9,9,9,9 | 0 |
| 56 | MG | AA | 1642 | 1/1 | 0.97 | 0.14 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3313 | 1/1 | 0.97 | 0.11 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3306 | 1/1 | 0.97 | 0.20 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3284 | 1/1 | 0.97 | 0.13 | 12,12,12,12 | 0 |
| 56 | MG | B1 | 101 | 1/1 | 0.97 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3239 | 1/1 | 0.97 | 0.25 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3123 | 1/1 | 0.97 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3319 | 1/1 | 0.97 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3105 | 1/1 | 0.97 | 0.19 | 13,13,13,13 | 0 |
| 56 | MG | DA | 3104 | 1/1 | 0.97 | 0.12 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3080 | 1/1 | 0.97 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3281 | 1/1 | 0.97 | 0.20 | 14,14,14,14 | 1 |
| 56 | MG | BB | 207 | 1/1 | 0.97 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | BA | 3291 | 1/1 | 0.97 | 0.05 | 12,12,12,12 | 0 |
| 58 | ZN | AN | 101 | 1/1 | 0.97 | 0.05 | 50,50,50,50 | 0 |
| 56 | MG | BA | 3297 | 1/1 | 0.97 | 0.24 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3196 | 1/1 | 0.97 | 0.24 | 18,18,18,18 | 0 |
| 56 | MG | AA | 1722 | 1/1 | 0.97 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | DA | 3317 | 1/1 | 0.97 | 0.06 | 11,11,11,11 | 1 |
| 56 | MG | BA | 3303 | 1/1 | 0.97 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | AA | 1641 | 1/1 | 0.97 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1740 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3345 | 1/1 | 0.97 | 0.21 | 17,17,17,17 | 0 |
| 56 | MG | CA | 1771 | 1/1 | 0.97 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3244 | 1/1 | 0.97 | 0.29 | 0,0,0,0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1806 | 1/1 | 0.97 | 0.23 | 24,24,24,24 | 0 |
| 56 | MG | AA | 1711 | 1/1 | 0.97 | 0.09 | 8,8,8,8 | 0 |
| 56 | MG | AA | 1774 | 1/1 | 0.97 | 0.08 | 9,9,9,9 | 0 |
| 56 | MG | DA | 3117 | 1/1 | 0.97 | 0.06 | 1,1,1,1 | 0 |
| 56 | MG | BA | 3115 | 1/1 | 0.97 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3336 | 1/1 | 0.97 | 0.17 | 3,3,3,3 | 1 |
| 56 | MG | DA | 3355 | 1/1 | 0.97 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3046 | 1/1 | 0.97 | 0.26 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1724 | 1/1 | 0.97 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3085 | 1/1 | 0.97 | 0.16 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3209 | 1/1 | 0.97 | 0.15 | 15,15,15,15 | 0 |
| 56 | MG | DA | 3190 | 1/1 | 0.97 | 0.07 | 2,2,2,2 | 0 |
| 56 | MG | AV | 105 | 1/1 | 0.97 | 0.13 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3424 | 1/1 | 0.97 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | CA | 1631 | 1/1 | 0.97 | 0.37 | 48,48,48,48 | 0 |
| 56 | MG | AA | 1662 | 1/1 | 0.97 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3362 | 1/1 | 0.97 | 0.21 | 10,10,10,10 | 1 |
| 56 | MG | CA | 1669 | 1/1 | 0.97 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | B2 | 105 | 1/1 | 0.97 | 0.16 | 0,0,0,0 | 0 |
| 56 | MG | DB | 206 | 1/1 | 0.97 | 0.09 | 0,0,0,0 | 1 |
| 56 | MG | CA | 1629 | 1/1 | 0.97 | 0.14 | 10,10,10,10 | 0 |
| 56 | MG | CA | 1754 | 1/1 | 0.97 | 0.14 | 6,6,6,6 | 0 |
| 56 | MG | CA | 1624 | 1/1 | 0.97 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | DS | 201 | 1/1 | 0.97 | 0.45 | 14,14,14,14 | 1 |
