



wwPDB X-ray Structure Validation Summary Report i

Sep 10, 2014 – 10:54 PM EDT

PDB ID : 1VY4
Title : Crystal structure of the Thermus thermophilus 70S ribosome in the pre-attack state of peptide bond formation containing acylated tRNA-substrates in the A and P sites.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

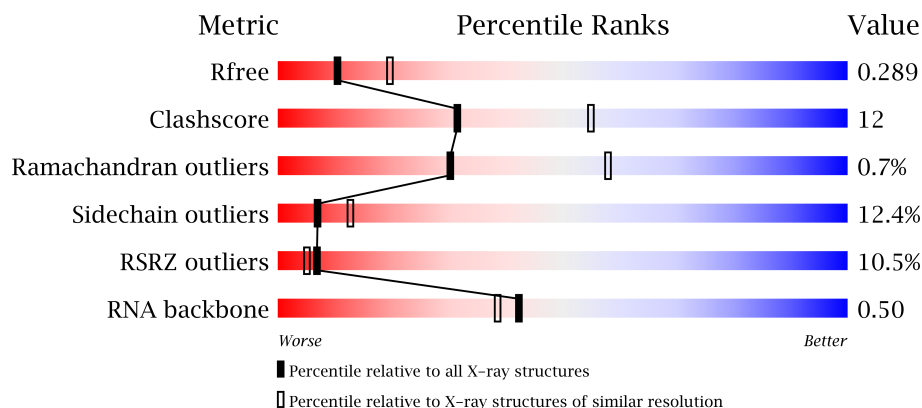
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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} | 66092 | 1718 (2.60-2.60) |
| Clashscore | 79885 | 2154 (2.60-2.60) |
| Ramachandran outliers | 78287 | 2113 (2.60-2.60) |
| Sidechain outliers | 78261 | 2113 (2.60-2.60) |
| RSRZ outliers | 66119 | 1718 (2.60-2.60) |
| RNA backbone | 1838 | 1002 (3.12-2.08) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AA | 1521 | |
| 1 | CA | 1521 | |
| 2 | AB | 256 | |
| 2 | CB | 256 | |
| 3 | AC | 239 | |
| 3 | CC | 239 | |
| 4 | AD | 209 | |
| 4 | CD | 209 | |
| 5 | AE | 162 | |
| 5 | CE | 162 | |
| 6 | AF | 101 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 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 | 76 | |
| 23 | CW | 76 | |
| 24 | AX | 77 | |
| 24 | CX | 77 | |
| 25 | AY | 76 | |
| 25 | CY | 76 | |
| 26 | BA | 2915 | |
| 26 | DA | 2915 | |
| 27 | BB | 121 | |







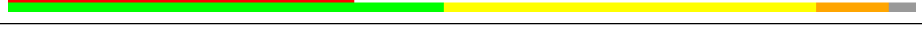


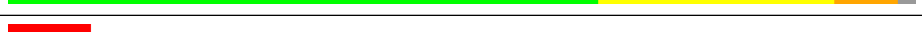

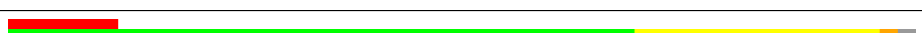


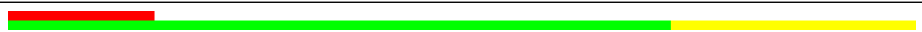


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27 | DB | 121 | |
| 28 | BD | 276 | |
| 28 | DD | 276 | |
| 29 | BE | 206 | |
| 29 | DE | 206 | |
| 30 | BF | 210 | |
| 30 | DF | 210 | |
| 31 | BG | 182 | |
| 31 | DG | 182 | |
| 32 | BH | 180 | |
| 32 | DH | 180 | |
| 33 | BI | 148 | |
| 33 | DI | 148 | |
| 34 | BN | 140 | |
| 34 | DN | 140 | |
| 35 | BO | 122 | |
| 35 | DO | 122 | |
| 36 | BP | 150 | |
| 36 | DP | 150 | |
| 37 | BQ | 141 | |
| 37 | DQ | 141 | |
| 38 | BR | 118 | |
| 38 | DR | 118 | |
| 39 | BS | 112 | |
| 39 | DS | 112 | |
| 40 | BT | 146 | |
| 40 | DT | 146 | |
| 41 | BU | 118 | |
| 41 | DU | 118 | |
| 42 | BV | 101 | |
| 42 | DV | 101 | |
| 43 | BW | 113 | |
| 43 | DW | 113 | |
| 44 | BX | 96 | |
| 44 | DX | 96 | |
| 45 | BY | 110 | |
| 45 | DY | 110 | |
| 46 | BZ | 206 | |
| 46 | DZ | 206 | |
| 47 | B0 | 85 | |
| 47 | D0 | 85 | |
| 48 | B1 | 98 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 48 | D1 | 98 |  |
| 49 | B2 | 72 |  |
| 49 | D2 | 72 |  |
| 50 | B3 | 60 |  |
| 50 | D3 | 60 |  |
| 51 | B4 | 71 |  |
| 51 | D4 | 71 |  |
| 52 | B5 | 60 |  |
| 52 | D5 | 60 |  |
| 53 | B6 | 54 |  |
| 53 | D6 | 54 |  |
| 54 | B7 | 49 |  |
| 54 | D7 | 49 |  |
| 55 | B8 | 65 |  |
| 55 | D8 | 65 |  |
| 56 | B9 | 37 |  |
| 56 | D9 | 37 |  |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297127 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1497 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32185 | 14324 | 5968 | 10396 | 1497 | | | |
| 1 | CA | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32312 | 14381 | 5990 | 10438 | 1503 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 976 | 302 | 273 | 1 | | | |
| 3 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1544 | 970 | 300 | 273 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | AD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1659 | 1040 | 326 | 286 | 7 | | | |
| 4 | CD | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1678 | 1052 | 333 | 286 | 7 | | | |

- 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 |
| | | | 812 | 514 | 146 | 149 | 3 | | | |
| 6 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 820 | 518 | 147 | 152 | 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 |
| | | | 986 | 626 | 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 |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10 | CJ | 96 | Total | C | N | O | | | |
| | | | 714 | 445 | 138 | 131 | 0 | 0 | 0 |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 13 | AM | 123 | Total | C | N | O | S | | |
| | | | 966 | 598 | 200 | 166 | 2 | 0 | 0 |
| 13 | CM | 122 | Total | C | N | O | S | | |
| | | | 950 | 586 | 197 | 165 | 2 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | | |
| | | | 728 | 456 | 144 | 126 | 2 | 0 | 0 |
| 15 | CO | 88 | Total | C | N | O | S | | |
| | | | 728 | 456 | 144 | 126 | 2 | 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 | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 661 | 423 | 122 | 114 | 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 |
| | | | 731 | 449 | 156 | 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 | 12 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 252 | 115 | 46 | 80 | 11 | | | |

- Molecule 23 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23 | AW | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1599 | 722 | 287 | 515 | 73 | 2 | | | |
| 23 | CW | 72 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1552 | 697 | 280 | 502 | 72 | 1 | | | |

- 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 |
| | | | 1635 | 731 | 296 | 530 | 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 | 74 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1581 | 707 | 285 | 515 | 73 | 1 | | | |
| 25 | CY | 73 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1561 | 698 | 283 | 507 | 72 | 1 | | | |

- 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 |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26 | DA | 2800 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60311 | 26840 | 11284 | 19388 | 2799 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28 | BD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2136 | 1349 | 423 | 361 | 3 | | | |
| 28 | DD | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2142 | 1352 | 426 | 361 | 3 | | | |

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

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

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

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

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

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

- 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 |
| | | | 1073 | 688 | 188 | 196 | 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 |
| | | | 1139 | 709 | 231 | 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 |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | DV | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

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

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

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

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

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

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

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

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

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

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

- 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 |
| | | | 558 | 352 | 102 | 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 |
| | | | 517 | 331 | 102 | 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 | B4 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | BA | 814 | Total | Mg | 0 | 0 |
| | | | 814 | 814 | | |
| 57 | AK | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | DQ | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | D3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | AB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DF | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | B8 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BE | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | AW | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | AN | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | AX | 15 | Total 15 | Mg 15 | 0 | 0 |
| 57 | DN | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CA | 169 | Total 169 | Mg 169 | 0 | 0 |
| 57 | B5 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | BB | 23 | Total 23 | Mg 23 | 0 | 0 |
| 57 | D8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | AE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DB | 13 | Total 13 | Mg 13 | 0 | 0 |
| 57 | CF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B9 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BF | 11 | Total 11 | Mg 11 | 0 | 0 |
| 57 | BX | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B2 | 1 | Total 1 | Mg 1 | 0 | 0 |

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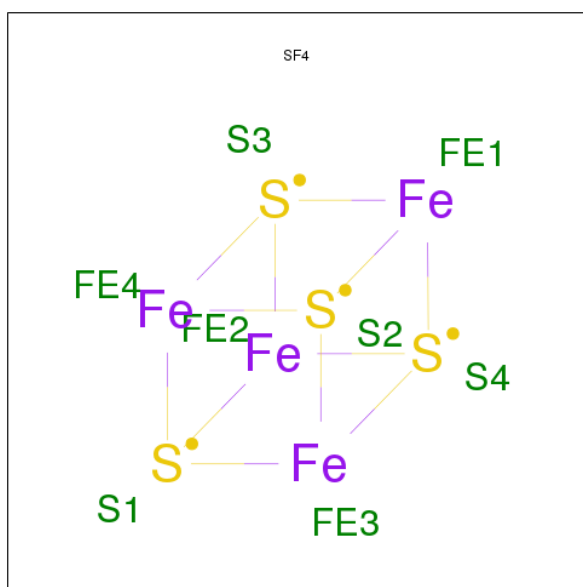
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | AA | 216 | Total 216 | Mg 216 | 0 | 0 |
| 57 | BQ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | CX | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B6 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | AM | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BU | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | DR | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BN | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | CT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | D0 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BG | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DE | 7 | Total 7 | Mg 7 | 0 | 0 |
| 57 | CJ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BR | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DA | 664 | Total 664 | Mg 664 | 0 | 0 |
| 57 | AU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B7 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | AL | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 57 | BV | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | DP | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DO | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BO | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BZ | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | DY | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CW | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | DG | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | CD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BD | 10 | Total 10 | Mg 10 | 0 | 0 |
| 57 | AT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | B0 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | CE | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | BW | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | AY | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | DD | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | CK | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | AF | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | BH | 1 | Total 1 | Mg 1 | 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 | B5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | CN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | BY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | B9 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | DY | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | AN | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | D6 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59 | D9 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 59 | B6 | 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 |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61 | AA | 210 | Total 210 | O 210 | 0 | 0 |
| 61 | AD | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | AE | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AJ | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | AL | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AM | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AV | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | AW | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | AX | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | AY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BA | 1405 | Total 1406 | O 1406 | 0 | 1 |
| 61 | BB | 37 | Total 37 | O 37 | 0 | 0 |
| 61 | BD | 15 | Total 15 | O 15 | 0 | 0 |
| 61 | BE | 17 | Total 17 | O 17 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 61 | BF | 11 | Total 11 | O 11 | 0 | 0 |
| 61 | BG | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BH | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BI | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BN | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | BO | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BP | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | BQ | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BR | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BS | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BT | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BU | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | BV | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | BW | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BX | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | BZ | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | B0 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | B1 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | B3 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | B5 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | B6 | 2 | Total 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | B7 | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | B8 | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | B9 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CA | 156 | Total 156 | O 156 | 0 | 0 |
| 61 | CE | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CH | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CJ | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CL | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | CW | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | CY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DA | 989 | Total 989 | O 989 | 0 | 0 |
| 61 | DB | 9 | Total 9 | O 9 | 0 | 0 |
| 61 | DD | 18 | Total 18 | O 18 | 0 | 0 |
| 61 | DE | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | DF | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | DN | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DP | 12 | Total 12 | O 12 | 0 | 0 |
| 61 | DQ | 1 | Total 1 | O 1 | 0 | 0 |

