



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 07:57 PM EST

PDB ID : 1VY7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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) : 2.36

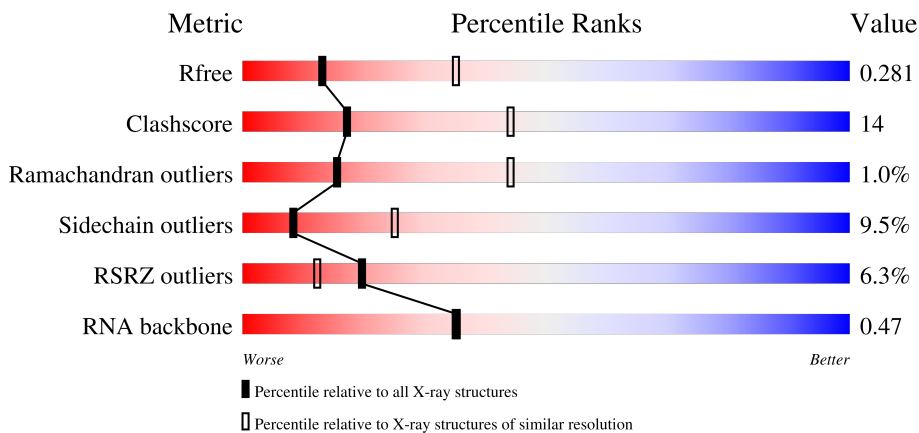
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 of 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 | 1521 | |
| 1 | CA | 1521 | |
| 2 | AB | 256 | |
| 2 | CB | 256 | |

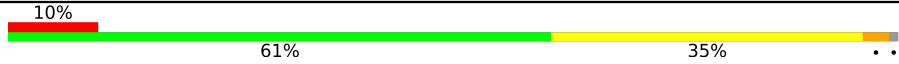

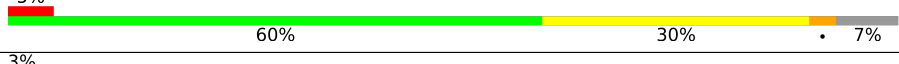



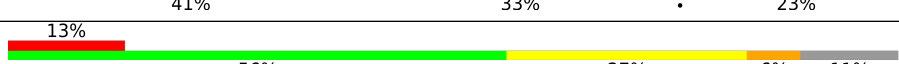
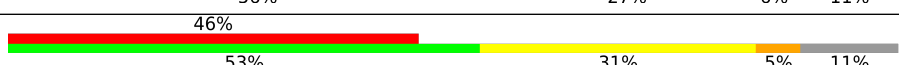
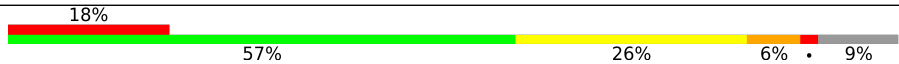



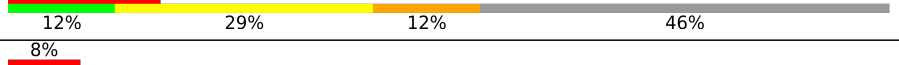

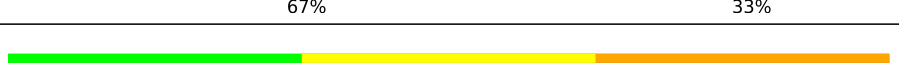
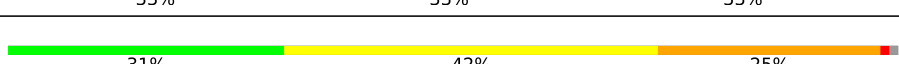
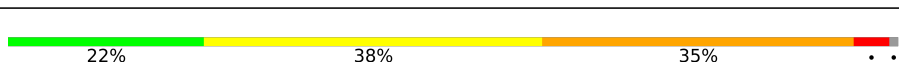
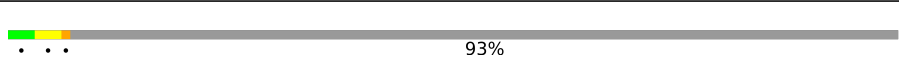
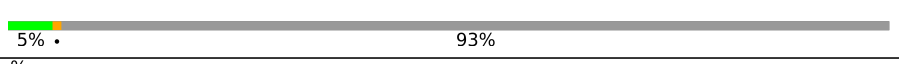
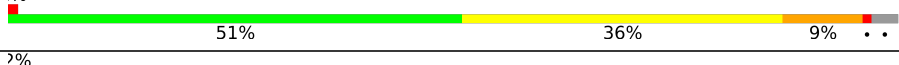


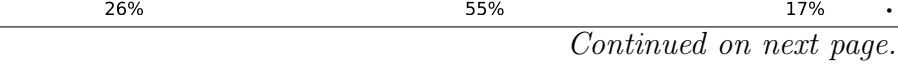


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 239 | |
| 3 | CC | 239 | |
| 4 | AD | 209 | |
| 4 | CD | 209 | |
| 5 | AE | 162 | |
| 5 | CE | 162 | |
| 6 | AF | 101 | |
| 6 | CF | 101 | |
| 7 | AG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




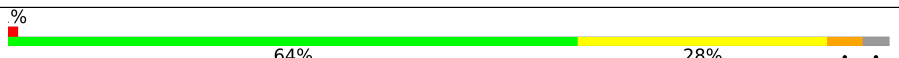
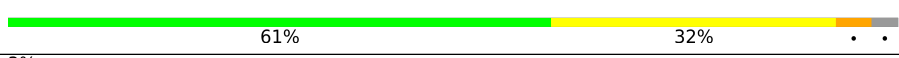

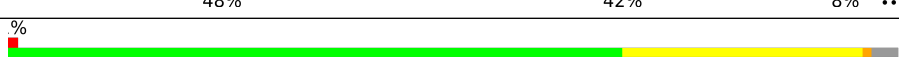



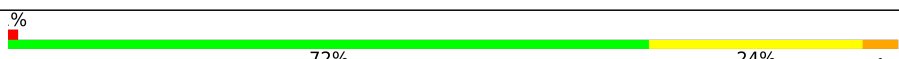



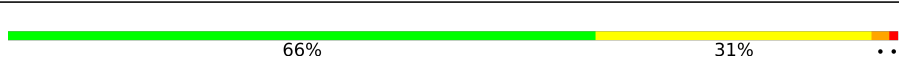

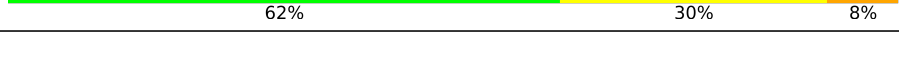






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | CO | 89 |  |
| 16 | AP | 88 |  |
| 16 | CP | 88 |  |
| 17 | AQ | 105 |  |
| 17 | CQ | 105 |  |
| 18 | AR | 88 |  |
| 18 | CR | 88 |  |
| 19 | AS | 93 |  |
| 19 | CS | 93 |  |
| 20 | AT | 106 |  |
| 20 | CT | 106 |  |
| 21 | AU | 27 |  |
| 21 | CU | 27 |  |
| 22 | AV | 24 |  |
| 22 | CV | 24 |  |
| 23 | AW | 3 |  |
| 23 | CW | 3 |  |
| 24 | AX | 77 |  |
| 24 | CX | 77 |  |
| 25 | AY | 76 |  |
| 25 | CY | 76 |  |
| 26 | BA | 2915 |  |
| 26 | DA | 2915 |  |
| 27 | BB | 121 |  |
| 27 | DB | 121 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | BD | 276 |  % 69% 29% |
| 28 | DD | 276 |  % 72% 25% |
| 29 | BE | 206 |  % 68% 25% 6% |
| 29 | DE | 206 |  % 67% 26% 5% |
| 30 | BF | 210 |  % 64% 28% |
| 30 | DF | 210 |  % 61% 32% |
| 31 | BG | 182 |  3% 67% 29% |
| 31 | DG | 182 |  27% 48% 42% 8% |
| 32 | BH | 180 |  % 69% 27% |
| 32 | DH | 180 |  21% 58% 34% |
| 33 | BI | 148 |  9% 66% 24% 8% |
| 33 | DI | 148 |  53% 57% 32% 9% |
| 34 | BN | 140 |  % 72% 25% |
| 34 | DN | 140 |  % 72% 24% |
| 35 | BO | 122 |  % 71% 25% |
| 35 | DO | 122 |  % 63% 34% |
| 36 | BP | 150 |  % 69% 27% |
| 36 | DP | 150 |  4% 61% 31% 7% |
| 37 | BQ | 141 |  % 66% 31% |
| 37 | DQ | 141 |  11% 70% 26% |
| 38 | BR | 118 |  % 62% 30% 8% |
| 38 | DR | 118 |  % 55% 36% 8% |
| 39 | BS | 112 |  % 69% 24% |
| 39 | DS | 112 | 10% 61% 34% |
| 40 | BT | 146 | % 58% 27% 10% |






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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------|
| 40 | DT | 146 | 55% 29% 5% 10% |
| 41 | BU | 118 | 69% 27% .. |
| 41 | DU | 118 | 69% 28% .. |
| 42 | BV | 101 | 61% 35% .. |
| 42 | DV | 101 | 13% 69% 27% .. |
| 43 | BW | 113 | 75% 21% .. |
| 43 | DW | 113 | 66% 31% .. |
| 44 | BX | 96 | 70% 26% .. |
| 44 | DX | 96 | 8% 70% 27% .. |
| 45 | BY | 110 | 64% 33% .. |
| 45 | DY | 110 | 13% 71% 23% .. |
| 46 | BZ | 206 | 2% 51% 29% . 17% |
| 46 | DZ | 206 | 29% 50% 30% 5% 16% |
| 47 | B0 | 85 | 78% 16% .. |
| 47 | D0 | 85 | 7% 72% 24% .. |
| 48 | B1 | 98 | 70% 23% 5% .. |
| 48 | D1 | 98 | 3% 70% 23% 5% .. |
| 49 | B2 | 72 | 71% 22% . .. |
| 49 | D2 | 72 | 6% 75% 21% .. |
| 50 | B3 | 60 | 65% 27% 7% . |
| 50 | D3 | 60 | 10% 62% 33% .. |
| 51 | B4 | 71 | 15% 49% 34% 11% .. |
| 51 | D4 | 71 | 34% 41% 48% 8% . |
| 52 | B5 | 60 | 2% 83% 13% .. |
| 52 | D5 | 60 | 78% 18% .. |

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

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | BF | 309 | - | - | - | X |
| 57 | MG | DA | 3069 | - | - | - | X |
| 57 | MG | DA | 3553 | - | - | - | X |
| 57 | MG | DV | 202 | - | - | - | X |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 290205 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 |
|-----|-------|----------|----------------|------------|-----------|------------|-----------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | AA | 1498 | Total 32205 | C 14333 | N 5970 | O 10404 | P 1498 | 0 | 0 | 0 |
| 1 | CA | 1503 | Total 32312 | C 14381 | N 5990 | O 10438 | P 1503 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | AB | 231 | Total 1846 | C 1179 | N 331 | O 331 | S 5 | 0 | 0 | 0 |
| 2 | CB | 231 | Total 1825 | C 1167 | N 326 | O 327 | S 5 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | AC | 206 | Total 1552 | C 976 | N 302 | O 273 | S 1 | 0 | 0 | 0 |
| 3 | CC | 206 | Total 1542 | C 968 | N 300 | O 273 | S 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | AD | 208 | Total 1659 | C 1040 | N 326 | O 286 | S 7 | 0 | 0 | 0 |
| 4 | CD | 208 | Total 1674 | C 1050 | N 333 | O 284 | S 7 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 213 | 198 | 4 | | | |
| 5 | CE | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 716 | 214 | 199 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 511 | 143 | 149 | 3 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 146 | 151 | 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 |
| | | | 1231 | 766 | 243 | 216 | 6 | | | |
| 7 | CG | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1235 | 769 | 244 | 216 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |
| 8 | CH | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1088 | 689 | 206 | 191 | 2 | | | |

- 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 |
| | | | 983 | 623 | 193 | 167 | | | |
| 9 | CI | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 978 | 619 | 190 | 169 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10 | AJ | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 709 | 440 | 138 | 131 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 10 | CJ | 96 | 714 | 445 | 138 | 131 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 11 | AK | 114 | 829 | 516 | 155 | 155 | 3 | 0 | 0 | 0 |
| 11 | CK | 114 | 833 | 519 | 156 | 155 | 3 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 12 | AL | 122 | 930 | 585 | 185 | 159 | 1 | 0 | 0 | 0 |
| 12 | CL | 122 | 930 | 585 | 185 | 159 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 13 | AM | 123 | 958 | 592 | 198 | 166 | 2 | 0 | 0 | 0 |
| 13 | CM | 122 | 950 | 586 | 197 | 165 | 2 | 0 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 15 | AO | 88 | 728 | 456 | 144 | 126 | 2 | 0 | 0 | 0 |
| 15 | CO | 88 | 728 | 456 | 144 | 126 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 681 | 433 | 134 | 113 | 1 | | | |
| 16 | CP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 677 | 430 | 133 | 113 | 1 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18 | AR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | |
| 18 | CR | 68 | Total | C | N | O | 0 | 0 | 0 |
| | | | 555 | 355 | 108 | 92 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 652 | 417 | 120 | 113 | 2 | | | |
| 19 | CS | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 646 | 412 | 119 | 113 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 446 | 156 | 124 | 2 | | | |
| 20 | CT | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 727 | 446 | 155 | 124 | 2 | | | |

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

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

- Molecule 22 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 22 | AV | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 125 | 51 | 88 | 13 | | | |
| 22 | CV | 6 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 129 | 58 | 24 | 41 | 6 | | | |

- Molecule 23 is a RNA chain called Cytidine-Puromycin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23 | AW | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 74 | 40 | 13 | 19 | 2 | | | |
| 23 | CW | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 74 | 40 | 13 | 19 | 2 | | | |

- Molecule 24 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 24 | AX | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1633 | 730 | 296 | 529 | 76 | 2 | | | |
| 24 | CX | 76 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | 2 | | | |

- Molecule 25 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 25 | AY | 5 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 104 | 47 | 19 | 33 | 5 | | | |
| 25 | CY | 5 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 104 | 47 | 19 | 33 | 5 | | | |

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26 | BA | 2819 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60729 | 27026 | 11370 | 19515 | 2818 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 26 | DA | 2800 | 60311 | 26840 | 11284 | 19388 | 2799 | 0 | 0 | 0 |

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 27 | BB | 120 | 2573 | 1146 | 476 | 832 | 119 | 0 | 0 | 0 |
| 27 | DB | 120 | 2573 | 1146 | 476 | 832 | 119 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 28 | BD | 275 | 2136 | 1349 | 423 | 361 | 3 | 0 | 0 | 0 |
| 28 | DD | 275 | 2136 | 1349 | 423 | 361 | 3 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 29 | BE | 204 | 1559 | 985 | 298 | 270 | 6 | 0 | 0 | 0 |
| 29 | DE | 204 | 1559 | 985 | 298 | 270 | 6 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 30 | BF | 203 | 1584 | 1009 | 298 | 275 | 2 | 0 | 0 | 1 |
| 30 | DF | 203 | 1580 | 1007 | 297 | 274 | 2 | 0 | 0 | 1 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 31 | BG | 181 | 1425 | 914 | 256 | 251 | 4 | 0 | 0 | 0 |
| 31 | DG | 181 | 1424 | 911 | 258 | 251 | 4 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | BH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |
| 32 | DH | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | BI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1085 | 693 | 189 | 202 | 1 | | | |
| 33 | DI | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1061 | 680 | 186 | 194 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | BN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |
| 34 | DN | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | BP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |
| 36 | DP | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1135 | 706 | 230 | 196 | 3 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 38 | DR | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39 | BS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | |
| 39 | DS | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 870 | 549 | 173 | 148 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1091 | 680 | 225 | 185 | 1 | | | |
| 40 | DT | 131 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1083 | 675 | 224 | 183 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |
| 41 | DU | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 959 | 608 | 201 | 149 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 42 | DV | 101 | 771 | 495 | 140 | 135 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 43 | BW | 112 | 886 | 557 | 174 | 153 | 2 | 0 | 0 | 0 |
| 43 | DW | 112 | 886 | 557 | 174 | 153 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 44 | BX | 95 | 750 | 488 | 135 | 126 | 1 | 0 | 0 | 0 |
| 44 | DX | 95 | 750 | 488 | 135 | 126 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 45 | BY | 107 | 806 | 517 | 152 | 131 | 6 | 0 | 0 | 0 |
| 45 | DY | 107 | 806 | 517 | 152 | 131 | 6 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 46 | BZ | 171 | 1349 | 862 | 243 | 242 | 2 | 0 | 0 | 0 |
| 46 | DZ | 174 | 1360 | 870 | 243 | 245 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 47 | B0 | 83 | 653 | 404 | 139 | 109 | 1 | 0 | 0 | 0 |
| 47 | D0 | 83 | 653 | 404 | 139 | 109 | 1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | B1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |
| 48 | D1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | B2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |
| 49 | D2 | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 588 | 365 | 118 | 103 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 50 | B3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |
| 50 | D3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 464 | 296 | 90 | 78 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51 | B4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 552 | 349 | 99 | 99 | 5 | | | |
| 51 | D4 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 97 | 91 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | B5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |
| 52 | D5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 455 | 285 | 89 | 76 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | B6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 53 | D6 | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 279 | 91 | 75 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54 | B7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 54 | D7 | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55 | B8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 511 | 328 | 99 | 82 | 2 | | | |
| 55 | D8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 56 | B9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 56 | D9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57 | AA | 207 | Total | Mg | 0 | 0 |
| | | | 207 | 207 | | |
| 57 | AD | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | AE | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | AF | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | AJ | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 57 | AK | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | AM | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | AN | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | AS | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | AV | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | AW | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | AX | 11 | Total Mg 11 11 | 0 | 0 |
| 57 | BA | 720 | Total Mg 720 720 | 0 | 0 |
| 57 | BB | 20 | Total Mg 20 20 | 0 | 0 |
| 57 | BD | 11 | Total Mg 11 11 | 0 | 0 |
| 57 | BE | 7 | Total Mg 7 7 | 0 | 0 |
| 57 | BF | 10 | Total Mg 10 10 | 0 | 0 |
| 57 | BG | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | BN | 6 | Total Mg 6 6 | 0 | 0 |
| 57 | BO | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | BP | 4 | Total Mg 4 4 | 0 | 0 |
| 57 | BQ | 5 | Total Mg 5 5 | 0 | 0 |
| 57 | BR | 3 | Total Mg 3 3 | 0 | 0 |
| 57 | BU | 8 | Total Mg 8 8 | 0 | 0 |
| 57 | BV | 4 | Total Mg 4 4 | 0 | 0 |
| 57 | BW | 5 | Total Mg 5 5 | 0 | 0 |

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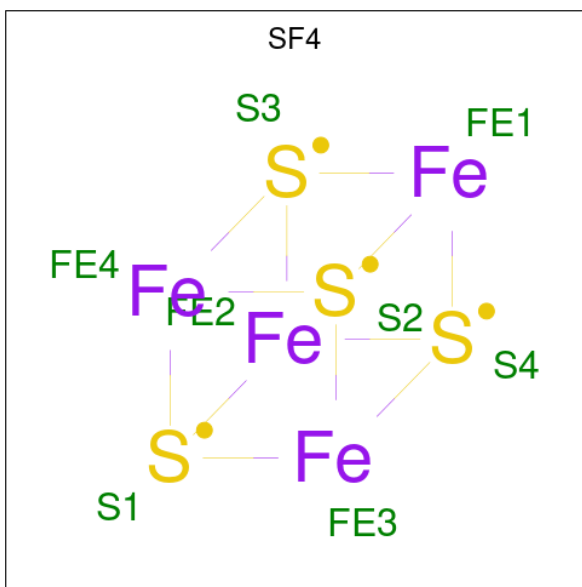
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | BX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BZ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B0 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | B1 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B2 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B3 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | B5 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | B7 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | B8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CA | 160 | Total 160 | Mg 160 | 0 | 0 |
| 57 | CE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DA | 629 | Total 629 | Mg 629 | 0 | 0 |
| 57 | DB | 10 | Total 10 | Mg 10 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 57 | DD | 7 | Total Mg 7 7 | 0 | 0 |
| 57 | DE | 4 | Total Mg 4 4 | 0 | 0 |
| 57 | DF | 4 | Total Mg 4 4 | 0 | 0 |
| 57 | DG | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | DN | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | DO | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | DP | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | DQ | 3 | Total Mg 3 3 | 0 | 0 |
| 57 | DR | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | DU | 4 | Total Mg 4 4 | 0 | 0 |
| 57 | DV | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | DW | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | DY | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | D3 | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | D5 | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | D8 | 2 | Total Mg 2 2 | 0 | 0 |

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 58 | AD | 1 | Total | Fe S | 0 | 0 |
| | | | 8 | 4 4 | | |
| 58 | CD | 1 | Total | Fe S | 0 | 0 |
| | | | 8 | 4 4 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59 | AN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | BY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | CN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | DY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59 | D6 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 60 | AX | 1 | Total 1 | K 1 | 0 | 0 |
| 60 | CX | 1 | Total 1 | K 1 | 0 | 0 |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61 | AA | 170 | Total 170 | O 170 | 0 | 0 |
| 61 | AL | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AO | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | AU | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | AV | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AW | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BA | 1102 | Total 1102 | O 1102 | 0 | 0 |
| 61 | BB | 36 | Total 36 | O 36 | 0 | 0 |
| 61 | BD | 8 | Total 8 | O 8 | 0 | 0 |
| 61 | BE | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | BF | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BG | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BI | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | BP | 15 | Total 15 | O 15 | 0 | 0 |
| 61 | BQ | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BR | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BS | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BT | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BU | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BV | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BW | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | B0 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | B1 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B3 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B5 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | B7 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B8 | 7 | Total 7 | O 7 | 0 | 0 |
| 61 | CA | 130 | Total 130 | O 130 | 0 | 0 |
| 61 | CE | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CJ | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CN | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CV | 1 | Total 1 | O 1 | 0 | 0 |

Continued on next page...

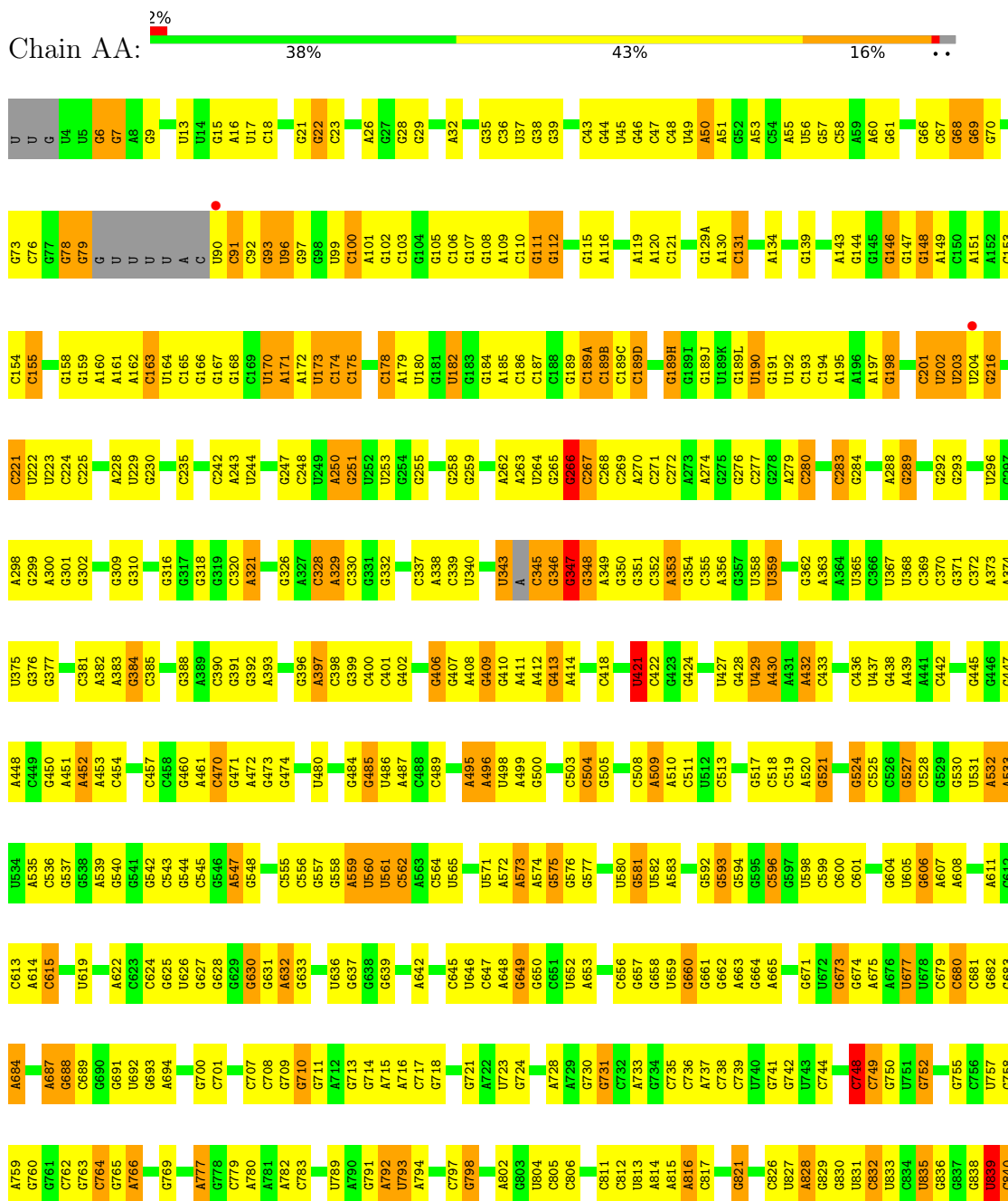
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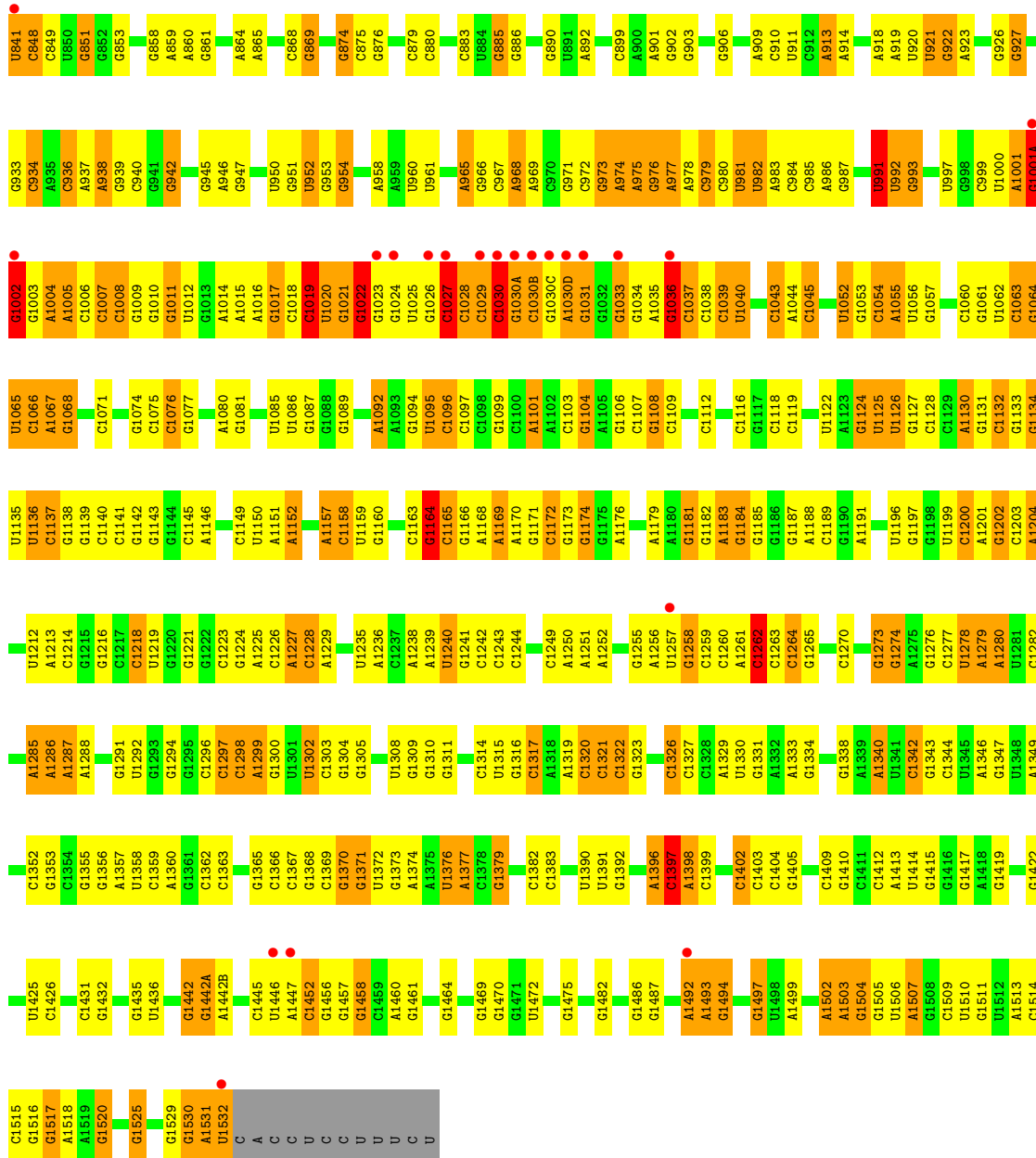
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | CW | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CX | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DA | 767 | Total 767 | O 767 | 0 | 0 |
| 61 | DB | 9 | Total 9 | O 9 | 0 | 0 |
| 61 | DD | 9 | Total 9 | O 9 | 0 | 0 |
| 61 | DE | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | DF | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | DN | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DP | 12 | Total 12 | O 12 | 0 | 0 |
| 61 | DR | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DT | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DU | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D0 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | D1 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D3 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | D7 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D8 | 4 | Total 4 | O 4 | 0 | 0 |

3 Residue-property plots

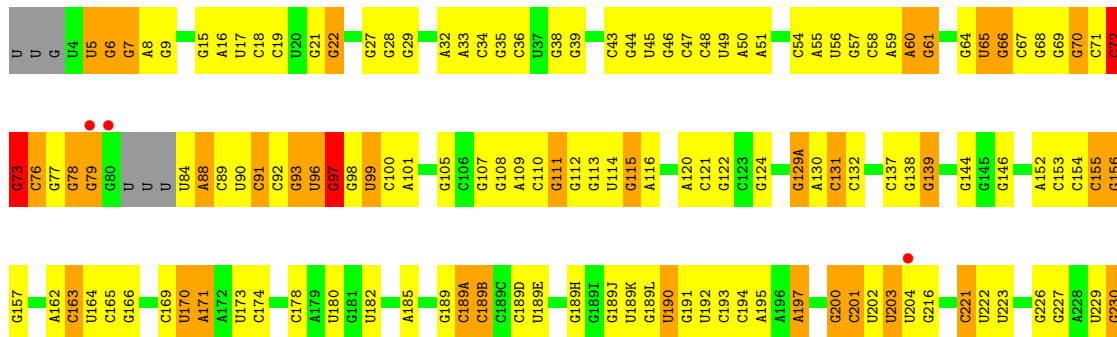
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ($RSRZ > 2$). 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.

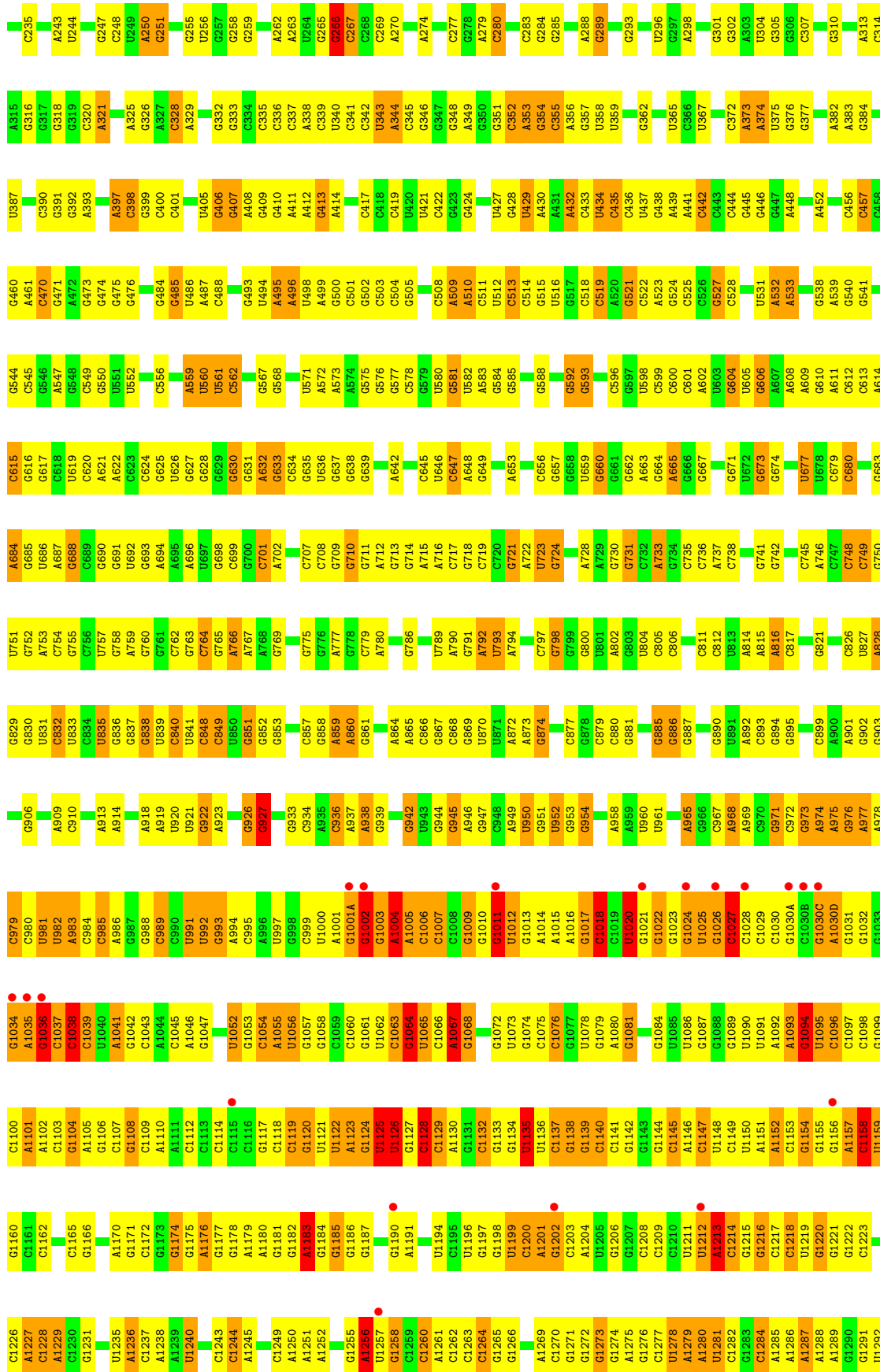
- Molecule 1: 16S Ribosomal RNA

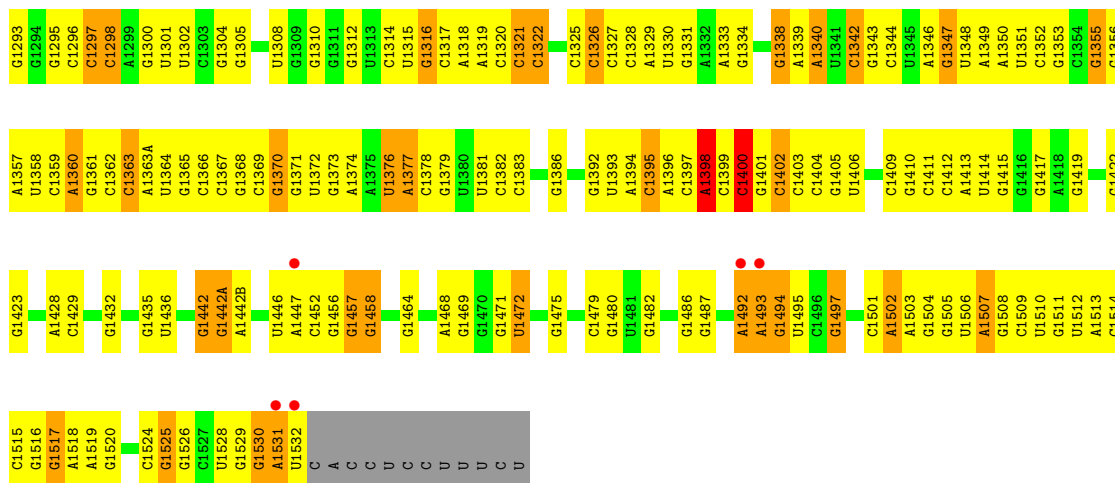




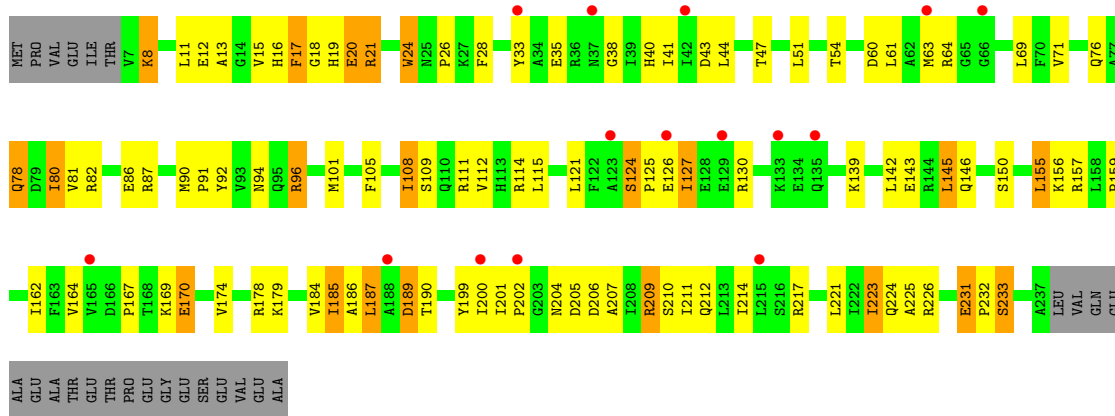
● Molecule 1: 16S Ribosomal RNA



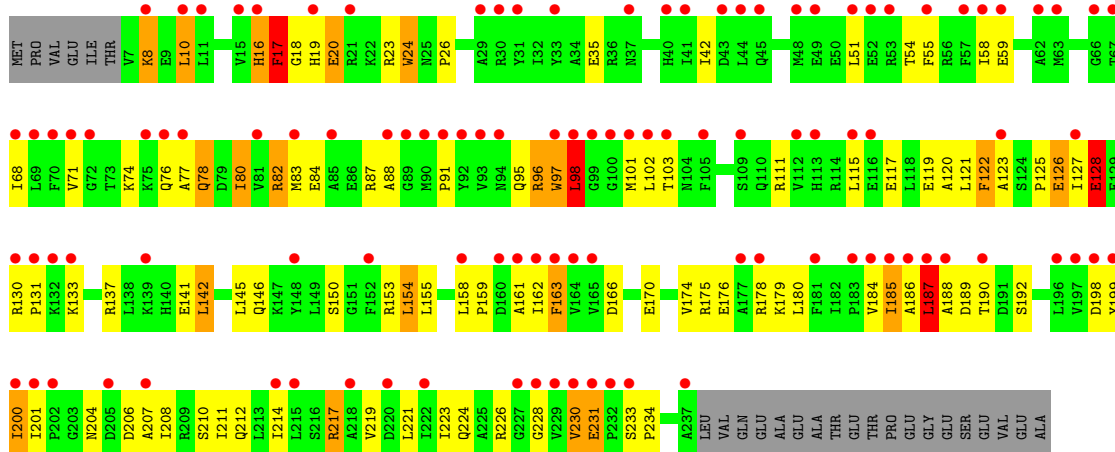
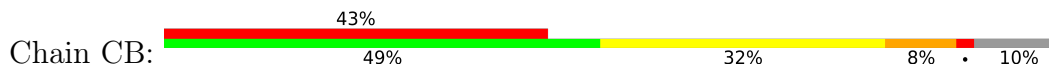