| 56 | MG | DA | 3397 | 1/1 | 0.97 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | DA | 3225 | 1/1 | 0.97 | 0.25 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3325 | 1/1 | 0.97 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | CW | 101 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | CA | 1770 | 1/1 | 0.98 | 0.08 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3097 | 1/1 | 0.98 | 0.12 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3035 | 1/1 | 0.98 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3079 | 1/1 | 0.98 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3077 | 1/1 | 0.98 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1664 | 1/1 | 0.98 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3079 | 1/1 | 0.98 | 0.14 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3077 | 1/1 | 0.98 | 0.22 | 6,6,6,6 | 0 |
| 56 | MG | DA | 3028 | 1/1 | 0.98 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1621 | 1/1 | 0.98 | 0.18 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3119 | 1/1 | 0.98 | 0.12 | 7,7,7,7 | 0 |
| 56 | MG | AA | 1707 | 1/1 | 0.98 | 0.08 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3013 | 1/1 | 0.98 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3003 | 1/1 | 0.98 | 0.07 | 26,26,26,26 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3041 | 1/1 | 0.98 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3177 | 1/1 | 0.98 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3263 | 1/1 | 0.98 | 0.16 | 30,30,30,30 | 0 |
| 58 | ZN | CD | 301 | 1/1 | 0.98 | 0.19 | 24,24,24,24 | 0 |
| 56 | MG | BB | 202 | 1/1 | 0.98 | 0.10 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3075 | 1/1 | 0.98 | 0.22 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3202 | 1/1 | 0.98 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3037 | 1/1 | 0.98 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3133 | 1/1 | 0.98 | 0.07 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3054 | 1/1 | 0.98 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3141 | 1/1 | 0.98 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3092 | 1/1 | 0.98 | 0.10 | 4,4,4,4 | 0 |
| 56 | MG | AA | 1649 | 1/1 | 0.98 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3036 | 1/1 | 0.98 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3127 | 1/1 | 0.98 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3124 | 1/1 | 0.98 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1759 | 1/1 | 0.98 | 0.11 | 5,5,5,5 | 1 |
| 56 | MG | BA | 3096 | 1/1 | 0.98 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3196 | 1/1 | 0.98 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3159 | 1/1 | 0.98 | 0.18 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3335 | 1/1 | 0.98 | 0.06 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3098 | 1/1 | 0.98 | 0.07 | 5,5,5,5 | 0 |
| 56 | MG | DA | 3178 | 1/1 | 0.98 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1713 | 1/1 | 0.98 | 0.13 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3131 | 1/1 | 0.98 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3107 | 1/1 | 0.98 | 0.27 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3179 | 1/1 | 0.98 | 0.05 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3357 | 1/1 | 0.98 | 0.07 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3221 | 1/1 | 0.98 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | CA | 1743 | 1/1 | 0.98 | 0.18 | 1,1,1,1 | 0 |
| 56 | MG | CA | 1613 | 1/1 | 0.98 | 0.21 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3027 | 1/1 | 0.98 | 0.07 | 8,8,8,8 | 0 |
| 56 | MG | DA | 3252 | 1/1 | 0.98 | 0.08 | 0,0,0,0 | 1 |