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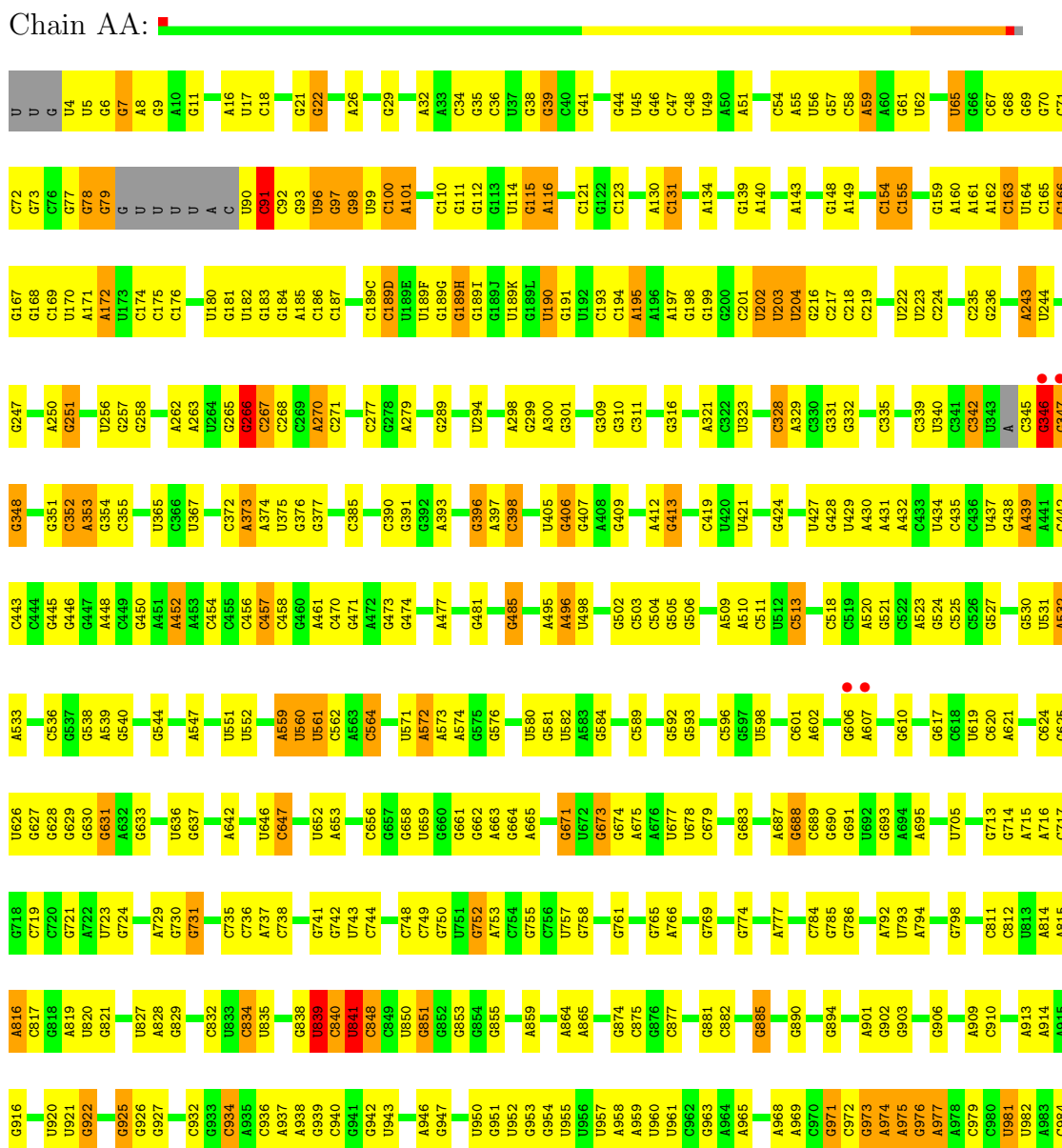
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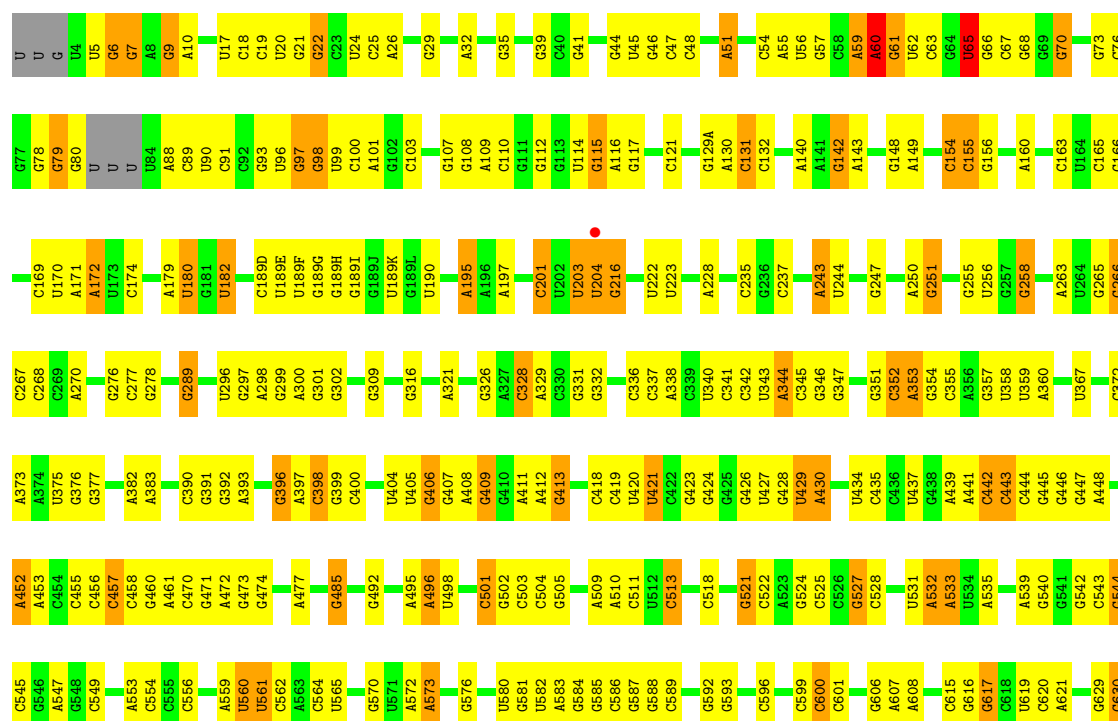
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 61 | DT | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | DU | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DW | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | DX | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | DY | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D0 | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | D1 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D3 | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | D5 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D6 | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | D8 | 3 | Total 3 | O 3 | 0 | 0 |

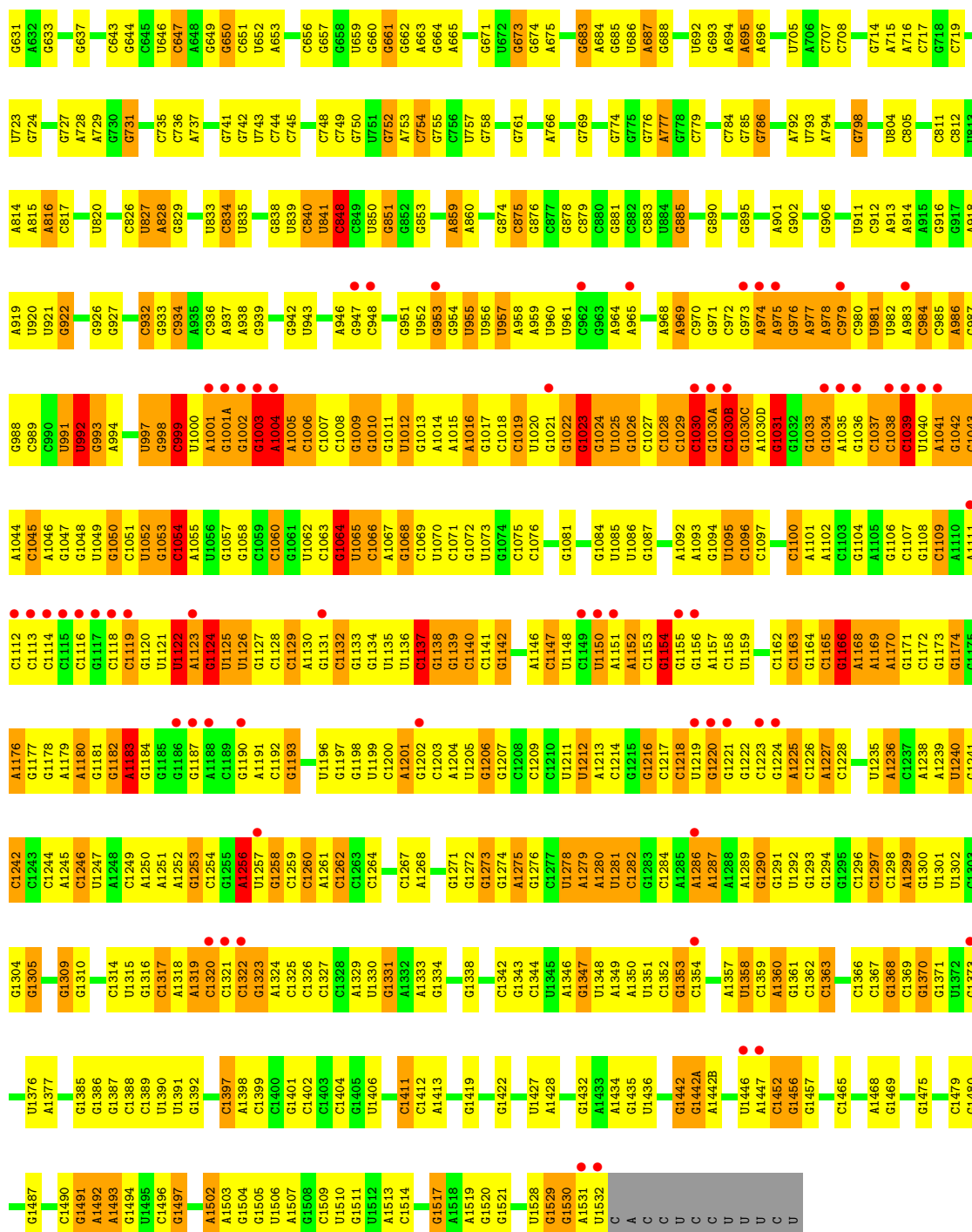
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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

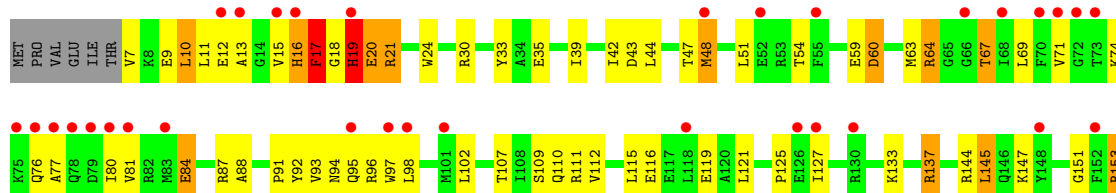


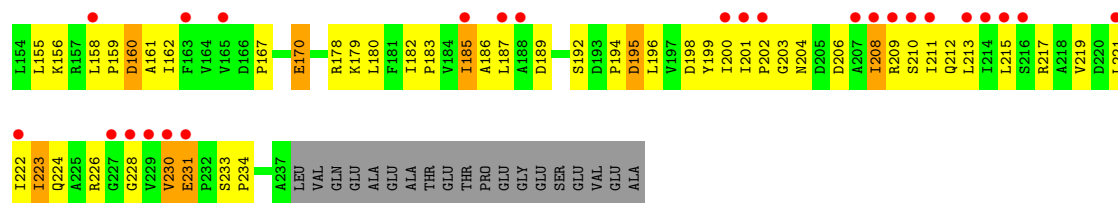




• Molecule 2: 30S ribosomal protein S2

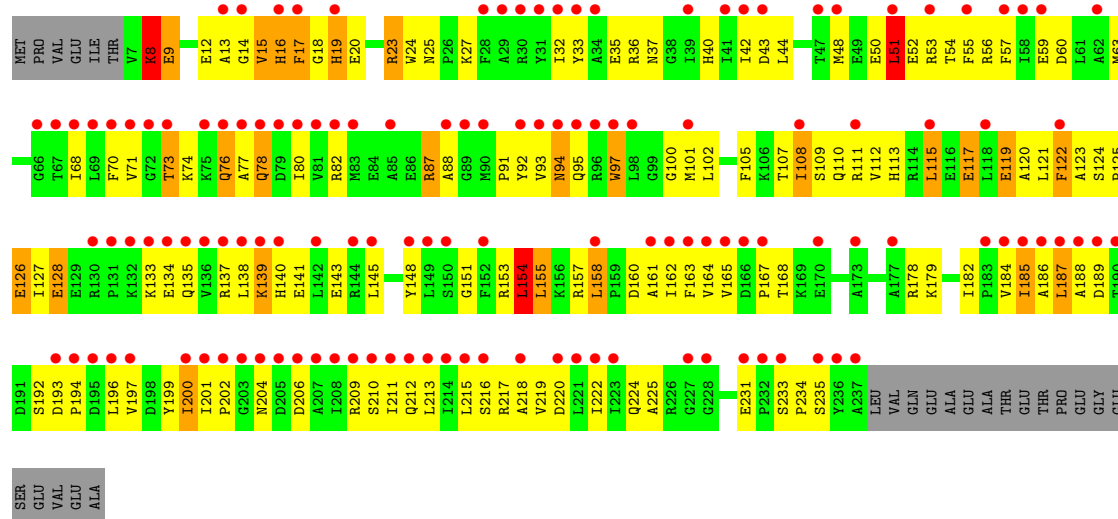
Chain AB:





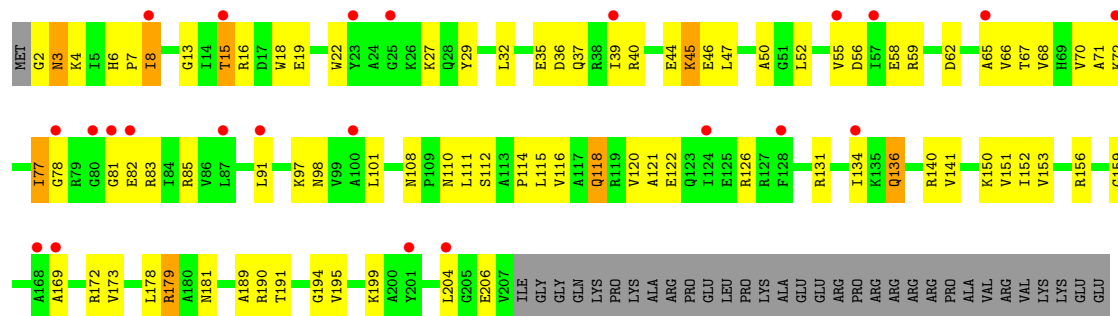
• Molecule 2: 30S ribosomal protein S2

Chain CB:



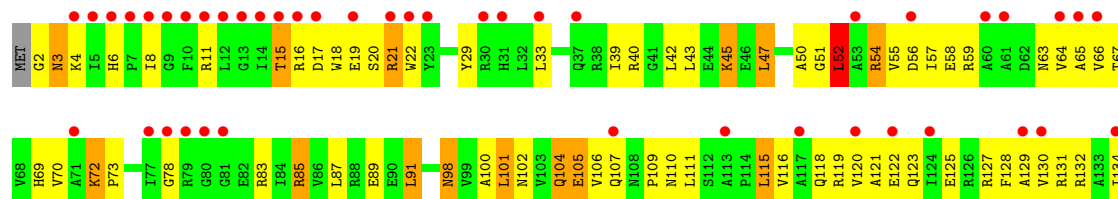
• Molecule 3: 30S ribosomal protein S3

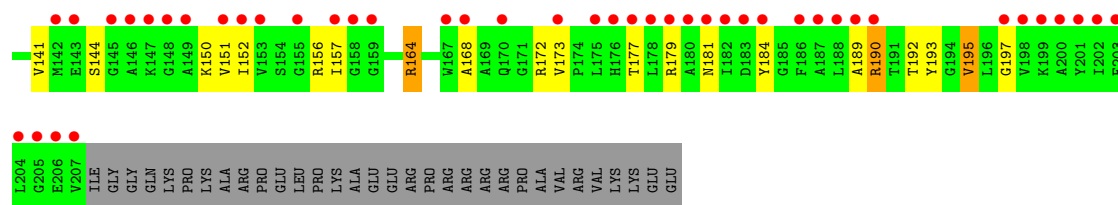
Chain AC:



• Molecule 3: 30S ribosomal protein S3

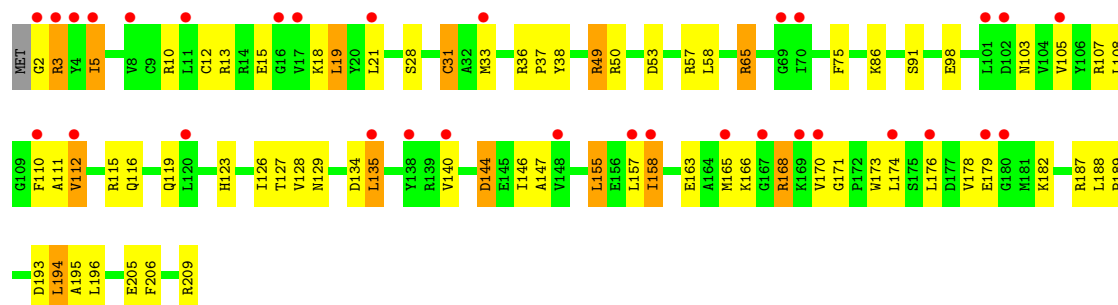
Chain CC:





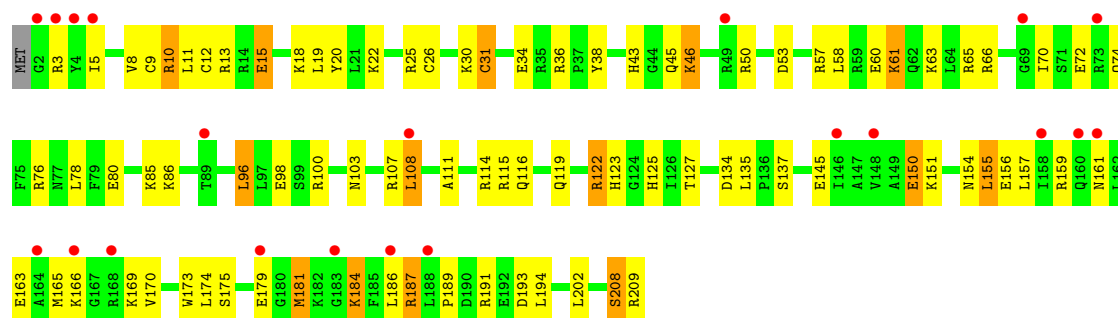
• Molecule 4: 30S ribosomal protein S4

Chain AD:



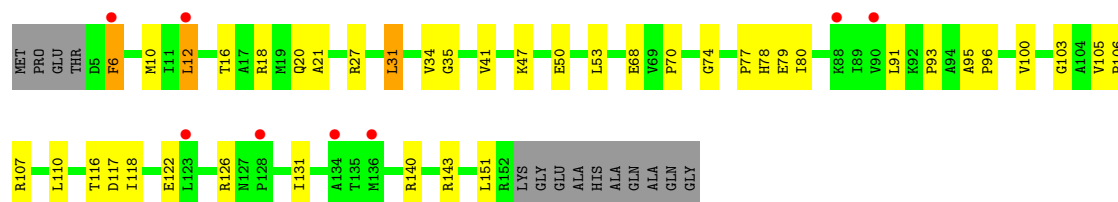
• Molecule 4: 30S ribosomal protein S4

Chain CD:



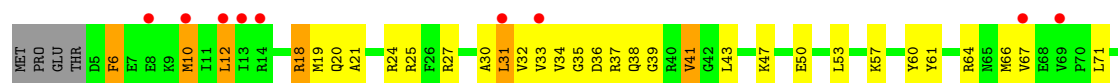
• Molecule 5: 30S ribosomal protein S5

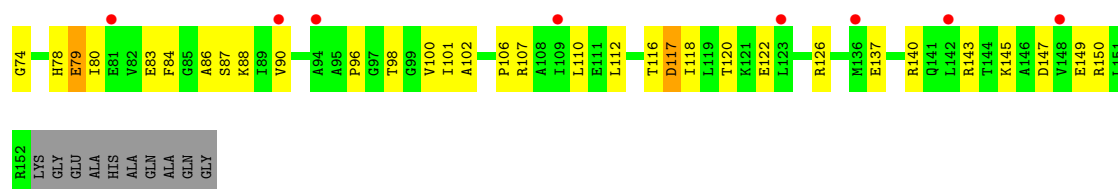
Chain AE:



• Molecule 5: 30S ribosomal protein S5

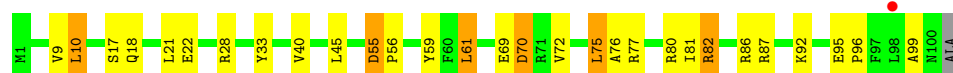
Chain CE:





- Molecule 6: 30S ribosomal protein S6

Chain AF:



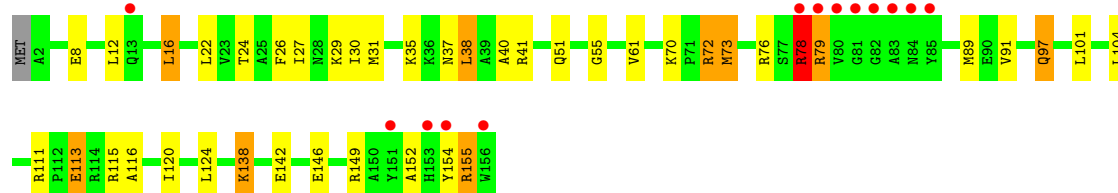
- Molecule 6: 30S ribosomal protein S6

Chain CF:



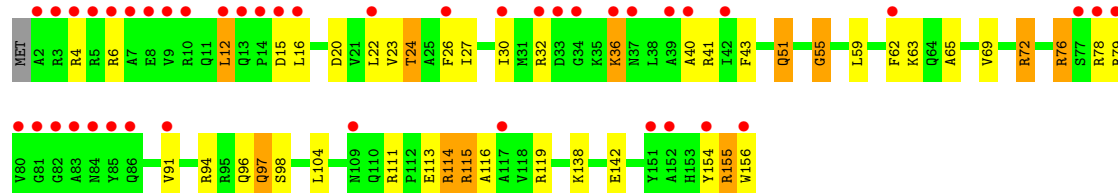
- Molecule 7: 30S ribosomal protein S7

Chain AG:



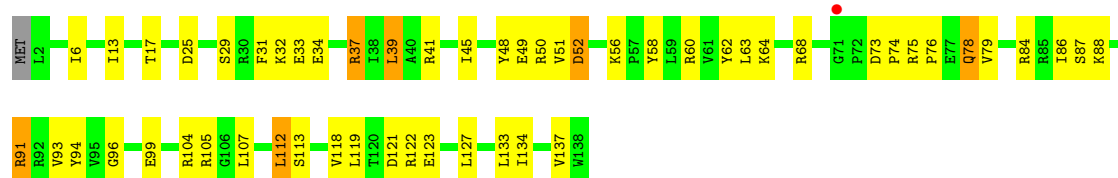
- Molecule 7: 30S ribosomal protein S7

Chain CG:



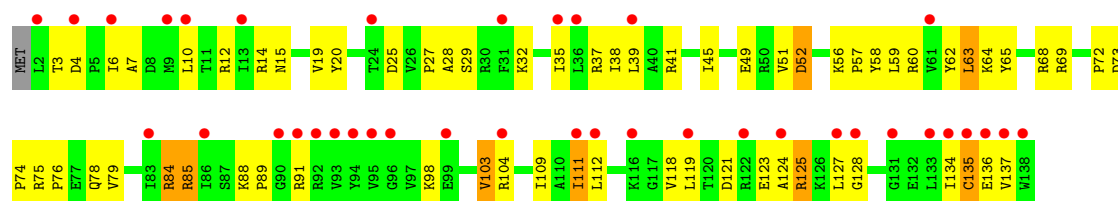
- Molecule 8: 30S ribosomal protein S8

Chain AH:



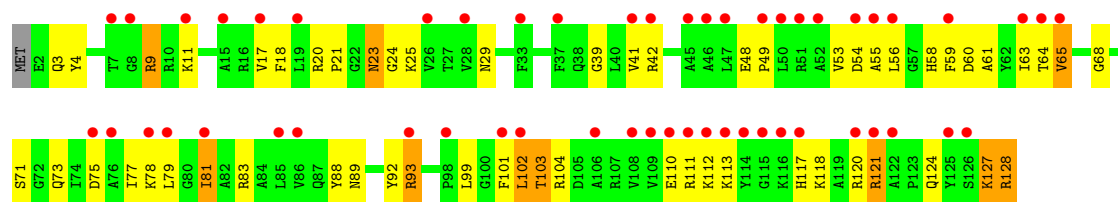
- Molecule 8: 30S ribosomal protein S8

Chain CH:



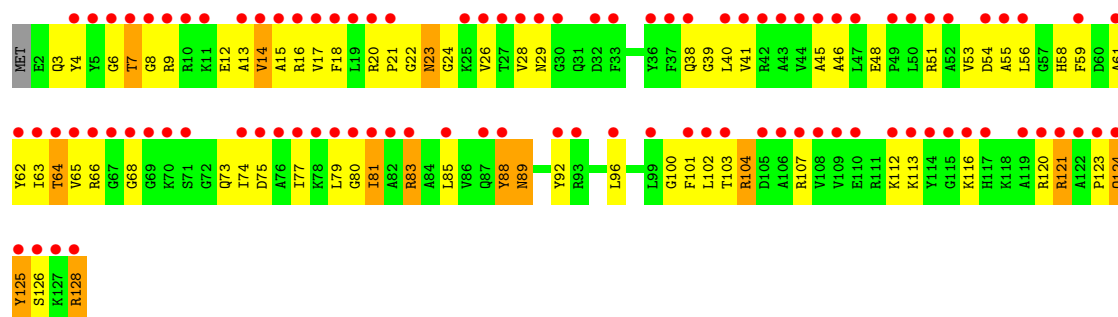
- Molecule 9: 30S ribosomal protein S9

Chain AI:



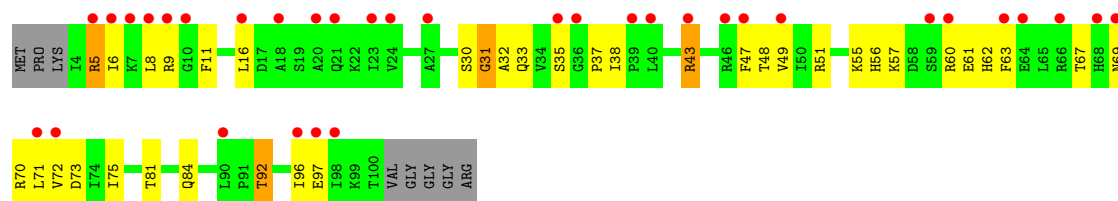
- Molecule 9: 30S ribosomal protein S9

Chain CI:



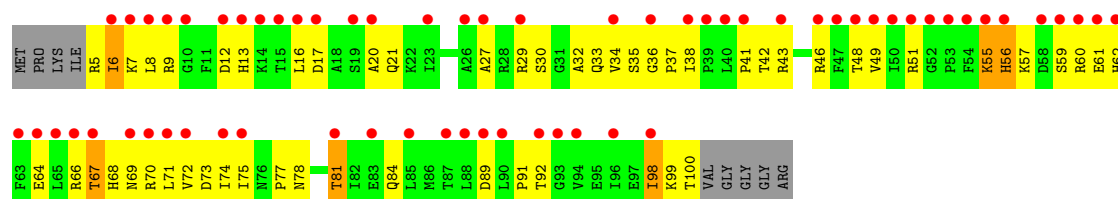
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



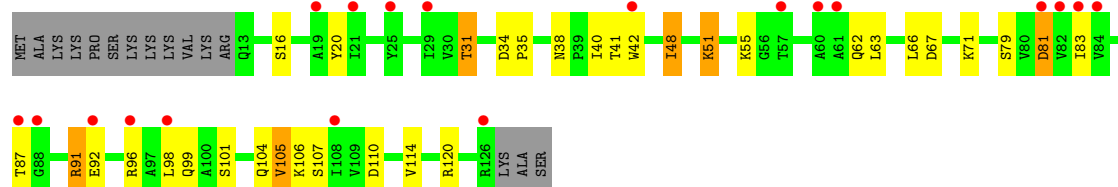
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