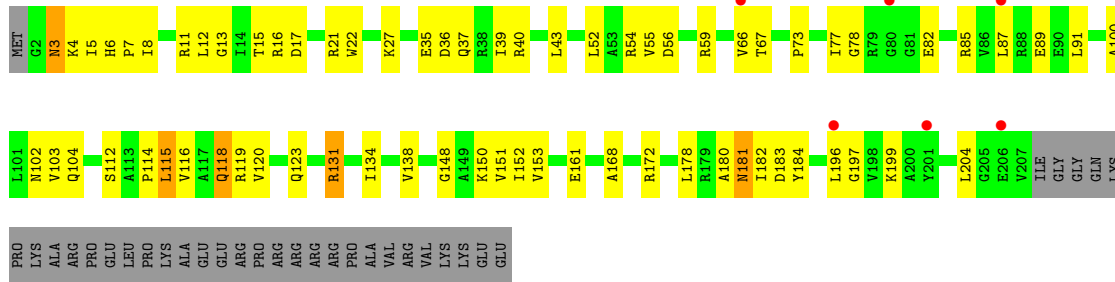
• Molecule 2: 30S ribosomal protein S2



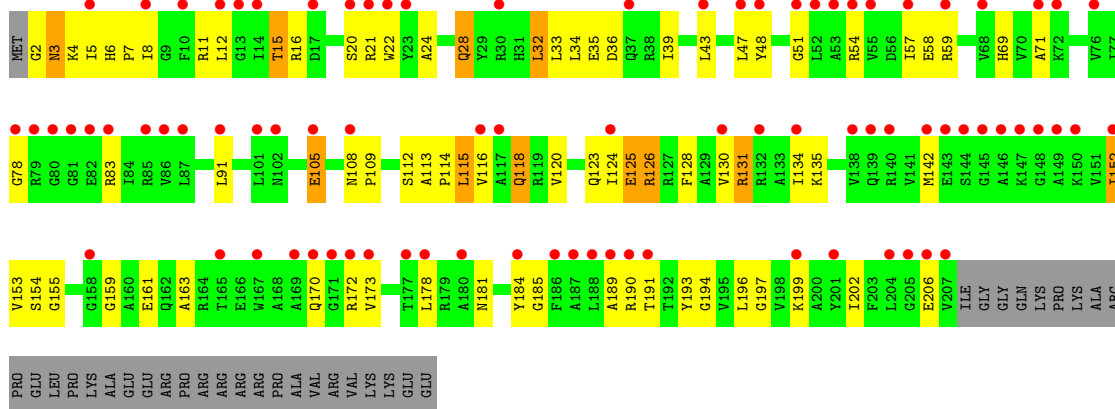
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

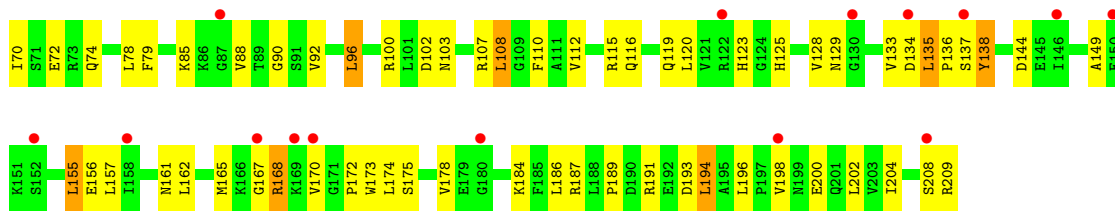


• Molecule 4: 30S ribosomal protein S4

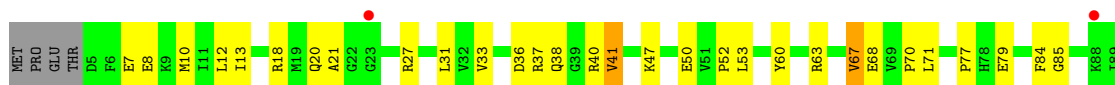


• Molecule 4: 30S ribosomal protein S4

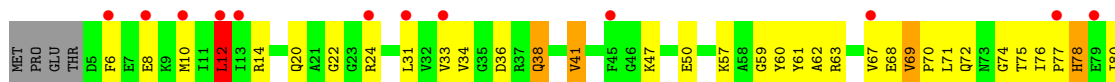




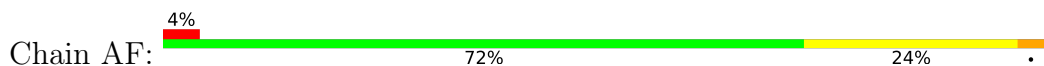
- Molecule 5: 30S ribosomal protein S5



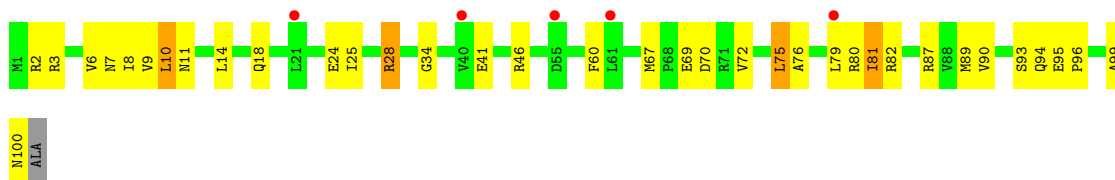
- Molecule 5: 30S ribosomal protein S5



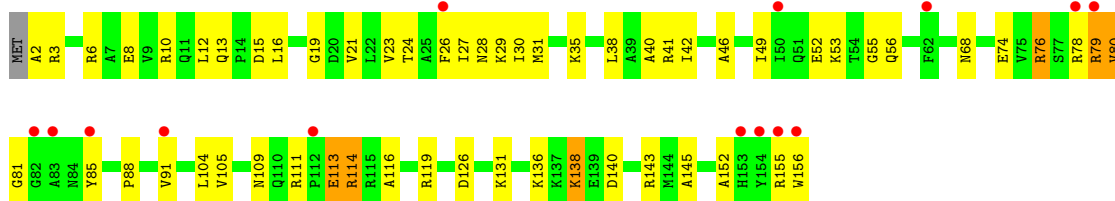
- Molecule 6: 30S ribosomal protein S6



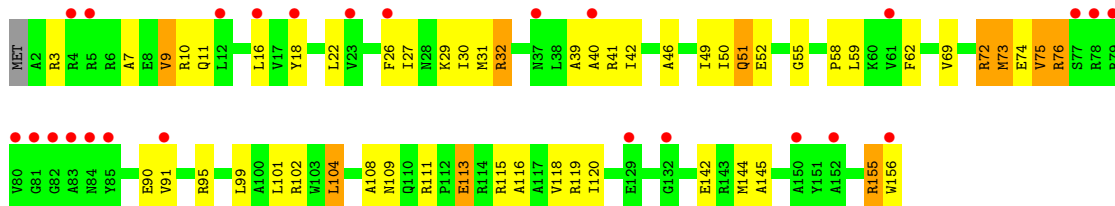
- Molecule 6: 30S ribosomal protein S6



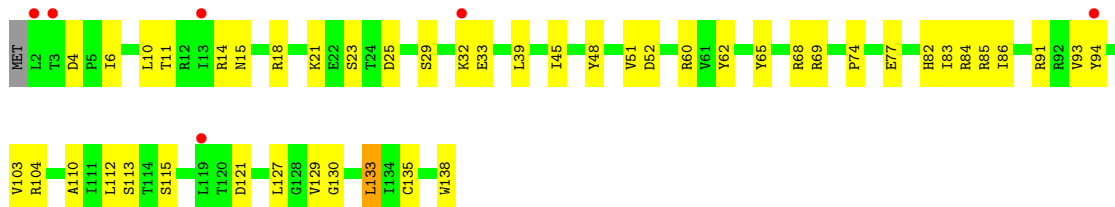
- Molecule 7: 30S ribosomal protein S7



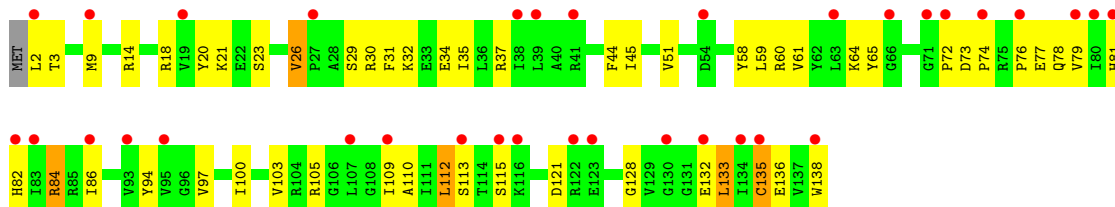
- Molecule 7: 30S ribosomal protein S7



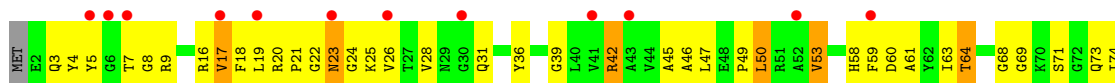
- Molecule 8: 30S ribosomal protein S8

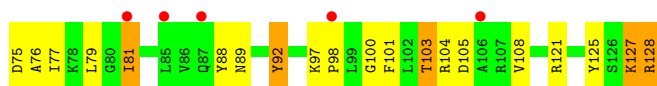


- Molecule 8: 30S ribosomal protein S8

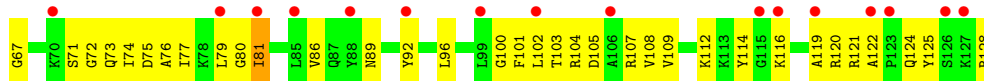
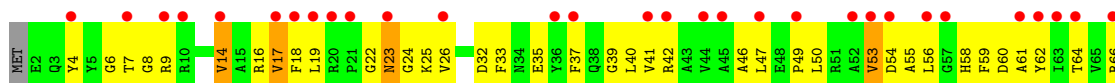
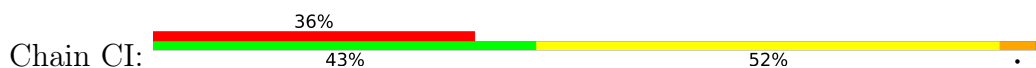


- Molecule 9: 30S ribosomal protein S9

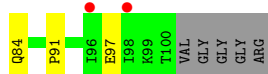




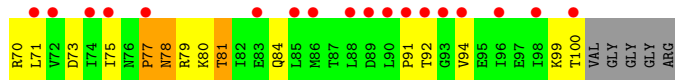
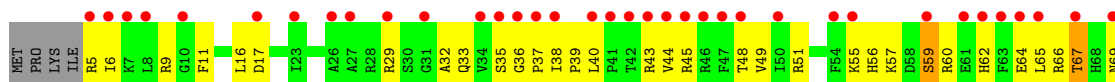
- Molecule 9: 30S ribosomal protein S9



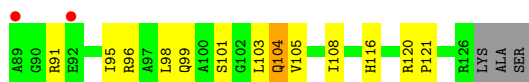
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

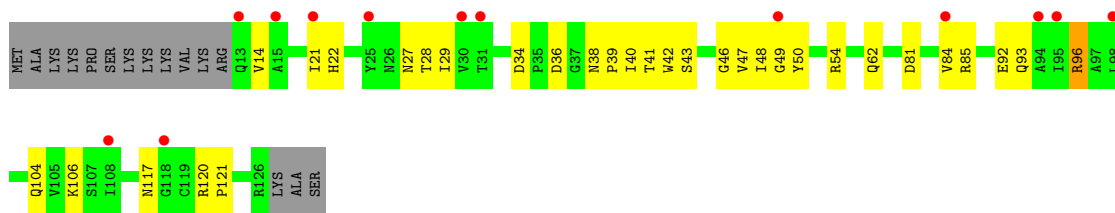


- Molecule 11: 30S ribosomal protein S11

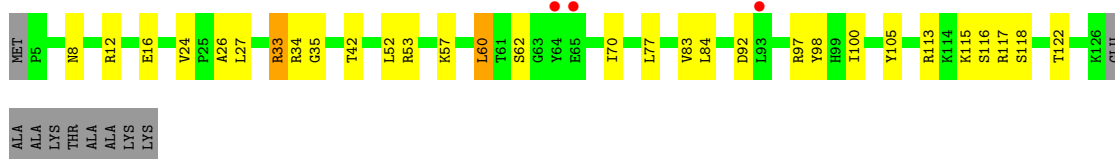


- Molecule 11: 30S ribosomal protein S11

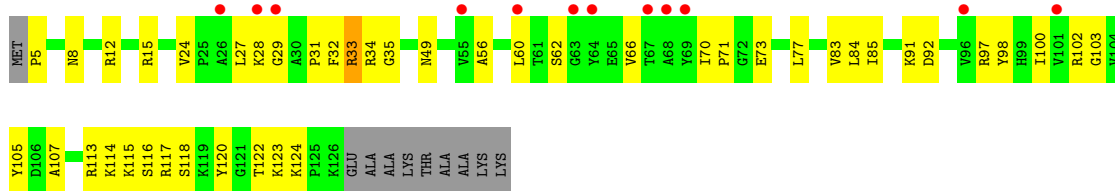




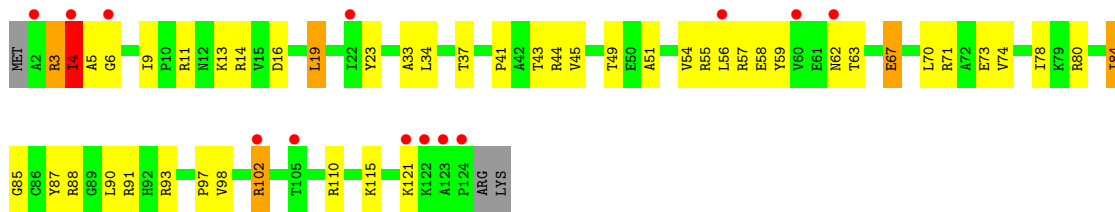
• Molecule 12: 30S ribosomal protein S12



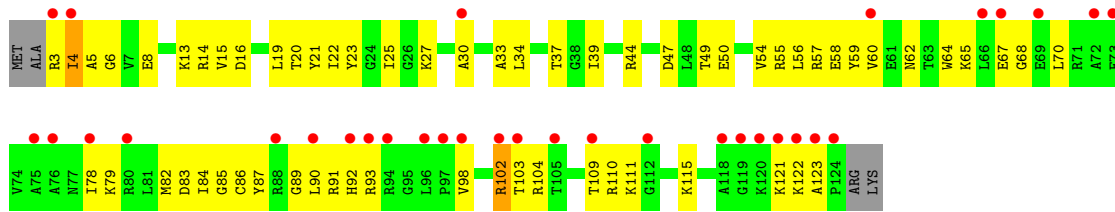
• Molecule 12: 30S ribosomal protein S12



• Molecule 13: 30S ribosomal protein S13



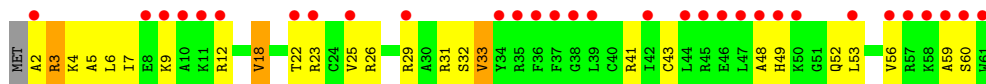
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14 type Z



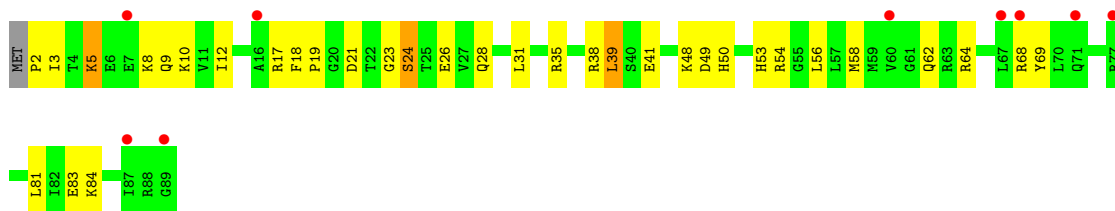
• Molecule 14: 30S ribosomal protein S14 type Z



• 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

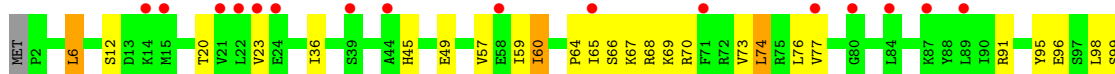
Chain AQ: 



ALA

- Molecule 17: 30S ribosomal protein S17

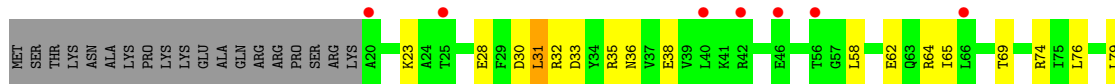
Chain CQ: 



K100
ARG
GLY
LYS
ALA

- Molecule 18: 30S ribosomal protein S18

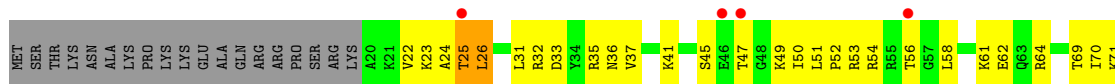
Chain AR: 



L85
V86
R87
LYS

- Molecule 18: 30S ribosomal protein S18

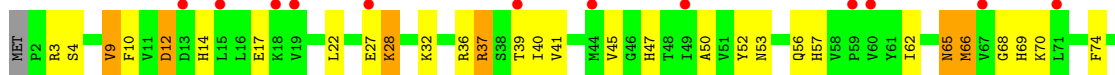
Chain CR: 

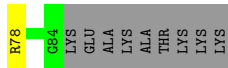


R72
A73
R74
L76
L79
P80
F81
K84
R87
LYS

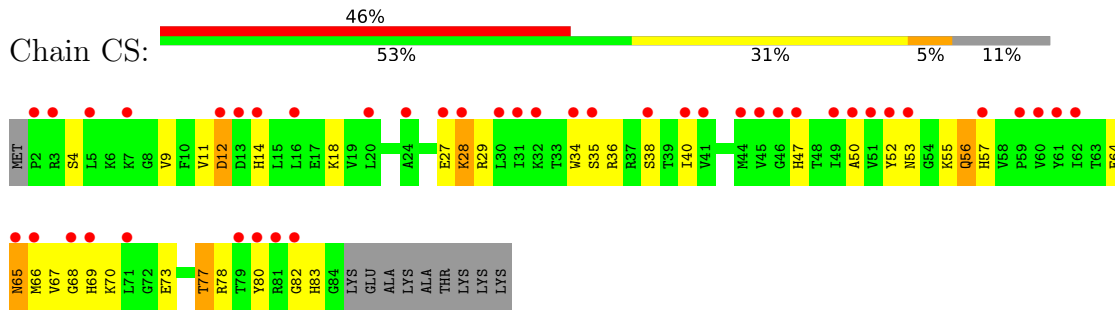
- Molecule 19: 30S ribosomal protein S19

Chain AS: 

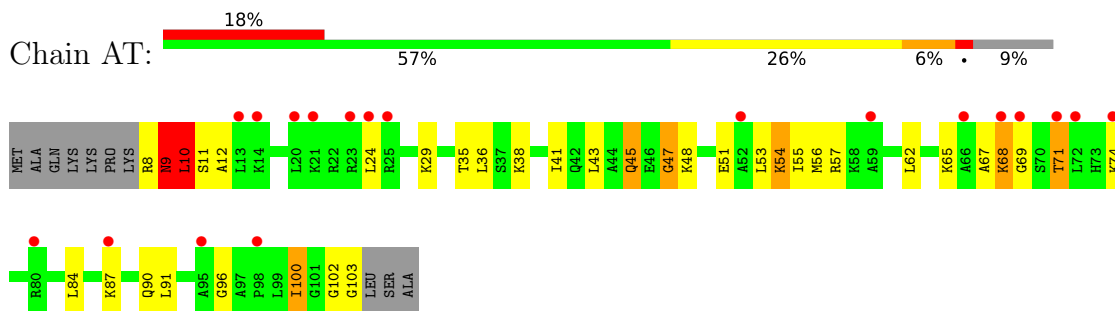




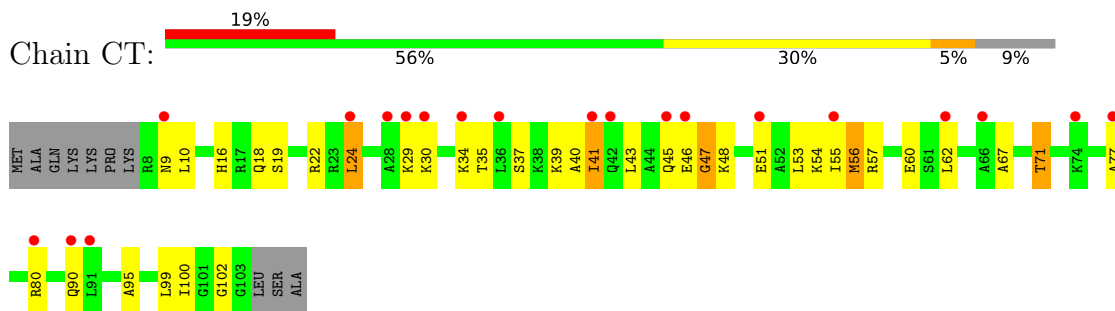
- Molecule 19: 30S ribosomal protein S19



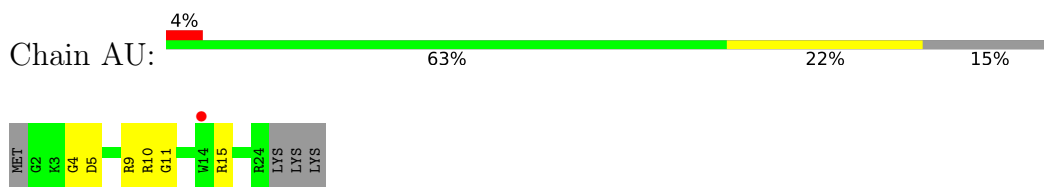
- Molecule 20: 30S ribosomal protein S20



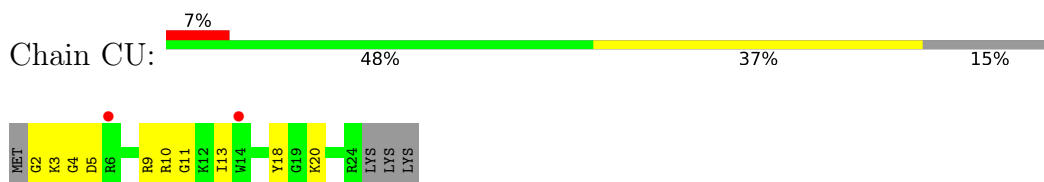
- Molecule 20: 30S ribosomal protein S20



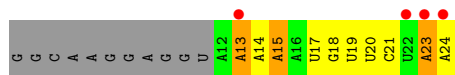
- Molecule 21: 30S ribosomal protein Thx



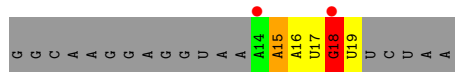
- Molecule 21: 30S ribosomal protein Thx



• Molecule 22: mRNA



• Molecule 22: mRNA



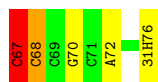
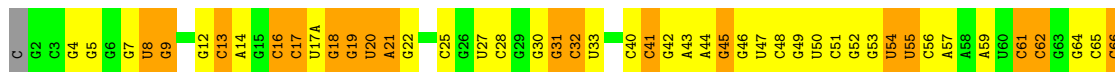
• Molecule 23: Cytidine-Puromycin



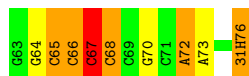
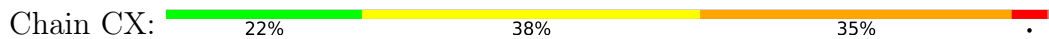
• Molecule 23: Cytidine-Puromycin