| 56 | MG | BA | 3083 | 1/1 | 0.98 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1705 | 1/1 | 0.98 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | DA | 3021 | 1/1 | 0.98 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3265 | 1/1 | 0.98 | 0.08 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3045 | 1/1 | 0.98 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3123 | 1/1 | 0.98 | 0.12 | 6,6,6,6 | 0 |
| 56 | MG | CA | 1678 | 1/1 | 0.98 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3161 | 1/1 | 0.98 | 0.08 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3445 | 1/1 | 0.98 | 0.14 | 52,52,52,52 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1652 | 1/1 | 0.98 | 0.09 | 7,7,7,7 | 0 |
| 56 | MG | DA | 3227 | 1/1 | 0.98 | 0.06 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3295 | 1/1 | 0.98 | 0.17 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3310 | 1/1 | 0.98 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | CA | 1699 | 1/1 | 0.98 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3089 | 1/1 | 0.98 | 0.11 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3130 | 1/1 | 0.98 | 0.05 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3131 | 1/1 | 0.98 | 0.18 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1689 | 1/1 | 0.98 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3238 | 1/1 | 0.98 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3176 | 1/1 | 0.98 | 0.07 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3076 | 1/1 | 0.98 | 0.15 | 4,4,4,4 | 0 |
| 56 | MG | CX | 105 | 1/1 | 0.98 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | CM | 201 | 1/1 | 0.98 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | AA | 1719 | 1/1 | 0.98 | 0.11 | 65,65,65,65 | 0 |
| 56 | MG | BA | 3137 | 1/1 | 0.98 | 0.17 | 6,6,6,6 | 0 |
| 56 | MG | DA | 3064 | 1/1 | 0.98 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1604 | 1/1 | 0.98 | 0.23 | 45,45,45,45 | 0 |
| 56 | MG | DA | 3181 | 1/1 | 0.98 | 0.10 | 17,17,17,17 | 0 |
| 56 | MG | DA | 3326 | 1/1 | 0.98 | 0.34 | 25,25,25,25 | 0 |
| 56 | MG | BA | 3321 | 1/1 | 0.98 | 0.20 | 4,4,4,4 | 0 |
| 56 | MG | AA | 1732 | 1/1 | 0.98 | 0.07 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3360 | 1/1 | 0.98 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | CA | 1623 | 1/1 | 0.98 | 0.09 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3334 | 1/1 | 0.98 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3315 | 1/1 | 0.98 | 0.06 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3097 | 1/1 | 0.98 | 0.07 | 2,2,2,2 | 0 |
| 56 | MG | CA | 1666 | 1/1 | 0.98 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3110 | 1/1 | 0.98 | 0.21 | 1,1,1,1 | 0 |
| 56 | MG | CA | 1630 | 1/1 | 0.98 | 0.10 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3385 | 1/1 | 0.98 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | BA | 3312 | 1/1 | 0.98 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1773 | 1/1 | 0.98 | 0.09 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3386 | 1/1 | 0.98 | 0.07 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3017 | 1/1 | 0.98 | 0.13 | 6,6,6,6 | 0 |
| 56 | MG | BA | 3182 | 1/1 | 0.98 | 0.09 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3127 | 1/1 | 0.98 | 0.11 | 8,8,8,8 | 0 |
| 56 | MG | CA | 1614 | 1/1 | 0.98 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | BA | 3443 | 1/1 | 0.98 | 0.04 | 20,20,20,20 | 0 |
| 56 | MG | AA | 1800 | 1/1 | 0.98 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3005 | 1/1 | 0.98 | 0.07 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3082 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58 | ZN | AD | 301 | 1/1 | 0.98 | 0.18 | 21,21,21,21 | 0 |