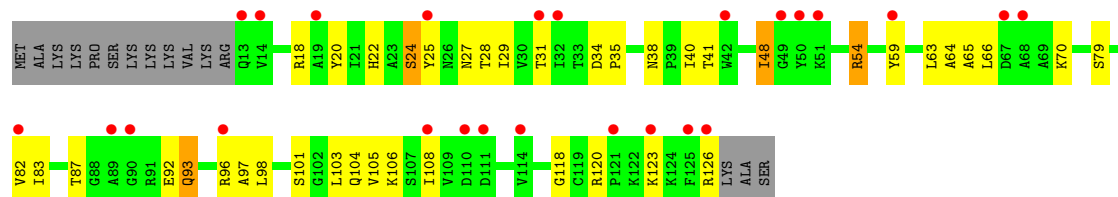
- Molecule 11: 30S ribosomal protein S11

Chain AK:



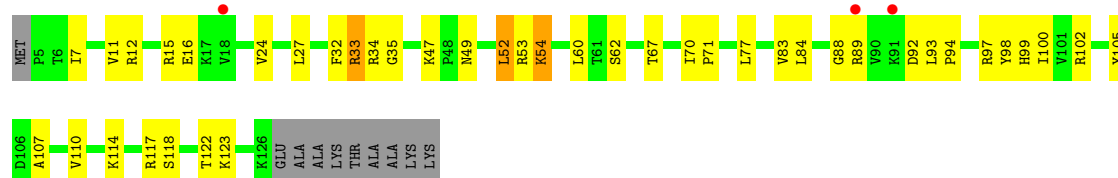
- Molecule 11: 30S ribosomal protein S11

Chain CK:



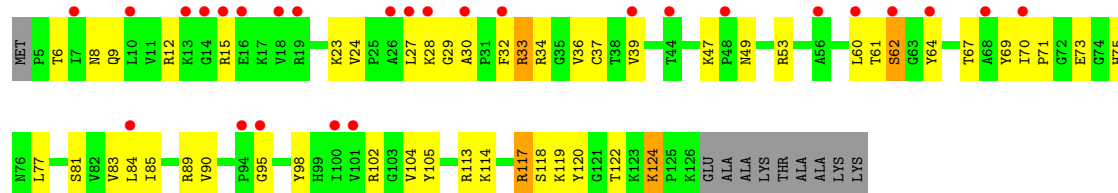
- Molecule 12: 30S ribosomal protein S12

Chain AL:



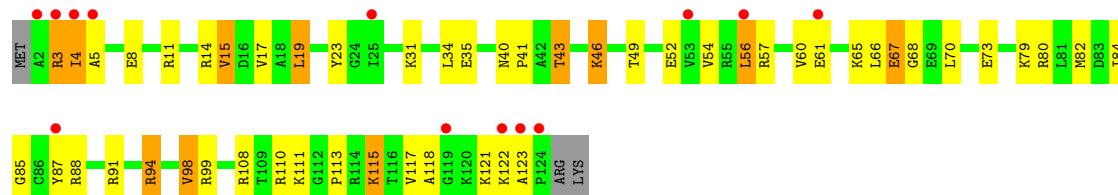
- Molecule 12: 30S ribosomal protein S12

Chain CL:



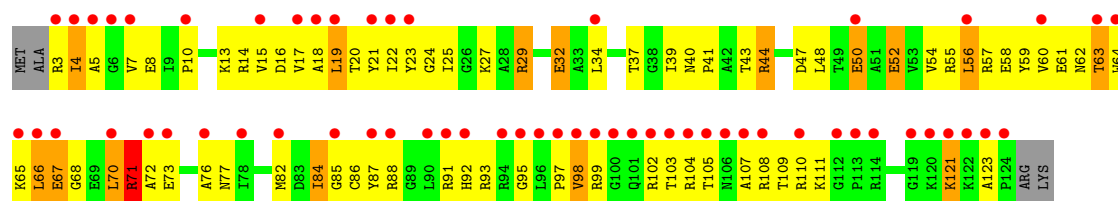
- Molecule 13: 30S ribosomal protein S13

Chain AM:



- Molecule 13: 30S ribosomal protein S13

Chain CM:



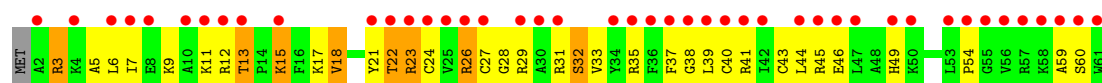
- Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



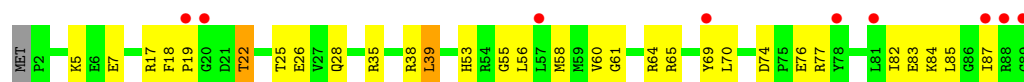
- Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



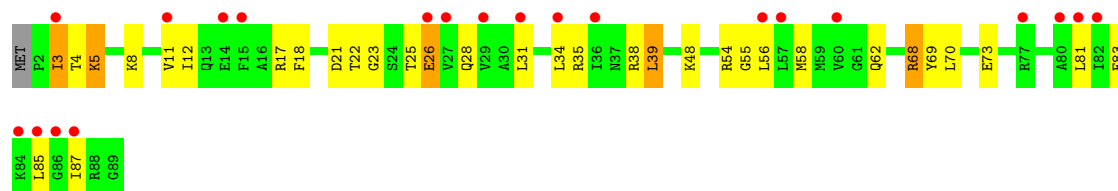
- Molecule 15: 30S ribosomal protein S15

Chain AO:



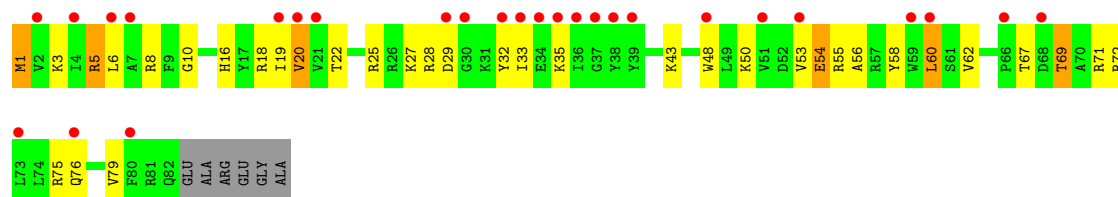
- Molecule 15: 30S ribosomal protein S15

Chain CO:



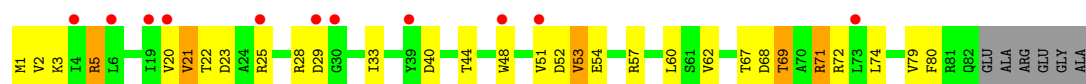
- Molecule 16: 30S ribosomal protein S16

Chain AP:



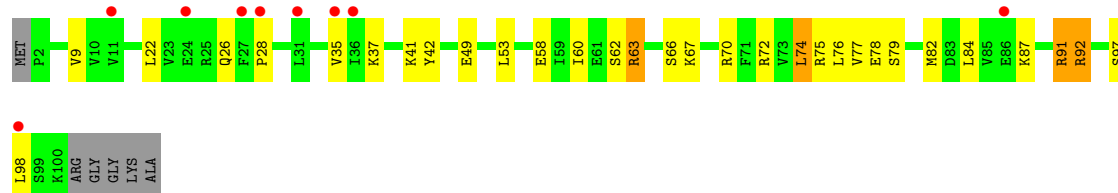
- Molecule 16: 30S ribosomal protein S16

Chain CP:



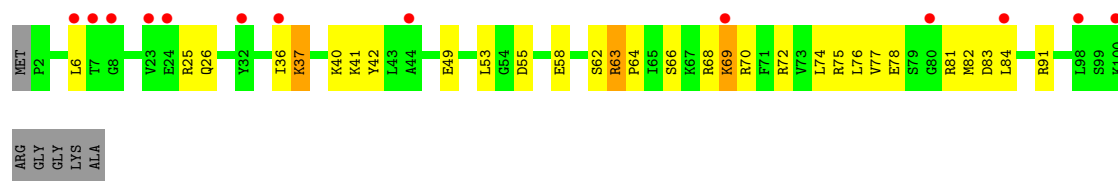
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



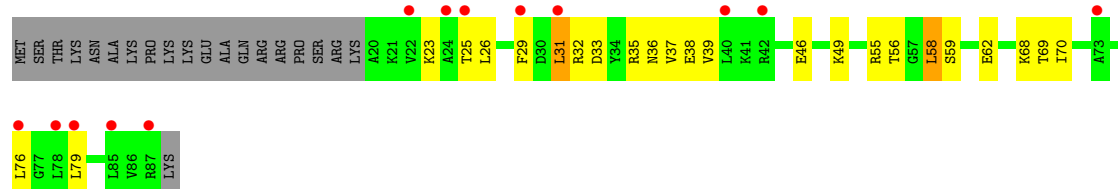
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



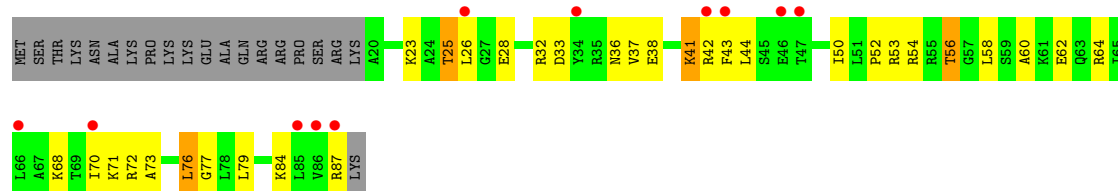
- Molecule 18: 30S ribosomal protein S18

Chain AR:



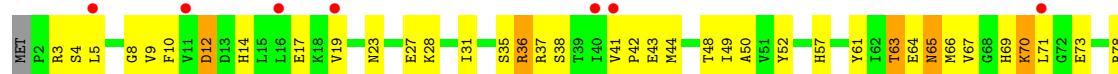
- Molecule 18: 30S ribosomal protein S18

Chain CR:



- Molecule 19: 30S ribosomal protein S19

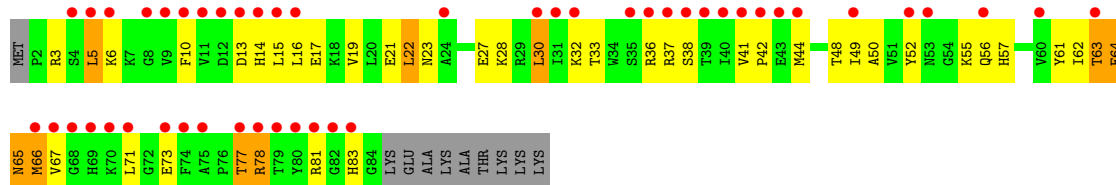
Chain AS:





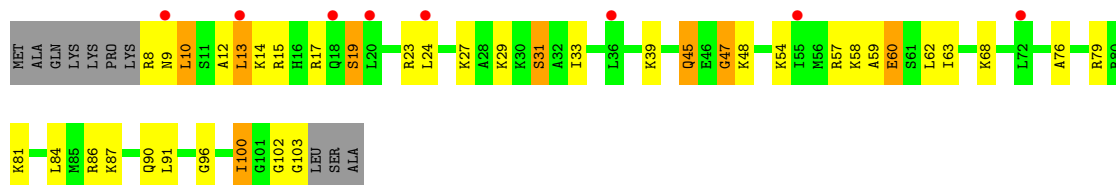
- Molecule 19: 30S ribosomal protein S19

Chain CS:



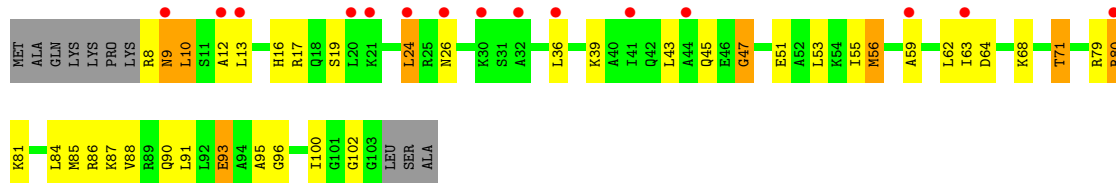
- Molecule 20: 30S ribosomal protein S20

Chain AT:



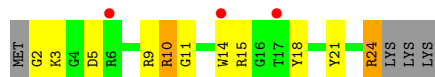
- Molecule 20: 30S ribosomal protein S20

Chain CT:



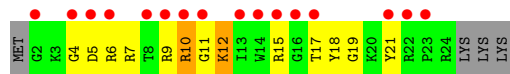
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



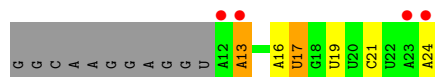
- Molecule 21: 30S ribosomal protein Thx

Chain CU:

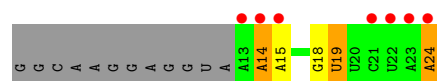


- Molecule 22: mRNA

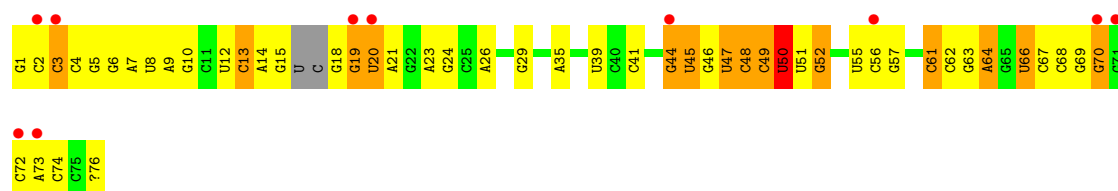
Chain AV:



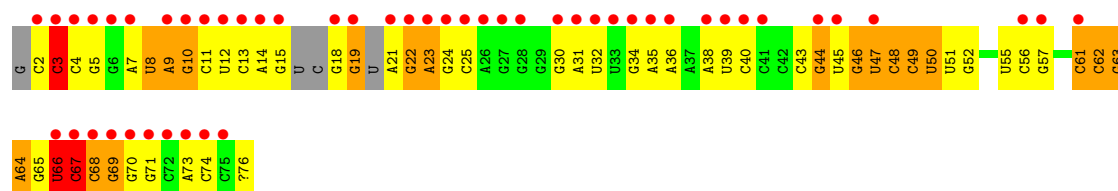
- Molecule 22: mRNA

Chain CV: 

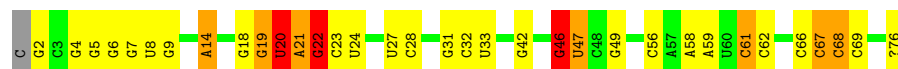
- Molecule 23: A-site tRNA

Chain AW: 

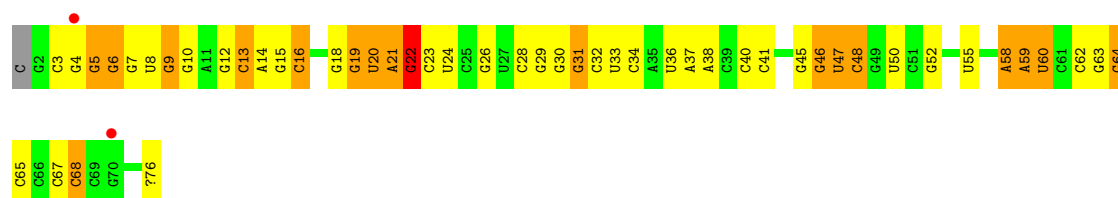
- Molecule 23: A-site tRNA

Chain CW: 

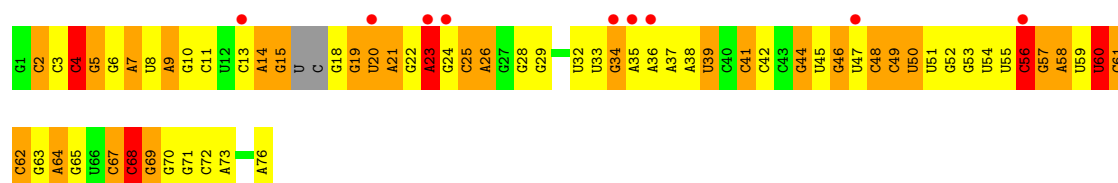
- Molecule 24: P-site tRNA

Chain AX: 

- Molecule 24: P-site tRNA

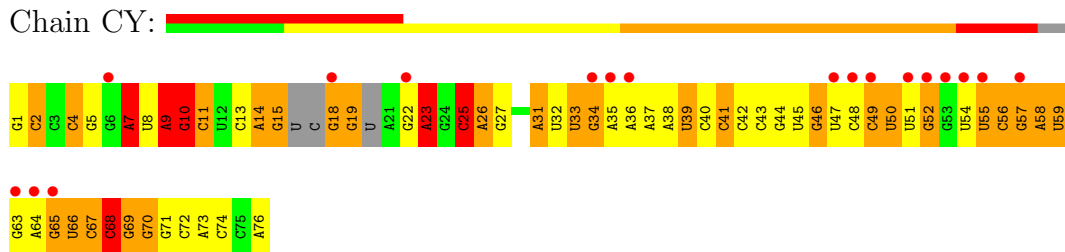
Chain CX: 

- Molecule 25: E-site tRNA

Chain AY: 

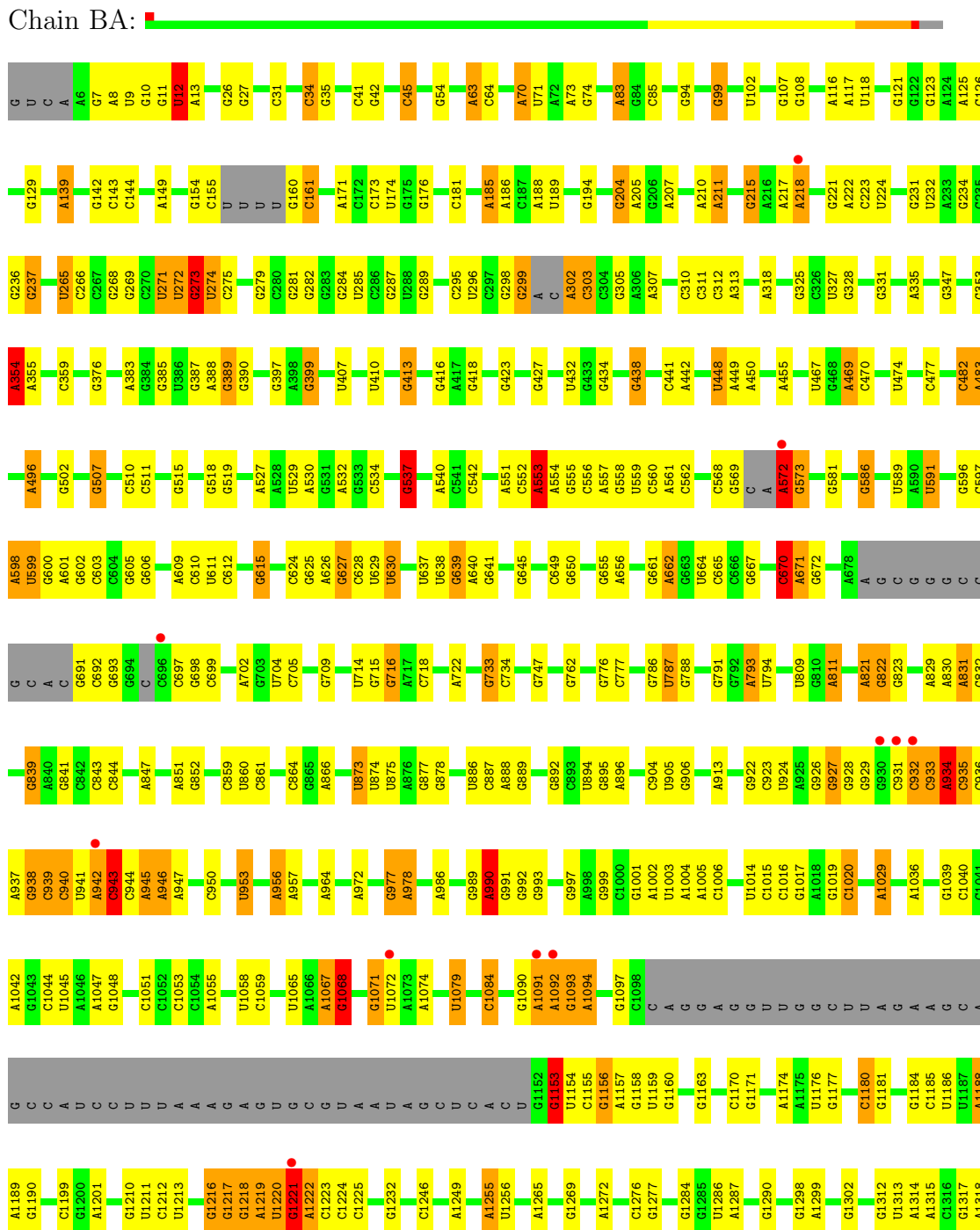
- Molecule 25: E-site tRNA

Chain CY:



- Molecule 26: 23S Ribosomal RNA

Chain BA:





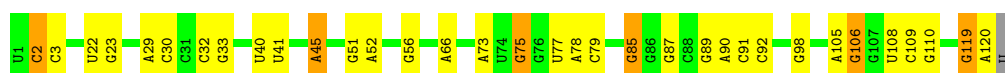


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| A2602 | C2494 | G2334 | A2170 | G1192 | A1566 | G1487 | U1288 |
| G2603 | A2425 | A2335 | A2171 | C1793 | A1567 | G1488 | |
| U2604 | G2429 | A2336 | A2172 | C1794 | G1568 | U1397 | U1396 |
| U2605 | A2430 | | A2173 | C1795 | A1668 | U1405 | C1291 |
| G2606 | U2431 | C2343 | C2174 | C1796 | A1669 | U1406 | U1292 |
| | | U2344 | C2175 | C1797 | A1674 | C1407 | C1293 |
| U2609 | A2434 | C2347 | A2176 | C1798 | | C1408 | G1297 |
| G2610 | A2435 | U2348 | C2177 | C1799 | A1576 | G1409 | G1298 |
| U2611 | A2436 | C2349 | C2178 | C1800 | U1497 | G1410 | G1299 |
| G2612 | A2439 | C2350 | C2179 | C1801 | A1579 | C1411 | A1300 |
| | U2440 | G2351 | U2180 | A1802 | A1580 | A1412 | U1301 |
| C2617 | C2441 | | G2181 | C1803 | G1581 | G1413 | A1302 |
| G2618 | | G2354 | C2182 | C1804 | A1507 | | G1303 |
| | G2445 | C2355 | C2183 | U1805 | A1508 | G1416 | |
| G2625 | G2446 | C2356 | G2184 | A1812 | C1417 | G1417 | A1308 |
| G2626 | G2447 | A2287 | C2185 | C1813 | A1584 | G1418 | G1309 |
| | A2448 | G2288 | A2186 | G1813 | A1586 | A1419 | G1310 |
| | U2449 | G2289 | G2187 | | A1587 | U1420 | |
| G2629 | U2450 | G2290 | C2188 | G1816 | G1588 | G1421 | U1313 |
| G2630 | A2450 | U2291 | C2189 | G1826 | A1509 | | C1314 |
| A2632 | G2455 | C2292 | U2190 | C1827 | A1509A | A1427 | C1315 |
| G2633 | G2456 | C2293 | G2191 | G1828 | A1509B | G1428 | U1316 |
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| | U2462 | G2295 | G2193 | C1830 | | C1430 | C1318 |
| | G2463 | U2296 | G2194 | | G1523 | U1431 | |
| A2639 | G2465 | C2297 | | G1740 | G1524 | | G1325 |
| | U2466 | A2298 | A2198 | A1741 | G1525 | A1434 | |
| G2645 | G2468 | G2299 | U2203 | U1833 | G1526 | A1435 | G1332 |
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| U2649 | | C2303 | G2207 | G1837 | A1528A | C1445A | U1341 |
| | | G2304 | A2208 | U1838 | G1529 | G1446 | |
| | | A2305 | U2218 | G1842 | C1530 | | U1352 |
| | | | U2219 | | C1531 | | |
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| A2654 | U2654 | G2307 | A2225 | A1844 | G1533 | G1450 | G1358 |
| | G2555 | C2308 | C2226 | | U | U1453 | A1359 |
| A2657 | G2556 | G2309 | C2227 | U1851 | A | | A1360 |
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| A2660 | | U2312 | G2230 | A1854 | G1622 | G1461 | A1366 |
| G2661 | U2562 | C2313 | U2232 | A1855 | G1628 | C1462 | A1367 |
| A2662 | A2566 | G2314 | U2233 | G1857 | U1629 | C1463 | G1368 |
| G2663 | G2567 | C2315 | G2238 | G1858 | A1637 | C1464 | G1369 |
| G2664 | C2568 | G2316 | G2239 | A1859 | C1638 | G1465 | C1370 |
| A2665 | G2569 | C2317 | C2240 | G1860 | A1545 | G1466 | G1371 |
| | | G2318 | | | C1546 | C1467 | U1372 |
| G2669 | C2573 | G2319 | U2243 | A1876 | C1547 | | |
| A2670 | | A2320 | U2244 | U1777 | | G1470 | A1378 |
| | | G2321 | | U1778 | C1560 | A1471 | A1379 |
| | | A2322 | C2248 | U1779 | | | G1380 |
| | G2578 | G2323 | G2252 | A1780 | G1645 | | |
| G2673 | G2674 | C2324 | U2253 | C1781 | G1646 | A1474 | |
| A2675 | A2675 | U2405 | G2253 | C1782 | G1647 | | |
| | | G2406 | G2253 | A1783 | A1554 | C1474 | |
| | C2586 | C2326 | | A1655 | G1555 | | A1384 |
| G2680 | U2590 | U2407 | C2261 | A1784 | C1556 | G1479 | G1385 |
| C2681 | G2505 | G2327 | U2102 | G1652 | C1557 | U1481 | C1386 |
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| | G2508 | | G2105 | C1790 | | | U1394 |
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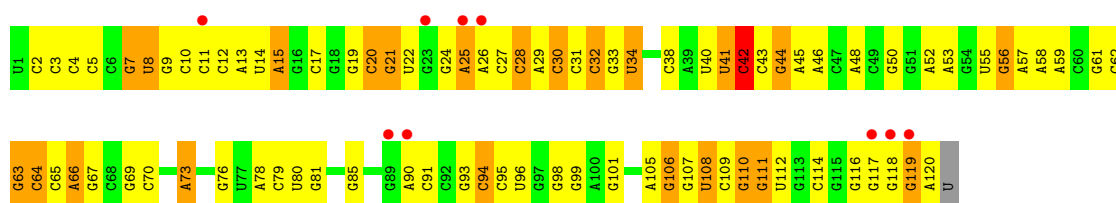
• Molecule 27: 5S Ribosomal RNA

Chain BB:



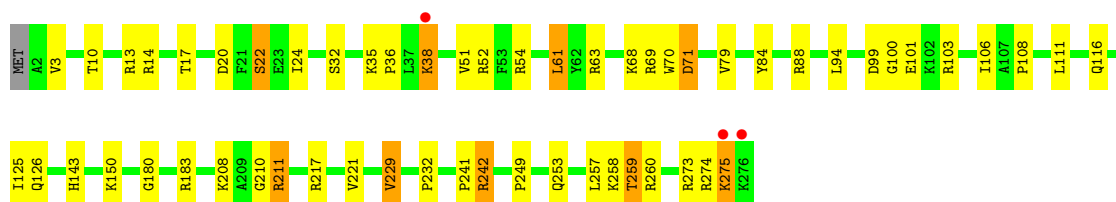
• Molecule 27: 5S Ribosomal RNA

Chain DB:



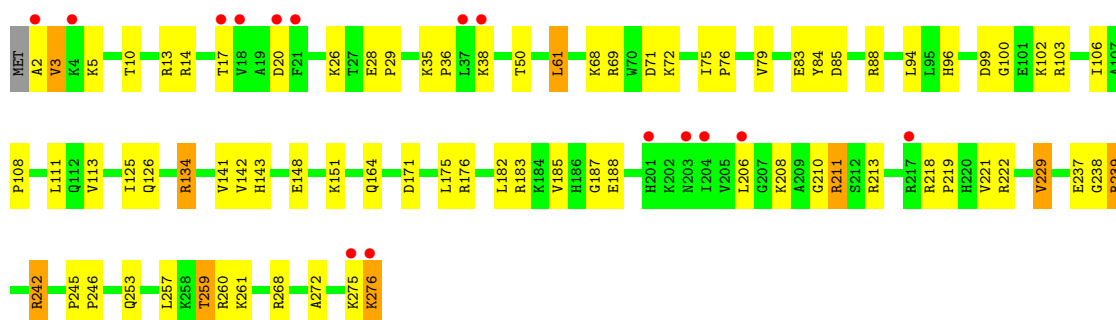
• Molecule 28: 50S ribosomal protein L2

Chain BD:



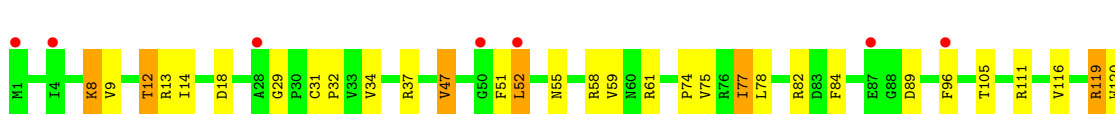
• Molecule 28: 50S ribosomal protein L2

Chain DD:



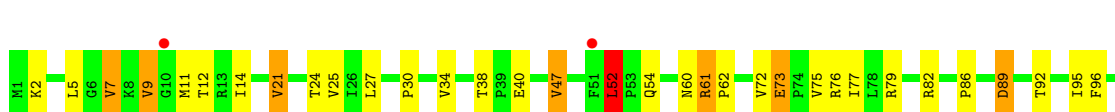
• Molecule 29: 50S ribosomal protein L3

Chain BE:



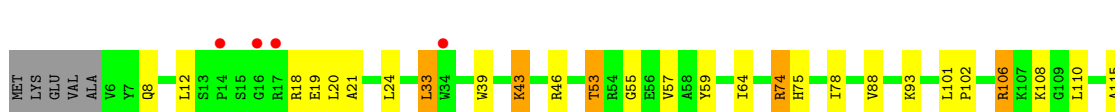
- Molecule 29: 50S ribosomal protein L3

Chain DE:



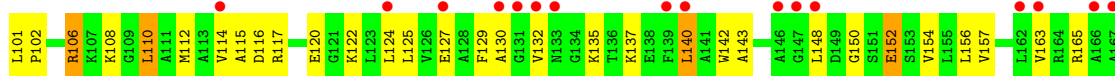
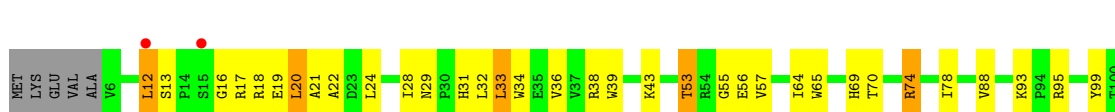
- Molecule 30: 50S ribosomal protein L4

Chain BF:



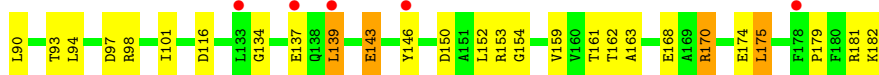
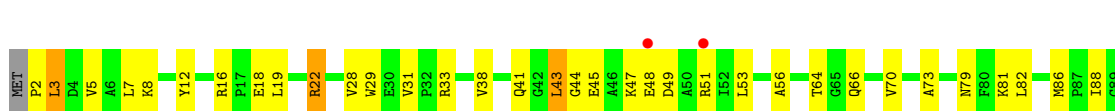
- Molecule 30: 50S ribosomal protein L4

Chain DF:



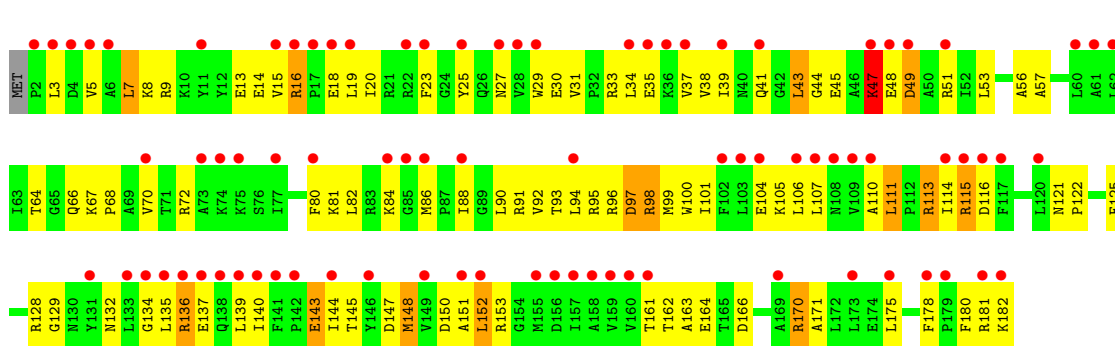
- Molecule 31: 50S ribosomal protein L5

Chain BG:



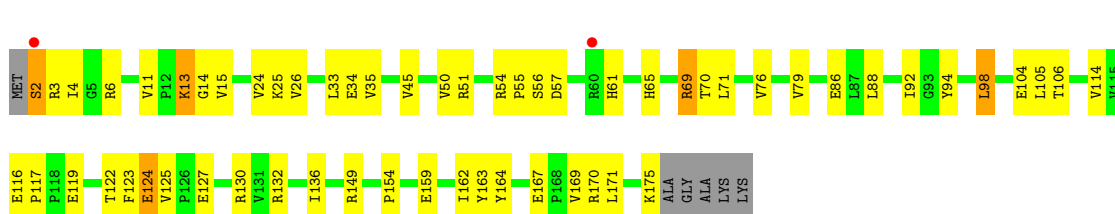
- Molecule 31: 50S ribosomal protein L5

Chain DG:



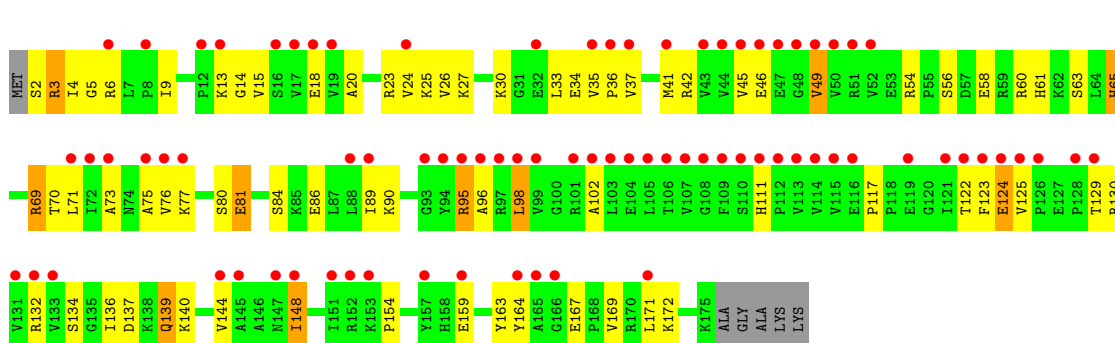
- Molecule 32: 50S ribosomal protein L6

Chain BH:



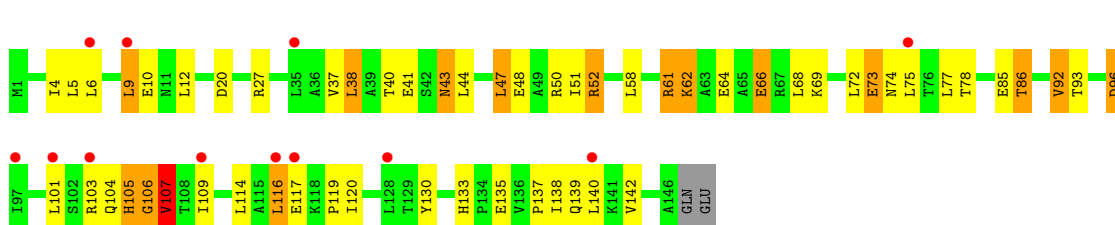
- Molecule 32: 50S ribosomal protein L6

Chain DH:



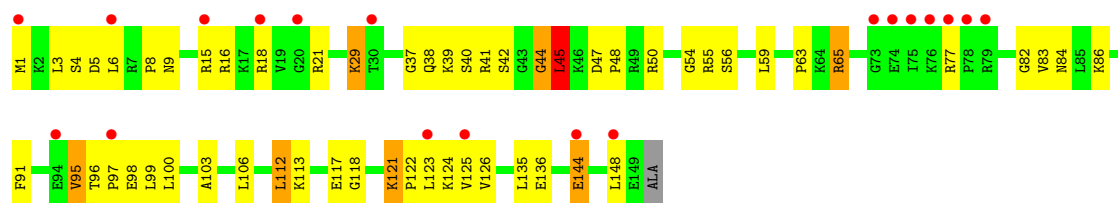
- Molecule 33: 50S ribosomal protein L9

Chain BI:



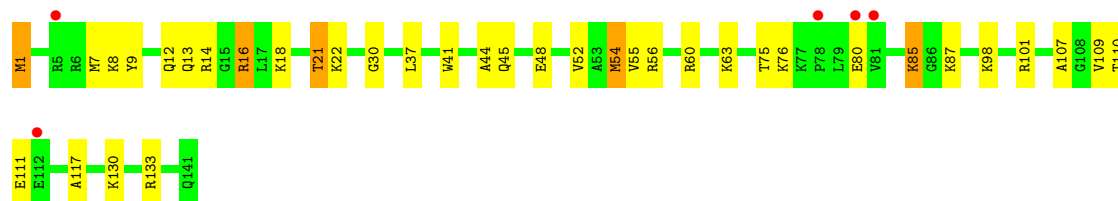
- Molecule 33: 50S ribosomal protein L9

Chain DI:



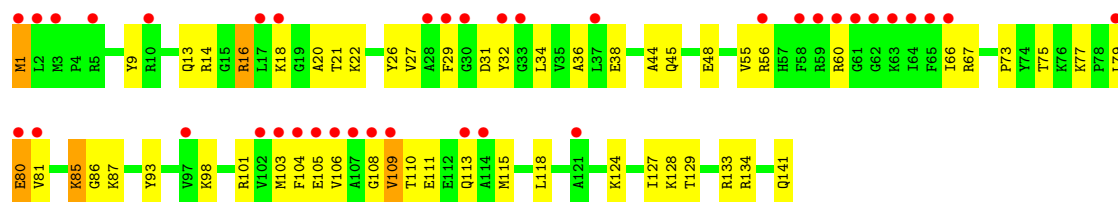
- Molecule 37: 50S ribosomal protein L16

Chain BQ:



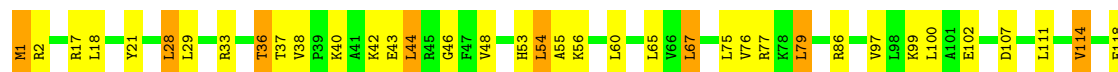
- Molecule 37: 50S ribosomal protein L16

Chain DQ:



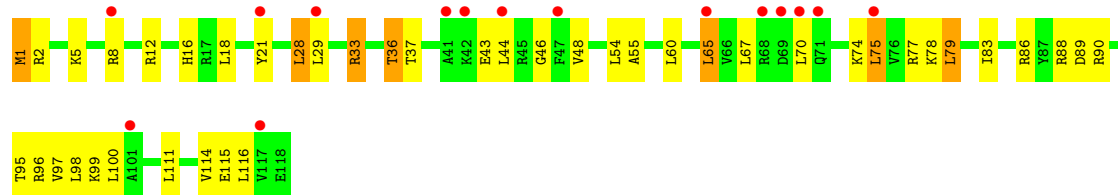
- Molecule 38: 50S ribosomal protein L17

Chain BR:



- Molecule 38: 50S ribosomal protein L17

Chain DR:



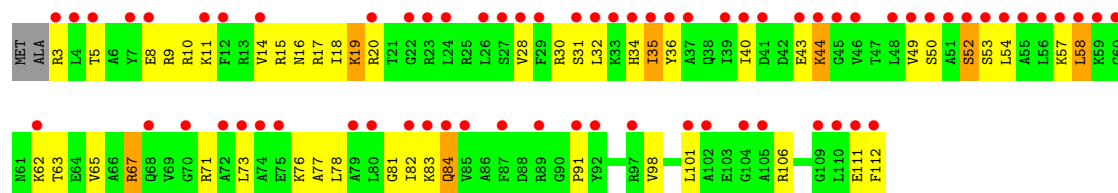
- Molecule 39: 50S ribosomal protein L18

Chain BS:



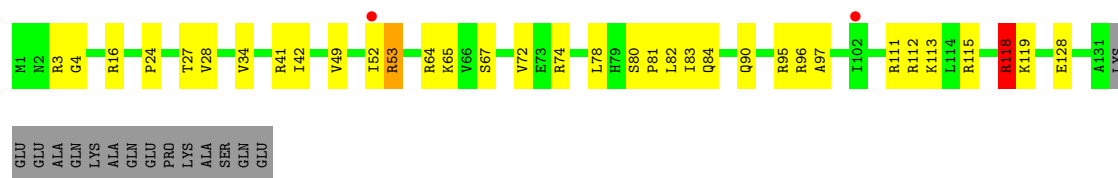
- Molecule 39: 50S ribosomal protein L18

Chain DS: 



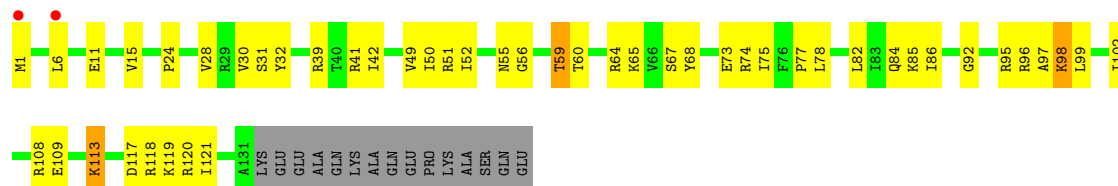
- Molecule 40: 50S ribosomal protein L19

Chain BT: 



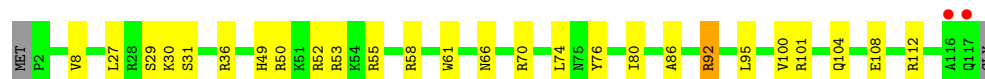
- Molecule 40: 50S ribosomal protein L19

Chain DT: 



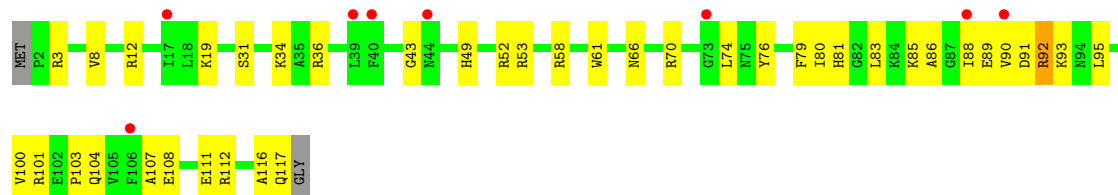
- Molecule 41: 50S ribosomal protein L20

Chain BU: 



- Molecule 41: 50S ribosomal protein L20

Chain DU: 



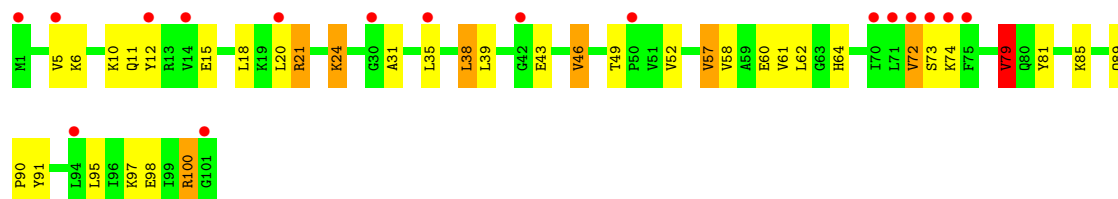
- Molecule 42: 50S ribosomal protein L21

Chain BV: 



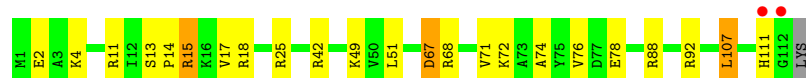
- Molecule 42: 50S ribosomal protein L21

Chain DV: 



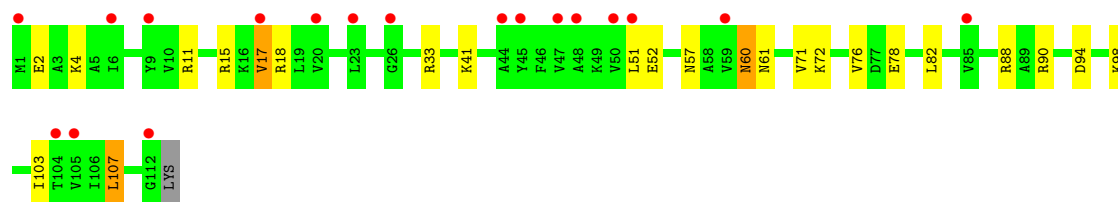
- Molecule 43: 50S ribosomal protein L22

Chain BW: 



- Molecule 43: 50S ribosomal protein L22

Chain DW: 



- Molecule 44: 50S ribosomal protein L23

Chain BX: 



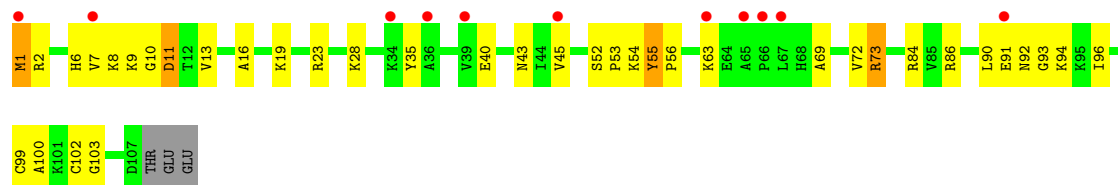
- Molecule 44: 50S ribosomal protein L23

Chain DX: 



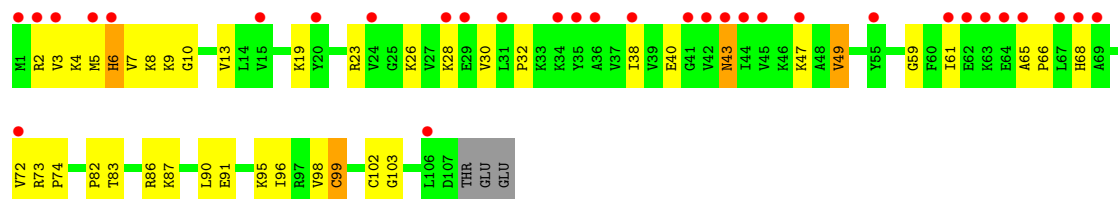
- Molecule 45: 50S ribosomal protein L24

Chain BY: 



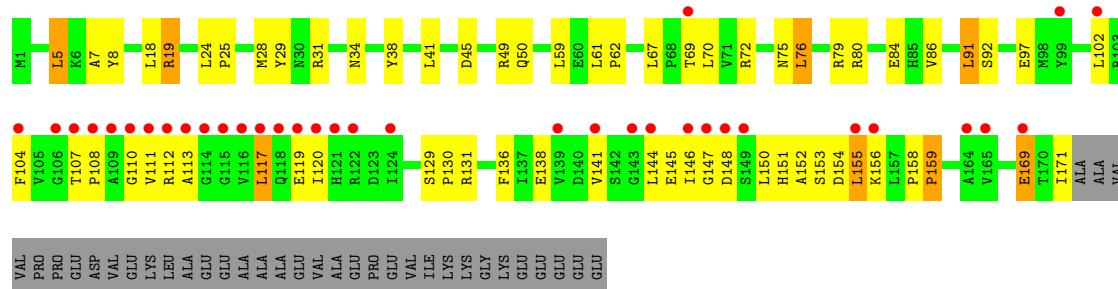
- Molecule 45: 50S ribosomal protein L24

Chain DY: 



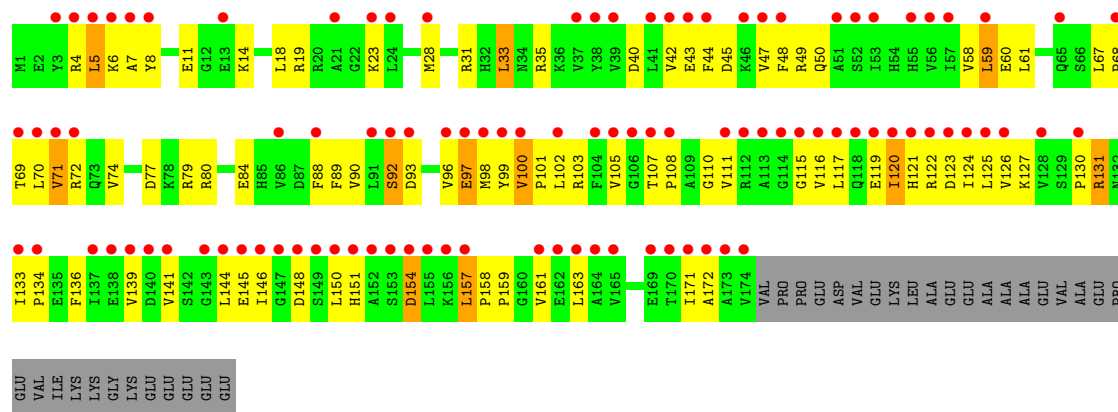
- Molecule 46: 50S ribosomal protein L25

Chain BZ: 



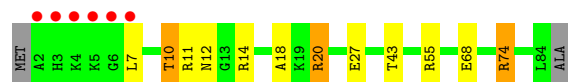
- Molecule 46: 50S ribosomal protein L25

Chain DZ: 



- Molecule 47: 50S ribosomal protein L27

Chain B0: 



- Molecule 47: 50S ribosomal protein L27

Chain D0: 





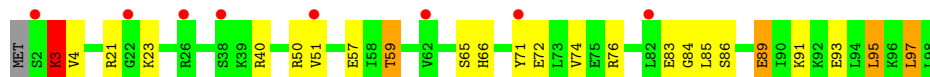
- Molecule 48: 50S ribosomal protein L28

Chain B1:



- Molecule 48: 50S ribosomal protein L28

Chain D1:



- Molecule 49: 50S ribosomal protein L29

Chain B2:



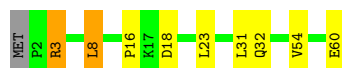
- Molecule 49: 50S ribosomal protein L29

Chain D2:



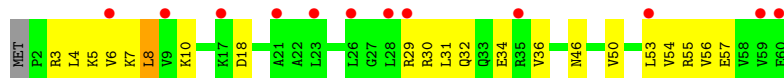
- Molecule 50: 50S ribosomal protein L30

Chain B3:



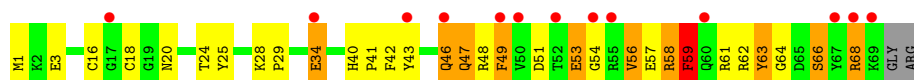
- Molecule 50: 50S ribosomal protein L30

Chain D3:



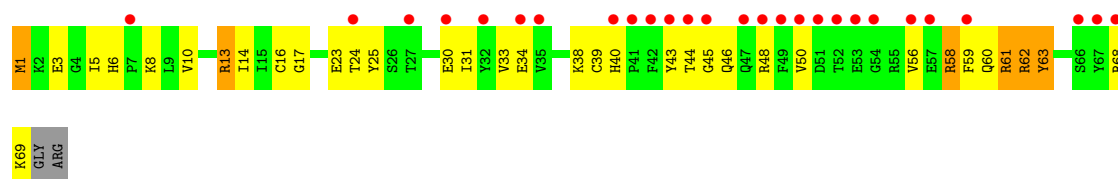
- Molecule 51: 50S ribosomal protein L31

Chain B4:



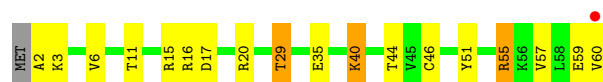
- Molecule 51: 50S ribosomal protein L31

Chain D4:



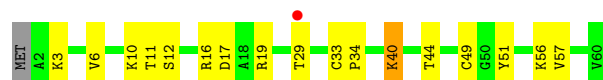
- Molecule 52: 50S ribosomal protein L32

Chain B5:



- Molecule 52: 50S ribosomal protein L32

Chain D5:



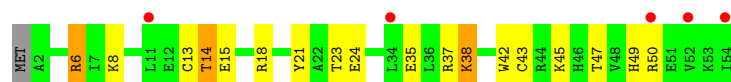
- Molecule 53: 50S ribosomal protein L33

Chain B6:



- Molecule 53: 50S ribosomal protein L33

Chain D6:



- Molecule 54: 50S ribosomal protein L34

Chain B7:



- Molecule 54: 50S ribosomal protein L34

Chain D7:



- Molecule 55: 50S ribosomal protein L35

Chain B8:



- Molecule 55: 50S ribosomal protein L35

Chain D8: 



- Molecule 56: 50S ribosomal protein L36

Chain B9: 