• Molecule 24: P-site tRNA

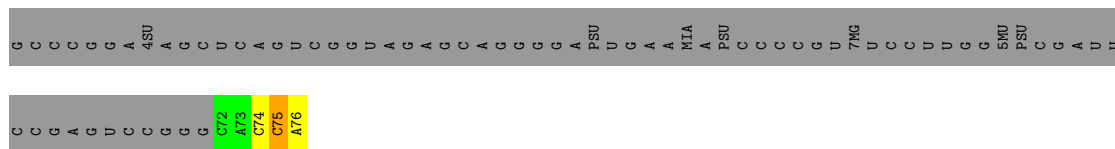


• Molecule 24: P-site tRNA

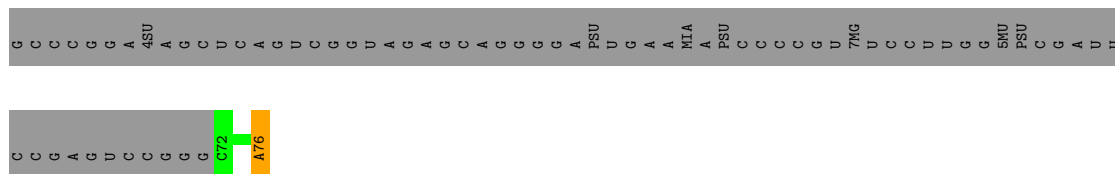


• Molecule 25: E-site tRNA

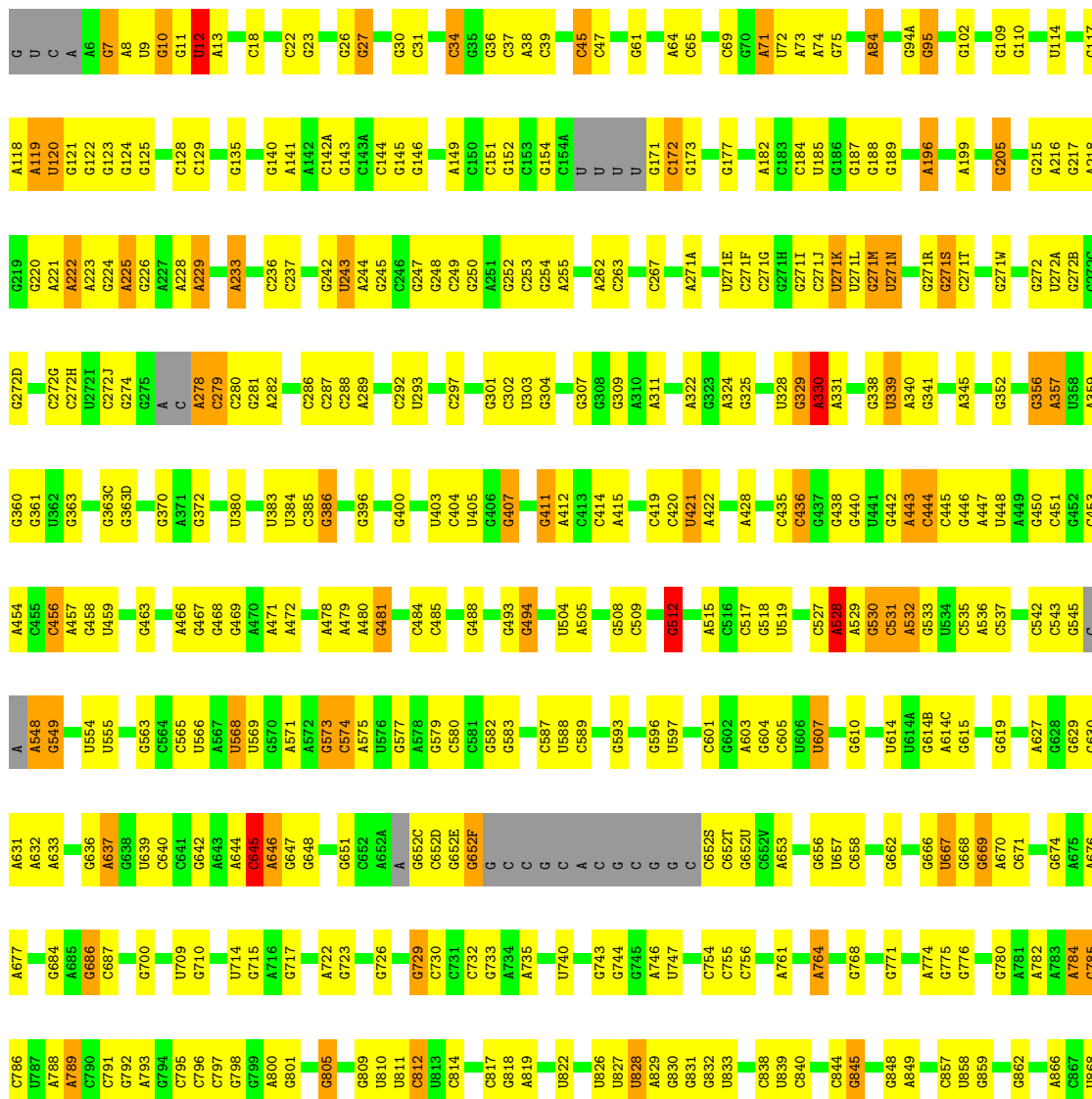




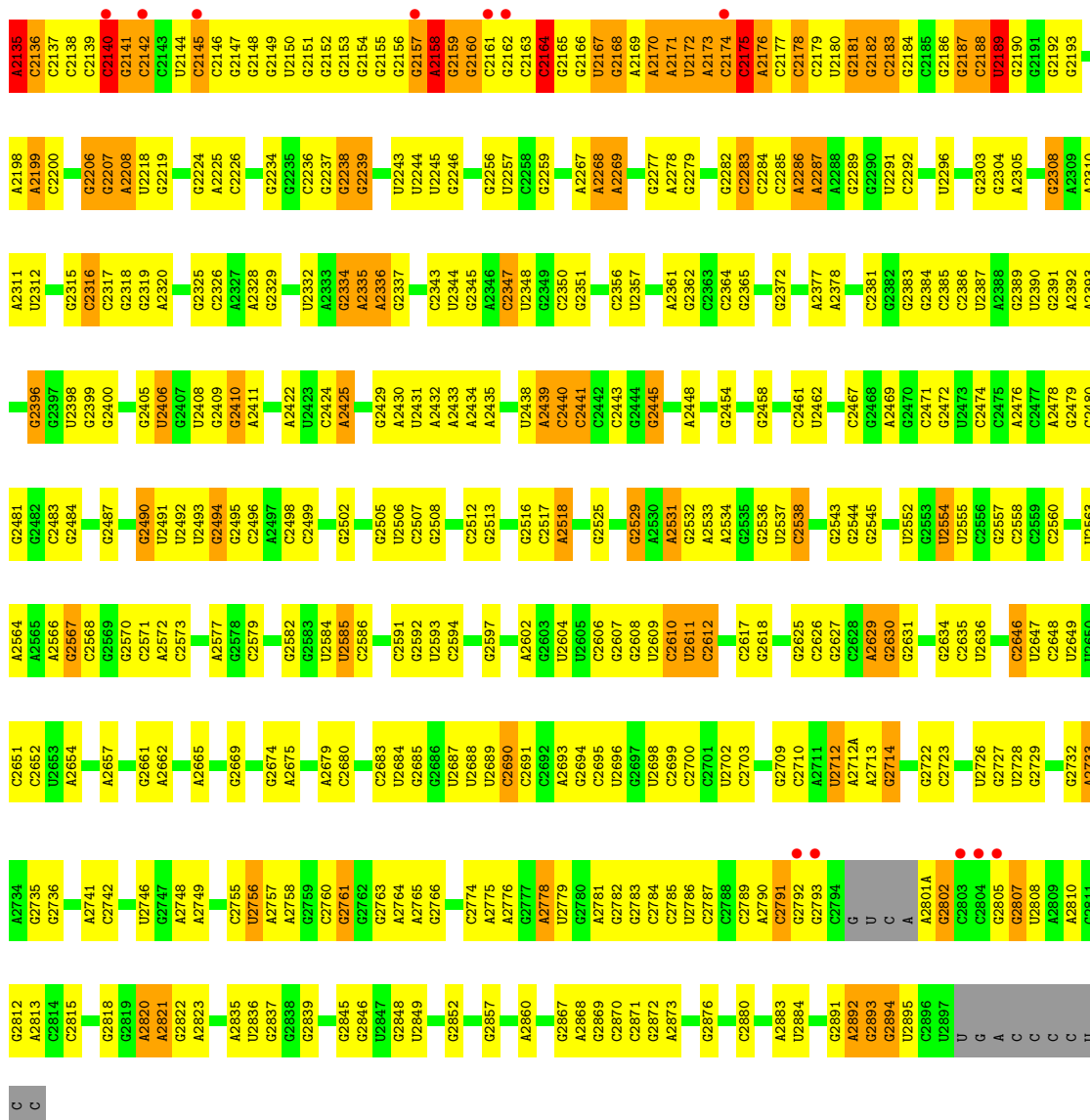
● Molecule 25: E-site tRNA



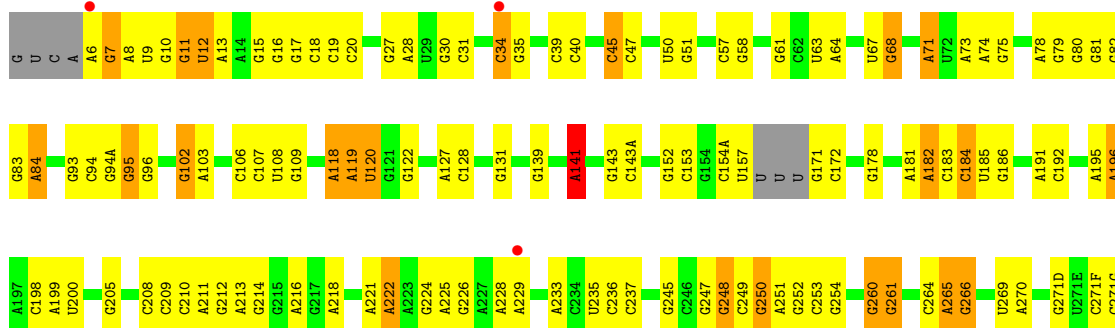
● Molecule 26: 23S Ribosomal RNA



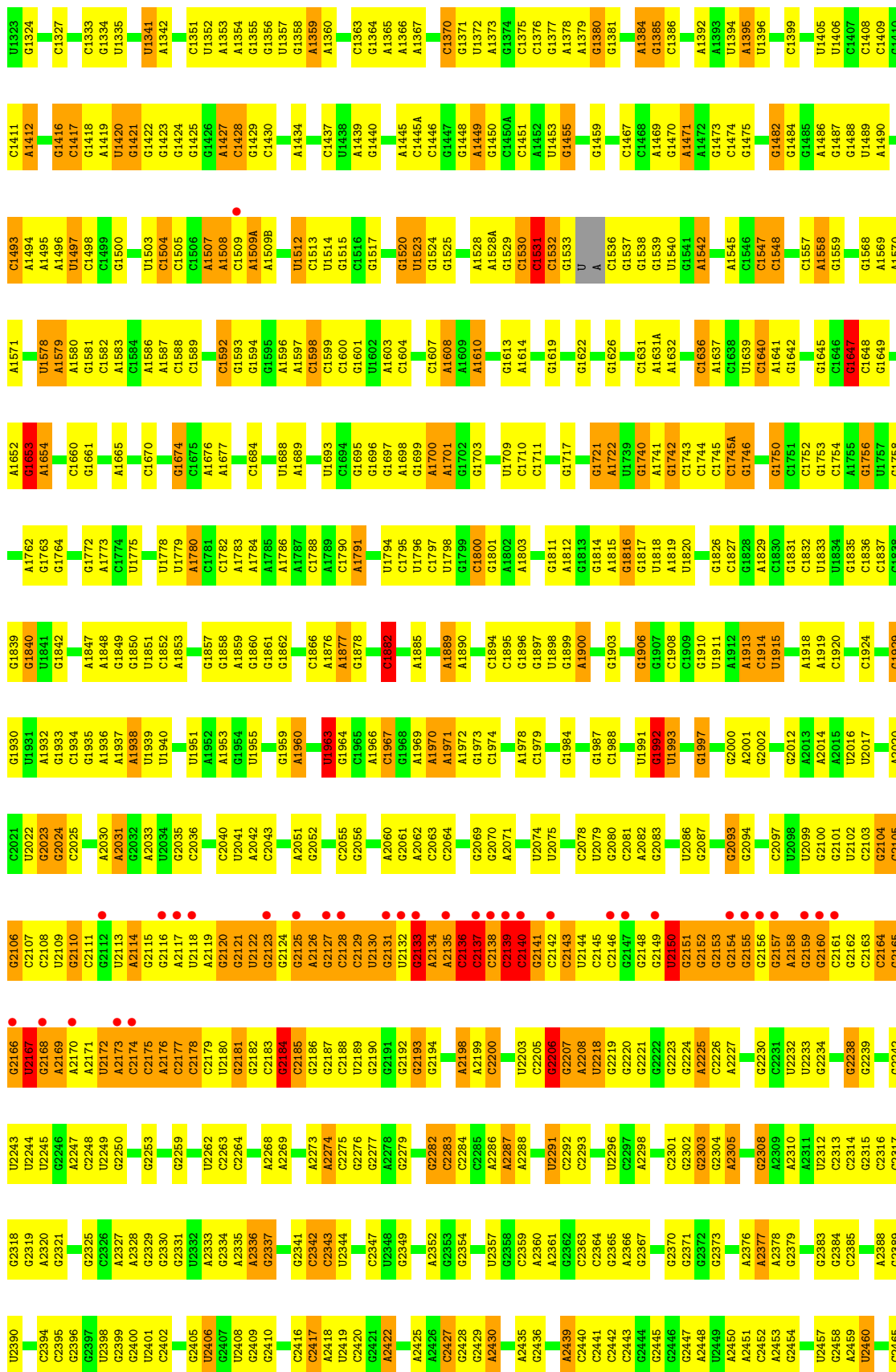
| | | | | | | | | | | | |
|-------|-------|-------|-------|-------|--------|--------|-------|-------|--------|-------|-------|
| G2056 | C1967 | U1864 | G1666 | G1555 | A1477 | A1392 | U1300 | A1194 | A1111 | C961 | G869 |
| A2060 | G1968 | G1865 | G1667 | C1586 | G1478 | A1393 | A1301 | A1194 | G1112 | G962 | A870 |
| A2062 | A1969 | A1877 | A1668 | A1557 | G1482 | U1394 | A1302 | G1195 | G1113 | U963 | U871 |
| C2065 | G1970 | G1878 | A1671 | A1566 | U1489 | U1396 | A1308 | C1201 | G1120 | U969 | G874 |
| C2066 | C1974 | C1782 | U1673 | A1567 | A1490 | C1398 | G1309 | A1204 | G1121 | C970 | G875 |
| G2069 | A1889 | A1784 | G1674 | G1568 | G1491 | U1405 | G1310 | G1309 | G1122 | A973 | C876 |
| U2074 | G1899 | A1786 | C1675 | A1569 | C1492 | U1406 | G1311 | C1208 | G1123 | G974 | G879 |
| U2075 | A1900 | A1787 | A1676 | A1570 | C1493 | U1407 | U1312 | G1209 | G1124 | G974 | G880 |
| G2080 | A1901 | G1788 | G1682 | A1571 | C1494 | C1408 | U1313 | A1210 | G1125 | G975A | G881 |
| U2086 | C1902 | U1688 | U1688 | U1578 | A1496 | A1408 | C1314 | U1211 | A1126 | A983 | C884 |
| U2087 | G1906 | A1689 | A1689 | A1579 | A1412 | A1412 | U1316 | C1218 | A1128 | C885 | C885 |
| G2093 | G1907 | G1690 | A1690 | G1580 | G1413 | G1413 | A1317 | C1219 | A1129 | C886 | C886 |
| G2094 | C1908 | C1691 | C1691 | G1581 | G1414 | G1414 | U1318 | G1219 | U1130 | A990 | C887 |
| C2095 | A1912 | U1692 | U1692 | A1582 | U1415 | U1415 | G1319 | A1220 | U1131 | G993 | C888 |
| U2096 | A1913 | U1693 | U1693 | A1583 | C1505 | G1416 | C1320 | G1224 | G1135 | C994 | C889 |
| C2097 | A1914 | C1694 | C1694 | A1584 | C1506 | C1417 | A1321 | A1226 | G1136 | C995 | C890 |
| U2098 | U1915 | G1695 | G1695 | A1585 | A1507 | A1418 | G1324 | A1226 | G1136 | A996 | A890 |
| U2099 | U1916 | U1696 | U1696 | A1586 | A1508 | A1419 | U1324 | A1226 | G1136 | G997 | G892 |
| G2100 | U1917 | A1697 | A1697 | A1587 | A1509 | U1420 | G1328 | C1230 | G1139 | C998 | U895 |
| U2102 | U1918 | G1698 | G1698 | A1588 | C1509 | U1421 | U1329 | G1231 | C1140 | C999 | A896 |
| C2103 | A1919 | U1699 | U1699 | A1589 | A1509B | G1422 | U1329 | G1232 | U1141 | A1000 | C897 |
| U2104 | C1924 | G1700 | G1700 | G1510 | G1423 | G1422 | C1333 | G1232 | U1142 | A1009 | C898 |
| A2013 | U1927 | A1701 | A1701 | G1511 | G1424 | G1424 | U1333 | G1239 | A1142A | C904 | C904 |
| A2014 | A1928 | A1702 | A1702 | G1512 | G1425 | G1425 | U1334 | U1240 | G1143 | U012 | U905 |
| A2015 | G1929 | G1703 | G1703 | C1513 | G1426 | G1426 | U1335 | U1241 | G1144 | U1012 | U905 |
| A2019 | U1930 | U1709 | U1709 | U1518 | A1427 | A1427 | G1338 | U1242 | C1145 | C1013 | G906 |
| U2109 | G1931 | C1710 | C1710 | U1519 | G1428 | G1428 | U1338 | G1243 | U1146 | U1014 | U907 |
| G2111 | A1932 | U1720 | U1720 | G1520 | G1429 | G1429 | U1341 | G1244 | C1147 | G1015 | A910 |
| G2112 | C1934 | G1721 | G1721 | A1521 | A1430 | A1430 | A1342 | G1280 | A1148 | G1016 | A910 |
| U2113 | G1935 | A1722 | A1722 | G1522 | U1431 | U1431 | A1342 | C1281 | G1149 | G1017 | A911 |
| A2114 | U1936 | U1723 | U1723 | C1530 | A1432 | A1432 | U1352 | G1281 | C1153 | C1018 | C914 |
| G2115 | A1937 | G1740 | G1740 | G1532 | U1433 | U1433 | U1352 | G1285 | G1154 | A1018 | C914 |
| G2116 | U1938 | A1741 | A1741 | G1532 | A1434 | A1434 | A1353 | A1253 | G1154 | U1019 | C914 |
| A2117 | G1939 | A1742 | A1742 | G1532 | A1434 | A1434 | A1354 | A1254 | A1020 | A1020 | A918 |
| U2118 | U1940 | G1746 | G1746 | A1532 | C1437 | C1437 | U1355 | U1255 | A1021 | A1021 | G919 |
| A2119 | C1941 | G1747 | G1747 | G1533 | A1445 | A1445 | G1356 | G1256 | G1025 | G1022 | G931 |
| G2120 | G1949 | U1748 | U1748 | C1533 | C1445A | C1445A | U1357 | C1257 | U1166 | U1026 | G932 |
| G2121 | G1950 | A1749 | A1749 | G1533 | G1446 | G1446 | G1358 | C1257 | U1167 | A1027 | G932 |
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| | | | | | | | G1386 | C1297 | G1187 | G1042 | G955 |
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| | | | | | | | | | | U1108 | U988 |
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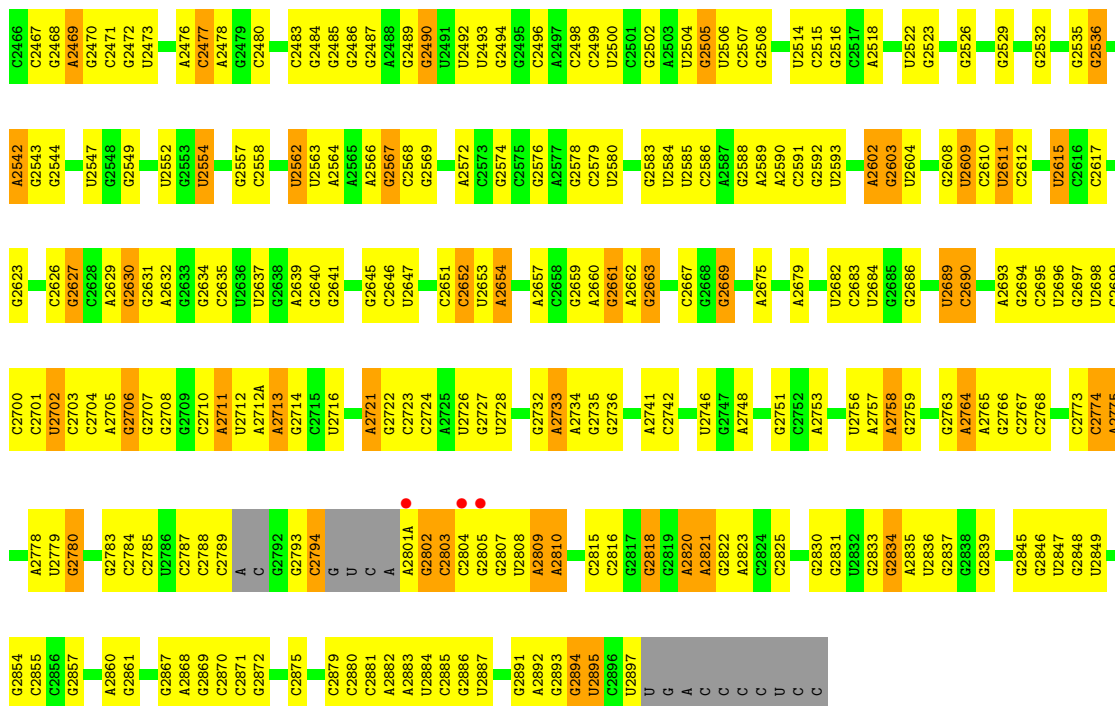


• Molecule 26: 23S Ribosomal RNA

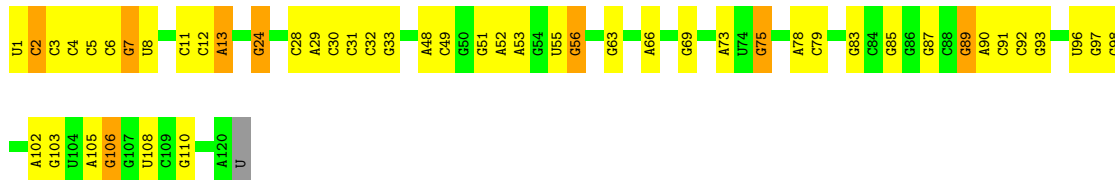


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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|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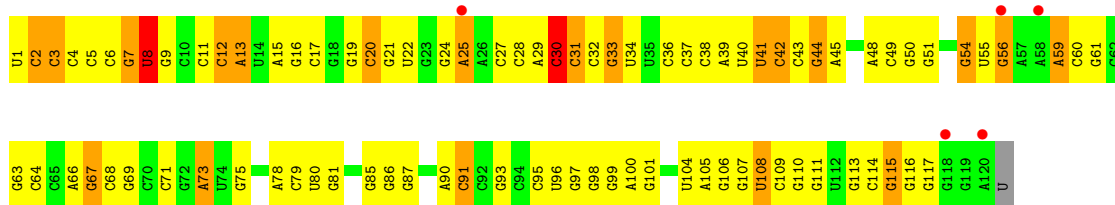




• Molecule 27: 5S Ribosomal RNA

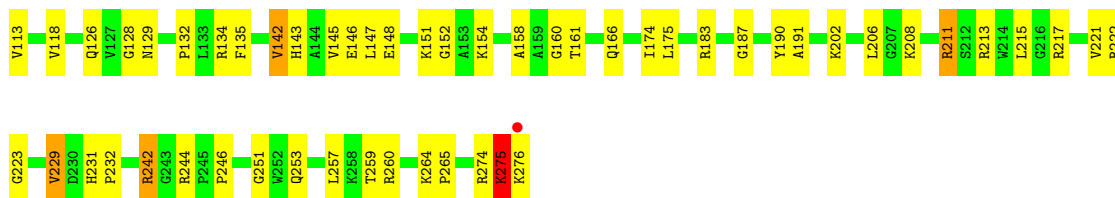


• Molecule 27: 5S Ribosomal RNA



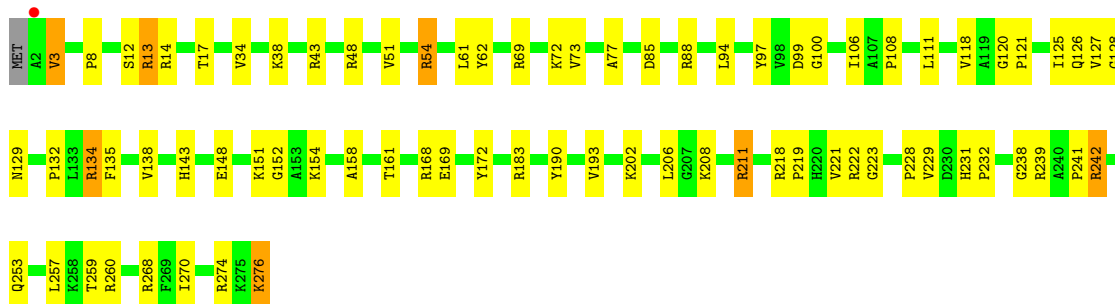
• Molecule 28: 50S ribosomal protein L2





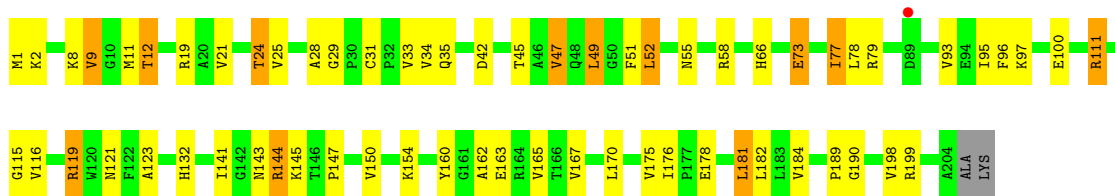
- Molecule 28: 50S ribosomal protein L2

Chain DD: 72% 25% .



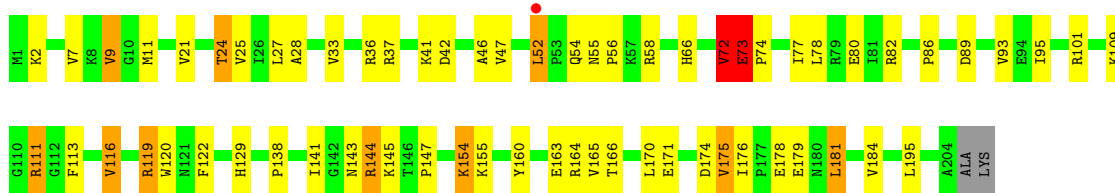
- Molecule 29: 50S ribosomal protein L3

Chain BE: 68% 25% 6% .



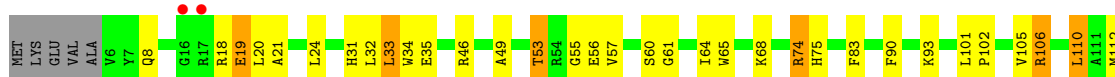
- Molecule 29: 50S ribosomal protein L3

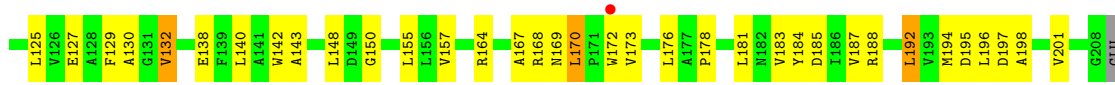
Chain DE: 67% 26% 5% ..



- Molecule 30: 50S ribosomal protein L4

Chain BF: % 64% 28% . .



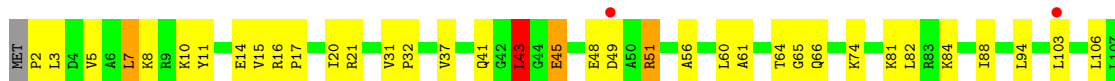


ALA

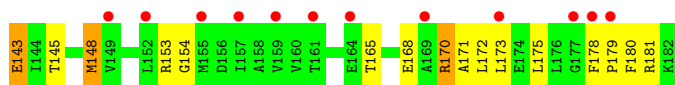
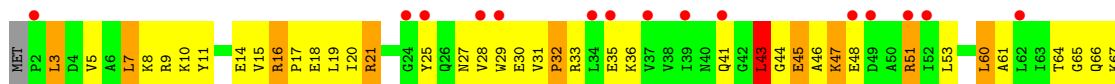
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

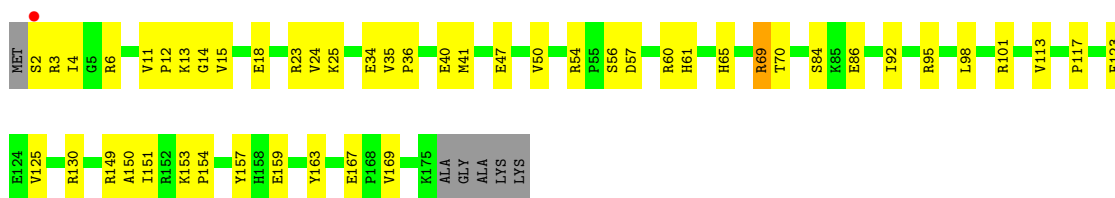


- Molecule 31: 50S ribosomal protein L5

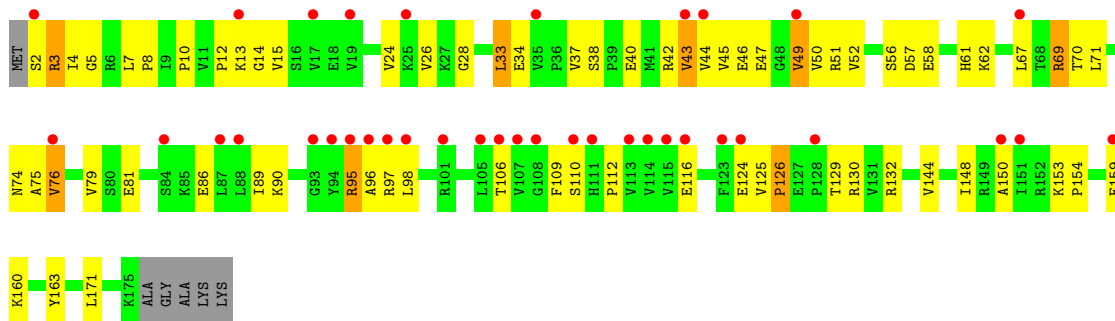


- Molecule 32: 50S ribosomal protein L6

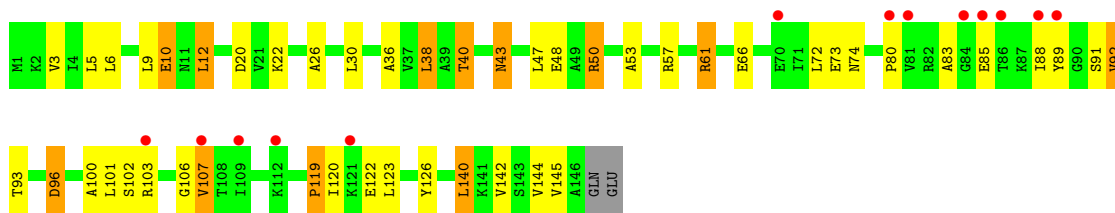




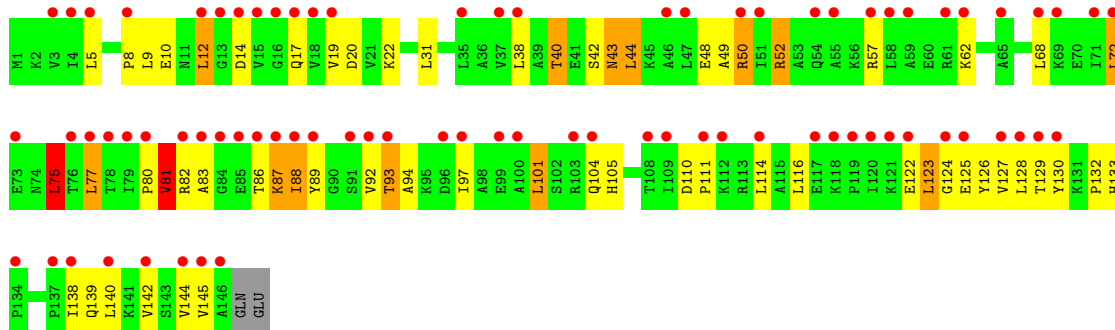
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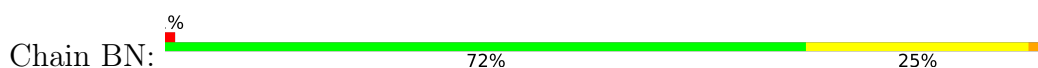
• Molecule 33: 50S ribosomal protein L9

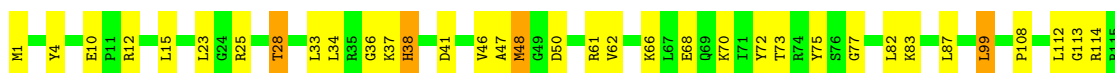


• Molecule 33: 50S ribosomal protein L9

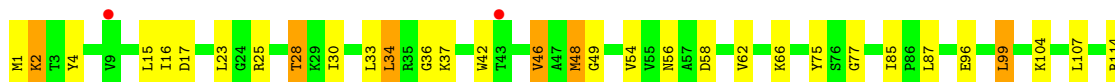
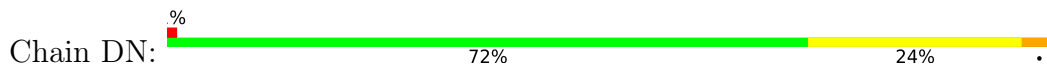


• Molecule 34: 50S ribosomal protein L13





- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L14

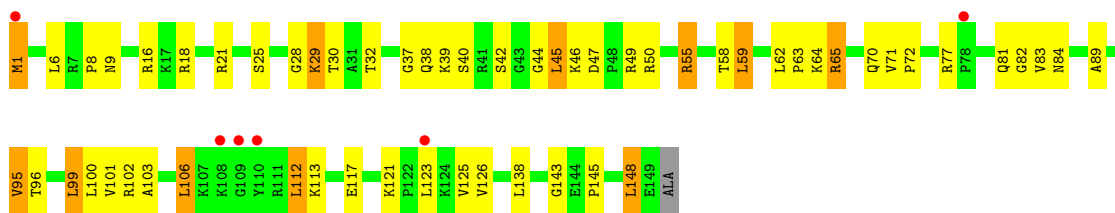


- Molecule 36: 50S ribosomal protein L15



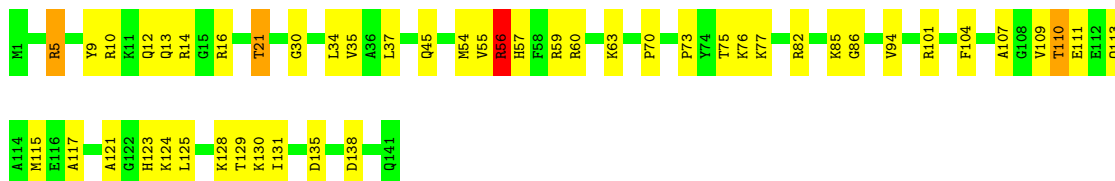
- Molecule 36: 50S ribosomal protein L15





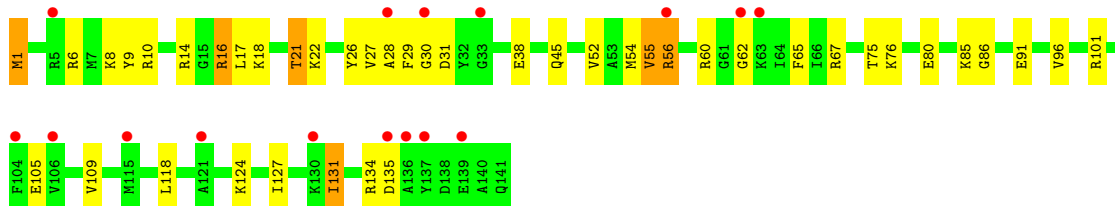
- Molecule 37: 50S ribosomal protein L16

Chain BQ: 66% 31% ..



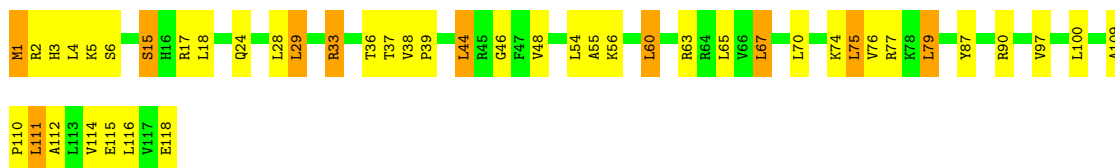
- Molecule 37: 50S ribosomal protein L16

Chain DQ: 11% 70% 26% .



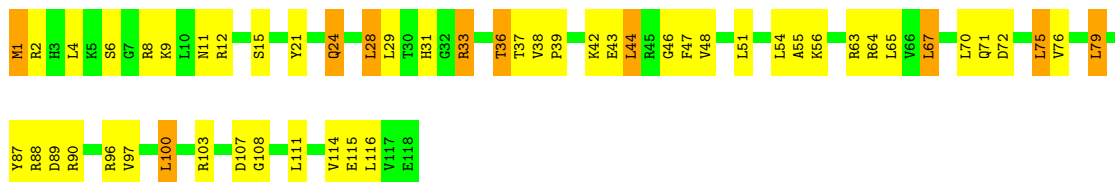
- Molecule 38: 50S ribosomal protein L17

Chain BR: 62% 30% 8%



- Molecule 38: 50S ribosomal protein L17

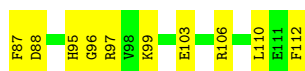
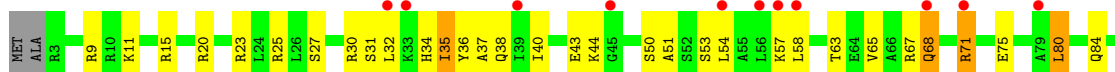
Chain DR: 55% 36% 8%



- Molecule 39: 50S ribosomal protein L18



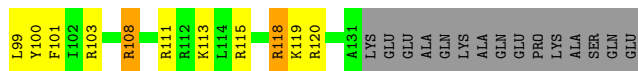
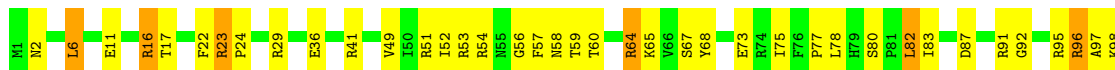
• Molecule 39: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L19

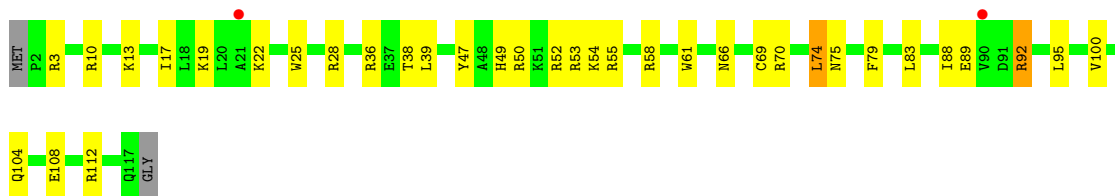


• Molecule 41: 50S ribosomal protein L20



• Molecule 41: 50S ribosomal protein L20





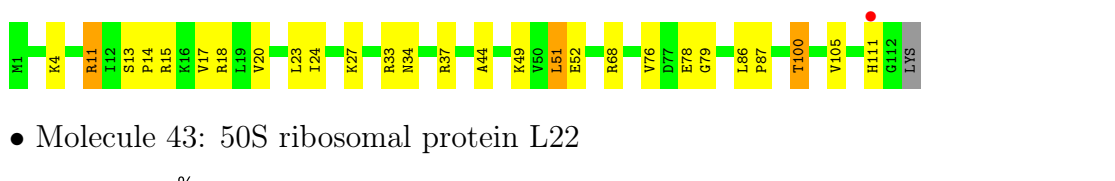
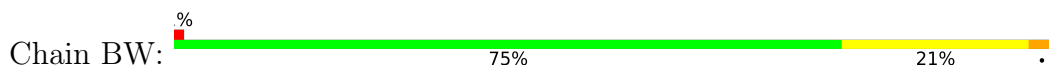
• Molecule 42: 50S ribosomal protein L21



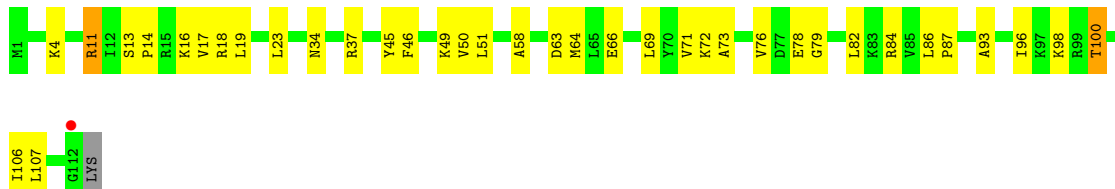
• Molecule 42: 50S ribosomal protein L21



• Molecule 43: 50S ribosomal protein L22

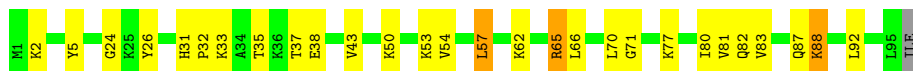


• Molecule 43: 50S ribosomal protein L22

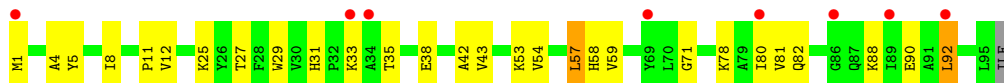


• Molecule 44: 50S ribosomal protein L23

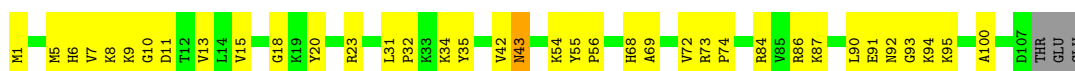




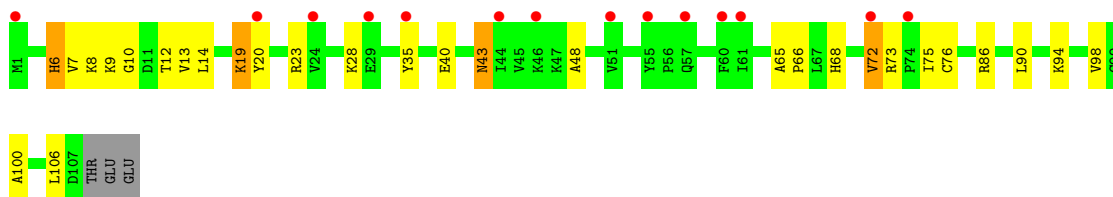
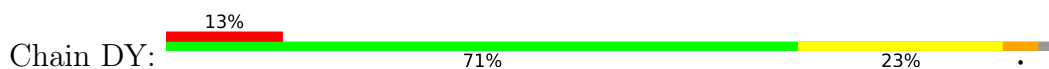
- Molecule 44: 50S ribosomal protein L23



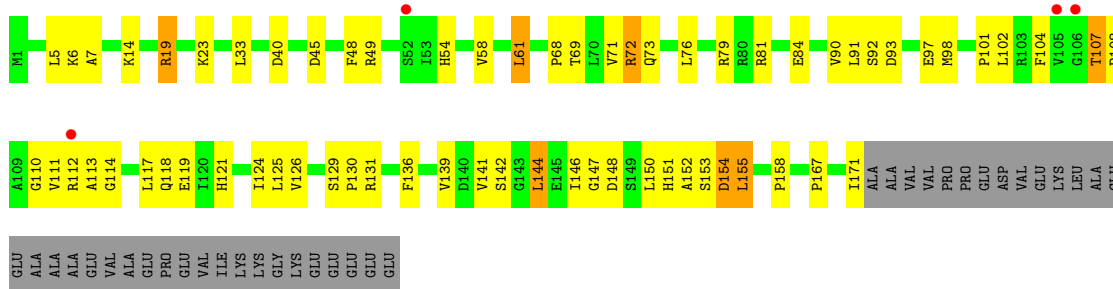
- Molecule 45: 50S ribosomal protein L24



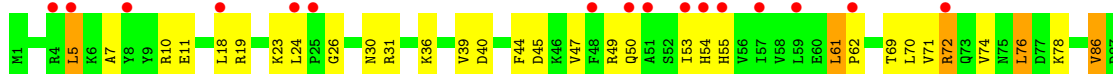
- Molecule 45: 50S ribosomal protein L24

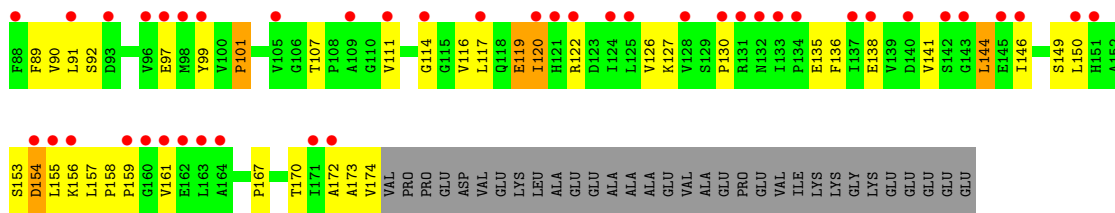


- Molecule 46: 50S ribosomal protein L25

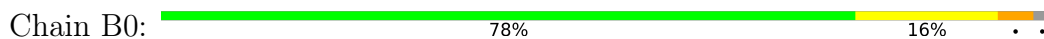


- Molecule 46: 50S ribosomal protein L25

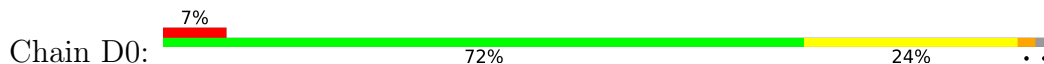




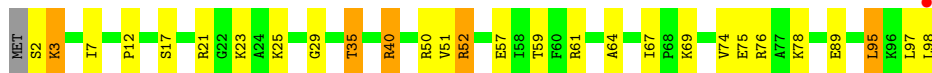
• Molecule 47: 50S ribosomal protein L27



• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L28



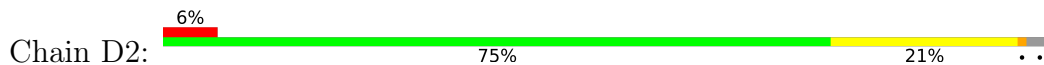
• Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L29



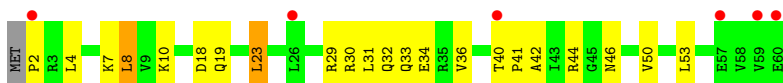
- Molecule 50: 50S ribosomal protein L30

Chain B3:  65% 27% 7%



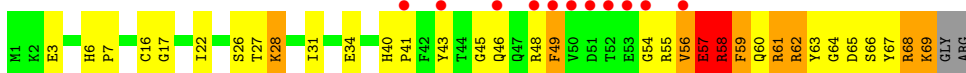
- Molecule 50: 50S ribosomal protein L30

Chain D3:  10% 62% 33%



- Molecule 51: 50S ribosomal protein L31

Chain B4:  15% 49% 34% 11%




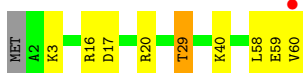
- Molecule 51: 50S ribosomal protein L31