| 56 | MG | DA | 3292 | 1/1 | 0.98 | 0.08 | 5,5,5,5 | 0 |
| 56 | MG | DA | 3286 | 1/1 | 0.98 | 0.10 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3158 | 1/1 | 0.98 | 0.10 | 5,5,5,5 | 0 |
| 56 | MG | CA | 1783 | 1/1 | 0.98 | 0.17 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3307 | 1/1 | 0.98 | 0.04 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3398 | 1/1 | 0.98 | 0.07 | 9,9,9,9 | 1 |
| 56 | MG | BE | 301 | 1/1 | 0.98 | 0.15 | 8,8,8,8 | 0 |
| 56 | MG | BA | 3089 | 1/1 | 0.98 | 0.17 | 6,6,6,6 | 0 |
| 56 | MG | BA | 3078 | 1/1 | 0.98 | 0.20 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3170 | 1/1 | 0.98 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3031 | 1/1 | 0.98 | 0.20 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3249 | 1/1 | 0.98 | 0.08 | 11,11,11,11 | 0 |
| 56 | MG | CA | 1606 | 1/1 | 0.98 | 0.18 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3343 | 1/1 | 0.98 | 0.11 | 4,4,4,4 | 0 |
| 56 | MG | CA | 1687 | 1/1 | 0.98 | 0.08 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3014 | 1/1 | 0.98 | 0.24 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3262 | 1/1 | 0.98 | 0.06 | 20,20,20,20 | 0 |
| 56 | MG | AX | 101 | 1/1 | 0.98 | 0.05 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3043 | 1/1 | 0.98 | 0.16 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3044 | 1/1 | 0.98 | 0.18 | 5,5,5,5 | 0 |
| 56 | MG | BA | 3007 | 1/1 | 0.98 | 0.24 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1797 | 1/1 | 0.98 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3135 | 1/1 | 0.98 | 0.19 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3113 | 1/1 | 0.98 | 0.24 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3134 | 1/1 | 0.98 | 0.21 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3042 | 1/1 | 0.98 | 0.08 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3025 | 1/1 | 0.98 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3050 | 1/1 | 0.98 | 0.31 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1761 | 1/1 | 0.98 | 0.15 | 16,16,16,16 | 0 |
| 56 | MG | BA | 3444 | 1/1 | 0.98 | 0.09 | 7,7,7,7 | 0 |
| 56 | MG | BA | 3359 | 1/1 | 0.98 | 0.05 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3163 | 1/1 | 0.98 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | BA | 3020 | 1/1 | 0.98 | 0.26 | 1,1,1,1 | 0 |
| 56 | MG | AA | 1744 | 1/1 | 0.98 | 0.30 | 18,18,18,18 | 0 |
| 56 | MG | DA | 3121 | 1/1 | 0.98 | 0.10 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3169 | 1/1 | 0.98 | 0.07 | 8,8,8,8 | 0 |
| 56 | MG | AA | 1813 | 1/1 | 0.98 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | DA | 3154 | 1/1 | 0.98 | 0.19 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3132 | 1/1 | 0.98 | 0.13 | 2,2,2,2 | 0 |
| 56 | MG | AA | 1692 | 1/1 | 0.98 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3299 | 1/1 | 0.98 | 0.10 | 0,0,0,0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3100 | 1/1 | 0.98 | 0.21 | 3,3,3,3 | 0 |
| 56 | MG | DA | 3091 | 1/1 | 0.98 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3270 | 1/1 | 0.98 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3065 | 1/1 | 0.98 | 0.25 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3067 | 1/1 | 0.98 | 0.11 | 5,5,5,5 | 0 |
| 56 | MG | CA | 1784 | 1/1 | 0.98 | 0.10 | 15,15,15,15 | 0 |