Chain D4:  34% 41% 48% 8%




- Molecule 52: 50S ribosomal protein L32

Chain B5:  2% 83% 13%



- Molecule 52: 50S ribosomal protein L32

Chain D5:  78% 18%

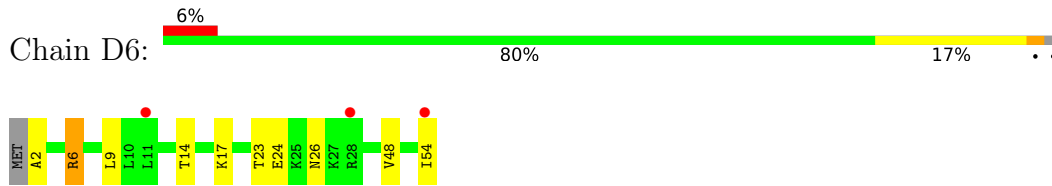


- Molecule 53: 50S ribosomal protein L33

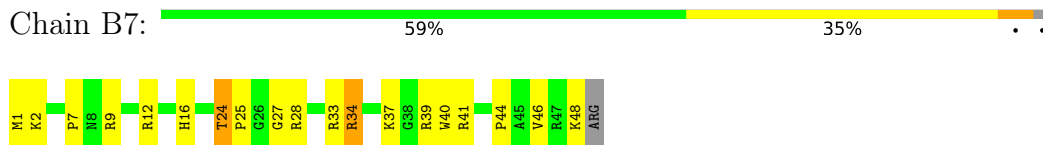
Chain B6:  59% 33% 6%



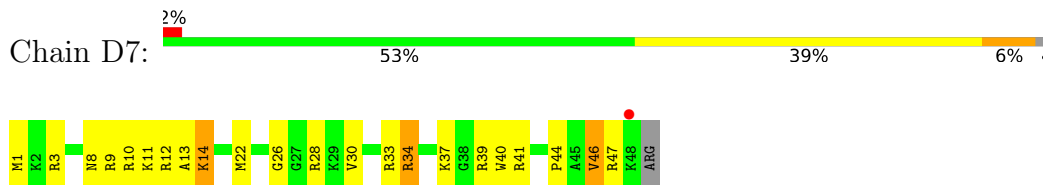
- Molecule 53: 50S ribosomal protein L33



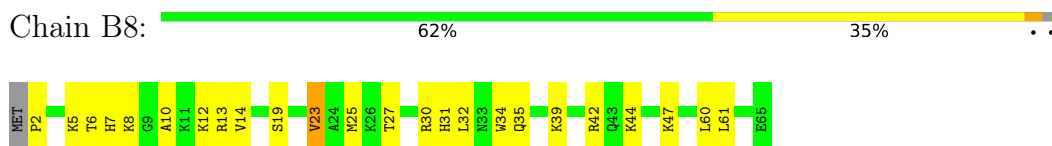
- Molecule 54: 50S ribosomal protein L34



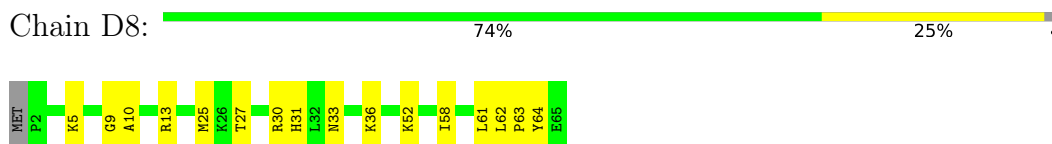
- Molecule 54: 50S ribosomal protein L34



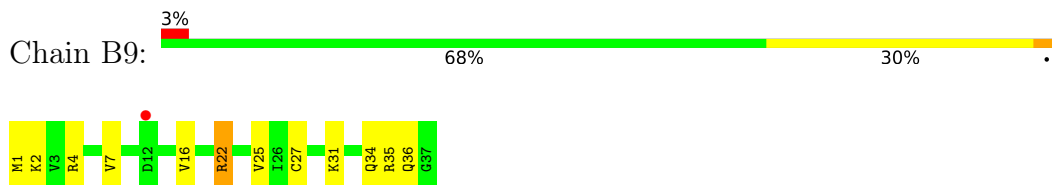
- Molecule 55: 50S ribosomal protein L35



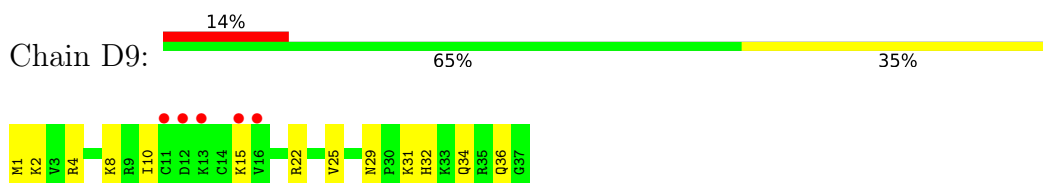
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 207.56Å 444.23Å 613.03Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 150.38 – 2.80 150.38 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | 98.0 (150.38-2.80) 98.0 (150.38-2.80) | Depositor EDS |
| R_{merge} | 0.18 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.29 (at 2.82Å) | Xtrriage |
| Refinement program | PHENIX 1.8.2_1309 | Depositor |
| R, R_{free} | 0.234 , 0.280 0.234 , 0.281 | Depositor DCC |
| R_{free} test set | 67651 reflections (5.03%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 50.1 | Xtrriage |
| Anisotropy | 0.204 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 61.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 290205 | wwPDB-VP |
| Average B, all atoms (Å ²) | 59.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PPU, 5MU, K, MG, 31H, SF4, PSU, 5MC, ZN, 4SU

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 | 0.41 | 4/36049 (0.0%) | 0.98 | 71/56261 (0.1%) |
| 1 | CA | 0.42 | 7/36170 (0.0%) | 1.05 | 147/56452 (0.3%) |
| 2 | AB | 0.29 | 0/1881 | 0.59 | 0/2542 |
| 2 | CB | 0.33 | 0/1860 | 0.68 | 3/2518 (0.1%) |
| 3 | AC | 0.28 | 0/1576 | 0.52 | 0/2130 |
| 3 | CC | 0.30 | 0/1566 | 0.58 | 0/2119 |
| 4 | AD | 0.28 | 0/1689 | 0.55 | 0/2267 |
| 4 | CD | 0.30 | 0/1704 | 0.56 | 0/2284 |
| 5 | AE | 0.29 | 0/1145 | 0.52 | 0/1543 |
| 5 | CE | 0.30 | 0/1149 | 0.58 | 1/1548 (0.1%) |
| 6 | AF | 0.29 | 0/819 | 0.50 | 0/1111 |
| 6 | CF | 0.30 | 0/829 | 0.49 | 0/1123 |
| 7 | AG | 0.27 | 0/1250 | 0.51 | 0/1679 |
| 7 | CG | 0.29 | 0/1254 | 0.53 | 0/1683 |
| 8 | AH | 0.27 | 0/1108 | 0.51 | 0/1494 |
| 8 | CH | 0.27 | 0/1108 | 0.55 | 0/1494 |
| 9 | AI | 0.28 | 0/1002 | 0.54 | 0/1346 |
| 9 | CI | 0.30 | 0/997 | 0.56 | 0/1343 |
| 10 | AJ | 0.27 | 0/722 | 0.60 | 0/982 |
| 10 | CJ | 0.30 | 0/727 | 0.57 | 0/988 |
| 11 | AK | 0.29 | 0/844 | 0.50 | 0/1145 |
| 11 | CK | 0.27 | 0/848 | 0.50 | 0/1149 |
| 12 | AL | 0.29 | 0/946 | 0.51 | 0/1274 |
| 12 | CL | 0.29 | 0/946 | 0.56 | 0/1274 |
| 13 | AM | 0.28 | 0/969 | 0.58 | 0/1302 |
| 13 | CM | 0.29 | 0/961 | 0.57 | 0/1291 |
| 14 | AN | 0.30 | 0/501 | 0.55 | 0/664 |
| 14 | CN | 0.32 | 0/501 | 0.55 | 0/664 |
| 15 | AO | 0.27 | 0/739 | 0.53 | 0/985 |
| 15 | CO | 0.30 | 0/739 | 0.54 | 0/985 |
| 16 | AP | 0.29 | 0/697 | 0.53 | 0/939 |
| 16 | CP | 0.28 | 0/693 | 0.54 | 0/935 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.29 | 0/836 | 0.55 | 0/1117 |
| 17 | CQ | 0.29 | 0/836 | 0.53 | 0/1117 |
| 18 | AR | 0.27 | 0/560 | 0.48 | 0/746 |
| 18 | CR | 0.28 | 0/560 | 0.52 | 0/746 |
| 19 | AS | 0.28 | 0/667 | 0.54 | 0/900 |
| 19 | CS | 0.30 | 0/661 | 0.68 | 0/893 |
| 20 | AT | 0.27 | 0/730 | 0.58 | 0/965 |
| 20 | CT | 0.27 | 0/729 | 0.52 | 0/965 |
| 21 | AU | 0.29 | 0/203 | 0.56 | 0/266 |
| 21 | CU | 0.32 | 0/203 | 0.48 | 0/266 |
| 22 | AV | 0.49 | 0/310 | 0.95 | 1/480 (0.2%) |
| 22 | CV | 1.15 | 3/144 (2.1%) | 3.12 | 11/222 (5.0%) |
| 23 | AW | 0.45 | 0/40 | 1.07 | 0/60 |
| 23 | CW | 0.35 | 0/40 | 1.09 | 0/60 |
| 24 | AX | 0.53 | 2/1700 (0.1%) | 1.24 | 23/2650 (0.9%) |
| 24 | CX | 0.54 | 0/1700 | 1.36 | 19/2650 (0.7%) |
| 25 | AY | 0.33 | 0/115 | 0.82 | 0/176 |
| 25 | CY | 0.29 | 0/115 | 0.95 | 0/176 |
| 26 | BA | 0.50 | 4/68013 (0.0%) | 0.93 | 70/106165 (0.1%) |
| 26 | DA | 0.42 | 0/67542 | 0.94 | 88/105428 (0.1%) |
| 27 | BB | 0.41 | 0/2878 | 0.91 | 2/4490 (0.0%) |
| 27 | DB | 0.41 | 0/2878 | 1.00 | 8/4490 (0.2%) |
| 28 | BD | 0.37 | 0/2186 | 0.57 | 0/2944 |
| 28 | DD | 0.34 | 0/2186 | 0.56 | 0/2944 |
| 29 | BE | 0.36 | 0/1592 | 0.53 | 0/2149 |
| 29 | DE | 0.34 | 0/1592 | 0.59 | 1/2149 (0.0%) |
| 30 | BF | 0.35 | 0/1619 | 0.53 | 0/2193 |
| 30 | DF | 0.33 | 0/1615 | 0.56 | 0/2188 |
| 31 | BG | 0.29 | 0/1450 | 0.54 | 0/1959 |
| 31 | DG | 0.32 | 0/1449 | 0.57 | 0/1958 |
| 32 | BH | 0.30 | 0/1356 | 0.51 | 0/1834 |
| 32 | DH | 0.29 | 0/1356 | 0.51 | 0/1834 |
| 33 | BI | 0.31 | 0/1100 | 0.59 | 0/1501 |
| 33 | DI | 0.37 | 0/1076 | 0.78 | 4/1471 (0.3%) |
| 34 | BN | 0.34 | 0/1144 | 0.54 | 0/1543 |
| 34 | DN | 0.31 | 0/1144 | 0.52 | 0/1543 |
| 35 | BO | 0.34 | 0/943 | 0.56 | 0/1269 |
| 35 | DO | 0.33 | 0/943 | 0.55 | 1/1269 (0.1%) |
| 36 | BP | 0.35 | 0/1152 | 0.57 | 0/1533 |
| 36 | DP | 0.32 | 0/1152 | 0.63 | 0/1533 |
| 37 | BQ | 0.35 | 0/1143 | 0.59 | 1/1527 (0.1%) |
| 37 | DQ | 0.32 | 0/1143 | 0.54 | 0/1527 |
| 38 | BR | 0.36 | 0/982 | 0.57 | 0/1312 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DR | 0.29 | 0/982 | 0.55 | 0/1312 |
| 39 | BS | 0.32 | 0/887 | 0.57 | 1/1180 (0.1%) |
| 39 | DS | 0.29 | 0/880 | 0.57 | 0/1172 |
| 40 | BT | 0.34 | 0/1105 | 0.61 | 0/1477 |
| 40 | DT | 0.30 | 0/1097 | 0.53 | 0/1468 |
| 41 | BU | 0.35 | 0/977 | 0.53 | 0/1301 |
| 41 | DU | 0.28 | 0/977 | 0.50 | 0/1301 |
| 42 | BV | 0.36 | 0/782 | 0.55 | 0/1049 |
| 42 | DV | 0.29 | 0/782 | 0.54 | 0/1049 |
| 43 | BW | 0.35 | 0/897 | 0.53 | 0/1205 |
| 43 | DW | 0.30 | 0/897 | 0.49 | 0/1205 |
| 44 | BX | 0.39 | 0/764 | 0.58 | 1/1025 (0.1%) |
| 44 | DX | 0.32 | 0/764 | 0.53 | 1/1025 (0.1%) |
| 45 | BY | 0.34 | 0/819 | 0.59 | 0/1095 |
| 45 | DY | 0.30 | 0/819 | 0.55 | 0/1095 |
| 46 | BZ | 0.32 | 0/1379 | 0.58 | 0/1873 |
| 46 | DZ | 0.29 | 0/1390 | 0.54 | 0/1890 |
| 47 | B0 | 0.36 | 0/662 | 0.60 | 0/881 |
| 47 | D0 | 0.30 | 0/662 | 0.50 | 0/881 |
| 48 | B1 | 0.32 | 0/762 | 0.53 | 0/1014 |
| 48 | D1 | 0.31 | 0/762 | 0.53 | 0/1014 |
| 49 | B2 | 0.32 | 0/590 | 0.57 | 0/781 |
| 49 | D2 | 0.26 | 0/590 | 0.49 | 0/781 |
| 50 | B3 | 0.35 | 0/474 | 0.52 | 0/635 |
| 50 | D3 | 0.31 | 0/469 | 0.54 | 0/630 |
| 51 | B4 | 0.34 | 0/565 | 0.70 | 0/761 |
| 51 | D4 | 0.32 | 0/545 | 0.67 | 0/737 |
| 52 | B5 | 0.37 | 0/469 | 0.62 | 1/635 (0.2%) |
| 52 | D5 | 0.32 | 0/469 | 0.54 | 0/635 |
| 53 | B6 | 0.36 | 0/460 | 0.53 | 0/613 |
| 53 | D6 | 0.34 | 0/456 | 0.51 | 0/608 |
| 54 | B7 | 0.36 | 0/426 | 0.56 | 0/561 |
| 54 | D7 | 0.34 | 0/426 | 0.49 | 0/561 |
| 55 | B8 | 0.37 | 0/519 | 0.54 | 0/684 |
| 55 | D8 | 0.31 | 0/525 | 0.50 | 0/691 |
| 56 | B9 | 0.43 | 0/310 | 0.65 | 0/407 |
| 56 | D9 | 0.33 | 0/310 | 0.59 | 0/407 |
| All | All | 0.41 | 20/310421 (0.0%) | 0.88 | 455/464361 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | AB | 0 | 1 |
| 7 | AG | 0 | 1 |
| 20 | AT | 0 | 1 |
| 29 | DE | 0 | 1 |
| 33 | DI | 0 | 1 |
| 39 | BS | 0 | 1 |
| 46 | BZ | 0 | 1 |
| 51 | B4 | 0 | 2 |
| 51 | D4 | 0 | 1 |
| All | All | 0 | 10 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | CA | 1154 | G | C6-N1 | -12.37 | 1.30 | 1.39 |
| 1 | AA | 1172 | C | N3-C4 | -10.50 | 1.26 | 1.33 |
| 1 | CA | 1154 | G | N1-C2 | -10.41 | 1.29 | 1.37 |
| 1 | AA | 1172 | C | C2-N3 | -8.49 | 1.28 | 1.35 |
| 1 | AA | 1164 | G | N1-C2 | -6.91 | 1.32 | 1.37 |

The worst 5 of 455 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | AA | 1172 | C | N1-C2-O2 | 39.76 | 142.76 | 118.90 |
| 1 | CA | 1119 | C | N1-C2-O2 | 26.84 | 135.00 | 118.90 |
| 1 | AA | 1172 | C | N3-C2-O2 | -25.31 | 104.18 | 121.90 |
| 1 | CA | 1154 | G | C5-C6-O6 | 24.22 | 143.13 | 128.60 |
| 1 | CA | 1154 | G | N1-C2-N2 | -23.61 | 94.95 | 116.20 |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | AB | 8 | LYS | Peptide |
| 7 | AG | 79 | ARG | Peptide |
| 20 | AT | 9 | ASN | Peptide |
| 39 | BS | 58 | LEU | Peptide |
| 46 | BZ | 158 | PRO | Peptide |

5.2 Too-close contacts [i](#)

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 | 32205 | 0 | 16255 | 743 | 1 |
| 1 | CA | 32312 | 0 | 16307 | 964 | 1 |
| 2 | AB | 1846 | 0 | 1867 | 74 | 0 |
| 2 | CB | 1825 | 0 | 1828 | 76 | 0 |
| 3 | AC | 1552 | 0 | 1546 | 49 | 0 |
| 3 | CC | 1542 | 0 | 1517 | 58 | 0 |
| 4 | AD | 1659 | 0 | 1676 | 74 | 0 |
| 4 | CD | 1674 | 0 | 1714 | 83 | 0 |
| 5 | AE | 1129 | 0 | 1184 | 33 | 0 |
| 5 | CE | 1133 | 0 | 1191 | 39 | 0 |
| 6 | AF | 806 | 0 | 793 | 16 | 0 |
| 6 | CF | 816 | 0 | 808 | 23 | 0 |
| 7 | AG | 1231 | 0 | 1238 | 37 | 0 |
| 7 | CG | 1235 | 0 | 1249 | 38 | 0 |
| 8 | AH | 1088 | 0 | 1126 | 35 | 0 |
| 8 | CH | 1088 | 0 | 1126 | 40 | 0 |
| 9 | AI | 983 | 0 | 986 | 48 | 0 |
| 9 | CI | 978 | 0 | 966 | 53 | 0 |
| 10 | AJ | 709 | 0 | 650 | 35 | 0 |
| 10 | CJ | 714 | 0 | 672 | 38 | 0 |
| 11 | AK | 829 | 0 | 825 | 23 | 0 |
| 11 | CK | 833 | 0 | 836 | 20 | 0 |
| 12 | AL | 930 | 0 | 980 | 21 | 0 |
| 12 | CL | 930 | 0 | 980 | 33 | 0 |
| 13 | AM | 958 | 0 | 1002 | 37 | 0 |
| 13 | CM | 950 | 0 | 988 | 47 | 0 |
| 14 | AN | 492 | 0 | 529 | 27 | 0 |
| 14 | CN | 492 | 0 | 529 | 23 | 0 |
| 15 | AO | 728 | 0 | 760 | 22 | 0 |
| 15 | CO | 728 | 0 | 760 | 27 | 0 |
| 16 | AP | 681 | 0 | 697 | 27 | 0 |
| 16 | CP | 677 | 0 | 686 | 26 | 0 |
| 17 | AQ | 823 | 0 | 891 | 23 | 0 |
| 17 | CQ | 823 | 0 | 891 | 18 | 0 |
| 18 | AR | 555 | 0 | 618 | 11 | 0 |
| 18 | CR | 555 | 0 | 618 | 23 | 0 |
| 19 | AS | 652 | 0 | 662 | 29 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | CS | 646 | 0 | 644 | 40 | 0 |
| 20 | AT | 728 | 0 | 798 | 27 | 0 |
| 20 | CT | 727 | 0 | 796 | 23 | 0 |
| 21 | AU | 199 | 0 | 208 | 5 | 0 |
| 21 | CU | 199 | 0 | 208 | 8 | 0 |
| 22 | AV | 277 | 0 | 140 | 7 | 0 |
| 22 | CV | 129 | 0 | 65 | 16 | 0 |
| 23 | AW | 74 | 0 | 51 | 5 | 0 |
| 23 | CW | 74 | 0 | 51 | 11 | 0 |
| 24 | AX | 1633 | 0 | 836 | 35 | 0 |
| 24 | CX | 1635 | 0 | 838 | 83 | 0 |
| 25 | AY | 104 | 0 | 56 | 3 | 0 |
| 25 | CY | 104 | 0 | 56 | 2 | 0 |
| 26 | BA | 60729 | 0 | 30620 | 950 | 0 |
| 26 | DA | 60311 | 0 | 30412 | 1223 | 1 |
| 27 | BB | 2573 | 0 | 1306 | 32 | 0 |
| 27 | DB | 2573 | 0 | 1306 | 87 | 0 |
| 28 | BD | 2136 | 0 | 2218 | 67 | 0 |
| 28 | DD | 2136 | 0 | 2218 | 74 | 0 |
| 29 | BE | 1559 | 0 | 1618 | 43 | 0 |
| 29 | DE | 1559 | 0 | 1618 | 56 | 0 |
| 30 | BF | 1584 | 0 | 1625 | 49 | 0 |
| 30 | DF | 1580 | 0 | 1619 | 55 | 0 |
| 31 | BG | 1425 | 0 | 1443 | 37 | 0 |
| 31 | DG | 1424 | 0 | 1434 | 73 | 0 |
| 32 | BH | 1330 | 0 | 1407 | 29 | 0 |
| 32 | DH | 1330 | 0 | 1407 | 44 | 0 |
| 33 | BI | 1085 | 0 | 1114 | 28 | 1 |
| 33 | DI | 1061 | 0 | 1080 | 50 | 0 |
| 34 | BN | 1117 | 0 | 1184 | 21 | 0 |
| 34 | DN | 1117 | 0 | 1184 | 29 | 0 |
| 35 | BO | 933 | 0 | 996 | 27 | 0 |
| 35 | DO | 933 | 0 | 996 | 38 | 0 |
| 36 | BP | 1135 | 0 | 1212 | 53 | 0 |
| 36 | DP | 1135 | 0 | 1212 | 61 | 0 |
| 37 | BQ | 1122 | 0 | 1179 | 38 | 0 |
| 37 | DQ | 1122 | 0 | 1179 | 33 | 0 |
| 38 | BR | 968 | 0 | 1033 | 26 | 1 |
| 38 | DR | 968 | 0 | 1033 | 36 | 0 |
| 39 | BS | 877 | 0 | 938 | 28 | 0 |
| 39 | DS | 870 | 0 | 923 | 29 | 0 |
| 40 | BT | 1091 | 0 | 1151 | 37 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | DT | 1083 | 0 | 1136 | 39 | 0 |
| 41 | BU | 959 | 0 | 1019 | 24 | 0 |
| 41 | DU | 959 | 0 | 1018 | 29 | 0 |
| 42 | BV | 771 | 0 | 830 | 21 | 1 |
| 42 | DV | 771 | 0 | 830 | 24 | 0 |
| 43 | BW | 886 | 0 | 940 | 15 | 0 |
| 43 | DW | 886 | 0 | 940 | 20 | 0 |
| 44 | BX | 750 | 0 | 814 | 24 | 0 |
| 44 | DX | 750 | 0 | 814 | 19 | 0 |
| 45 | BY | 806 | 0 | 881 | 24 | 0 |
| 45 | DY | 806 | 0 | 881 | 19 | 0 |
| 46 | BZ | 1349 | 0 | 1355 | 38 | 0 |
| 46 | DZ | 1360 | 0 | 1363 | 47 | 0 |
| 47 | B0 | 653 | 0 | 674 | 20 | 0 |
| 47 | D0 | 653 | 0 | 674 | 19 | 0 |
| 48 | B1 | 755 | 0 | 826 | 19 | 0 |
| 48 | D1 | 755 | 0 | 826 | 20 | 0 |
| 49 | B2 | 588 | 0 | 643 | 8 | 0 |
| 49 | D2 | 588 | 0 | 643 | 9 | 0 |
| 50 | B3 | 469 | 0 | 518 | 15 | 0 |
| 50 | D3 | 464 | 0 | 514 | 15 | 0 |
| 51 | B4 | 552 | 0 | 533 | 32 | 0 |
| 51 | D4 | 532 | 0 | 503 | 28 | 0 |
| 52 | B5 | 455 | 0 | 465 | 8 | 0 |
| 52 | D5 | 455 | 0 | 465 | 10 | 0 |
| 53 | B6 | 453 | 0 | 473 | 13 | 0 |
| 53 | D6 | 449 | 0 | 469 | 6 | 0 |
| 54 | B7 | 418 | 0 | 467 | 19 | 0 |
| 54 | D7 | 418 | 0 | 467 | 15 | 0 |
| 55 | B8 | 511 | 0 | 571 | 29 | 0 |
| 55 | D8 | 517 | 0 | 582 | 14 | 0 |
| 56 | B9 | 307 | 0 | 335 | 8 | 0 |
| 56 | D9 | 307 | 0 | 335 | 10 | 0 |
| 57 | AA | 207 | 0 | 0 | 0 | 0 |
| 57 | AD | 2 | 0 | 0 | 0 | 0 |
| 57 | AE | 2 | 0 | 0 | 0 | 0 |
| 57 | AF | 1 | 0 | 0 | 0 | 0 |
| 57 | AJ | 1 | 0 | 0 | 0 | 0 |
| 57 | AK | 1 | 0 | 0 | 0 | 0 |
| 57 | AM | 1 | 0 | 0 | 0 | 0 |
| 57 | AN | 2 | 0 | 0 | 0 | 0 |
| 57 | AS | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | AV | 1 | 0 | 0 | 0 | 0 |
| 57 | AW | 1 | 0 | 0 | 0 | 0 |
| 57 | AX | 11 | 0 | 0 | 0 | 0 |
| 57 | B0 | 4 | 0 | 0 | 0 | 0 |
| 57 | B1 | 1 | 0 | 0 | 0 | 0 |
| 57 | B2 | 1 | 0 | 0 | 0 | 0 |
| 57 | B3 | 2 | 0 | 0 | 0 | 0 |
| 57 | B5 | 2 | 0 | 0 | 0 | 0 |
| 57 | B7 | 3 | 0 | 0 | 0 | 0 |
| 57 | B8 | 1 | 0 | 0 | 0 | 0 |
| 57 | B9 | 1 | 0 | 0 | 0 | 0 |
| 57 | BA | 720 | 0 | 0 | 0 | 0 |
| 57 | BB | 20 | 0 | 0 | 0 | 0 |
| 57 | BD | 11 | 0 | 0 | 0 | 0 |
| 57 | BE | 7 | 0 | 0 | 0 | 0 |
| 57 | BF | 10 | 0 | 0 | 0 | 0 |
| 57 | BG | 2 | 0 | 0 | 0 | 0 |
| 57 | BN | 6 | 0 | 0 | 0 | 0 |
| 57 | BO | 1 | 0 | 0 | 0 | 0 |
| 57 | BP | 4 | 0 | 0 | 0 | 0 |
| 57 | BQ | 5 | 0 | 0 | 0 | 0 |
| 57 | BR | 3 | 0 | 0 | 0 | 0 |
| 57 | BU | 8 | 0 | 0 | 0 | 0 |
| 57 | BV | 4 | 0 | 0 | 0 | 0 |
| 57 | BW | 5 | 0 | 0 | 0 | 0 |
| 57 | BX | 1 | 0 | 0 | 0 | 0 |
| 57 | BY | 1 | 0 | 0 | 0 | 0 |
| 57 | BZ | 1 | 0 | 0 | 0 | 0 |
| 57 | CA | 160 | 0 | 0 | 0 | 0 |
| 57 | CE | 1 | 0 | 0 | 0 | 0 |
| 57 | CF | 1 | 0 | 0 | 0 | 0 |
| 57 | CJ | 1 | 0 | 0 | 0 | 0 |
| 57 | CK | 1 | 0 | 0 | 0 | 0 |
| 57 | CT | 1 | 0 | 0 | 0 | 0 |
| 57 | CW | 1 | 0 | 0 | 0 | 0 |
| 57 | CX | 2 | 0 | 0 | 0 | 0 |
| 57 | D3 | 1 | 0 | 0 | 0 | 0 |
| 57 | D5 | 1 | 0 | 0 | 0 | 0 |
| 57 | D8 | 2 | 0 | 0 | 0 | 0 |
| 57 | DA | 629 | 0 | 0 | 0 | 0 |
| 57 | DB | 10 | 0 | 0 | 0 | 0 |
| 57 | DD | 7 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | DE | 4 | 0 | 0 | 0 | 0 |
| 57 | DF | 4 | 0 | 0 | 0 | 0 |
| 57 | DG | 1 | 0 | 0 | 0 | 0 |
| 57 | DN | 1 | 0 | 0 | 0 | 0 |
| 57 | DO | 1 | 0 | 0 | 0 | 0 |
| 57 | DP | 2 | 0 | 0 | 0 | 0 |
| 57 | DQ | 3 | 0 | 0 | 0 | 0 |
| 57 | DR | 2 | 0 | 0 | 0 | 0 |
| 57 | DU | 4 | 0 | 0 | 0 | 0 |
| 57 | DV | 2 | 0 | 0 | 0 | 0 |
| 57 | DW | 2 | 0 | 0 | 0 | 0 |
| 57 | DY | 1 | 0 | 0 | 0 | 0 |
| 58 | AD | 8 | 0 | 0 | 1 | 0 |
| 58 | CD | 8 | 0 | 0 | 1 | 0 |
| 59 | AN | 1 | 0 | 0 | 0 | 0 |
| 59 | B4 | 1 | 0 | 0 | 0 | 0 |
| 59 | B5 | 1 | 0 | 0 | 0 | 0 |
| 59 | B6 | 1 | 0 | 0 | 0 | 0 |
| 59 | B9 | 1 | 0 | 0 | 0 | 0 |
| 59 | BY | 1 | 0 | 0 | 0 | 0 |
| 59 | CN | 1 | 0 | 0 | 0 | 0 |
| 59 | D4 | 1 | 0 | 0 | 0 | 0 |
| 59 | D5 | 1 | 0 | 0 | 0 | 0 |
| 59 | D6 | 1 | 0 | 0 | 0 | 0 |
| 59 | D9 | 1 | 0 | 0 | 0 | 0 |
| 59 | DY | 1 | 0 | 0 | 0 | 0 |
| 60 | AX | 1 | 0 | 0 | 0 | 0 |
| 60 | CX | 1 | 0 | 0 | 0 | 0 |
| 61 | AA | 170 | 0 | 0 | 16 | 0 |
| 61 | AL | 2 | 0 | 0 | 1 | 0 |
| 61 | AO | 1 | 0 | 0 | 0 | 0 |
| 61 | AU | 1 | 0 | 0 | 1 | 0 |
| 61 | AV | 2 | 0 | 0 | 0 | 0 |
| 61 | AW | 3 | 0 | 0 | 0 | 0 |
| 61 | B0 | 4 | 0 | 0 | 0 | 0 |
| 61 | B1 | 1 | 0 | 0 | 0 | 0 |
| 61 | B3 | 1 | 0 | 0 | 0 | 0 |
| 61 | B5 | 5 | 0 | 0 | 0 | 0 |
| 61 | B7 | 1 | 0 | 0 | 1 | 0 |
| 61 | B8 | 7 | 0 | 0 | 0 | 0 |
| 61 | BA | 1102 | 0 | 0 | 59 | 0 |
| 61 | BB | 36 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | BD | 8 | 0 | 0 | 1 | 0 |
| 61 | BE | 13 | 0 | 0 | 5 | 0 |
| 61 | BF | 4 | 0 | 0 | 0 | 0 |
| 61 | BG | 3 | 0 | 0 | 0 | 0 |
| 61 | BI | 1 | 0 | 0 | 0 | 0 |
| 61 | BP | 15 | 0 | 0 | 1 | 0 |
| 61 | BQ | 3 | 0 | 0 | 0 | 0 |
| 61 | BR | 1 | 0 | 0 | 1 | 0 |
| 61 | BS | 1 | 0 | 0 | 0 | 0 |
| 61 | BT | 3 | 0 | 0 | 0 | 0 |
| 61 | BU | 1 | 0 | 0 | 1 | 0 |
| 61 | BV | 4 | 0 | 0 | 0 | 0 |
| 61 | BW | 2 | 0 | 0 | 0 | 0 |
| 61 | BX | 2 | 0 | 0 | 0 | 0 |
| 61 | CA | 130 | 0 | 0 | 8 | 0 |
| 61 | CE | 1 | 0 | 0 | 0 | 0 |
| 61 | CJ | 2 | 0 | 0 | 0 | 0 |
| 61 | CN | 1 | 0 | 0 | 0 | 0 |
| 61 | CT | 1 | 0 | 0 | 0 | 0 |
| 61 | CV | 1 | 0 | 0 | 0 | 0 |
| 61 | CW | 1 | 0 | 0 | 0 | 0 |
| 61 | CX | 1 | 0 | 0 | 1 | 0 |
| 61 | D0 | 5 | 0 | 0 | 1 | 0 |
| 61 | D1 | 1 | 0 | 0 | 0 | 0 |
| 61 | D3 | 2 | 0 | 0 | 0 | 0 |
| 61 | D7 | 1 | 0 | 0 | 0 | 0 |
| 61 | D8 | 4 | 0 | 0 | 0 | 0 |
| 61 | DA | 767 | 0 | 0 | 55 | 0 |
| 61 | DB | 9 | 0 | 0 | 0 | 0 |
| 61 | DD | 9 | 0 | 0 | 3 | 0 |
| 61 | DE | 5 | 0 | 0 | 0 | 0 |
| 61 | DF | 6 | 0 | 0 | 0 | 0 |
| 61 | DN | 2 | 0 | 0 | 0 | 0 |
| 61 | DP | 12 | 0 | 0 | 3 | 0 |
| 61 | DR | 2 | 0 | 0 | 1 | 0 |
| 61 | DT | 1 | 0 | 0 | 0 | 0 |
| 61 | DU | 2 | 0 | 0 | 0 | 0 |
| 61 | DV | 1 | 0 | 0 | 1 | 0 |
| 61 | DX | 2 | 0 | 0 | 0 | 0 |
| 61 | DY | 1 | 0 | 0 | 1 | 0 |
| All | All | 290205 | 0 | 193167 | 6242 | 3 |

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 14.