| 56 | MG | BA | 3355 | 1/1 | 0.98 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | CA | 1701 | 1/1 | 0.98 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | AW | 104 | 1/1 | 0.98 | 0.04 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3073 | 1/1 | 0.98 | 0.10 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3239 | 1/1 | 0.98 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | BA | 3369 | 1/1 | 0.98 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3303 | 1/1 | 0.98 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | AA | 1718 | 1/1 | 0.98 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3087 | 1/1 | 0.98 | 0.30 | 23,23,23,23 | 0 |
| 56 | MG | AW | 107 | 1/1 | 0.98 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3366 | 1/1 | 0.98 | 0.10 | 3,3,3,3 | 0 |
| 56 | MG | AW | 117 | 1/1 | 0.98 | 0.21 | 24,24,24,24 | 0 |
| 56 | MG | DA | 3030 | 1/1 | 0.98 | 0.10 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3210 | 1/1 | 0.98 | 0.15 | 11,11,11,11 | 0 |
| 56 | MG | DA | 3395 | 1/1 | 0.98 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | BA | 3340 | 1/1 | 0.98 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | DA | 3090 | 1/1 | 0.98 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3038 | 1/1 | 0.98 | 0.13 | 17,17,17,17 | 0 |
| 56 | MG | BA | 3059 | 1/1 | 0.98 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | DA | 3095 | 1/1 | 0.98 | 0.22 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3094 | 1/1 | 0.98 | 0.22 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1774 | 1/1 | 0.98 | 0.16 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3391 | 1/1 | 0.98 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | DA | 3108 | 1/1 | 0.98 | 0.25 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3224 | 1/1 | 0.98 | 0.29 | 2,2,2,2 | 0 |
| 56 | MG | DA | 3386 | 1/1 | 0.98 | 0.28 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3125 | 1/1 | 0.98 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3032 | 1/1 | 0.98 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | BA | 3427 | 1/1 | 0.98 | 0.06 | 12,12,12,12 | 0 |
| 56 | MG | AA | 1675 | 1/1 | 0.98 | 0.23 | 4,4,4,4 | 0 |
| 56 | MG | DA | 3049 | 1/1 | 0.98 | 0.18 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1707 | 1/1 | 0.98 | 0.19 | 6,6,6,6 | 0 |
| 56 | MG | AA | 1746 | 1/1 | 0.98 | 0.11 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3273 | 1/1 | 0.98 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | B5 | 101 | 1/1 | 0.98 | 0.15 | 6,6,6,6 | 0 |
| 56 | MG | DA | 3306 | 1/1 | 0.98 | 0.22 | 6,6,6,6 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | BA | 3244 | 1/1 | 0.98 | 0.11 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1757 | 1/1 | 0.98 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1679 | 1/1 | 0.98 | 0.07 | 5,5,5,5 | 1 |
| 56 | MG | BA | 3232 | 1/1 | 0.98 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | AA | 1639 | 1/1 | 0.98 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3237 | 1/1 | 0.98 | 0.06 | 15,15,15,15 | 0 |
| 56 | MG | AA | 1624 | 1/1 | 0.98 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | BA | 3198 | 1/1 | 0.98 | 0.08 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3156 | 1/1 | 0.98 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3128 | 1/1 | 0.98 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1653 | 1/1 | 0.98 | 0.05 | 60,60,60,60 | 0 |
| 56 | MG | BA | 3145 | 1/1 | 0.98 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3251 | 1/1 | 0.98 | 0.15 | 11,11,11,11 | 0 |
| 56 | MG | BA | 3328 | 1/1 | 0.98 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | DA | 3198 | 1/1 | 0.98 | 0.09 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3213 | 1/1 | 0.98 | 0.23 | 19,19,19,19 | 0 |
| 56 | MG | DA | 3072 | 1/1 | 0.98 | 0.05 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3338 | 1/1 | 0.98 | 0.06 | 22,22,22,22 | 1 |
| 56 | MG | BA | 3437 | 1/1 | 0.98 | 0.06 | 4,4,4,4 | 0 |
| 56 | MG | CA | 1703 | 1/1 | 0.98 | 0.06 | 19,19,19,19 | 0 |
| 56 | MG | AA | 1625 | 1/1 | 0.99 | 0.09 | 3,3,3,3 | 0 |
| 56 | MG | DA | 3378 | 1/1 | 0.99 | 0.10 | 8,8,8,8 | 0 |
| 56 | MG | CA | 1740 | 1/1 | 0.99 | 0.07 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3188 | 1/1 | 0.99 | 0.21 | 13,13,13,13 | 0 |
| 56 | MG | B7 | 101 | 1/1 | 0.99 | 0.07 | 7,7,7,7 | 0 |
| 56 | MG | AA | 1704 | 1/1 | 0.99 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1613 | 1/1 | 0.99 | 0.22 | 2,2,2,2 | 0 |
| 56 | MG | CX | 101 | 1/1 | 0.99 | 0.15 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3385 | 1/1 | 0.99 | 0.06 | 12,12,12,12 | 0 |
| 56 | MG | BB | 216 | 1/1 | 0.99 | 0.27 | 11,11,11,11 | 1 |
| 56 | MG | DA | 3356 | 1/1 | 0.99 | 0.08 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3289 | 1/1 | 0.99 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | BA | 3175 | 1/1 | 0.99 | 0.07 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3404 | 1/1 | 0.99 | 0.29 | 17,17,17,17 | 0 |
| 56 | MG | AA | 1712 | 1/1 | 0.99 | 0.06 | 22,22,22,22 | 0 |
| 56 | MG | BA | 3081 | 1/1 | 0.99 | 0.13 | 10,10,10,10 | 0 |
| 56 | MG | BA | 3274 | 1/1 | 0.99 | 0.06 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3192 | 1/1 | 0.99 | 0.11 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1771 | 1/1 | 0.99 | 0.07 | 6,6,6,6 | 0 |
| 56 | MG | DA | 3025 | 1/1 | 0.99 | 0.15 | 6,6,6,6 | 0 |
| 56 | MG | AA | 1659 | 1/1 | 0.99 | 0.10 | 14,14,14,14 | 1 |
| 56 | MG | DA | 3055 | 1/1 | 0.99 | 0.20 | 0,0,0,0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | AA | 1672 | 1/1 | 0.99 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3290 | 1/1 | 0.99 | 0.08 | 2,2,2,2 | 0 |
| 56 | MG | DA | 3372 | 1/1 | 0.99 | 0.09 | 12,12,12,12 | 0 |
| 56 | MG | BA | 3066 | 1/1 | 0.99 | 0.08 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3013 | 1/1 | 0.99 | 0.12 | 1,1,1,1 | 0 |
| 56 | MG | BA | 3053 | 1/1 | 0.99 | 0.16 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1696 | 1/1 | 0.99 | 0.09 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3294 | 1/1 | 0.99 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DD | 301 | 1/1 | 0.99 | 0.14 | 1,1,1,1 | 0 |
| 56 | MG | DA | 3259 | 1/1 | 0.99 | 0.17 | 14,14,14,14 | 0 |
| 56 | MG | DA | 3051 | 1/1 | 0.99 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3356 | 1/1 | 0.99 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | BA | 3224 | 1/1 | 0.99 | 0.21 | 2,2,2,2 | 0 |
| 56 | MG | DA | 3062 | 1/1 | 0.99 | 0.27 | 13,13,13,13 | 0 |
| 56 | MG | AA | 1646 | 1/1 | 0.99 | 0.17 | 3,3,3,3 | 0 |
| 56 | MG | BA | 3352 | 1/1 | 0.99 | 0.10 | 30,30,30,30 | 1 |
| 56 | MG | BA | 3397 | 1/1 | 0.99 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1728 | 1/1 | 0.99 | 0.08 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3084 | 1/1 | 0.99 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3078 | 1/1 | 0.99 | 0.20 | 2,2,2,2 | 0 |
| 56 | MG | DA | 3023 | 1/1 | 0.99 | 0.26 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1610 | 1/1 | 0.99 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3092 | 1/1 | 0.99 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1679 | 1/1 | 0.99 | 0.05 | 4,4,4,4 | 0 |
| 56 | MG | BA | 3095 | 1/1 | 0.99 | 0.12 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3390 | 1/1 | 0.99 | 0.08 | 73,73,73,73 | 0 |