The worst 5 of 6242 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:CA:1002:G:H1 | 1:CA:1038:C:N4 | 1.48 | 1.11 |
| 26:DA:2121:G:H1 | 26:DA:2177:C:N4 | 1.52 | 1.06 |
| 1:AA:1164:G:N2 | 1:AA:1165:C:C5 | 2.24 | 1.06 |
| 1:CA:72:C:N4 | 1:CA:97:G:N1 | 2.04 | 1.05 |
| 26:DA:2139:C:N4 | 26:DA:2152:G:H1 | 1.55 | 1.04 |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:AA:1043:C:O2' | 26:DA:2137:C:O2'[2_655] | 2.08 | 0.12 |
| 33:BI:89:TYR:O | 1:CA:357:G:O2'[3_654] | 2.10 | 0.10 |
| 38:BR:33:ARG:NH2 | 42:BV:53:GLU:OE2[4_445] | 2.19 | 0.01 |

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 | 229/256 (90%) | 204 (89%) | 21 (9%) | 4 (2%) | 9 | 29 |
| 2 | CB | 229/256 (90%) | 204 (89%) | 14 (6%) | 11 (5%) | 2 | 7 |
| 3 | AC | 204/239 (85%) | 189 (93%) | 13 (6%) | 2 (1%) | 15 | 44 |
| 3 | CC | 204/239 (85%) | 188 (92%) | 15 (7%) | 1 (0%) | 29 | 61 |
| 4 | AD | 206/209 (99%) | 198 (96%) | 7 (3%) | 1 (0%) | 29 | 61 |
| 4 | CD | 206/209 (99%) | 196 (95%) | 7 (3%) | 3 (2%) | 10 | 33 |
| 5 | AE | 146/162 (90%) | 136 (93%) | 9 (6%) | 1 (1%) | 22 | 53 |
| 5 | CE | 146/162 (90%) | 135 (92%) | 10 (7%) | 1 (1%) | 22 | 53 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 6 | AF | 98/101 (97%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | CF | 98/101 (97%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 7 | AG | 153/156 (98%) | 143 (94%) | 7 (5%) | 3 (2%) | 7 | 24 |
| 7 | CG | 153/156 (98%) | 143 (94%) | 9 (6%) | 1 (1%) | 22 | 53 |
| 8 | AH | 135/138 (98%) | 133 (98%) | 2 (2%) | 0 | 100 | 100 |
| 8 | CH | 135/138 (98%) | 130 (96%) | 4 (3%) | 1 (1%) | 22 | 53 |
| 9 | AI | 125/128 (98%) | 118 (94%) | 7 (6%) | 0 | 100 | 100 |
| 9 | CI | 125/128 (98%) | 118 (94%) | 6 (5%) | 1 (1%) | 19 | 49 |
| 10 | AJ | 95/105 (90%) | 83 (87%) | 5 (5%) | 7 (7%) | 1 | 2 |
| 10 | CJ | 94/105 (90%) | 83 (88%) | 6 (6%) | 5 (5%) | 2 | 6 |
| 11 | AK | 112/129 (87%) | 106 (95%) | 5 (4%) | 1 (1%) | 17 | 46 |
| 11 | CK | 112/129 (87%) | 105 (94%) | 6 (5%) | 1 (1%) | 17 | 46 |
| 12 | AL | 120/132 (91%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 12 | CL | 120/132 (91%) | 113 (94%) | 7 (6%) | 0 | 100 | 100 |
| 13 | AM | 121/126 (96%) | 113 (93%) | 6 (5%) | 2 (2%) | 9 | 29 |
| 13 | CM | 120/126 (95%) | 110 (92%) | 9 (8%) | 1 (1%) | 19 | 49 |
| 14 | AN | 58/61 (95%) | 57 (98%) | 1 (2%) | 0 | 100 | 100 |
| 14 | CN | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 15 | AO | 86/89 (97%) | 85 (99%) | 1 (1%) | 0 | 100 | 100 |
| 15 | CO | 86/89 (97%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | AP | 80/88 (91%) | 75 (94%) | 5 (6%) | 0 | 100 | 100 |
| 16 | CP | 80/88 (91%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 17 | AQ | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 17 | CQ | 97/105 (92%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 18 | AR | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 18 | CR | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 19 | AS | 81/93 (87%) | 70 (86%) | 11 (14%) | 0 | 100 | 100 |
| 19 | CS | 81/93 (87%) | 71 (88%) | 8 (10%) | 2 (2%) | 5 | 19 |
| 20 | AT | 94/106 (89%) | 85 (90%) | 3 (3%) | 6 (6%) | 1 | 3 |
| 20 | CT | 94/106 (89%) | 84 (89%) | 6 (6%) | 4 (4%) | 2 | 8 |
| 21 | AU | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 21 | CU | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 28 | BD | 273/276 (99%) | 263 (96%) | 9 (3%) | 1 (0%) | 34 | 66 |
| 28 | DD | 273/276 (99%) | 261 (96%) | 10 (4%) | 2 (1%) | 22 | 53 |
| 29 | BE | 202/206 (98%) | 194 (96%) | 7 (4%) | 1 (0%) | 29 | 61 |
| 29 | DE | 202/206 (98%) | 193 (96%) | 7 (4%) | 2 (1%) | 15 | 44 |
| 30 | BF | 201/210 (96%) | 197 (98%) | 3 (2%) | 1 (0%) | 29 | 61 |
| 30 | DF | 201/210 (96%) | 197 (98%) | 2 (1%) | 2 (1%) | 15 | 44 |
| 31 | BG | 179/182 (98%) | 166 (93%) | 9 (5%) | 4 (2%) | 6 | 22 |
| 31 | DG | 179/182 (98%) | 166 (93%) | 9 (5%) | 4 (2%) | 6 | 22 |
| 32 | BH | 172/180 (96%) | 161 (94%) | 9 (5%) | 2 (1%) | 13 | 39 |
| 32 | DH | 172/180 (96%) | 163 (95%) | 7 (4%) | 2 (1%) | 13 | 39 |
| 33 | BI | 144/148 (97%) | 132 (92%) | 9 (6%) | 3 (2%) | 7 | 23 |
| 33 | DI | 144/148 (97%) | 130 (90%) | 12 (8%) | 2 (1%) | 11 | 34 |
| 34 | BN | 138/140 (99%) | 134 (97%) | 4 (3%) | 0 | 100 | 100 |
| 34 | DN | 138/140 (99%) | 132 (96%) | 5 (4%) | 1 (1%) | 22 | 53 |
| 35 | BO | 120/122 (98%) | 114 (95%) | 5 (4%) | 1 (1%) | 19 | 49 |
| 35 | DO | 120/122 (98%) | 115 (96%) | 4 (3%) | 1 (1%) | 19 | 49 |
| 36 | BP | 147/150 (98%) | 138 (94%) | 8 (5%) | 1 (1%) | 22 | 53 |
| 36 | DP | 147/150 (98%) | 133 (90%) | 13 (9%) | 1 (1%) | 22 | 53 |
| 37 | BQ | 139/141 (99%) | 133 (96%) | 6 (4%) | 0 | 100 | 100 |
| 37 | DQ | 139/141 (99%) | 134 (96%) | 5 (4%) | 0 | 100 | 100 |
| 38 | BR | 116/118 (98%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 38 | DR | 116/118 (98%) | 111 (96%) | 5 (4%) | 0 | 100 | 100 |
| 39 | BS | 108/112 (96%) | 104 (96%) | 4 (4%) | 0 | 100 | 100 |
| 39 | DS | 108/112 (96%) | 104 (96%) | 3 (3%) | 1 (1%) | 17 | 46 |
| 40 | BT | 129/146 (88%) | 121 (94%) | 8 (6%) | 0 | 100 | 100 |
| 40 | DT | 129/146 (88%) | 125 (97%) | 3 (2%) | 1 (1%) | 19 | 49 |
| 41 | BU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 41 | DU | 114/118 (97%) | 113 (99%) | 1 (1%) | 0 | 100 | 100 |
| 42 | BV | 99/101 (98%) | 94 (95%) | 4 (4%) | 1 (1%) | 15 | 44 |
| 42 | DV | 99/101 (98%) | 95 (96%) | 3 (3%) | 1 (1%) | 15 | 44 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 43 | BW | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 43 | DW | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | BX | 93/96 (97%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 44 | DX | 93/96 (97%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 45 | BY | 105/110 (96%) | 95 (90%) | 10 (10%) | 0 | 100 | 100 |
| 45 | DY | 105/110 (96%) | 99 (94%) | 6 (6%) | 0 | 100 | 100 |
| 46 | BZ | 169/206 (82%) | 148 (88%) | 19 (11%) | 2 (1%) | 13 | 39 |
| 46 | DZ | 172/206 (84%) | 156 (91%) | 14 (8%) | 2 (1%) | 13 | 39 |
| 47 | B0 | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 47 | D0 | 81/85 (95%) | 77 (95%) | 4 (5%) | 0 | 100 | 100 |
| 48 | B1 | 95/98 (97%) | 94 (99%) | 0 | 1 (1%) | 14 | 41 |
| 48 | D1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 14 | 41 |
| 49 | B2 | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 49 | D2 | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 50 | B3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 50 | D3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 51 | B4 | 67/71 (94%) | 54 (81%) | 8 (12%) | 5 (8%) | 1 | 2 |
| 51 | D4 | 67/71 (94%) | 53 (79%) | 10 (15%) | 4 (6%) | 1 | 4 |
| 52 | B5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 52 | D5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | B6 | 51/54 (94%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | D6 | 51/54 (94%) | 50 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | B7 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 54 | D7 | 46/49 (94%) | 45 (98%) | 0 | 1 (2%) | 6 | 22 |
| 55 | B8 | 62/65 (95%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 55 | D8 | 62/65 (95%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 56 | B9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 56 | D9 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| All | All | 11409/12128 (94%) | 10783 (94%) | 516 (4%) | 110 (1%) | 15 | 44 |

5 of 110 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 231 | GLU |
| 4 | AD | 166 | LYS |
| 7 | AG | 80 | VAL |
| 10 | AJ | 55 | LYS |
| 20 | AT | 10 | LEU |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|-------------|
| 2 | AB | 192/220 (87%) | 161 (84%) | 31 (16%) | 2 7 |
| 2 | CB | 187/220 (85%) | 161 (86%) | 26 (14%) | 3 11 |
| 3 | AC | 143/188 (76%) | 131 (92%) | 12 (8%) | 11 31 |
| 3 | CC | 140/188 (74%) | 127 (91%) | 13 (9%) | 9 26 |
| 4 | AD | 170/181 (94%) | 153 (90%) | 17 (10%) | 7 22 |
| 4 | CD | 173/181 (96%) | 157 (91%) | 16 (9%) | 9 27 |
| 5 | AE | 113/123 (92%) | 106 (94%) | 7 (6%) | 18 47 |
| 5 | CE | 114/123 (93%) | 105 (92%) | 9 (8%) | 12 34 |
| 6 | AF | 83/90 (92%) | 78 (94%) | 5 (6%) | 19 48 |
| 6 | CF | 85/90 (94%) | 79 (93%) | 6 (7%) | 14 39 |
| 7 | AG | 119/127 (94%) | 107 (90%) | 12 (10%) | 7 22 |
| 7 | CG | 120/127 (94%) | 108 (90%) | 12 (10%) | 7 22 |
| 8 | AH | 114/119 (96%) | 109 (96%) | 5 (4%) | 28 61 |
| 8 | CH | 114/119 (96%) | 106 (93%) | 8 (7%) | 15 40 |
| 9 | AI | 90/99 (91%) | 76 (84%) | 14 (16%) | 2 8 |
| 9 | CI | 89/99 (90%) | 78 (88%) | 11 (12%) | 4 14 |
| 10 | AJ | 66/92 (72%) | 60 (91%) | 6 (9%) | 9 27 |
| 10 | CJ | 69/92 (75%) | 63 (91%) | 6 (9%) | 10 30 |
| 11 | AK | 82/99 (83%) | 76 (93%) | 6 (7%) | 14 38 |
| 11 | CK | 83/99 (84%) | 79 (95%) | 4 (5%) | 25 58 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 12 | AL | 97/109 (89%) | 91 (94%) | 6 (6%) | 18 | 47 |
| 12 | CL | 97/109 (89%) | 94 (97%) | 3 (3%) | 40 | 74 |
| 13 | AM | 93/101 (92%) | 82 (88%) | 11 (12%) | 5 | 16 |
| 13 | CM | 92/101 (91%) | 81 (88%) | 11 (12%) | 5 | 15 |
| 14 | AN | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 | 15 |
| 14 | CN | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 | 15 |
| 15 | AO | 78/80 (98%) | 66 (85%) | 12 (15%) | 2 | 8 |
| 15 | CO | 78/80 (98%) | 70 (90%) | 8 (10%) | 7 | 21 |
| 16 | AP | 69/74 (93%) | 60 (87%) | 9 (13%) | 4 | 13 |
| 16 | CP | 68/74 (92%) | 62 (91%) | 6 (9%) | 10 | 29 |
| 17 | AQ | 94/97 (97%) | 91 (97%) | 3 (3%) | 39 | 73 |
| 17 | CQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 37 |
| 18 | AR | 59/77 (77%) | 54 (92%) | 5 (8%) | 10 | 31 |
| 18 | CR | 59/77 (77%) | 54 (92%) | 5 (8%) | 10 | 31 |
| 19 | AS | 69/80 (86%) | 61 (88%) | 8 (12%) | 5 | 17 |
| 19 | CS | 67/80 (84%) | 62 (92%) | 5 (8%) | 13 | 37 |
| 20 | AT | 70/82 (85%) | 60 (86%) | 10 (14%) | 3 | 10 |
| 20 | CT | 70/82 (85%) | 63 (90%) | 7 (10%) | 7 | 22 |
| 21 | AU | 18/22 (82%) | 16 (89%) | 2 (11%) | 6 | 19 |
| 21 | CU | 18/22 (82%) | 17 (94%) | 1 (6%) | 21 | 51 |
| 28 | BD | 215/218 (99%) | 201 (94%) | 14 (6%) | 17 | 44 |
| 28 | DD | 215/218 (99%) | 200 (93%) | 15 (7%) | 15 | 40 |
| 29 | BE | 164/166 (99%) | 144 (88%) | 20 (12%) | 5 | 15 |
| 29 | DE | 164/166 (99%) | 147 (90%) | 17 (10%) | 7 | 21 |
| 30 | BF | 160/166 (96%) | 145 (91%) | 15 (9%) | 8 | 26 |
| 30 | DF | 159/166 (96%) | 146 (92%) | 13 (8%) | 11 | 33 |
| 31 | BG | 143/156 (92%) | 128 (90%) | 15 (10%) | 7 | 20 |
| 31 | DG | 142/156 (91%) | 122 (86%) | 20 (14%) | 3 | 10 |
| 32 | BH | 144/148 (97%) | 138 (96%) | 6 (4%) | 30 | 63 |
| 32 | DH | 144/148 (97%) | 132 (92%) | 12 (8%) | 11 | 32 |
| 33 | BI | 110/124 (89%) | 90 (82%) | 20 (18%) | 1 | 5 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 33 | DI | 104/124 (84%) | 87 (84%) | 17 (16%) | 2 | 7 |
| 34 | BN | 118/119 (99%) | 103 (87%) | 15 (13%) | 4 | 14 |
| 34 | DN | 118/119 (99%) | 108 (92%) | 10 (8%) | 10 | 31 |
| 35 | BO | 100/100 (100%) | 94 (94%) | 6 (6%) | 19 | 48 |
| 35 | DO | 100/100 (100%) | 96 (96%) | 4 (4%) | 31 | 65 |
| 36 | BP | 115/116 (99%) | 105 (91%) | 10 (9%) | 10 | 30 |
| 36 | DP | 115/116 (99%) | 103 (90%) | 12 (10%) | 7 | 21 |
| 37 | BQ | 111/111 (100%) | 100 (90%) | 11 (10%) | 8 | 23 |
| 37 | DQ | 111/111 (100%) | 100 (90%) | 11 (10%) | 8 | 23 |
| 38 | BR | 101/101 (100%) | 82 (81%) | 19 (19%) | 1 | 5 |
| 38 | DR | 101/101 (100%) | 84 (83%) | 17 (17%) | 2 | 6 |
| 39 | BS | 87/88 (99%) | 79 (91%) | 8 (9%) | 9 | 27 |
| 39 | DS | 85/88 (97%) | 75 (88%) | 10 (12%) | 5 | 16 |
| 40 | BT | 115/127 (91%) | 106 (92%) | 9 (8%) | 12 | 35 |
| 40 | DT | 113/127 (89%) | 103 (91%) | 10 (9%) | 10 | 29 |
| 41 | BU | 93/94 (99%) | 86 (92%) | 7 (8%) | 13 | 37 |
| 41 | DU | 93/94 (99%) | 88 (95%) | 5 (5%) | 22 | 53 |
| 42 | BV | 80/82 (98%) | 68 (85%) | 12 (15%) | 3 | 9 |
| 42 | DV | 80/82 (98%) | 72 (90%) | 8 (10%) | 7 | 22 |
| 43 | BW | 90/92 (98%) | 84 (93%) | 6 (7%) | 16 | 43 |
| 43 | DW | 90/92 (98%) | 82 (91%) | 8 (9%) | 9 | 28 |
| 44 | BX | 77/78 (99%) | 74 (96%) | 3 (4%) | 32 | 66 |
| 44 | DX | 77/78 (99%) | 72 (94%) | 5 (6%) | 17 | 44 |
| 45 | BY | 85/91 (93%) | 77 (91%) | 8 (9%) | 8 | 26 |
| 45 | DY | 85/91 (93%) | 78 (92%) | 7 (8%) | 11 | 33 |
| 46 | BZ | 145/179 (81%) | 131 (90%) | 14 (10%) | 8 | 24 |
| 46 | DZ | 145/179 (81%) | 127 (88%) | 18 (12%) | 4 | 14 |
| 47 | B0 | 65/67 (97%) | 62 (95%) | 3 (5%) | 27 | 60 |
| 47 | D0 | 65/67 (97%) | 62 (95%) | 3 (5%) | 27 | 60 |
| 48 | B1 | 80/83 (96%) | 72 (90%) | 8 (10%) | 7 | 22 |
| 48 | D1 | 80/83 (96%) | 73 (91%) | 7 (9%) | 10 | 29 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|----|
| 49 | B2 | 65/67 (97%) | 56 (86%) | 9 (14%) | 3 | 11 |
| 49 | D2 | 65/67 (97%) | 59 (91%) | 6 (9%) | 9 | 27 |
| 50 | B3 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 16 |
| 50 | D3 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 48 |
| 51 | B4 | 59/63 (94%) | 47 (80%) | 12 (20%) | 1 | 4 |
| 51 | D4 | 53/63 (84%) | 46 (87%) | 7 (13%) | 4 | 12 |
| 52 | B5 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 65 |
| 52 | D5 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 65 |
| 53 | B6 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 | 11 |
| 53 | D6 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 65 |
| 54 | B7 | 41/42 (98%) | 38 (93%) | 3 (7%) | 14 | 38 |
| 54 | D7 | 41/42 (98%) | 38 (93%) | 3 (7%) | 14 | 38 |
| 55 | B8 | 53/55 (96%) | 49 (92%) | 4 (8%) | 13 | 37 |
| 55 | D8 | 54/55 (98%) | 53 (98%) | 1 (2%) | 57 | 85 |
| 56 | B9 | 34/34 (100%) | 31 (91%) | 3 (9%) | 10 | 29 |
| 56 | D9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 76 |
| All | All | 9319/10066 (93%) | 8433 (90%) | 886 (10%) | 8 | 25 |

5 of 886 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | CB | 17 | PHE |
| 12 | CL | 33 | ARG |
| 52 | D5 | 29 | THR |
| 40 | DT | 118 | ARG |
| 2 | CB | 150 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | DP | 70 | GLN |
| 38 | DR | 71 | GLN |
| 33 | BI | 43 | ASN |
| 31 | BG | 108 | ASN |
| 40 | DT | 58 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1495/1521 (98%) | 407 (27%) | 26 (1%) |
| 1 | CA | 1501/1521 (98%) | 413 (27%) | 28 (1%) |
| 22 | AV | 12/24 (50%) | 7 (58%) | 0 |
| 22 | CV | 5/24 (20%) | 4 (80%) | 0 |
| 23 | AW | 1/3 (33%) | 0 | 0 |
| 23 | CW | 1/3 (33%) | 0 | 0 |
| 24 | AX | 74/77 (96%) | 26 (35%) | 2 (2%) |
| 24 | CX | 74/77 (96%) | 31 (41%) | 4 (5%) |
| 25 | AY | 4/76 (5%) | 1 (25%) | 0 |
| 25 | CY | 4/76 (5%) | 1 (25%) | 0 |
| 26 | BA | 2811/2915 (96%) | 529 (18%) | 30 (1%) |
| 26 | DA | 2791/2915 (95%) | 595 (21%) | 30 (1%) |
| 27 | BB | 120/121 (99%) | 16 (13%) | 2 (1%) |
| 27 | DB | 119/121 (98%) | 31 (26%) | 0 |
| All | All | 9012/9474 (95%) | 2061 (22%) | 122 (1%) |

5 of 2061 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 6 | G |
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 15 | G |
| 1 | AA | 22 | G |

5 of 122 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | BA | 2893 | G |
| 26 | DA | 1913 | A |
| 1 | CA | 687 | A |
| 26 | DA | 1653 | G |
| 26 | DA | 2439 | A |

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

12 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 |
| 24 | PSU | AX | 55 | 24 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.90 | 3 (13%) |
| 24 | 5MC | AX | 32 | 24 | 18,22,23 | 1.01 | 2 (11%) | 26,32,35 | 1.27 | 3 (11%) |
| 24 | 5MC | CX | 32 | 24 | 18,22,23 | 0.94 | 1 (5%) | 26,32,35 | 1.06 | 2 (7%) |
| 24 | 31H | AX | 76 | 24,57 | 26,32,35 | 1.15 | 3 (11%) | 22,45,50 | 1.70 | 3 (13%) |
| 24 | 31H | CX | 76 | 24,60,57 | 28,34,35 | 1.26 | 4 (14%) | 23,47,50 | 1.67 | 3 (13%) |
| 24 | 5MU | AX | 54 | 24 | 19,22,23 | 1.38 | 5 (26%) | 28,32,35 | 2.18 | 6 (21%) |
| 23 | PPU | AW | 76 | 23,26 | 32,40,41 | 0.97 | 1 (3%) | 33,57,60 | 1.53 | 7 (21%) |
| 23 | PPU | CW | 76 | 23,26 | 32,40,41 | 0.92 | 1 (3%) | 33,57,60 | 1.76 | 9 (27%) |
| 24 | 4SU | CX | 8 | 24 | 18,21,22 | 1.89 | 5 (27%) | 26,30,33 | 1.61 | 5 (19%) |
| 24 | 5MU | CX | 54 | 24 | 19,22,23 | 1.35 | 5 (26%) | 28,32,35 | 2.22 | 6 (21%) |
| 24 | PSU | CX | 55 | 24 | 18,21,22 | 1.31 | 2 (11%) | 22,30,33 | 1.81 | 4 (18%) |
| 24 | 4SU | AX | 8 | 24 | 18,21,22 | 2.14 | 5 (27%) | 26,30,33 | 1.67 | 4 (15%) |

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 |
|-----|------|-------|-----|----------|---------|------------|---------|
| 24 | PSU | AX | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 5MC | AX | 32 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 5MC | CX | 32 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 31H | AX | 76 | 24,57 | - | 7/15/37/41 | 0/3/3/3 |
| 24 | 31H | CX | 76 | 24,60,57 | - | 9/18/40/41 | 0/3/3/3 |
| 24 | 5MU | AX | 54 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 23 | PPU | AW | 76 | 23,26 | - | 4/21/43/44 | 0/4/4/4 |
| 23 | PPU | CW | 76 | 23,26 | - | 5/21/43/44 | 0/4/4/4 |
| 24 | 4SU | CX | 8 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 5MU | CX | 54 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | PSU | CX | 55 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 4SU | AX | 8 | 24 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 36 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 24 | AX | 8 | 4SU | C4-N3 | -4.97 | 1.32 | 1.37 |
| 24 | CX | 8 | 4SU | C4-S4 | -4.41 | 1.60 | 1.68 |
| 24 | AX | 8 | 4SU | C4-S4 | -4.37 | 1.60 | 1.68 |
| 24 | CX | 8 | 4SU | C4-N3 | -3.86 | 1.33 | 1.37 |
| 24 | AX | 8 | 4SU | C5-C4 | -3.66 | 1.37 | 1.42 |

The worst 5 of 55 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 24 | AX | 55 | PSU | N1-C2-N3 | 5.94 | 121.86 | 115.13 |
| 24 | AX | 76 | 31H | N3-C2-N1 | -5.77 | 119.67 | 128.68 |
| 24 | CX | 76 | 31H | N3-C2-N1 | -5.68 | 119.81 | 128.68 |
| 24 | CX | 55 | PSU | N1-C2-N3 | 5.60 | 121.48 | 115.13 |
| 24 | AX | 54 | 5MU | N3-C2-N1 | 5.50 | 122.20 | 114.89 |

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 24 | AX | 76 | 31H | C3'-C4'-C5'-O5' |
| 24 | CX | 76 | 31H | C3'-C4'-C5'-O5' |
| 24 | CX | 76 | 31H | C-CA-CB-CG |
| 24 | CX | 76 | 31H | N-CA-CB-CG |
| 24 | CX | 76 | 31H | OCN-CN-N-CA |

There are no ring outliers.

11 monomers are involved in 32 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24 | AX | 55 | PSU | 1 | 0 |
| 24 | AX | 32 | 5MC | 2 | 0 |
| 24 | CX | 32 | 5MC | 3 | 0 |
| 24 | CX | 76 | 31H | 4 | 0 |
| 24 | AX | 54 | 5MU | 1 | 0 |
| 23 | AW | 76 | PPU | 5 | 0 |
| 23 | CW | 76 | PPU | 11 | 0 |
| 24 | CX | 8 | 4SU | 2 | 0 |
| 24 | CX | 54 | 5MU | 2 | 0 |
| 24 | CX | 55 | PSU | 1 | 0 |
| 24 | AX | 8 | 4SU | 2 | 0 |

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1916 ligands modelled in this entry, 1914 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 58 | SF4 | AD | 302 | 4 | 0,12,12 | - | - | - | | |
| 58 | SF4 | CD | 501 | 4 | 0,12,12 | - | - | - | | |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 58 | SF4 | AD | 302 | 4 | - | - | 0/6/5/5 |
| 58 | SF4 | CD | 501 | 4 | - | - | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 58 | AD | 302 | SF4 | 1 | 0 |
| 58 | CD | 501 | SF4 | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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 | 1498/1521 (98%) | 0.20 | 23 (1%) 73 68 | 39, 73, 93, 105 | 0 |
| 1 | CA | 1503/1521 (98%) | 0.15 | 27 (1%) 68 61 | 41, 75, 94, 106 | 0 |
| 2 | AB | 231/256 (90%) | 0.52 | 15 (6%) 18 11 | 69, 82, 91, 101 | 0 |
| 2 | CB | 231/256 (90%) | 2.17 | 109 (47%) 0 0 | 71, 84, 93, 101 | 0 |
| 3 | AC | 206/239 (86%) | 0.45 | 6 (2%) 51 41 | 67, 79, 89, 95 | 0 |
| 3 | CC | 206/239 (86%) | 1.88 | 84 (40%) 0 0 | 70, 81, 91, 95 | 0 |
| 4 | AD | 208/209 (99%) | 0.58 | 13 (6%) 20 12 | 57, 74, 85, 91 | 0 |
| 4 | CD | 208/209 (99%) | 0.80 | 21 (10%) 7 4 | 57, 75, 85, 92 | 0 |
| 5 | AE | 148/162 (91%) | 0.51 | 5 (3%) 45 35 | 59, 71, 82, 90 | 0 |
| 5 | CE | 148/162 (91%) | 1.02 | 29 (19%) 1 0 | 59, 73, 84, 91 | 0 |
| 6 | AF | 100/101 (99%) | 0.43 | 4 (4%) 38 28 | 54, 69, 78, 83 | 0 |
| 6 | CF | 100/101 (99%) | 0.26 | 5 (5%) 28 19 | 56, 71, 80, 83 | 0 |
| 7 | AG | 155/156 (99%) | 0.57 | 14 (9%) 9 5 | 64, 76, 86, 92 | 0 |
| 7 | CG | 155/156 (99%) | 1.08 | 25 (16%) 1 1 | 67, 78, 88, 92 | 0 |
| 8 | AH | 137/138 (99%) | 0.41 | 6 (4%) 34 24 | 60, 72, 80, 85 | 0 |
| 8 | CH | 137/138 (99%) | 1.35 | 34 (24%) 0 0 | 62, 74, 82, 85 | 0 |
| 9 | AI | 127/128 (99%) | 0.83 | 17 (13%) 3 1 | 64, 83, 91, 96 | 0 |
| 9 | CI | 127/128 (99%) | 1.62 | 46 (36%) 0 0 | 69, 84, 91, 98 | 0 |
| 10 | AJ | 97/105 (92%) | 0.72 | 10 (10%) 6 3 | 66, 83, 92, 94 | 0 |
| 10 | CJ | 96/105 (91%) | 2.07 | 54 (56%) 0 0 | 69, 85, 93, 94 | 0 |
| 11 | AK | 114/129 (88%) | 0.68 | 9 (7%) 12 7 | 46, 70, 81, 85 | 0 |
| 11 | CK | 114/129 (88%) | 0.62 | 13 (11%) 5 3 | 50, 71, 82, 85 | 0 |
| 12 | AL | 122/132 (92%) | 0.53 | 3 (2%) 57 47 | 50, 64, 73, 81 | 0 |
| 12 | CL | 122/132 (92%) | 0.71 | 12 (9%) 7 4 | 52, 65, 75, 81 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 123/126 (97%) | 0.64 | 13 (10%) 6 3 | 58, 72, 83, 90 | 0 |
| 13 | CM | 122/126 (96%) | 1.49 | 33 (27%) 0 0 | 72, 85, 93, 100 | 0 |
| 14 | AN | 60/61 (98%) | 0.63 | 6 (10%) 7 4 | 65, 75, 81, 82 | 0 |
| 14 | CN | 60/61 (98%) | 2.22 | 31 (51%) 0 0 | 69, 78, 83, 86 | 0 |
| 15 | AO | 88/89 (98%) | 0.75 | 2 (2%) 60 51 | 54, 69, 81, 85 | 0 |
| 15 | CO | 88/89 (98%) | 0.60 | 9 (10%) 6 3 | 53, 71, 82, 87 | 0 |
| 16 | AP | 82/88 (93%) | 0.81 | 10 (12%) 4 2 | 59, 72, 82, 85 | 0 |
| 16 | CP | 82/88 (93%) | 0.52 | 4 (4%) 29 20 | 57, 71, 81, 85 | 0 |
| 17 | AQ | 99/105 (94%) | 0.62 | 3 (3%) 50 40 | 58, 71, 80, 83 | 0 |
| 17 | CQ | 99/105 (94%) | 1.13 | 17 (17%) 1 1 | 56, 72, 81, 83 | 0 |
| 18 | AR | 68/88 (77%) | 0.82 | 8 (11%) 4 2 | 59, 70, 80, 84 | 0 |
| 18 | CR | 68/88 (77%) | 0.55 | 7 (10%) 6 3 | 60, 71, 82, 85 | 0 |
| 19 | AS | 83/93 (89%) | 0.84 | 12 (14%) 2 1 | 72, 82, 89, 93 | 0 |
| 19 | CS | 83/93 (89%) | 2.22 | 43 (51%) 0 0 | 73, 84, 91, 95 | 0 |
| 20 | AT | 96/106 (90%) | 1.07 | 19 (19%) 1 0 | 60, 71, 83, 85 | 0 |
| 20 | CT | 96/106 (90%) | 1.09 | 20 (20%) 1 0 | 56, 71, 83, 85 | 0 |
| 21 | AU | 23/27 (85%) | 0.88 | 1 (4%) 35 25 | 69, 74, 79, 85 | 0 |
| 21 | CU | 23/27 (85%) | 0.56 | 2 (8%) 10 5 | 71, 76, 84, 86 | 0 |
| 22 | AV | 13/24 (54%) | 1.75 | 4 (30%) 0 0 | 56, 88, 93, 97 | 0 |
| 22 | CV | 6/24 (25%) | 1.12 | 2 (33%) 0 0 | 59, 76, 95, 96 | 0 |
| 23 | AW | 2/3 (66%) | 0.33 | 0 100 100 | 30, 30, 30, 37 | 0 |
| 23 | CW | 2/3 (66%) | 0.65 | 0 100 100 | 50, 50, 50, 57 | 0 |
| 24 | AX | 71/77 (92%) | 0.18 | 0 100 100 | 27, 70, 84, 92 | 0 |
| 24 | CX | 71/77 (92%) | 0.24 | 0 100 100 | 30, 75, 86, 93 | 0 |
| 25 | AY | 5/76 (6%) | 0.06 | 0 100 100 | 51, 76, 87, 94 | 0 |
| 25 | CY | 5/76 (6%) | 1.35 | 0 100 100 | 60, 79, 90, 91 | 0 |
| 26 | BA | 2819/2915 (96%) | 0.22 | 22 (0%) 86 81 | 20, 42, 89, 107 | 0 |
| 26 | DA | 2800/2915 (96%) | -0.04 | 50 (1%) 68 61 | 22, 46, 90, 107 | 0 |
| 27 | BB | 120/121 (99%) | 0.07 | 0 100 100 | 37, 63, 77, 88 | 0 |
| 27 | DB | 120/121 (99%) | 0.10 | 5 (4%) 36 26 | 42, 68, 80, 91 | 0 |
| 28 | BD | 275/276 (99%) | 0.20 | 2 (0%) 87 84 | 21, 41, 58, 78 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DD | 275/276 (99%) | 0.00 | 1 (0%) 92 91 | 23, 43, 61, 80 | 0 |
| 29 | BE | 204/206 (99%) | 0.20 | 1 (0%) 91 88 | 21, 46, 65, 82 | 0 |
| 29 | DE | 204/206 (99%) | -0.06 | 1 (0%) 91 88 | 23, 48, 67, 84 | 0 |
| 30 | BF | 203/210 (96%) | 0.22 | 3 (1%) 73 68 | 22, 51, 73, 87 | 0 |
| 30 | DF | 203/210 (96%) | 0.06 | 1 (0%) 91 88 | 24, 54, 74, 86 | 0 |
| 31 | BG | 181/182 (99%) | 0.36 | 6 (3%) 46 36 | 55, 70, 82, 93 | 0 |
| 31 | DG | 181/182 (99%) | 1.34 | 49 (27%) 0 0 | 59, 74, 85, 93 | 0 |
| 32 | BH | 174/180 (96%) | 0.13 | 1 (0%) 89 86 | 49, 65, 77, 81 | 0 |
| 32 | DH | 174/180 (96%) | 1.24 | 37 (21%) 0 0 | 52, 70, 80, 84 | 0 |
| 33 | BI | 146/148 (98%) | 0.71 | 13 (8%) 9 5 | 47, 81, 90, 95 | 0 |
| 33 | DI | 146/148 (98%) | 3.00 | 79 (54%) 0 0 | 46, 84, 94, 99 | 0 |
| 34 | BN | 140/140 (100%) | 0.25 | 1 (0%) 87 84 | 29, 49, 72, 82 | 0 |
| 34 | DN | 140/140 (100%) | 0.08 | 2 (1%) 75 70 | 33, 53, 74, 83 | 0 |
| 35 | BO | 122/122 (100%) | -0.02 | 0 100 100 | 26, 42, 61, 65 | 0 |
| 35 | DO | 122/122 (100%) | -0.04 | 0 100 100 | 36, 57, 70, 79 | 0 |
| 36 | BP | 149/150 (99%) | 0.32 | 2 (1%) 77 72 | 25, 52, 76, 85 | 0 |
| 36 | DP | 149/150 (99%) | 0.52 | 6 (4%) 38 28 | 28, 54, 78, 86 | 0 |
| 37 | BQ | 141/141 (100%) | 0.24 | 0 100 100 | 29, 51, 65, 78 | 0 |
| 37 | DQ | 141/141 (100%) | 0.70 | 16 (11%) 5 3 | 31, 55, 69, 79 | 0 |
| 38 | BR | 118/118 (100%) | -0.11 | 0 100 100 | 23, 37, 56, 63 | 0 |
| 38 | DR | 118/118 (100%) | 0.17 | 0 100 100 | 31, 50, 64, 71 | 0 |
| 39 | BS | 110/112 (98%) | 0.18 | 1 (0%) 84 80 | 33, 51, 63, 76 | 0 |
| 39 | DS | 110/112 (98%) | 0.79 | 11 (10%) 7 4 | 55, 76, 86, 89 | 0 |
| 40 | BT | 131/146 (89%) | -0.19 | 0 100 100 | 27, 44, 73, 86 | 0 |
| 40 | DT | 131/146 (89%) | 0.04 | 0 100 100 | 42, 59, 78, 86 | 0 |
| 41 | BU | 116/118 (98%) | -0.07 | 1 (0%) 84 80 | 18, 32, 52, 73 | 0 |
| 41 | DU | 116/118 (98%) | 0.26 | 2 (1%) 70 63 | 37, 58, 75, 80 | 0 |
| 42 | BV | 101/101 (100%) | -0.03 | 0 100 100 | 20, 42, 61, 76 | 0 |
| 42 | DV | 101/101 (100%) | 0.84 | 13 (12%) 3 2 | 36, 67, 81, 87 | 0 |
| 43 | BW | 112/113 (99%) | 0.05 | 1 (0%) 84 80 | 20, 33, 51, 84 | 0 |
| 43 | DW | 112/113 (99%) | 0.29 | 1 (0%) 84 80 | 32, 47, 65, 100 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | BX | 95/96 (98%) | 0.11 | 0 100 100 | 22, 37, 57, 82 | 0 |
| 44 | DX | 95/96 (98%) | 0.69 | 8 (8%) 11 5 | 39, 59, 73, 82 | 0 |
| 45 | BY | 107/110 (97%) | 0.00 | 0 100 100 | 32, 48, 70, 81 | 0 |
| 45 | DY | 107/110 (97%) | 0.97 | 14 (13%) 3 2 | 48, 68, 78, 89 | 0 |
| 46 | BZ | 171/206 (83%) | 0.46 | 4 (2%) 60 51 | 40, 63, 83, 88 | 0 |
| 46 | DZ | 174/206 (84%) | 1.68 | 59 (33%) 0 0 | 64, 82, 94, 97 | 0 |
| 47 | B0 | 83/85 (97%) | -0.07 | 0 100 100 | 23, 38, 52, 66 | 0 |
| 47 | D0 | 83/85 (97%) | 0.77 | 6 (7%) 15 8 | 36, 61, 72, 81 | 0 |
| 48 | B1 | 97/98 (98%) | 0.02 | 1 (1%) 82 77 | 21, 42, 65, 74 | 0 |
| 48 | D1 | 97/98 (98%) | 0.41 | 3 (3%) 49 39 | 30, 54, 76, 82 | 0 |
| 49 | B2 | 70/72 (97%) | 0.10 | 0 100 100 | 32, 48, 63, 87 | 0 |
| 49 | D2 | 70/72 (97%) | 0.48 | 4 (5%) 23 15 | 50, 67, 78, 83 | 0 |
| 50 | B3 | 59/60 (98%) | -0.12 | 0 100 100 | 21, 37, 62, 81 | 0 |
| 50 | D3 | 59/60 (98%) | 0.99 | 6 (10%) 6 3 | 44, 60, 77, 87 | 0 |
| 51 | B4 | 69/71 (97%) | 0.62 | 11 (15%) 1 1 | 54, 76, 90, 98 | 0 |
| 51 | D4 | 69/71 (97%) | 1.54 | 24 (34%) 0 0 | 80, 90, 95, 99 | 0 |
| 52 | B5 | 59/60 (98%) | -0.10 | 1 (1%) 70 63 | 19, 33, 53, 65 | 0 |
| 52 | D5 | 59/60 (98%) | -0.04 | 0 100 100 | 28, 48, 69, 72 | 0 |
| 53 | B6 | 53/54 (98%) | -0.06 | 0 100 100 | 28, 40, 60, 64 | 0 |
| 53 | D6 | 53/54 (98%) | 0.45 | 3 (5%) 23 15 | 43, 59, 72, 82 | 0 |
| 54 | B7 | 48/49 (97%) | -0.06 | 0 100 100 | 18, 25, 54, 63 | 0 |
| 54 | D7 | 48/49 (97%) | -0.00 | 1 (2%) 63 54 | 29, 39, 63, 81 | 0 |
| 55 | B8 | 64/65 (98%) | -0.04 | 0 100 100 | 23, 32, 46, 61 | 0 |
| 55 | D8 | 64/65 (98%) | 0.42 | 0 100 100 | 37, 55, 66, 70 | 0 |
| 56 | B9 | 37/37 (100%) | 0.48 | 1 (2%) 54 44 | 27, 49, 67, 71 | 0 |
| 56 | D9 | 37/37 (100%) | 0.88 | 5 (13%) 3 1 | 46, 54, 67, 74 | 0 |
| All | All | 20640/21602 (95%) | 0.40 | 1309 (6%) 20 12 | 18, 63, 89, 107 | 0 |

The worst 5 of 1309 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33 | DI | 65 | ALA | 11.9 |
| 33 | DI | 119 | PRO | 11.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33 | DI | 146 | ALA | 10.9 |
| 33 | DI | 128 | LEU | 10.8 |
| 33 | DI | 85 | GLU | 10.6 |