| 56 | MG | BA | 3074 | 1/1 | 0.99 | 0.19 | 10,10,10,10 | 0 |
| 56 | MG | DA | 3176 | 1/1 | 0.99 | 0.20 | 13,13,13,13 | 0 |
| 56 | MG | BA | 3047 | 1/1 | 0.99 | 0.27 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1778 | 1/1 | 0.99 | 0.11 | 3,3,3,3 | 0 |
| 56 | MG | AA | 1751 | 1/1 | 0.99 | 0.08 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3062 | 1/1 | 0.99 | 0.23 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1777 | 1/1 | 0.99 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3047 | 1/1 | 0.99 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1656 | 1/1 | 0.99 | 0.16 | 12,12,12,12 | 0 |
| 56 | MG | DA | 3174 | 1/1 | 0.99 | 0.23 | 26,26,26,26 | 0 |
| 56 | MG | BA | 3134 | 1/1 | 0.99 | 0.11 | 1,1,1,1 | 0 |
| 56 | MG | BA | 3225 | 1/1 | 0.99 | 0.17 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3378 | 1/1 | 0.99 | 0.04 | 54,54,54,54 | 1 |
| 56 | MG | DA | 3327 | 1/1 | 0.99 | 0.08 | 6,6,6,6 | 0 |
| 56 | MG | AA | 1805 | 1/1 | 0.99 | 0.23 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3056 | 1/1 | 0.99 | 0.17 | 0,0,0,0 | 0 |

Continued on next page...

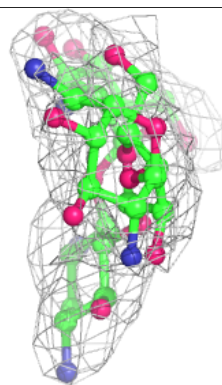
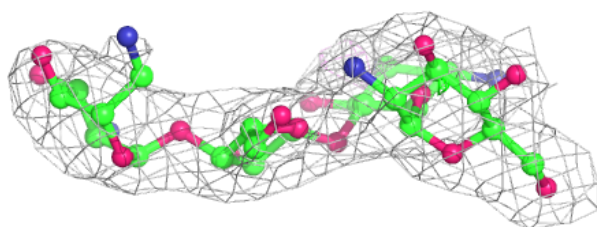
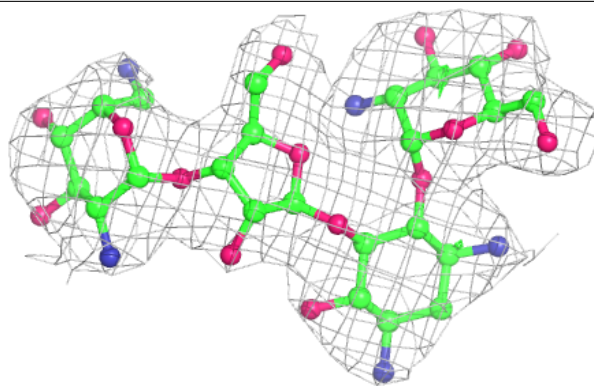
Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3015 | 1/1 | 0.99 | 0.10 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3050 | 1/1 | 0.99 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3059 | 1/1 | 0.99 | 0.21 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3121 | 1/1 | 0.99 | 0.12 | 2,2,2,2 | 0 |
| 56 | MG | CA | 1628 | 1/1 | 0.99 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | AA | 1699 | 1/1 | 0.99 | 0.14 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3382 | 1/1 | 0.99 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | BA | 3099 | 1/1 | 0.99 | 0.21 | 1,1,1,1 | 0 |
| 56 | MG | DA | 3129 | 1/1 | 0.99 | 0.17 | 6,6,6,6 | 0 |
| 56 | MG | BA | 3106 | 1/1 | 0.99 | 0.18 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3058 | 1/1 | 0.99 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | CA | 1659 | 1/1 | 0.99 | 0.06 | 9,9,9,9 | 0 |
| 58 | ZN | CN | 101 | 1/1 | 0.99 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | BA | 3284 | 1/1 | 0.99 | 0.19 | 14,14,14,14 | 0 |
| 56 | MG | BA | 3046 | 1/1 | 0.99 | 0.25 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3295 | 1/1 | 0.99 | 0.06 | 6,6,6,6 | 0 |
| 56 | MG | BA | 3060 | 1/1 | 0.99 | 0.22 | 0,0,0,0 | 0 |
| 56 | MG | AA | 1637 | 1/1 | 0.99 | 0.15 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3085 | 1/1 | 0.99 | 0.20 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3242 | 1/1 | 0.99 | 0.14 | 9,9,9,9 | 0 |
| 56 | MG | BA | 3281 | 1/1 | 0.99 | 0.13 | 0,0,0,0 | 0 |
| 56 | MG | BA | 3039 | 1/1 | 0.99 | 0.31 | 31,31,31,31 | 0 |
| 56 | MG | BA | 3187 | 1/1 | 0.99 | 0.15 | 2,2,2,2 | 0 |
| 56 | MG | BA | 3341 | 1/1 | 0.99 | 0.17 | 21,21,21,21 | 0 |
| 56 | MG | BA | 3365 | 1/1 | 0.99 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | DB | 201 | 1/1 | 0.99 | 0.06 | 19,19,19,19 | 0 |
| 56 | MG | BA | 3048 | 1/1 | 1.00 | 0.19 | 0,0,0,0 | 0 |
| 56 | MG | DA | 3039 | 1/1 | 1.00 | 0.17 | 10,10,10,10 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

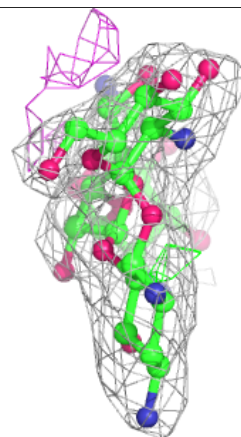
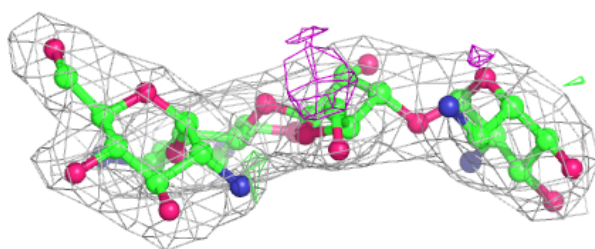
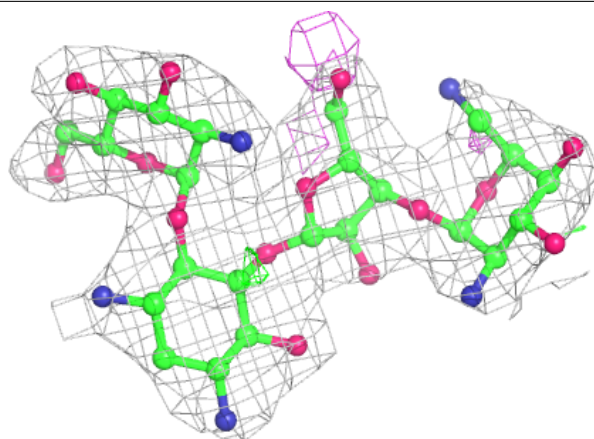
Electron density around PAR AA 1816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR CA 1790:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.