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 24 | 5MC | CX | 32 | 21/22 | 0.85 | 0.22 | 68,80,88,99 | 0 |
| 24 | 4SU | CX | 8 | 20/21 | 0.90 | 0.17 | 61,80,93,118 | 0 |
| 24 | PSU | CX | 55 | 20/21 | 0.91 | 0.16 | 61,72,81,89 | 0 |
| 24 | 5MU | CX | 54 | 21/22 | 0.92 | 0.13 | 71,79,92,107 | 0 |
| 24 | PSU | AX | 55 | 20/21 | 0.93 | 0.16 | 58,70,77,82 | 0 |
| 24 | 5MU | AX | 54 | 21/22 | 0.95 | 0.16 | 57,67,82,96 | 0 |
| 24 | 4SU | AX | 8 | 20/21 | 0.95 | 0.17 | 47,59,67,84 | 0 |
| 24 | 5MC | AX | 32 | 21/22 | 0.95 | 0.18 | 46,55,75,77 | 0 |
| 24 | 31H | CX | 76 | 32/33 | 0.95 | 0.23 | 23,42,61,84 | 10 |
| 24 | 31H | AX | 76 | 30/33 | 0.96 | 0.26 | 14,31,55,77 | 8 |
| 23 | PPU | CW | 76 | 37/38 | 0.97 | 0.23 | 27,41,53,63 | 0 |
| 23 | PPU | AW | 76 | 37/38 | 0.97 | 0.20 | 12,29,37,42 | 0 |

6.3 Carbohydrates [i](#)

There are no monosaccharides 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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | AA | 3063 | 1/1 | 0.17 | 0.12 | 89,89,89,89 | 0 |
| 57 | MG | DA | 3553 | 1/1 | 0.35 | 0.40 | 75,75,75,75 | 0 |
| 57 | MG | BA | 3502 | 1/1 | 0.50 | 0.23 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3674 | 1/1 | 0.55 | 0.19 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3160 | 1/1 | 0.57 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | AA | 3166 | 1/1 | 0.61 | 0.20 | 70,70,70,70 | 0 |
| 57 | MG | DW | 201 | 1/1 | 0.62 | 0.20 | 70,70,70,70 | 0 |
| 57 | MG | DA | 3069 | 1/1 | 0.63 | 0.49 | 59,59,59,59 | 0 |
| 57 | MG | DV | 202 | 1/1 | 0.63 | 0.79 | 75,75,75,75 | 0 |
| 57 | MG | CA | 3148 | 1/1 | 0.63 | 0.18 | 81,81,81,81 | 0 |
| 57 | MG | CA | 3116 | 1/1 | 0.64 | 0.33 | 74,74,74,74 | 0 |
| 57 | MG | DA | 3135 | 1/1 | 0.65 | 0.18 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3548 | 1/1 | 0.66 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3025 | 1/1 | 0.66 | 0.18 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3609 | 1/1 | 0.67 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | AA | 3041 | 1/1 | 0.67 | 0.19 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3519 | 1/1 | 0.67 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | AA | 3007 | 1/1 | 0.68 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3233 | 1/1 | 0.68 | 0.31 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3004 | 1/1 | 0.68 | 0.23 | 70,70,70,70 | 0 |
| 57 | MG | AA | 3100 | 1/1 | 0.69 | 0.17 | 69,69,69,69 | 0 |
| 57 | MG | AA | 3064 | 1/1 | 0.69 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3390 | 1/1 | 0.70 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | BF | 309 | 1/1 | 0.71 | 0.41 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3306 | 1/1 | 0.71 | 0.20 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3113 | 1/1 | 0.71 | 0.23 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3603 | 1/1 | 0.71 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3054 | 1/1 | 0.71 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3008 | 1/1 | 0.72 | 0.13 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3003 | 1/1 | 0.72 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | AF | 3001 | 1/1 | 0.73 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | CX | 3002 | 1/1 | 0.73 | 0.35 | 75,75,75,75 | 0 |
| 57 | MG | DA | 3550 | 1/1 | 0.73 | 0.28 | 63,63,63,63 | 0 |
| 57 | MG | AA | 3122 | 1/1 | 0.73 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3580 | 1/1 | 0.73 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | AA | 3085 | 1/1 | 0.73 | 0.15 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3639 | 1/1 | 0.73 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3198 | 1/1 | 0.73 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3102 | 1/1 | 0.74 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3106 | 1/1 | 0.74 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3260 | 1/1 | 0.74 | 0.20 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3130 | 1/1 | 0.74 | 0.23 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3044 | 1/1 | 0.75 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3056 | 1/1 | 0.75 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | AA | 3040 | 1/1 | 0.75 | 0.21 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AN | 502 | 1/1 | 0.75 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | AA | 3109 | 1/1 | 0.75 | 0.26 | 75,75,75,75 | 0 |
| 57 | MG | DB | 3008 | 1/1 | 0.75 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3062 | 1/1 | 0.75 | 0.26 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3114 | 1/1 | 0.75 | 0.31 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3293 | 1/1 | 0.76 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3342 | 1/1 | 0.76 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3578 | 1/1 | 0.76 | 0.23 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3374 | 1/1 | 0.76 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3027 | 1/1 | 0.76 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3407 | 1/1 | 0.76 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | AA | 3126 | 1/1 | 0.76 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3158 | 1/1 | 0.76 | 0.18 | 66,66,66,66 | 0 |
| 59 | ZN | D4 | 501 | 1/1 | 0.76 | 0.19 | 154,154,154,154 | 0 |
| 57 | MG | CA | 3107 | 1/1 | 0.77 | 0.21 | 89,89,89,89 | 0 |
| 57 | MG | DA | 3111 | 1/1 | 0.77 | 0.25 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3190 | 1/1 | 0.77 | 0.12 | 75,75,75,75 | 0 |
| 57 | MG | BA | 3470 | 1/1 | 0.78 | 0.13 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3328 | 1/1 | 0.78 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3565 | 1/1 | 0.78 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3145 | 1/1 | 0.78 | 0.23 | 71,71,71,71 | 0 |
| 57 | MG | BA | 3303 | 1/1 | 0.78 | 0.23 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3082 | 1/1 | 0.78 | 0.14 | 71,71,71,71 | 0 |
| 57 | MG | CA | 3085 | 1/1 | 0.78 | 0.32 | 71,71,71,71 | 0 |
| 57 | MG | DG | 3001 | 1/1 | 0.78 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3457 | 1/1 | 0.78 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3158 | 1/1 | 0.78 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3080 | 1/1 | 0.78 | 0.16 | 82,82,82,82 | 0 |
| 57 | MG | CA | 3040 | 1/1 | 0.79 | 0.26 | 67,67,67,67 | 0 |
| 57 | MG | AA | 3042 | 1/1 | 0.79 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3276 | 1/1 | 0.79 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3303 | 1/1 | 0.79 | 0.19 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3604 | 1/1 | 0.79 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | AA | 3111 | 1/1 | 0.79 | 0.13 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3158 | 1/1 | 0.79 | 0.29 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3328 | 1/1 | 0.79 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | DE | 303 | 1/1 | 0.79 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3216 | 1/1 | 0.79 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | AA | 3146 | 1/1 | 0.79 | 0.11 | 81,81,81,81 | 0 |
| 57 | MG | BA | 3587 | 1/1 | 0.79 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3545 | 1/1 | 0.79 | 0.18 | 70,70,70,70 | 0 |
| 57 | MG | AA | 3001 | 1/1 | 0.80 | 0.13 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | CA | 3113 | 1/1 | 0.80 | 0.17 | 75,75,75,75 | 0 |
| 57 | MG | BA | 3261 | 1/1 | 0.80 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3422 | 1/1 | 0.80 | 0.15 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3042 | 1/1 | 0.80 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3467 | 1/1 | 0.80 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | AA | 3125 | 1/1 | 0.80 | 0.11 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3520 | 1/1 | 0.80 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3487 | 1/1 | 0.80 | 0.11 | 70,70,70,70 | 0 |
| 57 | MG | AA | 3181 | 1/1 | 0.80 | 0.07 | 82,82,82,82 | 0 |
| 57 | MG | DA | 3307 | 1/1 | 0.80 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | CA | 3066 | 1/1 | 0.81 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3436 | 1/1 | 0.81 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | AA | 3043 | 1/1 | 0.81 | 0.27 | 59,59,59,59 | 0 |
| 57 | MG | BZ | 3001 | 1/1 | 0.81 | 0.28 | 56,56,56,56 | 0 |
| 57 | MG | AX | 3008 | 1/1 | 0.81 | 0.11 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3533 | 1/1 | 0.81 | 0.49 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3134 | 1/1 | 0.81 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3199 | 1/1 | 0.81 | 0.27 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3015 | 1/1 | 0.81 | 0.11 | 61,61,61,61 | 0 |
| 57 | MG | CA | 3137 | 1/1 | 0.81 | 0.17 | 81,81,81,81 | 0 |
| 57 | MG | DA | 3162 | 1/1 | 0.81 | 0.43 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3608 | 1/1 | 0.81 | 0.09 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3570 | 1/1 | 0.81 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | CE | 3001 | 1/1 | 0.81 | 0.19 | 80,80,80,80 | 0 |
| 57 | MG | DA | 3304 | 1/1 | 0.81 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | DD | 307 | 1/1 | 0.81 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3651 | 1/1 | 0.81 | 0.25 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3003 | 1/1 | 0.81 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3579 | 1/1 | 0.81 | 0.32 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3054 | 1/1 | 0.81 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | BB | 3020 | 1/1 | 0.81 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3351 | 1/1 | 0.82 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3410 | 1/1 | 0.82 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3396 | 1/1 | 0.82 | 0.24 | 20,20,20,20 | 0 |
| 57 | MG | DA | 3446 | 1/1 | 0.82 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | AA | 3069 | 1/1 | 0.82 | 0.11 | 75,75,75,75 | 0 |
| 57 | MG | DA | 3119 | 1/1 | 0.82 | 0.20 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3175 | 1/1 | 0.82 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3132 | 1/1 | 0.82 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3097 | 1/1 | 0.82 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3002 | 1/1 | 0.82 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3127 | 1/1 | 0.82 | 0.28 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CA | 3133 | 1/1 | 0.82 | 0.19 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3555 | 1/1 | 0.82 | 0.15 | 70,70,70,70 | 0 |
| 57 | MG | CA | 3005 | 1/1 | 0.82 | 0.12 | 81,81,81,81 | 0 |
| 57 | MG | BA | 3020 | 1/1 | 0.82 | 0.30 | 55,55,55,55 | 0 |
| 57 | MG | AA | 3008 | 1/1 | 0.82 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3608 | 1/1 | 0.82 | 0.15 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3079 | 1/1 | 0.82 | 0.23 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3030 | 1/1 | 0.82 | 0.10 | 75,75,75,75 | 0 |
| 57 | MG | CA | 3038 | 1/1 | 0.82 | 0.13 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3109 | 1/1 | 0.82 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3105 | 1/1 | 0.82 | 0.26 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3331 | 1/1 | 0.82 | 0.26 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3087 | 1/1 | 0.82 | 0.14 | 65,65,65,65 | 0 |
| 59 | ZN | CN | 501 | 1/1 | 0.82 | 0.07 | 101,101,101,101 | 0 |
| 57 | MG | DA | 3406 | 1/1 | 0.82 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3366 | 1/1 | 0.83 | 0.22 | 38,38,38,38 | 0 |
| 57 | MG | CA | 3092 | 1/1 | 0.83 | 0.16 | 76,76,76,76 | 0 |
| 57 | MG | CA | 3096 | 1/1 | 0.83 | 0.17 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3439 | 1/1 | 0.83 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3019 | 1/1 | 0.83 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | CA | 3023 | 1/1 | 0.83 | 0.10 | 88,88,88,88 | 0 |
| 57 | MG | AA | 3170 | 1/1 | 0.83 | 0.15 | 70,70,70,70 | 0 |
| 57 | MG | CA | 3126 | 1/1 | 0.83 | 0.36 | 73,73,73,73 | 0 |
| 57 | MG | BA | 3700 | 1/1 | 0.83 | 0.20 | 69,69,69,69 | 0 |
| 57 | MG | CA | 3033 | 1/1 | 0.83 | 0.15 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3546 | 1/1 | 0.83 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3166 | 1/1 | 0.83 | 0.27 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3193 | 1/1 | 0.83 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3217 | 1/1 | 0.83 | 0.35 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3224 | 1/1 | 0.83 | 0.29 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3252 | 1/1 | 0.83 | 0.12 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3221 | 1/1 | 0.83 | 0.25 | 59,59,59,59 | 0 |
| 57 | MG | BQ | 3003 | 1/1 | 0.83 | 0.74 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3283 | 1/1 | 0.83 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3297 | 1/1 | 0.83 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3624 | 1/1 | 0.83 | 0.28 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3130 | 1/1 | 0.83 | 0.38 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3052 | 1/1 | 0.83 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | CA | 3055 | 1/1 | 0.83 | 0.13 | 66,66,66,66 | 0 |
| 57 | MG | DF | 3001 | 1/1 | 0.83 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3258 | 1/1 | 0.83 | 0.22 | 35,35,35,35 | 0 |
| 57 | MG | CA | 3058 | 1/1 | 0.83 | 0.35 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3611 | 1/1 | 0.83 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3180 | 1/1 | 0.83 | 0.27 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3105 | 1/1 | 0.83 | 0.21 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3013 | 1/1 | 0.84 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3067 | 1/1 | 0.84 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3056 | 1/1 | 0.84 | 0.31 | 66,66,66,66 | 0 |
| 57 | MG | CA | 3031 | 1/1 | 0.84 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3072 | 1/1 | 0.84 | 0.37 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3547 | 1/1 | 0.84 | 0.25 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3177 | 1/1 | 0.84 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3035 | 1/1 | 0.84 | 0.28 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3178 | 1/1 | 0.84 | 0.24 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3554 | 1/1 | 0.84 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3474 | 1/1 | 0.84 | 0.17 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3347 | 1/1 | 0.84 | 0.22 | 32,32,32,32 | 0 |
| 57 | MG | CA | 3043 | 1/1 | 0.84 | 0.13 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3337 | 1/1 | 0.84 | 0.22 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3007 | 1/1 | 0.84 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3368 | 1/1 | 0.84 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3135 | 1/1 | 0.84 | 0.11 | 85,85,85,85 | 0 |
| 57 | MG | BA | 3136 | 1/1 | 0.84 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3507 | 1/1 | 0.84 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3148 | 1/1 | 0.84 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3543 | 1/1 | 0.84 | 0.11 | 69,69,69,69 | 0 |
| 57 | MG | AA | 3051 | 1/1 | 0.84 | 0.27 | 51,51,51,51 | 0 |
| 57 | MG | CA | 3059 | 1/1 | 0.84 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3191 | 1/1 | 0.84 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3004 | 1/1 | 0.84 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3495 | 1/1 | 0.84 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3445 | 1/1 | 0.85 | 0.21 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3367 | 1/1 | 0.85 | 0.15 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3299 | 1/1 | 0.85 | 0.20 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3369 | 1/1 | 0.85 | 0.26 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3070 | 1/1 | 0.85 | 0.22 | 35,35,35,35 | 0 |
| 57 | MG | AA | 3121 | 1/1 | 0.85 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3083 | 1/1 | 0.85 | 0.24 | 30,30,30,30 | 0 |
| 57 | MG | CA | 3054 | 1/1 | 0.85 | 0.36 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3090 | 1/1 | 0.85 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3425 | 1/1 | 0.85 | 0.13 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3430 | 1/1 | 0.85 | 0.21 | 26,26,26,26 | 0 |
| 57 | MG | BD | 308 | 1/1 | 0.85 | 0.32 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3304 | 1/1 | 0.85 | 0.26 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3052 | 1/1 | 0.85 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3110 | 1/1 | 0.85 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3494 | 1/1 | 0.85 | 0.22 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3114 | 1/1 | 0.85 | 0.14 | 51,51,51,51 | 0 |
| 57 | MG | B7 | 103 | 1/1 | 0.85 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | CA | 3003 | 1/1 | 0.85 | 0.13 | 74,74,74,74 | 0 |
| 57 | MG | BA | 3326 | 1/1 | 0.85 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | AA | 3141 | 1/1 | 0.85 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3047 | 1/1 | 0.85 | 0.21 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3549 | 1/1 | 0.85 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3012 | 1/1 | 0.85 | 0.34 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3334 | 1/1 | 0.85 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | CA | 3114 | 1/1 | 0.85 | 0.24 | 96,96,96,96 | 0 |
| 57 | MG | CA | 3017 | 1/1 | 0.85 | 0.29 | 69,69,69,69 | 0 |
| 57 | MG | CA | 3120 | 1/1 | 0.85 | 0.27 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3568 | 1/1 | 0.85 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3577 | 1/1 | 0.85 | 0.18 | 25,25,25,25 | 0 |
| 57 | MG | DA | 3197 | 1/1 | 0.85 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3091 | 1/1 | 0.85 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3130 | 1/1 | 0.85 | 0.16 | 88,88,88,88 | 0 |
| 57 | MG | BA | 3094 | 1/1 | 0.85 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3355 | 1/1 | 0.85 | 0.12 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3628 | 1/1 | 0.85 | 0.56 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3266 | 1/1 | 0.85 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3172 | 1/1 | 0.85 | 0.28 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3287 | 1/1 | 0.85 | 0.27 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3610 | 1/1 | 0.85 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3406 | 1/1 | 0.85 | 0.22 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3618 | 1/1 | 0.85 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3413 | 1/1 | 0.85 | 0.09 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3041 | 1/1 | 0.85 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3112 | 1/1 | 0.85 | 0.29 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3263 | 1/1 | 0.86 | 0.30 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3416 | 1/1 | 0.86 | 0.15 | 73,73,73,73 | 0 |
| 57 | MG | BA | 3623 | 1/1 | 0.86 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3625 | 1/1 | 0.86 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3005 | 1/1 | 0.86 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3058 | 1/1 | 0.86 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3127 | 1/1 | 0.86 | 0.33 | 76,76,76,76 | 0 |
| 57 | MG | DA | 3139 | 1/1 | 0.86 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3444 | 1/1 | 0.86 | 0.25 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3144 | 1/1 | 0.86 | 0.19 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3154 | 1/1 | 0.86 | 0.16 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3491 | 1/1 | 0.86 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3680 | 1/1 | 0.86 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3499 | 1/1 | 0.86 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3513 | 1/1 | 0.86 | 0.11 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3021 | 1/1 | 0.86 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3029 | 1/1 | 0.86 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3189 | 1/1 | 0.86 | 0.19 | 57,57,57,57 | 0 |
| 57 | MG | AA | 3151 | 1/1 | 0.86 | 0.16 | 72,72,72,72 | 0 |
| 57 | MG | AA | 3205 | 1/1 | 0.86 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | BG | 3002 | 1/1 | 0.86 | 0.12 | 65,65,65,65 | 0 |
| 57 | MG | CW | 101 | 1/1 | 0.86 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3223 | 1/1 | 0.86 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3066 | 1/1 | 0.86 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3244 | 1/1 | 0.86 | 0.22 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3163 | 1/1 | 0.86 | 0.17 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3182 | 1/1 | 0.86 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3566 | 1/1 | 0.86 | 0.08 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3001 | 1/1 | 0.86 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3043 | 1/1 | 0.86 | 0.15 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3011 | 1/1 | 0.86 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3284 | 1/1 | 0.86 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3602 | 1/1 | 0.86 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3059 | 1/1 | 0.86 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | AX | 3003 | 1/1 | 0.86 | 0.33 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3619 | 1/1 | 0.86 | 0.41 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3062 | 1/1 | 0.86 | 0.09 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3625 | 1/1 | 0.86 | 0.26 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3103 | 1/1 | 0.86 | 0.49 | 62,62,62,62 | 0 |
| 57 | MG | DB | 3002 | 1/1 | 0.86 | 0.07 | 75,75,75,75 | 0 |
| 57 | MG | DA | 3311 | 1/1 | 0.86 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3134 | 1/1 | 0.86 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3081 | 1/1 | 0.86 | 0.13 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3380 | 1/1 | 0.86 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3366 | 1/1 | 0.86 | 0.16 | 40,40,40,40 | 0 |
| 57 | MG | CA | 3084 | 1/1 | 0.86 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3385 | 1/1 | 0.86 | 0.27 | 34,34,34,34 | 0 |
| 57 | MG | AA | 3123 | 1/1 | 0.86 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | AA | 3087 | 1/1 | 0.86 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3492 | 1/1 | 0.87 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | AA | 3076 | 1/1 | 0.87 | 0.19 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3243 | 1/1 | 0.87 | 0.23 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3153 | 1/1 | 0.87 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3514 | 1/1 | 0.87 | 0.37 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3370 | 1/1 | 0.87 | 0.12 | 72,72,72,72 | 0 |
| 57 | MG | BU | 201 | 1/1 | 0.87 | 0.11 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3060 | 1/1 | 0.87 | 0.16 | 78,78,78,78 | 0 |
| 57 | MG | DA | 3088 | 1/1 | 0.87 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3515 | 1/1 | 0.87 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | B5 | 101 | 1/1 | 0.87 | 0.21 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3412 | 1/1 | 0.87 | 0.09 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3421 | 1/1 | 0.87 | 0.07 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3527 | 1/1 | 0.87 | 0.17 | 37,37,37,37 | 0 |
| 57 | MG | AA | 3113 | 1/1 | 0.87 | 0.29 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3548 | 1/1 | 0.87 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3360 | 1/1 | 0.87 | 0.16 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3566 | 1/1 | 0.87 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3164 | 1/1 | 0.87 | 0.28 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3120 | 1/1 | 0.87 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3281 | 1/1 | 0.87 | 0.26 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3062 | 1/1 | 0.87 | 0.23 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3097 | 1/1 | 0.87 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3295 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3137 | 1/1 | 0.87 | 0.28 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3412 | 1/1 | 0.87 | 0.40 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3141 | 1/1 | 0.87 | 0.23 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3298 | 1/1 | 0.87 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3124 | 1/1 | 0.87 | 0.17 | 57,57,57,57 | 0 |
| 57 | MG | AA | 3180 | 1/1 | 0.87 | 0.21 | 61,61,61,61 | 0 |
| 57 | MG | CA | 3026 | 1/1 | 0.87 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | CA | 3029 | 1/1 | 0.87 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3187 | 1/1 | 0.87 | 0.23 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3104 | 1/1 | 0.87 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3425 | 1/1 | 0.87 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3558 | 1/1 | 0.87 | 0.09 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3032 | 1/1 | 0.87 | 0.42 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3139 | 1/1 | 0.87 | 0.09 | 82,82,82,82 | 0 |
| 57 | MG | DA | 3205 | 1/1 | 0.87 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3142 | 1/1 | 0.87 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | AA | 3066 | 1/1 | 0.87 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | CA | 3149 | 1/1 | 0.87 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3587 | 1/1 | 0.87 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3600 | 1/1 | 0.87 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3154 | 1/1 | 0.87 | 0.14 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | CA | 3155 | 1/1 | 0.87 | 0.16 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3259 | 1/1 | 0.87 | 0.14 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3060 | 1/1 | 0.87 | 0.22 | 59,59,59,59 | 0 |
| 57 | MG | AA | 3156 | 1/1 | 0.87 | 0.15 | 86,86,86,86 | 0 |
| 57 | MG | AA | 3028 | 1/1 | 0.87 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3482 | 1/1 | 0.87 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3689 | 1/1 | 0.87 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3291 | 1/1 | 0.87 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3011 | 1/1 | 0.87 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3691 | 1/1 | 0.87 | 0.32 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3078 | 1/1 | 0.87 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3036 | 1/1 | 0.87 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3037 | 1/1 | 0.87 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3312 | 1/1 | 0.87 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | CA | 3050 | 1/1 | 0.87 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3046 | 1/1 | 0.87 | 0.33 | 50,50,50,50 | 0 |
| 57 | MG | CA | 3099 | 1/1 | 0.88 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3204 | 1/1 | 0.88 | 0.19 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3102 | 1/1 | 0.88 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3106 | 1/1 | 0.88 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3452 | 1/1 | 0.88 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3455 | 1/1 | 0.88 | 0.35 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3219 | 1/1 | 0.88 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3458 | 1/1 | 0.88 | 0.08 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3461 | 1/1 | 0.88 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | AX | 3010 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3350 | 1/1 | 0.88 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3496 | 1/1 | 0.88 | 0.19 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3226 | 1/1 | 0.88 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3503 | 1/1 | 0.88 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3509 | 1/1 | 0.88 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | BE | 3002 | 1/1 | 0.88 | 0.45 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3077 | 1/1 | 0.88 | 0.19 | 58,58,58,58 | 0 |
| 57 | MG | BF | 305 | 1/1 | 0.88 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3583 | 1/1 | 0.88 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3070 | 1/1 | 0.88 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3291 | 1/1 | 0.88 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3143 | 1/1 | 0.88 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | AS | 101 | 1/1 | 0.88 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | AA | 3104 | 1/1 | 0.88 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3293 | 1/1 | 0.88 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3234 | 1/1 | 0.88 | 0.43 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3615 | 1/1 | 0.88 | 0.13 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3235 | 1/1 | 0.88 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3564 | 1/1 | 0.88 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3305 | 1/1 | 0.88 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3117 | 1/1 | 0.88 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3242 | 1/1 | 0.88 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3574 | 1/1 | 0.88 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3129 | 1/1 | 0.88 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3122 | 1/1 | 0.88 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3636 | 1/1 | 0.88 | 0.29 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3152 | 1/1 | 0.88 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3591 | 1/1 | 0.88 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3596 | 1/1 | 0.88 | 0.25 | 71,71,71,71 | 0 |
| 57 | MG | DA | 3597 | 1/1 | 0.88 | 0.09 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3345 | 1/1 | 0.88 | 0.19 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3601 | 1/1 | 0.88 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3353 | 1/1 | 0.88 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3605 | 1/1 | 0.88 | 0.08 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3356 | 1/1 | 0.88 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3247 | 1/1 | 0.88 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3615 | 1/1 | 0.88 | 0.15 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3534 | 1/1 | 0.88 | 0.28 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3542 | 1/1 | 0.88 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | AA | 3065 | 1/1 | 0.88 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3683 | 1/1 | 0.88 | 0.27 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3022 | 1/1 | 0.88 | 0.28 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3063 | 1/1 | 0.88 | 0.14 | 39,39,39,39 | 0 |
| 57 | MG | DD | 305 | 1/1 | 0.88 | 0.35 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3402 | 1/1 | 0.88 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3333 | 1/1 | 0.88 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3143 | 1/1 | 0.88 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3023 | 1/1 | 0.88 | 0.21 | 35,35,35,35 | 0 |
| 57 | MG | CA | 3088 | 1/1 | 0.88 | 0.11 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3709 | 1/1 | 0.88 | 0.33 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3719 | 1/1 | 0.88 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3098 | 1/1 | 0.88 | 0.07 | 76,76,76,76 | 0 |
| 57 | MG | AA | 3073 | 1/1 | 0.89 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3447 | 1/1 | 0.89 | 0.13 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3138 | 1/1 | 0.89 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | AD | 303 | 1/1 | 0.89 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3316 | 1/1 | 0.89 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3146 | 1/1 | 0.89 | 0.11 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | BA | 3223 | 1/1 | 0.89 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3229 | 1/1 | 0.89 | 0.51 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3665 | 1/1 | 0.89 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3231 | 1/1 | 0.89 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3161 | 1/1 | 0.89 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3011 | 1/1 | 0.89 | 0.18 | 32,32,32,32 | 0 |
| 57 | MG | AA | 3090 | 1/1 | 0.89 | 0.20 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3337 | 1/1 | 0.89 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3146 | 1/1 | 0.89 | 0.19 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3048 | 1/1 | 0.89 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3349 | 1/1 | 0.89 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3088 | 1/1 | 0.89 | 0.42 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3001 | 1/1 | 0.89 | 0.37 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3519 | 1/1 | 0.89 | 0.16 | 26,26,26,26 | 0 |
| 57 | MG | BB | 3004 | 1/1 | 0.89 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3523 | 1/1 | 0.89 | 0.14 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3525 | 1/1 | 0.89 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3162 | 1/1 | 0.89 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3533 | 1/1 | 0.89 | 0.28 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3248 | 1/1 | 0.89 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3162 | 1/1 | 0.89 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3256 | 1/1 | 0.89 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3027 | 1/1 | 0.89 | 1.04 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3361 | 1/1 | 0.89 | 0.08 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3047 | 1/1 | 0.89 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3267 | 1/1 | 0.89 | 0.28 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3053 | 1/1 | 0.89 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3562 | 1/1 | 0.89 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3281 | 1/1 | 0.89 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3056 | 1/1 | 0.89 | 0.08 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3372 | 1/1 | 0.89 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3287 | 1/1 | 0.89 | 0.29 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3061 | 1/1 | 0.89 | 0.28 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3575 | 1/1 | 0.89 | 0.21 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3292 | 1/1 | 0.89 | 0.12 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3063 | 1/1 | 0.89 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3064 | 1/1 | 0.89 | 0.31 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3066 | 1/1 | 0.89 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3565 | 1/1 | 0.89 | 0.10 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3592 | 1/1 | 0.89 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3595 | 1/1 | 0.89 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3033 | 1/1 | 0.89 | 0.16 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3047 | 1/1 | 0.89 | 0.23 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3308 | 1/1 | 0.89 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3571 | 1/1 | 0.89 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | CA | 3094 | 1/1 | 0.89 | 0.09 | 80,80,80,80 | 0 |
| 57 | MG | DA | 3314 | 1/1 | 0.89 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3322 | 1/1 | 0.89 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | CA | 3095 | 1/1 | 0.89 | 0.25 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3610 | 1/1 | 0.89 | 0.16 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3577 | 1/1 | 0.89 | 0.24 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3388 | 1/1 | 0.89 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3188 | 1/1 | 0.89 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | AA | 3150 | 1/1 | 0.89 | 0.09 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3626 | 1/1 | 0.89 | 0.22 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3595 | 1/1 | 0.89 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3362 | 1/1 | 0.89 | 0.27 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3601 | 1/1 | 0.89 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | CA | 3109 | 1/1 | 0.89 | 0.19 | 61,61,61,61 | 0 |
| 57 | MG | AA | 3193 | 1/1 | 0.89 | 0.31 | 77,77,77,77 | 0 |
| 57 | MG | BA | 3183 | 1/1 | 0.89 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | AA | 3168 | 1/1 | 0.89 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3203 | 1/1 | 0.89 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | DO | 5001 | 1/1 | 0.89 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3204 | 1/1 | 0.89 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3429 | 1/1 | 0.89 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | D8 | 102 | 1/1 | 0.89 | 0.25 | 63,63,63,63 | 0 |
| 57 | MG | CA | 3027 | 1/1 | 0.89 | 0.08 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3129 | 1/1 | 0.89 | 0.21 | 83,83,83,83 | 0 |
| 57 | MG | DA | 3428 | 1/1 | 0.90 | 0.19 | 46,46,46,46 | 0 |
| 57 | MG | BB | 3005 | 1/1 | 0.90 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3014 | 1/1 | 0.90 | 0.14 | 73,73,73,73 | 0 |
| 57 | MG | BA | 3257 | 1/1 | 0.90 | 0.30 | 40,40,40,40 | 0 |
| 57 | MG | CJ | 5001 | 1/1 | 0.90 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | AA | 3124 | 1/1 | 0.90 | 0.21 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3448 | 1/1 | 0.90 | 0.25 | 36,36,36,36 | 0 |
| 57 | MG | BE | 3006 | 1/1 | 0.90 | 0.34 | 72,72,72,72 | 0 |
| 57 | MG | BF | 304 | 1/1 | 0.90 | 0.26 | 35,35,35,35 | 0 |
| 57 | MG | CA | 3057 | 1/1 | 0.90 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3196 | 1/1 | 0.90 | 0.23 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3007 | 1/1 | 0.90 | 0.08 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3201 | 1/1 | 0.90 | 0.27 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3008 | 1/1 | 0.90 | 0.22 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3574 | 1/1 | 0.90 | 0.12 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3453 | 1/1 | 0.90 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3465 | 1/1 | 0.90 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3508 | 1/1 | 0.90 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | BN | 3002 | 1/1 | 0.90 | 0.25 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3028 | 1/1 | 0.90 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3515 | 1/1 | 0.90 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3034 | 1/1 | 0.90 | 0.26 | 46,46,46,46 | 0 |
| 57 | MG | CA | 3064 | 1/1 | 0.90 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3581 | 1/1 | 0.90 | 0.08 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3539 | 1/1 | 0.90 | 0.26 | 52,52,52,52 | 0 |
| 57 | MG | BR | 202 | 1/1 | 0.90 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3255 | 1/1 | 0.90 | 0.28 | 34,34,34,34 | 0 |
| 57 | MG | CA | 3078 | 1/1 | 0.90 | 0.18 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3466 | 1/1 | 0.90 | 0.25 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3139 | 1/1 | 0.90 | 0.32 | 45,45,45,45 | 0 |
| 57 | MG | B0 | 103 | 1/1 | 0.90 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | AA | 3089 | 1/1 | 0.90 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | B7 | 102 | 1/1 | 0.90 | 0.32 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3557 | 1/1 | 0.90 | 0.07 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3280 | 1/1 | 0.90 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3173 | 1/1 | 0.90 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3214 | 1/1 | 0.90 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3031 | 1/1 | 0.90 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3067 | 1/1 | 0.90 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3068 | 1/1 | 0.90 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3217 | 1/1 | 0.90 | 0.36 | 57,57,57,57 | 0 |
| 57 | MG | AA | 3017 | 1/1 | 0.90 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3501 | 1/1 | 0.90 | 0.07 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3371 | 1/1 | 0.90 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3154 | 1/1 | 0.90 | 0.19 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3155 | 1/1 | 0.90 | 0.24 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3381 | 1/1 | 0.90 | 0.17 | 30,30,30,30 | 0 |
| 57 | MG | CA | 3110 | 1/1 | 0.90 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3095 | 1/1 | 0.90 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3632 | 1/1 | 0.90 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3103 | 1/1 | 0.90 | 0.32 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3598 | 1/1 | 0.90 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | AA | 3005 | 1/1 | 0.90 | 0.16 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3232 | 1/1 | 0.90 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | CA | 3119 | 1/1 | 0.90 | 0.09 | 74,74,74,74 | 0 |
| 57 | MG | BA | 3650 | 1/1 | 0.90 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3061 | 1/1 | 0.90 | 0.10 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3116 | 1/1 | 0.90 | 0.22 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3526 | 1/1 | 0.90 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3669 | 1/1 | 0.90 | 0.19 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3364 | 1/1 | 0.90 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3111 | 1/1 | 0.90 | 0.29 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3532 | 1/1 | 0.90 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3322 | 1/1 | 0.90 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3627 | 1/1 | 0.90 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | AA | 3098 | 1/1 | 0.90 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3238 | 1/1 | 0.90 | 0.27 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3419 | 1/1 | 0.90 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3375 | 1/1 | 0.90 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3380 | 1/1 | 0.90 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | DE | 301 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3140 | 1/1 | 0.90 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | AA | 3033 | 1/1 | 0.90 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3147 | 1/1 | 0.90 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3712 | 1/1 | 0.90 | 0.11 | 30,30,30,30 | 0 |
| 57 | MG | DQ | 3003 | 1/1 | 0.90 | 0.28 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3143 | 1/1 | 0.90 | 0.21 | 47,47,47,47 | 0 |
| 57 | MG | AA | 3039 | 1/1 | 0.90 | 0.28 | 62,62,62,62 | 0 |
| 57 | MG | DW | 202 | 1/1 | 0.90 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | BB | 3001 | 1/1 | 0.90 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3426 | 1/1 | 0.90 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3426 | 1/1 | 0.90 | 0.34 | 38,38,38,38 | 0 |
| 59 | ZN | D9 | 501 | 1/1 | 0.90 | 0.07 | 75,75,75,75 | 0 |
| 57 | MG | DA | 3147 | 1/1 | 0.91 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3427 | 1/1 | 0.91 | 0.20 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3556 | 1/1 | 0.91 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3171 | 1/1 | 0.91 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3218 | 1/1 | 0.91 | 0.59 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3149 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | AX | 3006 | 1/1 | 0.91 | 0.27 | 59,59,59,59 | 0 |
| 57 | MG | BB | 3009 | 1/1 | 0.91 | 0.18 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3178 | 1/1 | 0.91 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3449 | 1/1 | 0.91 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3053 | 1/1 | 0.91 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3453 | 1/1 | 0.91 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | BB | 3019 | 1/1 | 0.91 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | AA | 3055 | 1/1 | 0.91 | 0.31 | 53,53,53,53 | 0 |
| 57 | MG | BD | 306 | 1/1 | 0.91 | 0.30 | 30,30,30,30 | 0 |
| 57 | MG | AA | 3026 | 1/1 | 0.91 | 0.08 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3484 | 1/1 | 0.91 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | BD | 310 | 1/1 | 0.91 | 0.39 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3492 | 1/1 | 0.91 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3001 | 1/1 | 0.91 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3018 | 1/1 | 0.91 | 0.33 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3497 | 1/1 | 0.91 | 0.18 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3019 | 1/1 | 0.91 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3021 | 1/1 | 0.91 | 0.13 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3149 | 1/1 | 0.91 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3152 | 1/1 | 0.91 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3511 | 1/1 | 0.91 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3584 | 1/1 | 0.91 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3032 | 1/1 | 0.91 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | AA | 3084 | 1/1 | 0.91 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3590 | 1/1 | 0.91 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3522 | 1/1 | 0.91 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3524 | 1/1 | 0.91 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3527 | 1/1 | 0.91 | 0.26 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3069 | 1/1 | 0.91 | 0.33 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3038 | 1/1 | 0.91 | 0.11 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3075 | 1/1 | 0.91 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3257 | 1/1 | 0.91 | 0.34 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3185 | 1/1 | 0.91 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3598 | 1/1 | 0.91 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3263 | 1/1 | 0.91 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3265 | 1/1 | 0.91 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3241 | 1/1 | 0.91 | 0.32 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3083 | 1/1 | 0.91 | 0.27 | 71,71,71,71 | 0 |
| 57 | MG | AA | 3027 | 1/1 | 0.91 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | BU | 206 | 1/1 | 0.91 | 0.36 | 39,39,39,39 | 0 |
| 57 | MG | AA | 3086 | 1/1 | 0.91 | 0.13 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3563 | 1/1 | 0.91 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3018 | 1/1 | 0.91 | 0.21 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3500 | 1/1 | 0.91 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3173 | 1/1 | 0.91 | 0.27 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3288 | 1/1 | 0.91 | 0.25 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3569 | 1/1 | 0.91 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3572 | 1/1 | 0.91 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3613 | 1/1 | 0.91 | 0.09 | 74,74,74,74 | 0 |
| 57 | MG | CA | 3097 | 1/1 | 0.91 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3576 | 1/1 | 0.91 | 0.27 | 46,46,46,46 | 0 |
| 57 | MG | B9 | 502 | 1/1 | 0.91 | 0.12 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3174 | 1/1 | 0.91 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3616 | 1/1 | 0.91 | 0.17 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3081 | 1/1 | 0.91 | 0.31 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3092 | 1/1 | 0.91 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3509 | 1/1 | 0.91 | 0.32 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3374 | 1/1 | 0.91 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3379 | 1/1 | 0.91 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3091 | 1/1 | 0.91 | 0.21 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3093 | 1/1 | 0.91 | 0.13 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3319 | 1/1 | 0.91 | 0.33 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3635 | 1/1 | 0.91 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3326 | 1/1 | 0.91 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3327 | 1/1 | 0.91 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3013 | 1/1 | 0.91 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3160 | 1/1 | 0.91 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3117 | 1/1 | 0.91 | 0.13 | 100,100,100,100 | 0 |
| 57 | MG | DA | 3611 | 1/1 | 0.91 | 0.18 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3613 | 1/1 | 0.91 | 0.38 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3016 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3617 | 1/1 | 0.91 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3099 | 1/1 | 0.91 | 0.33 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3622 | 1/1 | 0.91 | 1.08 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3122 | 1/1 | 0.91 | 0.09 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3024 | 1/1 | 0.91 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3125 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3656 | 1/1 | 0.91 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3658 | 1/1 | 0.91 | 0.22 | 16,16,16,16 | 0 |
| 57 | MG | AA | 3070 | 1/1 | 0.91 | 0.24 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3404 | 1/1 | 0.91 | 0.22 | 30,30,30,30 | 0 |
| 57 | MG | DB | 3009 | 1/1 | 0.91 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3129 | 1/1 | 0.91 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | AA | 3072 | 1/1 | 0.91 | 0.08 | 65,65,65,65 | 0 |
| 57 | MG | AA | 3096 | 1/1 | 0.91 | 0.06 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3133 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3389 | 1/1 | 0.91 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3535 | 1/1 | 0.91 | 0.25 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3394 | 1/1 | 0.91 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3032 | 1/1 | 0.91 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3210 | 1/1 | 0.91 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3692 | 1/1 | 0.91 | 0.17 | 64,64,64,64 | 0 |
| 57 | MG | CA | 3036 | 1/1 | 0.91 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3699 | 1/1 | 0.91 | 0.10 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3417 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | AJ | 201 | 1/1 | 0.91 | 0.08 | 67,67,67,67 | 0 |
| 57 | MG | AA | 3046 | 1/1 | 0.91 | 0.18 | 72,72,72,72 | 0 |
| 57 | MG | CA | 3018 | 1/1 | 0.92 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3510 | 1/1 | 0.92 | 0.24 | 20,20,20,20 | 0 |
| 57 | MG | CA | 3136 | 1/1 | 0.92 | 0.11 | 68,68,68,68 | 0 |
| 57 | MG | DA | 3415 | 1/1 | 0.92 | 0.37 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3020 | 1/1 | 0.92 | 0.06 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3511 | 1/1 | 0.92 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3422 | 1/1 | 0.92 | 0.26 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3513 | 1/1 | 0.92 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3024 | 1/1 | 0.92 | 0.07 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3105 | 1/1 | 0.92 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3018 | 1/1 | 0.92 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | AM | 201 | 1/1 | 0.92 | 0.05 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3431 | 1/1 | 0.92 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3675 | 1/1 | 0.92 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3153 | 1/1 | 0.92 | 0.15 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3176 | 1/1 | 0.92 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3155 | 1/1 | 0.92 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3015 | 1/1 | 0.92 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3684 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3450 | 1/1 | 0.92 | 0.17 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3688 | 1/1 | 0.92 | 0.34 | 46,46,46,46 | 0 |
| 57 | MG | CF | 3001 | 1/1 | 0.92 | 0.17 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3017 | 1/1 | 0.92 | 0.23 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3182 | 1/1 | 0.92 | 0.39 | 52,52,52,52 | 0 |
| 57 | MG | CT | 3001 | 1/1 | 0.92 | 0.07 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3262 | 1/1 | 0.92 | 0.27 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3473 | 1/1 | 0.92 | 0.20 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3115 | 1/1 | 0.92 | 0.48 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3488 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3698 | 1/1 | 0.92 | 0.30 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3194 | 1/1 | 0.92 | 0.28 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3266 | 1/1 | 0.92 | 0.21 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3279 | 1/1 | 0.92 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3198 | 1/1 | 0.92 | 0.08 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3498 | 1/1 | 0.92 | 0.07 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3702 | 1/1 | 0.92 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3704 | 1/1 | 0.92 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | CA | 3045 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3212 | 1/1 | 0.92 | 0.08 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3216 | 1/1 | 0.92 | 0.29 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3120 | 1/1 | 0.92 | 0.36 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3514 | 1/1 | 0.92 | 0.20 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3284 | 1/1 | 0.92 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3517 | 1/1 | 0.92 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3221 | 1/1 | 0.92 | 0.13 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3397 | 1/1 | 0.92 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3521 | 1/1 | 0.92 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3122 | 1/1 | 0.92 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3123 | 1/1 | 0.92 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3411 | 1/1 | 0.92 | 0.23 | 24,24,24,24 | 0 |
| 57 | MG | DA | 3530 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3246 | 1/1 | 0.92 | 0.30 | 57,57,57,57 | 0 |
| 57 | MG | BB | 3008 | 1/1 | 0.92 | 0.11 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3543 | 1/1 | 0.92 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3250 | 1/1 | 0.92 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3559 | 1/1 | 0.92 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3035 | 1/1 | 0.92 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | BB | 3012 | 1/1 | 0.92 | 0.16 | 33,33,33,33 | 0 |
| 57 | MG | BB | 3018 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3003 | 1/1 | 0.92 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3040 | 1/1 | 0.92 | 0.42 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3068 | 1/1 | 0.92 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3264 | 1/1 | 0.92 | 0.10 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3415 | 1/1 | 0.92 | 0.22 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3207 | 1/1 | 0.92 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3135 | 1/1 | 0.92 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3268 | 1/1 | 0.92 | 0.12 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3271 | 1/1 | 0.92 | 0.21 | 47,47,47,47 | 0 |
| 57 | MG | BD | 311 | 1/1 | 0.92 | 0.36 | 60,60,60,60 | 0 |
| 57 | MG | CA | 3070 | 1/1 | 0.92 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3300 | 1/1 | 0.92 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3062 | 1/1 | 0.92 | 0.24 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3158 | 1/1 | 0.92 | 0.09 | 72,72,72,72 | 0 |
| 57 | MG | DA | 3285 | 1/1 | 0.92 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | BF | 302 | 1/1 | 0.92 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3075 | 1/1 | 0.92 | 0.35 | 45,45,45,45 | 0 |
| 57 | MG | AV | 3001 | 1/1 | 0.92 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3437 | 1/1 | 0.92 | 0.23 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3022 | 1/1 | 0.92 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3317 | 1/1 | 0.92 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3192 | 1/1 | 0.92 | 0.12 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3075 | 1/1 | 0.92 | 0.11 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3597 | 1/1 | 0.92 | 0.30 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3454 | 1/1 | 0.92 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3455 | 1/1 | 0.92 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | BU | 208 | 1/1 | 0.92 | 0.43 | 39,39,39,39 | 0 |
| 57 | MG | BW | 201 | 1/1 | 0.92 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | BW | 203 | 1/1 | 0.92 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3317 | 1/1 | 0.92 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3607 | 1/1 | 0.92 | 0.18 | 73,73,73,73 | 0 |
| 57 | MG | BA | 3324 | 1/1 | 0.92 | 0.21 | 61,61,61,61 | 0 |
| 57 | MG | B0 | 102 | 1/1 | 0.92 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3094 | 1/1 | 0.92 | 0.19 | 38,38,38,38 | 0 |
| 57 | MG | AA | 3059 | 1/1 | 0.92 | 0.30 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3099 | 1/1 | 0.92 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | AA | 3068 | 1/1 | 0.92 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3230 | 1/1 | 0.92 | 0.35 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3343 | 1/1 | 0.92 | 0.10 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3344 | 1/1 | 0.92 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3104 | 1/1 | 0.92 | 0.19 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3346 | 1/1 | 0.92 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3347 | 1/1 | 0.92 | 0.19 | 32,32,32,32 | 0 |
| 57 | MG | AA | 3199 | 1/1 | 0.92 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3476 | 1/1 | 0.92 | 0.14 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3107 | 1/1 | 0.92 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | DB | 3003 | 1/1 | 0.92 | 0.06 | 76,76,76,76 | 0 |
| 57 | MG | DA | 3109 | 1/1 | 0.92 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3155 | 1/1 | 0.92 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | DB | 3010 | 1/1 | 0.92 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | AX | 3011 | 1/1 | 0.92 | 0.37 | 73,73,73,73 | 0 |
| 57 | MG | DA | 3113 | 1/1 | 0.92 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3342 | 1/1 | 0.92 | 0.20 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3344 | 1/1 | 0.92 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3371 | 1/1 | 0.92 | 0.23 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3497 | 1/1 | 0.92 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | AA | 3176 | 1/1 | 0.92 | 0.09 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3379 | 1/1 | 0.92 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | DU | 3004 | 1/1 | 0.92 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | CA | 3010 | 1/1 | 0.92 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3383 | 1/1 | 0.92 | 0.13 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3031 | 1/1 | 0.92 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | D8 | 101 | 1/1 | 0.92 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3125 | 1/1 | 0.92 | 0.11 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3237 | 1/1 | 0.92 | 0.15 | 36,36,36,36 | 0 |
| 57 | MG | AA | 3032 | 1/1 | 0.92 | 0.11 | 80,80,80,80 | 0 |
| 57 | MG | BA | 3168 | 1/1 | 0.92 | 0.19 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3388 | 1/1 | 0.93 | 0.21 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3055 | 1/1 | 0.93 | 0.20 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3179 | 1/1 | 0.93 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3050 | 1/1 | 0.93 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3105 | 1/1 | 0.93 | 0.16 | 76,76,76,76 | 0 |
| 57 | MG | BA | 3547 | 1/1 | 0.93 | 0.18 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3268 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3273 | 1/1 | 0.93 | 0.17 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3411 | 1/1 | 0.93 | 0.09 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3552 | 1/1 | 0.93 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3413 | 1/1 | 0.93 | 0.29 | 30,30,30,30 | 0 |
| 57 | MG | CA | 3111 | 1/1 | 0.93 | 0.08 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3555 | 1/1 | 0.93 | 0.08 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3419 | 1/1 | 0.93 | 0.20 | 37,37,37,37 | 0 |
| 57 | MG | AA | 3202 | 1/1 | 0.93 | 0.06 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3557 | 1/1 | 0.93 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3399 | 1/1 | 0.93 | 0.15 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3564 | 1/1 | 0.93 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3142 | 1/1 | 0.93 | 0.23 | 50,50,50,50 | 0 |
| 57 | MG | BN | 3003 | 1/1 | 0.93 | 0.25 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3401 | 1/1 | 0.93 | 0.28 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3019 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3432 | 1/1 | 0.93 | 0.12 | 33,33,33,33 | 0 |
| 57 | MG | BR | 203 | 1/1 | 0.93 | 0.28 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3006 | 1/1 | 0.93 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | BU | 205 | 1/1 | 0.93 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | CA | 3128 | 1/1 | 0.93 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3409 | 1/1 | 0.93 | 0.27 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3159 | 1/1 | 0.93 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3410 | 1/1 | 0.93 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3286 | 1/1 | 0.93 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3064 | 1/1 | 0.93 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3167 | 1/1 | 0.93 | 0.17 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3170 | 1/1 | 0.93 | 0.37 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3065 | 1/1 | 0.93 | 0.27 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3205 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3020 | 1/1 | 0.93 | 0.19 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3585 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3297 | 1/1 | 0.93 | 0.22 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3490 | 1/1 | 0.93 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3421 | 1/1 | 0.93 | 0.18 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3591 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3134 | 1/1 | 0.93 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3151 | 1/1 | 0.93 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3424 | 1/1 | 0.93 | 0.21 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3200 | 1/1 | 0.93 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3213 | 1/1 | 0.93 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3501 | 1/1 | 0.93 | 0.24 | 47,47,47,47 | 0 |
| 57 | MG | AE | 3001 | 1/1 | 0.93 | 0.37 | 85,85,85,85 | 0 |
| 57 | MG | BA | 3301 | 1/1 | 0.93 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3431 | 1/1 | 0.93 | 0.22 | 25,25,25,25 | 0 |
| 57 | MG | DA | 3213 | 1/1 | 0.93 | 0.30 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3605 | 1/1 | 0.93 | 0.24 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3433 | 1/1 | 0.93 | 0.12 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3434 | 1/1 | 0.93 | 0.21 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3220 | 1/1 | 0.93 | 0.21 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3215 | 1/1 | 0.93 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | CA | 3016 | 1/1 | 0.93 | 0.05 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3021 | 1/1 | 0.93 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3225 | 1/1 | 0.93 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3138 | 1/1 | 0.93 | 0.26 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3234 | 1/1 | 0.93 | 0.30 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3528 | 1/1 | 0.93 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3450 | 1/1 | 0.93 | 0.07 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3308 | 1/1 | 0.93 | 0.15 | 14,14,14,14 | 0 |
| 57 | MG | DA | 3537 | 1/1 | 0.93 | 0.21 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3538 | 1/1 | 0.93 | 0.22 | 77,77,77,77 | 0 |
| 57 | MG | BA | 3621 | 1/1 | 0.93 | 0.13 | 18,18,18,18 | 0 |
| 57 | MG | BA | 3310 | 1/1 | 0.93 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3251 | 1/1 | 0.93 | 0.28 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3313 | 1/1 | 0.93 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3628 | 1/1 | 0.93 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3460 | 1/1 | 0.93 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3025 | 1/1 | 0.93 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3106 | 1/1 | 0.93 | 0.07 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3320 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3262 | 1/1 | 0.93 | 0.08 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3641 | 1/1 | 0.93 | 0.18 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3642 | 1/1 | 0.93 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3222 | 1/1 | 0.93 | 0.20 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3034 | 1/1 | 0.93 | 0.27 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 3006 | 1/1 | 0.93 | 0.17 | 62,62,62,62 | 0 |
| 57 | MG | BA | 3224 | 1/1 | 0.93 | 0.45 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3228 | 1/1 | 0.93 | 0.28 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3660 | 1/1 | 0.93 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3278 | 1/1 | 0.93 | 0.07 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3571 | 1/1 | 0.93 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3128 | 1/1 | 0.93 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3666 | 1/1 | 0.93 | 0.17 | 79,79,79,79 | 0 |
| 57 | MG | DA | 3048 | 1/1 | 0.93 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3131 | 1/1 | 0.93 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3671 | 1/1 | 0.93 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3672 | 1/1 | 0.93 | 0.10 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3673 | 1/1 | 0.93 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3581 | 1/1 | 0.93 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3582 | 1/1 | 0.93 | 0.16 | 24,24,24,24 | 0 |
| 57 | MG | AA | 3034 | 1/1 | 0.93 | 0.08 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3590 | 1/1 | 0.93 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3051 | 1/1 | 0.93 | 0.30 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3336 | 1/1 | 0.93 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3593 | 1/1 | 0.93 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3499 | 1/1 | 0.93 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3093 | 1/1 | 0.93 | 0.16 | 23,23,23,23 | 0 |
| 57 | MG | AX | 3005 | 1/1 | 0.93 | 0.32 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3156 | 1/1 | 0.93 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3505 | 1/1 | 0.93 | 0.20 | 16,16,16,16 | 0 |
| 57 | MG | AA | 3037 | 1/1 | 0.93 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3098 | 1/1 | 0.93 | 0.59 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3603 | 1/1 | 0.93 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3076 | 1/1 | 0.93 | 0.34 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3048 | 1/1 | 0.93 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3195 | 1/1 | 0.93 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3318 | 1/1 | 0.93 | 0.19 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3082 | 1/1 | 0.93 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | AA | 3197 | 1/1 | 0.93 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3357 | 1/1 | 0.93 | 0.20 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3049 | 1/1 | 0.93 | 0.25 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3616 | 1/1 | 0.93 | 0.13 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3089 | 1/1 | 0.93 | 0.19 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3331 | 1/1 | 0.93 | 0.26 | 54,54,54,54 | 0 |
| 57 | MG | CA | 3068 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3338 | 1/1 | 0.93 | 0.11 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3516 | 1/1 | 0.93 | 0.14 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | BA | 3710 | 1/1 | 0.93 | 0.11 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3107 | 1/1 | 0.93 | 0.28 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3715 | 1/1 | 0.93 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3097 | 1/1 | 0.93 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3717 | 1/1 | 0.93 | 0.43 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3350 | 1/1 | 0.93 | 0.36 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3521 | 1/1 | 0.93 | 0.28 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3522 | 1/1 | 0.93 | 0.11 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3360 | 1/1 | 0.93 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3249 | 1/1 | 0.93 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3524 | 1/1 | 0.93 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3250 | 1/1 | 0.93 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3090 | 1/1 | 0.93 | 0.43 | 64,64,64,64 | 0 |
| 57 | MG | DF | 3003 | 1/1 | 0.93 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | DF | 3004 | 1/1 | 0.93 | 0.27 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3091 | 1/1 | 0.93 | 0.20 | 75,75,75,75 | 0 |
| 57 | MG | BA | 3108 | 1/1 | 0.93 | 0.15 | 36,36,36,36 | 0 |
| 57 | MG | DP | 202 | 1/1 | 0.93 | 0.28 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3093 | 1/1 | 0.93 | 0.16 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3112 | 1/1 | 0.93 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | AA | 3115 | 1/1 | 0.93 | 0.33 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3377 | 1/1 | 0.93 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3376 | 1/1 | 0.93 | 0.24 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3115 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3378 | 1/1 | 0.93 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3381 | 1/1 | 0.93 | 0.22 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3054 | 1/1 | 0.93 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3384 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3678 | 1/1 | 0.94 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3679 | 1/1 | 0.94 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3148 | 1/1 | 0.94 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3682 | 1/1 | 0.94 | 0.19 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3353 | 1/1 | 0.94 | 0.08 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3508 | 1/1 | 0.94 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3377 | 1/1 | 0.94 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | CA | 3063 | 1/1 | 0.94 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3240 | 1/1 | 0.94 | 0.33 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3023 | 1/1 | 0.94 | 0.16 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3080 | 1/1 | 0.94 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3108 | 1/1 | 0.94 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3083 | 1/1 | 0.94 | 0.18 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3364 | 1/1 | 0.94 | 0.21 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3084 | 1/1 | 0.94 | 0.14 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3391 | 1/1 | 0.94 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3367 | 1/1 | 0.94 | 0.06 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3369 | 1/1 | 0.94 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3703 | 1/1 | 0.94 | 0.10 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3087 | 1/1 | 0.94 | 0.21 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3408 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3409 | 1/1 | 0.94 | 0.08 | 70,70,70,70 | 0 |
| 57 | MG | BA | 3708 | 1/1 | 0.94 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3157 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3118 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3251 | 1/1 | 0.94 | 0.27 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3086 | 1/1 | 0.94 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3711 | 1/1 | 0.94 | 0.19 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3418 | 1/1 | 0.94 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | AA | 3094 | 1/1 | 0.94 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3713 | 1/1 | 0.94 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | BA | 3089 | 1/1 | 0.94 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3260 | 1/1 | 0.94 | 0.26 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3090 | 1/1 | 0.94 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3530 | 1/1 | 0.94 | 0.26 | 20,20,20,20 | 0 |
| 57 | MG | AX | 3002 | 1/1 | 0.94 | 0.18 | 67,67,67,67 | 0 |
| 57 | MG | AA | 3130 | 1/1 | 0.94 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | BB | 3007 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3387 | 1/1 | 0.94 | 0.15 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3434 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3435 | 1/1 | 0.94 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3172 | 1/1 | 0.94 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3437 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3537 | 1/1 | 0.94 | 0.18 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3442 | 1/1 | 0.94 | 0.23 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3443 | 1/1 | 0.94 | 0.18 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3540 | 1/1 | 0.94 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | DA | 3144 | 1/1 | 0.94 | 0.08 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3389 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3392 | 1/1 | 0.94 | 0.18 | 27,27,27,27 | 0 |
| 57 | MG | BD | 302 | 1/1 | 0.94 | 0.24 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3149 | 1/1 | 0.94 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3544 | 1/1 | 0.94 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3393 | 1/1 | 0.94 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | AA | 3044 | 1/1 | 0.94 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3133 | 1/1 | 0.94 | 0.16 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3459 | 1/1 | 0.94 | 0.43 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3460 | 1/1 | 0.94 | 0.07 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3398 | 1/1 | 0.94 | 0.25 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3467 | 1/1 | 0.94 | 0.16 | 28,28,28,28 | 0 |
| 57 | MG | CA | 3118 | 1/1 | 0.94 | 0.17 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3278 | 1/1 | 0.94 | 0.07 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3485 | 1/1 | 0.94 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3486 | 1/1 | 0.94 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | AA | 3015 | 1/1 | 0.94 | 0.16 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3035 | 1/1 | 0.94 | 0.21 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3558 | 1/1 | 0.94 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | DA | 3171 | 1/1 | 0.94 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3177 | 1/1 | 0.94 | 0.34 | 29,29,29,29 | 0 |
| 57 | MG | BF | 306 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3282 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3185 | 1/1 | 0.94 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | BG | 3001 | 1/1 | 0.94 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3188 | 1/1 | 0.94 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3502 | 1/1 | 0.94 | 0.14 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3561 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3506 | 1/1 | 0.94 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3563 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3044 | 1/1 | 0.94 | 0.07 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3510 | 1/1 | 0.94 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | CA | 3131 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | BN | 3006 | 1/1 | 0.94 | 0.63 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3134 | 1/1 | 0.94 | 0.18 | 72,72,72,72 | 0 |
| 57 | MG | BO | 5001 | 1/1 | 0.94 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3199 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 57 | MG | BP | 3001 | 1/1 | 0.94 | 0.43 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3100 | 1/1 | 0.94 | 0.20 | 40,40,40,40 | 0 |
| 57 | MG | AA | 3135 | 1/1 | 0.94 | 0.08 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3567 | 1/1 | 0.94 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3209 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3525 | 1/1 | 0.94 | 0.08 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3210 | 1/1 | 0.94 | 0.44 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3048 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3181 | 1/1 | 0.94 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3214 | 1/1 | 0.94 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3535 | 1/1 | 0.94 | 0.23 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3294 | 1/1 | 0.94 | 0.21 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3575 | 1/1 | 0.94 | 0.17 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3218 | 1/1 | 0.94 | 0.09 | 36,36,36,36 | 0 |
| 57 | MG | AA | 3030 | 1/1 | 0.94 | 0.28 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3544 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3417 | 1/1 | 0.94 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BX | 101 | 1/1 | 0.94 | 0.28 | 36,36,36,36 | 0 |
| 57 | MG | AX | 3012 | 1/1 | 0.94 | 0.21 | 15,15,15,15 | 0 |
| 57 | MG | CA | 3157 | 1/1 | 0.94 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | B0 | 101 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3552 | 1/1 | 0.94 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3159 | 1/1 | 0.94 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3227 | 1/1 | 0.94 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3228 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |
| 57 | MG | CA | 3160 | 1/1 | 0.94 | 0.39 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3236 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3559 | 1/1 | 0.94 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3561 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | AA | 3099 | 1/1 | 0.94 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3200 | 1/1 | 0.94 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | B1 | 101 | 1/1 | 0.94 | 0.41 | 37,37,37,37 | 0 |
| 57 | MG | CK | 3001 | 1/1 | 0.94 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3201 | 1/1 | 0.94 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3200 | 1/1 | 0.94 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3254 | 1/1 | 0.94 | 0.28 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3058 | 1/1 | 0.94 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | CX | 3003 | 1/1 | 0.94 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3059 | 1/1 | 0.94 | 0.29 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3002 | 1/1 | 0.94 | 0.31 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3430 | 1/1 | 0.94 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3144 | 1/1 | 0.94 | 0.28 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3203 | 1/1 | 0.94 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3116 | 1/1 | 0.94 | 0.28 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3118 | 1/1 | 0.94 | 0.24 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3017 | 1/1 | 0.94 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3443 | 1/1 | 0.94 | 0.24 | 38,38,38,38 | 0 |
| 57 | MG | CA | 3009 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3270 | 1/1 | 0.94 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3119 | 1/1 | 0.94 | 0.24 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3446 | 1/1 | 0.94 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3036 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | CA | 3014 | 1/1 | 0.94 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3448 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3282 | 1/1 | 0.94 | 0.19 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3318 | 1/1 | 0.94 | 0.18 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3614 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | AA | 3060 | 1/1 | 0.94 | 0.38 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3286 | 1/1 | 0.94 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3147 | 1/1 | 0.94 | 0.06 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3323 | 1/1 | 0.94 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3039 | 1/1 | 0.94 | 0.39 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3021 | 1/1 | 0.94 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3458 | 1/1 | 0.94 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3045 | 1/1 | 0.94 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3459 | 1/1 | 0.94 | 0.28 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3126 | 1/1 | 0.94 | 0.28 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3626 | 1/1 | 0.94 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3306 | 1/1 | 0.94 | 0.12 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3049 | 1/1 | 0.94 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3051 | 1/1 | 0.94 | 0.09 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3463 | 1/1 | 0.94 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3175 | 1/1 | 0.94 | 0.32 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3058 | 1/1 | 0.94 | 0.21 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3327 | 1/1 | 0.94 | 0.18 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3060 | 1/1 | 0.94 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | AA | 3067 | 1/1 | 0.94 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3469 | 1/1 | 0.94 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | DB | 3005 | 1/1 | 0.94 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3329 | 1/1 | 0.94 | 0.12 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3471 | 1/1 | 0.94 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3644 | 1/1 | 0.94 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | DD | 302 | 1/1 | 0.94 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3472 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | DD | 306 | 1/1 | 0.94 | 0.38 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3132 | 1/1 | 0.94 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3019 | 1/1 | 0.94 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | DE | 302 | 1/1 | 0.94 | 0.61 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3341 | 1/1 | 0.94 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | CA | 3039 | 1/1 | 0.94 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | DF | 3002 | 1/1 | 0.94 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | AA | 3079 | 1/1 | 0.94 | 0.06 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3074 | 1/1 | 0.94 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3483 | 1/1 | 0.94 | 0.15 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3661 | 1/1 | 0.94 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3664 | 1/1 | 0.94 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3335 | 1/1 | 0.94 | 0.09 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DR | 3001 | 1/1 | 0.94 | 1.12 | 66,66,66,66 | 0 |
| 57 | MG | DU | 3002 | 1/1 | 0.94 | 0.42 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3071 | 1/1 | 0.94 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3667 | 1/1 | 0.94 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3358 | 1/1 | 0.94 | 0.53 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3137 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |
| 57 | MG | D5 | 101 | 1/1 | 0.94 | 0.20 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3072 | 1/1 | 0.94 | 0.12 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3073 | 1/1 | 0.94 | 0.29 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3074 | 1/1 | 0.94 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3107 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | AA | 3092 | 1/1 | 0.94 | 0.15 | 36,36,36,36 | 0 |
| 60 | K | AX | 3001 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | AA | 3120 | 1/1 | 0.95 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | B8 | 101 | 1/1 | 0.95 | 0.15 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3163 | 1/1 | 0.95 | 0.27 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3165 | 1/1 | 0.95 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3166 | 1/1 | 0.95 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3400 | 1/1 | 0.95 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3424 | 1/1 | 0.95 | 0.08 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3150 | 1/1 | 0.95 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3648 | 1/1 | 0.95 | 0.13 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3174 | 1/1 | 0.95 | 0.19 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3649 | 1/1 | 0.95 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3045 | 1/1 | 0.95 | 0.21 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3180 | 1/1 | 0.95 | 0.30 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3046 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3184 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3151 | 1/1 | 0.95 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3186 | 1/1 | 0.95 | 0.08 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3312 | 1/1 | 0.95 | 0.15 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3225 | 1/1 | 0.95 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3440 | 1/1 | 0.95 | 0.27 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3441 | 1/1 | 0.95 | 0.27 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3314 | 1/1 | 0.95 | 0.25 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3190 | 1/1 | 0.95 | 0.27 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3663 | 1/1 | 0.95 | 0.24 | 36,36,36,36 | 0 |
| 57 | MG | AA | 3196 | 1/1 | 0.95 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3447 | 1/1 | 0.95 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | AA | 3142 | 1/1 | 0.95 | 0.30 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3002 | 1/1 | 0.95 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3096 | 1/1 | 0.95 | 0.18 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3668 | 1/1 | 0.95 | 0.19 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3050 | 1/1 | 0.95 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3049 | 1/1 | 0.95 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3159 | 1/1 | 0.95 | 0.27 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3202 | 1/1 | 0.95 | 0.48 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3325 | 1/1 | 0.95 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3538 | 1/1 | 0.95 | 0.17 | 25,25,25,25 | 0 |
| 57 | MG | DA | 3208 | 1/1 | 0.95 | 0.13 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3006 | 1/1 | 0.95 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3472 | 1/1 | 0.95 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3539 | 1/1 | 0.95 | 0.22 | 18,18,18,18 | 0 |
| 57 | MG | DA | 3475 | 1/1 | 0.95 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3478 | 1/1 | 0.95 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3479 | 1/1 | 0.95 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3481 | 1/1 | 0.95 | 0.12 | 69,69,69,69 | 0 |
| 57 | MG | DA | 3211 | 1/1 | 0.95 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3677 | 1/1 | 0.95 | 0.24 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3010 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | AA | 3074 | 1/1 | 0.95 | 0.26 | 38,38,38,38 | 0 |
| 57 | MG | AA | 3057 | 1/1 | 0.95 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3165 | 1/1 | 0.95 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3056 | 1/1 | 0.95 | 0.20 | 21,21,21,21 | 0 |
| 57 | MG | DA | 3493 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3093 | 1/1 | 0.95 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3171 | 1/1 | 0.95 | 0.36 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3035 | 1/1 | 0.95 | 0.38 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3008 | 1/1 | 0.95 | 0.11 | 22,22,22,22 | 0 |
| 57 | MG | BA | 3436 | 1/1 | 0.95 | 0.22 | 21,21,21,21 | 0 |
| 57 | MG | AA | 3207 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3693 | 1/1 | 0.95 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3037 | 1/1 | 0.95 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | DA | 3504 | 1/1 | 0.95 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3695 | 1/1 | 0.95 | 0.20 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3229 | 1/1 | 0.95 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3230 | 1/1 | 0.95 | 0.22 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3439 | 1/1 | 0.95 | 0.16 | 12,12,12,12 | 0 |
| 57 | MG | BA | 3012 | 1/1 | 0.95 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3338 | 1/1 | 0.95 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3560 | 1/1 | 0.95 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3041 | 1/1 | 0.95 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3042 | 1/1 | 0.95 | 0.32 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3340 | 1/1 | 0.95 | 0.10 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3013 | 1/1 | 0.95 | 0.28 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3707 | 1/1 | 0.95 | 0.36 | 34,34,34,34 | 0 |
| 57 | MG | CA | 3046 | 1/1 | 0.95 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3253 | 1/1 | 0.95 | 0.23 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3449 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3345 | 1/1 | 0.95 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3052 | 1/1 | 0.95 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3529 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3053 | 1/1 | 0.95 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3532 | 1/1 | 0.95 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3452 | 1/1 | 0.95 | 0.18 | 15,15,15,15 | 0 |
| 57 | MG | DA | 3055 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 57 | MG | AD | 301 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | AA | 3174 | 1/1 | 0.95 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3714 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3540 | 1/1 | 0.95 | 0.09 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3110 | 1/1 | 0.95 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3067 | 1/1 | 0.95 | 0.25 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3576 | 1/1 | 0.95 | 0.26 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3274 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3275 | 1/1 | 0.95 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3720 | 1/1 | 0.95 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3277 | 1/1 | 0.95 | 0.44 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3551 | 1/1 | 0.95 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | AA | 3045 | 1/1 | 0.95 | 0.11 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3061 | 1/1 | 0.95 | 0.10 | 87,87,87,87 | 0 |
| 57 | MG | BA | 3578 | 1/1 | 0.95 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3069 | 1/1 | 0.95 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | BB | 3006 | 1/1 | 0.95 | 0.20 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3065 | 1/1 | 0.95 | 0.09 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3462 | 1/1 | 0.95 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3582 | 1/1 | 0.95 | 0.16 | 23,23,23,23 | 0 |
| 57 | MG | AA | 3152 | 1/1 | 0.95 | 0.09 | 64,64,64,64 | 0 |
| 57 | MG | BB | 3011 | 1/1 | 0.95 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3290 | 1/1 | 0.95 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3464 | 1/1 | 0.95 | 0.20 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3079 | 1/1 | 0.95 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3080 | 1/1 | 0.95 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | CA | 3071 | 1/1 | 0.95 | 0.40 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3299 | 1/1 | 0.95 | 0.13 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3300 | 1/1 | 0.95 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | CA | 3072 | 1/1 | 0.95 | 0.28 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BB | 3014 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3084 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3085 | 1/1 | 0.95 | 0.13 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3267 | 1/1 | 0.95 | 0.36 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3189 | 1/1 | 0.95 | 0.19 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3589 | 1/1 | 0.95 | 0.14 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3271 | 1/1 | 0.95 | 0.34 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3586 | 1/1 | 0.95 | 0.13 | 21,21,21,21 | 0 |
| 57 | MG | DA | 3313 | 1/1 | 0.95 | 0.05 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3589 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3198 | 1/1 | 0.95 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3594 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3277 | 1/1 | 0.95 | 0.29 | 34,34,34,34 | 0 |
| 57 | MG | AA | 3112 | 1/1 | 0.95 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3012 | 1/1 | 0.95 | 0.23 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3323 | 1/1 | 0.95 | 0.11 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3325 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BE | 3003 | 1/1 | 0.95 | 0.16 | 25,25,25,25 | 0 |
| 57 | MG | AN | 503 | 1/1 | 0.95 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3373 | 1/1 | 0.95 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3330 | 1/1 | 0.95 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3480 | 1/1 | 0.95 | 0.27 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3332 | 1/1 | 0.95 | 0.11 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3202 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3375 | 1/1 | 0.95 | 0.27 | 46,46,46,46 | 0 |
| 57 | MG | BF | 308 | 1/1 | 0.95 | 0.19 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3486 | 1/1 | 0.95 | 0.17 | 32,32,32,32 | 0 |
| 57 | MG | AA | 3061 | 1/1 | 0.95 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | DA | 3612 | 1/1 | 0.95 | 0.11 | 64,64,64,64 | 0 |
| 57 | MG | BA | 3612 | 1/1 | 0.95 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | CA | 3103 | 1/1 | 0.95 | 0.16 | 71,71,71,71 | 0 |
| 57 | MG | AA | 3189 | 1/1 | 0.95 | 0.12 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3077 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 57 | MG | BN | 3004 | 1/1 | 0.95 | 0.56 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3352 | 1/1 | 0.95 | 0.24 | 25,25,25,25 | 0 |
| 57 | MG | BA | 3289 | 1/1 | 0.95 | 0.13 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3355 | 1/1 | 0.95 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3028 | 1/1 | 0.95 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3208 | 1/1 | 0.95 | 0.10 | 33,33,33,33 | 0 |
| 57 | MG | CA | 3112 | 1/1 | 0.95 | 0.10 | 31,31,31,31 | 0 |
| 57 | MG | BP | 3002 | 1/1 | 0.95 | 0.20 | 32,32,32,32 | 0 |
| 57 | MG | BQ | 3001 | 1/1 | 0.95 | 0.32 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3121 | 1/1 | 0.95 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | AA | 3010 | 1/1 | 0.95 | 0.05 | 54,54,54,54 | 0 |
| 57 | MG | BQ | 3004 | 1/1 | 0.95 | 0.26 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3128 | 1/1 | 0.95 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | BQ | 3005 | 1/1 | 0.95 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3622 | 1/1 | 0.95 | 0.13 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3211 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | AA | 3191 | 1/1 | 0.95 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | BU | 202 | 1/1 | 0.95 | 0.10 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3391 | 1/1 | 0.95 | 0.24 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3082 | 1/1 | 0.95 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3629 | 1/1 | 0.95 | 0.19 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3630 | 1/1 | 0.95 | 0.13 | 72,72,72,72 | 0 |
| 57 | MG | BW | 202 | 1/1 | 0.95 | 0.60 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3631 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | AA | 3159 | 1/1 | 0.95 | 0.14 | 31,31,31,31 | 0 |
| 57 | MG | CA | 3132 | 1/1 | 0.95 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | DP | 201 | 1/1 | 0.95 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3633 | 1/1 | 0.95 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | DQ | 3001 | 1/1 | 0.95 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3634 | 1/1 | 0.95 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3395 | 1/1 | 0.95 | 0.18 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3396 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3118 | 1/1 | 0.95 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3404 | 1/1 | 0.95 | 0.08 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3638 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3138 | 1/1 | 0.95 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | B2 | 3001 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3156 | 1/1 | 0.95 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3157 | 1/1 | 0.95 | 0.18 | 44,44,44,44 | 0 |
| 59 | ZN | AN | 501 | 1/1 | 0.95 | 0.12 | 71,71,71,71 | 0 |
| 59 | ZN | B4 | 501 | 1/1 | 0.95 | 0.06 | 94,94,94,94 | 0 |
| 57 | MG | AX | 3007 | 1/1 | 0.95 | 0.26 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3036 | 1/1 | 0.95 | 0.63 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3145 | 1/1 | 0.95 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3414 | 1/1 | 0.95 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3394 | 1/1 | 0.96 | 0.18 | 22,22,22,22 | 0 |
| 57 | MG | BA | 3007 | 1/1 | 0.96 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | AA | 3206 | 1/1 | 0.96 | 0.06 | 62,62,62,62 | 0 |
| 57 | MG | CA | 3006 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3429 | 1/1 | 0.96 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3226 | 1/1 | 0.96 | 0.43 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3652 | 1/1 | 0.96 | 0.20 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3517 | 1/1 | 0.96 | 0.14 | 20,20,20,20 | 0 |
| 57 | MG | BA | 3657 | 1/1 | 0.96 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | CA | 3011 | 1/1 | 0.96 | 0.28 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3518 | 1/1 | 0.96 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3004 | 1/1 | 0.96 | 0.28 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3438 | 1/1 | 0.96 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3307 | 1/1 | 0.96 | 0.26 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3520 | 1/1 | 0.96 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3161 | 1/1 | 0.96 | 0.21 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3153 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3311 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3403 | 1/1 | 0.96 | 0.23 | 22,22,22,22 | 0 |
| 57 | MG | DA | 3014 | 1/1 | 0.96 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3077 | 1/1 | 0.96 | 0.27 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3405 | 1/1 | 0.96 | 0.24 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3178 | 1/1 | 0.96 | 0.19 | 67,67,67,67 | 0 |
| 57 | MG | DA | 3020 | 1/1 | 0.96 | 0.19 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3408 | 1/1 | 0.96 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3531 | 1/1 | 0.96 | 0.28 | 20,20,20,20 | 0 |
| 57 | MG | DA | 3025 | 1/1 | 0.96 | 0.18 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3456 | 1/1 | 0.96 | 0.35 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3026 | 1/1 | 0.96 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | AA | 3119 | 1/1 | 0.96 | 0.13 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3315 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3222 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3016 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3463 | 1/1 | 0.96 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3465 | 1/1 | 0.96 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3169 | 1/1 | 0.96 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3468 | 1/1 | 0.96 | 0.26 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3471 | 1/1 | 0.96 | 0.23 | 23,23,23,23 | 0 |
| 57 | MG | CA | 3028 | 1/1 | 0.96 | 0.31 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3170 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3319 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3476 | 1/1 | 0.96 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3477 | 1/1 | 0.96 | 0.10 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3236 | 1/1 | 0.96 | 0.15 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3681 | 1/1 | 0.96 | 0.22 | 42,42,42,42 | 0 |
| 57 | MG | AE | 3002 | 1/1 | 0.96 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | DA | 3232 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3541 | 1/1 | 0.96 | 0.17 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 3038 | 1/1 | 0.96 | 0.22 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3241 | 1/1 | 0.96 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3242 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3686 | 1/1 | 0.96 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | AA | 3184 | 1/1 | 0.96 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | AK | 3001 | 1/1 | 0.96 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | DA | 3494 | 1/1 | 0.96 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3249 | 1/1 | 0.96 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3545 | 1/1 | 0.96 | 0.24 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3423 | 1/1 | 0.96 | 0.25 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3114 | 1/1 | 0.96 | 0.24 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3253 | 1/1 | 0.96 | 0.23 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3500 | 1/1 | 0.96 | 0.16 | 32,32,32,32 | 0 |
| 57 | MG | AA | 3157 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3696 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3550 | 1/1 | 0.96 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3551 | 1/1 | 0.96 | 0.24 | 17,17,17,17 | 0 |
| 57 | MG | BA | 3244 | 1/1 | 0.96 | 0.39 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3701 | 1/1 | 0.96 | 0.19 | 17,17,17,17 | 0 |
| 57 | MG | DA | 3261 | 1/1 | 0.96 | 0.23 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3057 | 1/1 | 0.96 | 0.25 | 22,22,22,22 | 0 |
| 57 | MG | BA | 3246 | 1/1 | 0.96 | 0.23 | 46,46,46,46 | 0 |
| 57 | MG | AA | 3187 | 1/1 | 0.96 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3248 | 1/1 | 0.96 | 0.24 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3705 | 1/1 | 0.96 | 0.32 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3516 | 1/1 | 0.96 | 0.07 | 43,43,43,43 | 0 |
| 57 | MG | AA | 3140 | 1/1 | 0.96 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | AA | 3088 | 1/1 | 0.96 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3435 | 1/1 | 0.96 | 0.24 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3065 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3273 | 1/1 | 0.96 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | AA | 3022 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3562 | 1/1 | 0.96 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3526 | 1/1 | 0.96 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | AW | 101 | 1/1 | 0.96 | 0.24 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3438 | 1/1 | 0.96 | 0.16 | 19,19,19,19 | 0 |
| 57 | MG | BA | 3254 | 1/1 | 0.96 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3279 | 1/1 | 0.96 | 0.32 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3531 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3442 | 1/1 | 0.96 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3339 | 1/1 | 0.96 | 0.40 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3568 | 1/1 | 0.96 | 0.26 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | DA | 3536 | 1/1 | 0.96 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3444 | 1/1 | 0.96 | 0.23 | 32,32,32,32 | 0 |
| 57 | MG | AA | 3161 | 1/1 | 0.96 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3572 | 1/1 | 0.96 | 0.20 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3573 | 1/1 | 0.96 | 0.15 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3542 | 1/1 | 0.96 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3341 | 1/1 | 0.96 | 0.06 | 52,52,52,52 | 0 |
| 57 | MG | AA | 3082 | 1/1 | 0.96 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3184 | 1/1 | 0.96 | 0.26 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3188 | 1/1 | 0.96 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3074 | 1/1 | 0.96 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3086 | 1/1 | 0.96 | 0.08 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3549 | 1/1 | 0.96 | 0.20 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3295 | 1/1 | 0.96 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3127 | 1/1 | 0.96 | 0.24 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3076 | 1/1 | 0.96 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3451 | 1/1 | 0.96 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3195 | 1/1 | 0.96 | 0.28 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3264 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | DA | 3092 | 1/1 | 0.96 | 0.09 | 29,29,29,29 | 0 |
| 57 | MG | AA | 3075 | 1/1 | 0.96 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3352 | 1/1 | 0.96 | 0.14 | 29,29,29,29 | 0 |
| 57 | MG | BD | 301 | 1/1 | 0.96 | 0.38 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3309 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | AA | 3164 | 1/1 | 0.96 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3098 | 1/1 | 0.96 | 0.19 | 32,32,32,32 | 0 |
| 57 | MG | BD | 305 | 1/1 | 0.96 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3089 | 1/1 | 0.96 | 0.12 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3354 | 1/1 | 0.96 | 0.11 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3034 | 1/1 | 0.96 | 0.11 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3133 | 1/1 | 0.96 | 0.24 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3359 | 1/1 | 0.96 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | AA | 3101 | 1/1 | 0.96 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3324 | 1/1 | 0.96 | 0.25 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3167 | 1/1 | 0.96 | 0.06 | 65,65,65,65 | 0 |
| 57 | MG | BE | 3005 | 1/1 | 0.96 | 0.15 | 15,15,15,15 | 0 |
| 57 | MG | BA | 3363 | 1/1 | 0.96 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3081 | 1/1 | 0.96 | 0.14 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3599 | 1/1 | 0.96 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | CA | 3100 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3583 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3600 | 1/1 | 0.96 | 0.25 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3334 | 1/1 | 0.96 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3468 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3104 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3602 | 1/1 | 0.96 | 0.33 | 65,65,65,65 | 0 |
| 57 | MG | BA | 3365 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | BF | 310 | 1/1 | 0.96 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3038 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3206 | 1/1 | 0.96 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | BN | 3001 | 1/1 | 0.96 | 0.47 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3606 | 1/1 | 0.96 | 0.18 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3348 | 1/1 | 0.96 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3126 | 1/1 | 0.96 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3351 | 1/1 | 0.96 | 0.34 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3607 | 1/1 | 0.96 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3604 | 1/1 | 0.96 | 0.28 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3368 | 1/1 | 0.96 | 0.32 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3609 | 1/1 | 0.96 | 0.18 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3039 | 1/1 | 0.96 | 0.15 | 27,27,27,27 | 0 |
| 57 | MG | DA | 3357 | 1/1 | 0.96 | 0.19 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3040 | 1/1 | 0.96 | 0.14 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3478 | 1/1 | 0.96 | 0.15 | 22,22,22,22 | 0 |
| 57 | MG | BP | 3003 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3136 | 1/1 | 0.96 | 0.17 | 62,62,62,62 | 0 |
| 57 | MG | DA | 3365 | 1/1 | 0.96 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | BP | 3004 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3041 | 1/1 | 0.96 | 0.25 | 39,39,39,39 | 0 |
| 57 | MG | AX | 3009 | 1/1 | 0.96 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3621 | 1/1 | 0.96 | 0.46 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3288 | 1/1 | 0.96 | 0.10 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3623 | 1/1 | 0.96 | 0.16 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3484 | 1/1 | 0.96 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | BR | 201 | 1/1 | 0.96 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | DA | 3372 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3102 | 1/1 | 0.96 | 0.29 | 52,52,52,52 | 0 |
| 57 | MG | DA | 3145 | 1/1 | 0.96 | 0.20 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3619 | 1/1 | 0.96 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | AA | 3103 | 1/1 | 0.96 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3489 | 1/1 | 0.96 | 0.22 | 36,36,36,36 | 0 |
| 57 | MG | BU | 204 | 1/1 | 0.96 | 0.33 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3152 | 1/1 | 0.96 | 0.20 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3490 | 1/1 | 0.96 | 0.28 | 17,17,17,17 | 0 |
| 57 | MG | BA | 3491 | 1/1 | 0.96 | 0.16 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3387 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3292 | 1/1 | 0.96 | 0.17 | 26,26,26,26 | 0 |
| 57 | MG | AA | 3023 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3495 | 1/1 | 0.96 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | AA | 3201 | 1/1 | 0.96 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | AA | 3116 | 1/1 | 0.96 | 0.26 | 41,41,41,41 | 0 |
| 57 | MG | DE | 304 | 1/1 | 0.96 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3382 | 1/1 | 0.96 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3397 | 1/1 | 0.96 | 0.08 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3400 | 1/1 | 0.96 | 0.13 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3401 | 1/1 | 0.96 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3143 | 1/1 | 0.96 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3403 | 1/1 | 0.96 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3296 | 1/1 | 0.96 | 0.24 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3405 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3146 | 1/1 | 0.96 | 0.15 | 74,74,74,74 | 0 |
| 57 | MG | DQ | 3002 | 1/1 | 0.96 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | AA | 3117 | 1/1 | 0.96 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3220 | 1/1 | 0.96 | 0.23 | 54,54,54,54 | 0 |
| 57 | MG | DR | 3002 | 1/1 | 0.96 | 0.14 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3506 | 1/1 | 0.96 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3051 | 1/1 | 0.96 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | DV | 201 | 1/1 | 0.96 | 0.30 | 49,49,49,49 | 0 |
| 57 | MG | B3 | 3001 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3390 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3175 | 1/1 | 0.96 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | DY | 502 | 1/1 | 0.96 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | D3 | 3001 | 1/1 | 0.96 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | CA | 3153 | 1/1 | 0.96 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | B5 | 103 | 1/1 | 0.96 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | AA | 3204 | 1/1 | 0.96 | 0.23 | 64,64,64,64 | 0 |
| 57 | MG | AA | 3132 | 1/1 | 0.96 | 0.20 | 67,67,67,67 | 0 |
| 57 | MG | BA | 3302 | 1/1 | 0.96 | 0.17 | 50,50,50,50 | 0 |
| 59 | ZN | B9 | 501 | 1/1 | 0.96 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3420 | 1/1 | 0.96 | 0.09 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3646 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3647 | 1/1 | 0.96 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | CA | 3002 | 1/1 | 0.96 | 0.20 | 66,66,66,66 | 0 |
| 60 | K | CX | 3001 | 1/1 | 0.96 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3483 | 1/1 | 0.97 | 0.28 | 41,41,41,41 | 0 |
| 57 | MG | BD | 309 | 1/1 | 0.97 | 0.25 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3294 | 1/1 | 0.97 | 0.17 | 18,18,18,18 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3042 | 1/1 | 0.97 | 0.15 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3487 | 1/1 | 0.97 | 0.09 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3296 | 1/1 | 0.97 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3489 | 1/1 | 0.97 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3043 | 1/1 | 0.97 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3536 | 1/1 | 0.97 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3049 | 1/1 | 0.97 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3301 | 1/1 | 0.97 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3302 | 1/1 | 0.97 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3305 | 1/1 | 0.97 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | BE | 3004 | 1/1 | 0.97 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3141 | 1/1 | 0.97 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3186 | 1/1 | 0.97 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3187 | 1/1 | 0.97 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3142 | 1/1 | 0.97 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3640 | 1/1 | 0.97 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3102 | 1/1 | 0.97 | 0.26 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3151 | 1/1 | 0.97 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3012 | 1/1 | 0.97 | 0.08 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3505 | 1/1 | 0.97 | 0.07 | 41,41,41,41 | 0 |
| 57 | MG | BF | 307 | 1/1 | 0.97 | 0.24 | 25,25,25,25 | 0 |
| 57 | MG | DA | 3507 | 1/1 | 0.97 | 0.24 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3315 | 1/1 | 0.97 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3316 | 1/1 | 0.97 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3191 | 1/1 | 0.97 | 0.09 | 22,22,22,22 | 0 |
| 57 | MG | DA | 3016 | 1/1 | 0.97 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3512 | 1/1 | 0.97 | 0.13 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3192 | 1/1 | 0.97 | 0.09 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3320 | 1/1 | 0.97 | 0.12 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3321 | 1/1 | 0.97 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3194 | 1/1 | 0.97 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3546 | 1/1 | 0.97 | 0.25 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3456 | 1/1 | 0.97 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3108 | 1/1 | 0.97 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3196 | 1/1 | 0.97 | 0.27 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3383 | 1/1 | 0.97 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3523 | 1/1 | 0.97 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | BA | 3461 | 1/1 | 0.97 | 0.26 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3164 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 57 | MG | BN | 3005 | 1/1 | 0.97 | 0.22 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3654 | 1/1 | 0.97 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3333 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3030 | 1/1 | 0.97 | 0.39 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3384 | 1/1 | 0.97 | 0.29 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3033 | 1/1 | 0.97 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3172 | 1/1 | 0.97 | 0.09 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3173 | 1/1 | 0.97 | 0.34 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3534 | 1/1 | 0.97 | 0.12 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3554 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3197 | 1/1 | 0.97 | 0.19 | 32,32,32,32 | 0 |
| 57 | MG | DA | 3176 | 1/1 | 0.97 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3659 | 1/1 | 0.97 | 0.21 | 47,47,47,47 | 0 |
| 57 | MG | AA | 3091 | 1/1 | 0.97 | 0.24 | 35,35,35,35 | 0 |
| 57 | MG | AA | 3029 | 1/1 | 0.97 | 0.07 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3541 | 1/1 | 0.97 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3181 | 1/1 | 0.97 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3077 | 1/1 | 0.97 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | BQ | 3002 | 1/1 | 0.97 | 0.30 | 39,39,39,39 | 0 |
| 57 | MG | CA | 3079 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | CA | 3080 | 1/1 | 0.97 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3106 | 1/1 | 0.97 | 0.25 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3321 | 1/1 | 0.97 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3150 | 1/1 | 0.97 | 0.21 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3359 | 1/1 | 0.97 | 0.16 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3013 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | DA | 3361 | 1/1 | 0.97 | 0.18 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3259 | 1/1 | 0.97 | 0.29 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3192 | 1/1 | 0.97 | 0.23 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3071 | 1/1 | 0.97 | 0.39 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3556 | 1/1 | 0.97 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | BA | 3076 | 1/1 | 0.97 | 0.24 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3195 | 1/1 | 0.97 | 0.26 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3473 | 1/1 | 0.97 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3154 | 1/1 | 0.97 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3475 | 1/1 | 0.97 | 0.09 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3078 | 1/1 | 0.97 | 0.17 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3569 | 1/1 | 0.97 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | BV | 203 | 1/1 | 0.97 | 0.10 | 31,31,31,31 | 0 |
| 57 | MG | BV | 204 | 1/1 | 0.97 | 0.09 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3567 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3203 | 1/1 | 0.97 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3676 | 1/1 | 0.97 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3378 | 1/1 | 0.97 | 0.15 | 33,33,33,33 | 0 |
| 57 | MG | AA | 3024 | 1/1 | 0.97 | 0.24 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3573 | 1/1 | 0.97 | 0.08 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3207 | 1/1 | 0.97 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | AA | 3052 | 1/1 | 0.97 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3481 | 1/1 | 0.97 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3332 | 1/1 | 0.97 | 0.21 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3385 | 1/1 | 0.97 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | CA | 3101 | 1/1 | 0.97 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3209 | 1/1 | 0.97 | 0.22 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3402 | 1/1 | 0.97 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3485 | 1/1 | 0.97 | 0.11 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3585 | 1/1 | 0.97 | 0.27 | 45,45,45,45 | 0 |
| 57 | MG | DA | 3215 | 1/1 | 0.97 | 0.18 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3393 | 1/1 | 0.97 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3588 | 1/1 | 0.97 | 0.13 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3025 | 1/1 | 0.97 | 0.20 | 12,12,12,12 | 0 |
| 57 | MG | BA | 3270 | 1/1 | 0.97 | 0.42 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3488 | 1/1 | 0.97 | 0.05 | 34,34,34,34 | 0 |
| 57 | MG | DA | 3398 | 1/1 | 0.97 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | CA | 3108 | 1/1 | 0.97 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3594 | 1/1 | 0.97 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | B3 | 3002 | 1/1 | 0.97 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3053 | 1/1 | 0.97 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3160 | 1/1 | 0.97 | 0.25 | 23,23,23,23 | 0 |
| 57 | MG | BA | 3276 | 1/1 | 0.97 | 0.16 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3078 | 1/1 | 0.97 | 0.04 | 49,49,49,49 | 0 |
| 57 | MG | AA | 3148 | 1/1 | 0.97 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | BA | 3694 | 1/1 | 0.97 | 0.19 | 11,11,11,11 | 0 |
| 57 | MG | CA | 3115 | 1/1 | 0.97 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3493 | 1/1 | 0.97 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | AA | 3177 | 1/1 | 0.97 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | DA | 3606 | 1/1 | 0.97 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3697 | 1/1 | 0.97 | 0.16 | 23,23,23,23 | 0 |
| 57 | MG | DA | 3231 | 1/1 | 0.97 | 0.28 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3163 | 1/1 | 0.97 | 0.26 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3233 | 1/1 | 0.97 | 0.28 | 41,41,41,41 | 0 |
| 57 | MG | AA | 3009 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3416 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | DA | 3235 | 1/1 | 0.97 | 0.36 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3614 | 1/1 | 0.97 | 0.50 | 56,56,56,56 | 0 |
| 57 | MG | CA | 3121 | 1/1 | 0.97 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3237 | 1/1 | 0.97 | 0.31 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3498 | 1/1 | 0.97 | 0.23 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3618 | 1/1 | 0.97 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3343 | 1/1 | 0.97 | 0.18 | 18,18,18,18 | 0 |
| 57 | MG | DA | 3243 | 1/1 | 0.97 | 0.30 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3414 | 1/1 | 0.97 | 0.24 | 59,59,59,59 | 0 |
| 57 | MG | DA | 3245 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3085 | 1/1 | 0.97 | 0.15 | 18,18,18,18 | 0 |
| 57 | MG | DA | 3247 | 1/1 | 0.97 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3283 | 1/1 | 0.97 | 0.23 | 22,22,22,22 | 0 |
| 57 | MG | BA | 3219 | 1/1 | 0.97 | 0.43 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3418 | 1/1 | 0.97 | 0.23 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3629 | 1/1 | 0.97 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3348 | 1/1 | 0.97 | 0.12 | 17,17,17,17 | 0 |
| 57 | MG | DA | 3096 | 1/1 | 0.97 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | DB | 3004 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3420 | 1/1 | 0.97 | 0.11 | 23,23,23,23 | 0 |
| 57 | MG | DB | 3006 | 1/1 | 0.97 | 0.13 | 44,44,44,44 | 0 |
| 57 | MG | DB | 3007 | 1/1 | 0.97 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | BA | 3121 | 1/1 | 0.97 | 0.24 | 48,48,48,48 | 0 |
| 57 | MG | AA | 3179 | 1/1 | 0.97 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | DA | 3101 | 1/1 | 0.97 | 0.28 | 45,45,45,45 | 0 |
| 57 | MG | DD | 301 | 1/1 | 0.97 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3136 | 1/1 | 0.97 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | DD | 304 | 1/1 | 0.97 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3258 | 1/1 | 0.97 | 0.26 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3512 | 1/1 | 0.97 | 0.10 | 32,32,32,32 | 0 |
| 57 | MG | BA | 3124 | 1/1 | 0.97 | 0.12 | 31,31,31,31 | 0 |
| 57 | MG | AA | 3138 | 1/1 | 0.97 | 0.20 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3009 | 1/1 | 0.97 | 0.09 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3428 | 1/1 | 0.97 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | DA | 3445 | 1/1 | 0.97 | 0.09 | 59,59,59,59 | 0 |
| 57 | MG | BA | 3010 | 1/1 | 0.97 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | CA | 3141 | 1/1 | 0.97 | 0.15 | 69,69,69,69 | 0 |
| 57 | MG | BA | 3356 | 1/1 | 0.97 | 0.11 | 36,36,36,36 | 0 |
| 57 | MG | BB | 3002 | 1/1 | 0.97 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | CA | 3144 | 1/1 | 0.97 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | BA | 3227 | 1/1 | 0.97 | 0.19 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3432 | 1/1 | 0.97 | 0.26 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3454 | 1/1 | 0.97 | 0.27 | 28,28,28,28 | 0 |
| 57 | MG | DA | 3272 | 1/1 | 0.97 | 0.08 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3358 | 1/1 | 0.97 | 0.10 | 35,35,35,35 | 0 |
| 57 | MG | AA | 3183 | 1/1 | 0.97 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3617 | 1/1 | 0.97 | 0.13 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3131 | 1/1 | 0.97 | 0.38 | 31,31,31,31 | 0 |
| 57 | MG | DU | 3001 | 1/1 | 0.97 | 0.62 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3037 | 1/1 | 0.97 | 0.17 | 38,38,38,38 | 0 |
| 57 | MG | DU | 3003 | 1/1 | 0.97 | 0.20 | 60,60,60,60 | 0 |
| 57 | MG | BA | 3362 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3462 | 1/1 | 0.97 | 0.27 | 35,35,35,35 | 0 |
| 57 | MG | AA | 3165 | 1/1 | 0.97 | 0.24 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3095 | 1/1 | 0.97 | 0.23 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3124 | 1/1 | 0.97 | 0.26 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3624 | 1/1 | 0.97 | 0.11 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3470 | 1/1 | 0.97 | 0.14 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3529 | 1/1 | 0.97 | 0.28 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3127 | 1/1 | 0.97 | 0.35 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3440 | 1/1 | 0.97 | 0.23 | 40,40,40,40 | 0 |
| 58 | SF4 | CD | 501 | 8/8 | 0.97 | 0.12 | 59,71,83,91 | 0 |
| 57 | MG | DA | 3474 | 1/1 | 0.97 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | BA | 3627 | 1/1 | 0.97 | 0.09 | 28,28,28,28 | 0 |
| 57 | MG | BD | 303 | 1/1 | 0.97 | 0.32 | 42,42,42,42 | 0 |
| 57 | MG | AA | 3139 | 1/1 | 0.97 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | AX | 3004 | 1/1 | 0.97 | 0.13 | 45,45,45,45 | 0 |
| 57 | MG | BD | 307 | 1/1 | 0.97 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3480 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 57 | MG | AA | 3186 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3252 | 1/1 | 0.98 | 0.22 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3496 | 1/1 | 0.98 | 0.29 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3560 | 1/1 | 0.98 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3015 | 1/1 | 0.98 | 0.25 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3285 | 1/1 | 0.98 | 0.18 | 21,21,21,21 | 0 |
| 57 | MG | BA | 3457 | 1/1 | 0.98 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3185 | 1/1 | 0.98 | 0.49 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3386 | 1/1 | 0.98 | 0.25 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3593 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3643 | 1/1 | 0.98 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | BA | 3128 | 1/1 | 0.98 | 0.16 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3024 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3570 | 1/1 | 0.98 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | BA | 3645 | 1/1 | 0.98 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3255 | 1/1 | 0.98 | 0.06 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3596 | 1/1 | 0.98 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3503 | 1/1 | 0.98 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3029 | 1/1 | 0.98 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3123 | 1/1 | 0.98 | 0.16 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57 | MG | BA | 3706 | 1/1 | 0.98 | 0.25 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3504 | 1/1 | 0.98 | 0.24 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3086 | 1/1 | 0.98 | 0.22 | 15,15,15,15 | 0 |
| 57 | MG | DA | 3335 | 1/1 | 0.98 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | DA | 3336 | 1/1 | 0.98 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3290 | 1/1 | 0.98 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3584 | 1/1 | 0.98 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | AA | 3081 | 1/1 | 0.98 | 0.09 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3339 | 1/1 | 0.98 | 0.17 | 23,23,23,23 | 0 |
| 57 | MG | DA | 3340 | 1/1 | 0.98 | 0.17 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3653 | 1/1 | 0.98 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3464 | 1/1 | 0.98 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3427 | 1/1 | 0.98 | 0.16 | 23,23,23,23 | 0 |
| 57 | MG | DA | 3466 | 1/1 | 0.98 | 0.24 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3131 | 1/1 | 0.98 | 0.11 | 34,34,34,34 | 0 |
| 57 | MG | BA | 3553 | 1/1 | 0.98 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3469 | 1/1 | 0.98 | 0.31 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3014 | 1/1 | 0.98 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3190 | 1/1 | 0.98 | 0.23 | 24,24,24,24 | 0 |
| 57 | MG | BA | 3716 | 1/1 | 0.98 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3212 | 1/1 | 0.98 | 0.29 | 24,24,24,24 | 0 |
| 57 | MG | DA | 3349 | 1/1 | 0.98 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | BA | 3718 | 1/1 | 0.98 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3238 | 1/1 | 0.98 | 0.43 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3239 | 1/1 | 0.98 | 0.31 | 51,51,51,51 | 0 |
| 57 | MG | DA | 3240 | 1/1 | 0.98 | 0.24 | 36,36,36,36 | 0 |
| 57 | MG | CA | 3123 | 1/1 | 0.98 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3101 | 1/1 | 0.98 | 0.29 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3140 | 1/1 | 0.98 | 0.25 | 38,38,38,38 | 0 |
| 57 | MG | AA | 3194 | 1/1 | 0.98 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | BA | 3662 | 1/1 | 0.98 | 0.25 | 62,62,62,62 | 0 |
| 57 | MG | BU | 203 | 1/1 | 0.98 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3050 | 1/1 | 0.98 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3047 | 1/1 | 0.98 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3193 | 1/1 | 0.98 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | BB | 3003 | 1/1 | 0.98 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3265 | 1/1 | 0.98 | 0.14 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3117 | 1/1 | 0.98 | 0.17 | 24,24,24,24 | 0 |
| 57 | MG | DA | 3150 | 1/1 | 0.98 | 0.36 | 41,41,41,41 | 0 |
| 57 | MG | BV | 201 | 1/1 | 0.98 | 0.22 | 33,33,33,33 | 0 |
| 57 | MG | BV | 202 | 1/1 | 0.98 | 0.20 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3620 | 1/1 | 0.98 | 0.17 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 3182 | 1/1 | 0.98 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3057 | 1/1 | 0.98 | 0.18 | 21,21,21,21 | 0 |
| 57 | MG | DA | 3373 | 1/1 | 0.98 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3269 | 1/1 | 0.98 | 0.24 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3477 | 1/1 | 0.98 | 0.14 | 19,19,19,19 | 0 |
| 57 | MG | BB | 3010 | 1/1 | 0.98 | 0.10 | 28,28,28,28 | 0 |
| 57 | MG | BW | 204 | 1/1 | 0.98 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | BW | 205 | 1/1 | 0.98 | 0.14 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3670 | 1/1 | 0.98 | 0.11 | 25,25,25,25 | 0 |
| 57 | MG | DB | 3001 | 1/1 | 0.98 | 0.07 | 50,50,50,50 | 0 |
| 57 | MG | BY | 201 | 1/1 | 0.98 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | AA | 3095 | 1/1 | 0.98 | 0.15 | 44,44,44,44 | 0 |
| 57 | MG | DA | 3382 | 1/1 | 0.98 | 0.22 | 20,20,20,20 | 0 |
| 57 | MG | BB | 3013 | 1/1 | 0.98 | 0.18 | 43,43,43,43 | 0 |
| 57 | MG | BA | 3479 | 1/1 | 0.98 | 0.13 | 22,22,22,22 | 0 |
| 57 | MG | BB | 3015 | 1/1 | 0.98 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3269 | 1/1 | 0.98 | 0.16 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3071 | 1/1 | 0.98 | 0.15 | 42,42,42,42 | 0 |
| 57 | MG | B0 | 104 | 1/1 | 0.98 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | DA | 3168 | 1/1 | 0.98 | 0.32 | 50,50,50,50 | 0 |
| 57 | MG | DA | 3169 | 1/1 | 0.98 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | DD | 303 | 1/1 | 0.98 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | DA | 3392 | 1/1 | 0.98 | 0.23 | 40,40,40,40 | 0 |
| 57 | MG | DA | 3073 | 1/1 | 0.98 | 0.31 | 49,49,49,49 | 0 |
| 57 | MG | BB | 3016 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3518 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 57 | MG | BB | 3017 | 1/1 | 0.98 | 0.09 | 28,28,28,28 | 0 |
| 57 | MG | AA | 3137 | 1/1 | 0.98 | 0.28 | 66,66,66,66 | 0 |
| 57 | MG | BA | 3441 | 1/1 | 0.98 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | BA | 3620 | 1/1 | 0.98 | 0.12 | 35,35,35,35 | 0 |
| 57 | MG | CA | 3073 | 1/1 | 0.98 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | BA | 3370 | 1/1 | 0.98 | 0.21 | 32,32,32,32 | 0 |
| 57 | MG | CA | 3156 | 1/1 | 0.98 | 0.05 | 57,57,57,57 | 0 |
| 57 | MG | DA | 3179 | 1/1 | 0.98 | 0.24 | 50,50,50,50 | 0 |
| 57 | MG | B7 | 101 | 1/1 | 0.98 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | DN | 5001 | 1/1 | 0.98 | 0.06 | 53,53,53,53 | 0 |
| 57 | MG | BA | 3272 | 1/1 | 0.98 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3407 | 1/1 | 0.98 | 0.19 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3183 | 1/1 | 0.98 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | BD | 304 | 1/1 | 0.98 | 0.19 | 36,36,36,36 | 0 |
| 57 | MG | DA | 3289 | 1/1 | 0.98 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | AA | 3129 | 1/1 | 0.98 | 0.16 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3245 | 1/1 | 0.98 | 0.31 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3030 | 1/1 | 0.98 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | AA | 3083 | 1/1 | 0.98 | 0.30 | 38,38,38,38 | 0 |
| 57 | MG | BA | 3125 | 1/1 | 0.98 | 0.39 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3280 | 1/1 | 0.98 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | BA | 3685 | 1/1 | 0.98 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | BE | 3001 | 1/1 | 0.98 | 0.33 | 48,48,48,48 | 0 |
| 57 | MG | CA | 3087 | 1/1 | 0.98 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | BA | 3110 | 1/1 | 0.98 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3687 | 1/1 | 0.98 | 0.11 | 30,30,30,30 | 0 |
| 57 | MG | BA | 3580 | 1/1 | 0.98 | 0.27 | 13,13,13,13 | 0 |
| 57 | MG | DA | 3423 | 1/1 | 0.98 | 0.24 | 33,33,33,33 | 0 |
| 57 | MG | DA | 3005 | 1/1 | 0.98 | 0.20 | 29,29,29,29 | 0 |
| 57 | MG | BA | 3346 | 1/1 | 0.98 | 0.23 | 29,29,29,29 | 0 |
| 57 | MG | DA | 3100 | 1/1 | 0.98 | 0.20 | 38,38,38,38 | 0 |
| 58 | SF4 | AD | 302 | 8/8 | 0.98 | 0.14 | 59,71,78,78 | 0 |
| 57 | MG | BA | 3690 | 1/1 | 0.98 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | BF | 301 | 1/1 | 0.98 | 0.18 | 30,30,30,30 | 0 |
| 59 | ZN | BY | 202 | 1/1 | 0.98 | 0.12 | 70,70,70,70 | 0 |
| 57 | MG | DA | 3009 | 1/1 | 0.98 | 0.14 | 39,39,39,39 | 0 |
| 57 | MG | BA | 3145 | 1/1 | 0.98 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | DA | 3310 | 1/1 | 0.98 | 0.16 | 43,43,43,43 | 0 |
| 59 | ZN | DY | 501 | 1/1 | 0.98 | 0.10 | 88,88,88,88 | 0 |
| 57 | MG | BF | 303 | 1/1 | 0.98 | 0.18 | 35,35,35,35 | 0 |
| 59 | ZN | D6 | 501 | 1/1 | 0.98 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | DA | 3433 | 1/1 | 0.98 | 0.23 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3004 | 1/1 | 0.98 | 0.18 | 26,26,26,26 | 0 |
| 57 | MG | DA | 3206 | 1/1 | 0.98 | 0.22 | 37,37,37,37 | 0 |
| 57 | MG | DA | 3399 | 1/1 | 0.99 | 0.13 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3528 | 1/1 | 0.99 | 0.17 | 37,37,37,37 | 0 |
| 57 | MG | BA | 3239 | 1/1 | 0.99 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | BA | 3309 | 1/1 | 0.99 | 0.10 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3044 | 1/1 | 0.99 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3298 | 1/1 | 0.99 | 0.11 | 35,35,35,35 | 0 |
| 57 | MG | DA | 3022 | 1/1 | 0.99 | 0.09 | 27,27,27,27 | 0 |
| 57 | MG | BA | 3330 | 1/1 | 0.99 | 0.17 | 14,14,14,14 | 0 |
| 57 | MG | BA | 3026 | 1/1 | 0.99 | 0.24 | 36,36,36,36 | 0 |
| 57 | MG | BU | 207 | 1/1 | 0.99 | 0.16 | 23,23,23,23 | 0 |
| 57 | MG | DA | 3599 | 1/1 | 0.99 | 0.23 | 36,36,36,36 | 0 |
| 57 | MG | BE | 3007 | 1/1 | 0.99 | 0.10 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3376 | 1/1 | 0.99 | 0.21 | 21,21,21,21 | 0 |
| 57 | MG | DA | 3354 | 1/1 | 0.99 | 0.26 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3329 | 1/1 | 0.99 | 0.26 | 54,54,54,54 | 0 |
| 57 | MG | BA | 3586 | 1/1 | 0.99 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | BA | 3274 | 1/1 | 0.99 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | BA | 3588 | 1/1 | 0.99 | 0.18 | 19,19,19,19 | 0 |
| 57 | MG | DA | 3386 | 1/1 | 0.99 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | DA | 3031 | 1/1 | 0.99 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3637 | 1/1 | 0.99 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | BA | 3655 | 1/1 | 0.99 | 0.09 | 68,68,68,68 | 0 |
| 57 | MG | BA | 3275 | 1/1 | 0.99 | 0.10 | 38,38,38,38 | 0 |
| 57 | MG | DA | 3482 | 1/1 | 0.99 | 0.25 | 31,31,31,31 | 0 |
| 57 | MG | DA | 3579 | 1/1 | 0.99 | 0.29 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3451 | 1/1 | 0.99 | 0.21 | 39,39,39,39 | 0 |
| 59 | ZN | B5 | 102 | 1/1 | 0.99 | 0.16 | 41,41,41,41 | 0 |
| 59 | ZN | B6 | 501 | 1/1 | 0.99 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | DA | 3363 | 1/1 | 0.99 | 0.21 | 35,35,35,35 | 0 |
| 57 | MG | AA | 3169 | 1/1 | 0.99 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | BA | 3140 | 1/1 | 0.99 | 0.19 | 26,26,26,26 | 0 |
| 57 | MG | BA | 3592 | 1/1 | 0.99 | 0.18 | 14,14,14,14 | 0 |
| 59 | ZN | D5 | 102 | 1/1 | 0.99 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | DA | 3395 | 1/1 | 0.99 | 0.11 | 31,31,31,31 | 0 |
| 57 | MG | BA | 3167 | 1/1 | 0.99 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | BA | 3256 | 1/1 | 0.99 | 0.10 | 36,36,36,36 | 0 |
| 57 | MG | BA | 3147 | 1/1 | 0.99 | 0.23 | 34,34,34,34 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.