- Molecule 56: 50S ribosomal protein L36

Chain D9: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.45Å 448.85Å 619.02Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 151.90 – 2.60 224.43 – 2.60 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (151.90-2.60) 99.9 (224.43-2.60) | Depositor EDS |
| R_{merge} | 0.23 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.22 (at 2.62Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.2_1309) | Depositor |
| R, R_{free} | 0.223 , 0.264 0.248 , 0.289 | Depositor DCC |
| R_{free} test set | 43531 reflections (2.47%) | DCC |
| Wilson B-factor (Å ²) | 56.4 | Xtriage |
| Anisotropy | 0.077 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 38.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$ | Xtriage |
| Outliers | 0 of 1760092 reflections | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 297127 | wwPDB-VP |
| Average B, all atoms (Å ²) | 60.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | AA | 0.38 | 0/36027 | 0.91 | 43/56227 (0.1%) |
| 1 | CA | 0.41 | 8/36170 (0.0%) | 1.01 | 101/56452 (0.2%) |
| 2 | AB | 0.30 | 0/1881 | 0.62 | 0/2542 |
| 2 | CB | 0.33 | 0/1860 | 0.67 | 2/2518 (0.1%) |
| 3 | AC | 0.27 | 0/1576 | 0.52 | 0/2130 |
| 3 | CC | 0.31 | 0/1568 | 0.61 | 1/2122 (0.0%) |
| 4 | AD | 0.29 | 0/1689 | 0.55 | 0/2267 |
| 4 | CD | 0.30 | 0/1708 | 0.55 | 0/2289 |
| 5 | AE | 0.30 | 0/1145 | 0.54 | 0/1543 |
| 5 | CE | 0.33 | 0/1149 | 0.61 | 0/1548 |
| 6 | AF | 0.30 | 0/825 | 0.52 | 0/1118 |
| 6 | CF | 0.32 | 0/833 | 0.55 | 0/1128 |
| 7 | AG | 0.28 | 0/1250 | 0.50 | 0/1679 |
| 7 | CG | 0.27 | 0/1254 | 0.53 | 0/1683 |
| 8 | AH | 0.28 | 0/1108 | 0.52 | 0/1494 |
| 8 | CH | 0.29 | 0/1108 | 0.54 | 0/1494 |
| 9 | AI | 0.29 | 0/1005 | 0.57 | 0/1350 |
| 9 | CI | 0.31 | 0/997 | 0.64 | 0/1343 |
| 10 | AJ | 0.27 | 0/722 | 0.54 | 0/982 |
| 10 | CJ | 0.33 | 0/727 | 0.62 | 0/988 |
| 11 | AK | 0.28 | 0/848 | 0.51 | 0/1149 |
| 11 | CK | 0.28 | 0/848 | 0.53 | 0/1149 |
| 12 | AL | 0.33 | 0/946 | 0.52 | 0/1274 |
| 12 | CL | 0.30 | 0/946 | 0.58 | 0/1274 |
| 13 | AM | 0.31 | 0/977 | 0.60 | 0/1310 |
| 13 | CM | 0.31 | 0/961 | 0.62 | 1/1291 (0.1%) |
| 14 | AN | 0.32 | 0/501 | 0.53 | 0/664 |
| 14 | CN | 0.33 | 0/501 | 0.57 | 0/664 |
| 15 | AO | 0.28 | 0/739 | 0.52 | 0/985 |
| 15 | CO | 0.29 | 0/739 | 0.54 | 0/985 |
| 16 | AP | 0.31 | 0/697 | 0.54 | 0/939 |
| 16 | CP | 0.29 | 0/693 | 0.51 | 0/935 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AQ | 0.29 | 0/836 | 0.53 | 0/1117 |
| 17 | CQ | 0.29 | 0/836 | 0.50 | 0/1117 |
| 18 | AR | 0.27 | 0/560 | 0.54 | 0/746 |
| 18 | CR | 0.29 | 0/560 | 0.56 | 0/746 |
| 19 | AS | 0.30 | 0/676 | 0.58 | 0/911 |
| 19 | CS | 0.33 | 0/661 | 0.71 | 0/893 |
| 20 | AT | 0.29 | 0/730 | 0.57 | 0/965 |
| 20 | CT | 0.28 | 0/733 | 0.55 | 0/969 |
| 21 | AU | 0.27 | 0/203 | 0.50 | 0/266 |
| 21 | CU | 0.33 | 0/203 | 0.53 | 0/266 |
| 22 | AV | 0.39 | 0/310 | 0.96 | 1/480 (0.2%) |
| 22 | CV | 0.42 | 0/282 | 0.99 | 2/437 (0.5%) |
| 23 | AW | 0.47 | 0/1577 | 1.20 | 7/2454 (0.3%) |
| 23 | CW | 0.53 | 0/1531 | 1.28 | 9/2379 (0.4%) |
| 24 | AX | 0.53 | 2/1700 (0.1%) | 1.20 | 22/2650 (0.8%) |
| 24 | CX | 0.46 | 0/1700 | 1.15 | 6/2650 (0.2%) |
| 25 | AY | 0.58 | 0/1602 | 1.35 | 20/2493 (0.8%) |
| 25 | CY | 0.59 | 0/1579 | 1.40 | 25/2455 (1.0%) |
| 26 | BA | 0.50 | 1/68013 (0.0%) | 0.93 | 91/106165 (0.1%) |
| 26 | DA | 0.41 | 1/67542 (0.0%) | 0.92 | 74/105428 (0.1%) |
| 27 | BB | 0.41 | 0/2878 | 0.86 | 1/4490 (0.0%) |
| 27 | DB | 0.44 | 0/2878 | 0.92 | 2/4490 (0.0%) |
| 28 | BD | 0.37 | 0/2186 | 0.59 | 0/2944 |
| 28 | DD | 0.33 | 0/2192 | 0.57 | 0/2951 |
| 29 | BE | 0.37 | 0/1592 | 0.57 | 0/2149 |
| 29 | DE | 0.33 | 0/1592 | 0.55 | 0/2149 |
| 30 | BF | 0.34 | 0/1619 | 0.55 | 0/2193 |
| 30 | DF | 0.32 | 0/1615 | 0.55 | 0/2188 |
| 31 | BG | 0.31 | 0/1450 | 0.54 | 1/1959 (0.1%) |
| 31 | DG | 0.33 | 0/1449 | 0.60 | 0/1958 |
| 32 | BH | 0.33 | 0/1356 | 0.54 | 0/1834 |
| 32 | DH | 0.29 | 0/1356 | 0.54 | 0/1834 |
| 33 | BI | 0.28 | 0/1100 | 0.56 | 0/1501 |
| 33 | DI | 0.29 | 0/1088 | 0.55 | 0/1484 |
| 34 | BN | 0.34 | 0/1144 | 0.53 | 0/1543 |
| 34 | DN | 0.31 | 0/1144 | 0.52 | 0/1543 |
| 35 | BO | 0.37 | 0/943 | 0.57 | 0/1269 |
| 35 | DO | 0.31 | 0/943 | 0.55 | 1/1269 (0.1%) |
| 36 | BP | 0.35 | 0/1156 | 0.57 | 0/1537 |
| 36 | DP | 0.32 | 0/1152 | 0.61 | 1/1533 (0.1%) |
| 37 | BQ | 0.35 | 0/1143 | 0.53 | 0/1527 |
| 37 | DQ | 0.32 | 0/1143 | 0.53 | 0/1527 |
| 38 | BR | 0.36 | 0/982 | 0.58 | 0/1312 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DR | 0.30 | 0/982 | 0.53 | 0/1312 |
| 39 | BS | 0.31 | 0/887 | 0.56 | 0/1180 |
| 39 | DS | 0.28 | 0/880 | 0.56 | 0/1172 |
| 40 | BT | 0.34 | 0/1105 | 0.56 | 1/1477 (0.1%) |
| 40 | DT | 0.31 | 0/1097 | 0.53 | 0/1468 |
| 41 | BU | 0.39 | 0/977 | 0.56 | 0/1301 |
| 41 | DU | 0.30 | 0/977 | 0.54 | 0/1301 |
| 42 | BV | 0.36 | 0/782 | 0.58 | 0/1049 |
| 42 | DV | 0.32 | 0/782 | 0.57 | 1/1049 (0.1%) |
| 43 | BW | 0.39 | 0/897 | 0.56 | 0/1205 |
| 43 | DW | 0.31 | 0/897 | 0.52 | 0/1205 |
| 44 | BX | 0.38 | 0/764 | 0.57 | 1/1025 (0.1%) |
| 44 | DX | 0.33 | 0/764 | 0.58 | 1/1025 (0.1%) |
| 45 | BY | 0.35 | 0/819 | 0.57 | 0/1095 |
| 45 | DY | 0.32 | 0/819 | 0.55 | 0/1095 |
| 46 | BZ | 0.32 | 0/1379 | 0.58 | 0/1873 |
| 46 | DZ | 0.30 | 0/1390 | 0.56 | 0/1890 |
| 47 | B0 | 0.35 | 0/662 | 0.55 | 0/881 |
| 47 | D0 | 0.32 | 0/662 | 0.53 | 0/881 |
| 48 | B1 | 0.35 | 0/762 | 0.54 | 0/1014 |
| 48 | D1 | 0.31 | 0/762 | 0.53 | 0/1014 |
| 49 | B2 | 0.31 | 0/590 | 0.53 | 0/781 |
| 49 | D2 | 0.28 | 0/590 | 0.46 | 0/781 |
| 50 | B3 | 0.34 | 0/474 | 0.57 | 0/635 |
| 50 | D3 | 0.27 | 0/469 | 0.55 | 0/630 |
| 51 | B4 | 0.31 | 0/571 | 0.70 | 0/768 |
| 51 | D4 | 0.32 | 0/545 | 0.67 | 0/737 |
| 52 | B5 | 0.35 | 0/469 | 0.65 | 0/635 |
| 52 | D5 | 0.31 | 0/469 | 0.50 | 0/635 |
| 53 | B6 | 0.37 | 0/460 | 0.52 | 0/613 |
| 53 | D6 | 0.29 | 0/456 | 0.49 | 0/608 |
| 54 | B7 | 0.40 | 0/426 | 0.57 | 0/561 |
| 54 | D7 | 0.33 | 0/426 | 0.54 | 0/561 |
| 55 | B8 | 0.37 | 0/525 | 0.59 | 0/691 |
| 55 | D8 | 0.32 | 0/525 | 0.51 | 0/691 |
| 56 | B9 | 0.37 | 0/310 | 0.50 | 0/407 |
| 56 | D9 | 0.33 | 0/310 | 0.52 | 0/407 |
| All | All | 0.41 | 12/316594 (0.0%) | 0.87 | 415/473940 (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 | 2 |
| 2 | CB | 0 | 1 |
| 7 | AG | 0 | 2 |
| 20 | CT | 0 | 1 |
| 33 | BI | 0 | 1 |
| 35 | BO | 0 | 1 |
| 39 | BS | 0 | 1 |
| 51 | B4 | 0 | 1 |
| All | All | 0 | 10 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | CA | 1154 | G | N1-C2 | -10.90 | 1.29 | 1.37 |
| 1 | CA | 1119 | C | N3-C4 | -10.71 | 1.26 | 1.33 |
| 1 | CA | 1154 | G | C6-N1 | -10.47 | 1.32 | 1.39 |
| 26 | DA | 528 | A | N9-C4 | -6.80 | 1.33 | 1.37 |
| 1 | CA | 1154 | G | N7-C5 | -6.78 | 1.35 | 1.39 |

The worst 5 of 415 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | CA | 1119 | C | N1-C2-O2 | 35.97 | 140.48 | 118.90 |
| 1 | CA | 1154 | G | C5-C6-O6 | 25.44 | 143.86 | 128.60 |
| 1 | CA | 1154 | G | N3-C2-N2 | 24.34 | 136.94 | 119.90 |
| 1 | CA | 1154 | G | N1-C2-N2 | -21.83 | 96.56 | 116.20 |
| 1 | CA | 1119 | C | N3-C2-O2 | -21.82 | 106.63 | 121.90 |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | AB | 231 | GLU | Peptide |
| 2 | AB | 9 | GLU | Peptide |
| 7 | AG | 78 | ARG | Peptide |
| 7 | AG | 79 | ARG | Peptide |
| 33 | BI | 9 | LEU | Peptide |

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32185 | 0 | 16245 | 536 | 0 |
| 1 | CA | 32312 | 0 | 16307 | 762 | 0 |
| 2 | AB | 1846 | 0 | 1867 | 81 | 0 |
| 2 | CB | 1825 | 0 | 1828 | 119 | 0 |
| 3 | AC | 1552 | 0 | 1546 | 60 | 0 |
| 3 | CC | 1544 | 0 | 1524 | 70 | 0 |
| 4 | AD | 1659 | 0 | 1676 | 56 | 0 |
| 4 | CD | 1678 | 0 | 1718 | 67 | 0 |
| 5 | AE | 1129 | 0 | 1185 | 27 | 0 |
| 5 | CE | 1133 | 0 | 1191 | 46 | 0 |
| 6 | AF | 812 | 0 | 804 | 18 | 0 |
| 6 | CF | 820 | 0 | 814 | 19 | 0 |
| 7 | AG | 1231 | 0 | 1238 | 21 | 0 |
| 7 | CG | 1235 | 0 | 1249 | 39 | 0 |
| 8 | AH | 1088 | 0 | 1126 | 35 | 0 |
| 8 | CH | 1088 | 0 | 1126 | 40 | 0 |
| 9 | AI | 986 | 0 | 995 | 43 | 0 |
| 9 | CI | 978 | 0 | 966 | 55 | 0 |
| 10 | AJ | 709 | 0 | 650 | 34 | 0 |
| 10 | CJ | 714 | 0 | 672 | 44 | 0 |
| 11 | AK | 833 | 0 | 836 | 19 | 0 |
| 11 | CK | 833 | 0 | 836 | 22 | 0 |
| 12 | AL | 930 | 0 | 980 | 27 | 0 |
| 12 | CL | 930 | 0 | 980 | 33 | 0 |
| 13 | AM | 966 | 0 | 1024 | 40 | 0 |
| 13 | CM | 950 | 0 | 988 | 74 | 0 |
| 14 | AN | 492 | 0 | 529 | 26 | 0 |
| 14 | CN | 492 | 0 | 529 | 34 | 0 |
| 15 | AO | 728 | 0 | 760 | 20 | 0 |
| 15 | CO | 728 | 0 | 760 | 22 | 0 |
| 16 | AP | 681 | 0 | 697 | 27 | 0 |
| 16 | CP | 677 | 0 | 686 | 22 | 0 |
| 17 | AQ | 823 | 0 | 891 | 26 | 0 |
| 17 | CQ | 823 | 0 | 891 | 19 | 0 |
| 18 | AR | 555 | 0 | 618 | 12 | 0 |
| 18 | CR | 555 | 0 | 618 | 24 | 0 |
| 19 | AS | 661 | 0 | 675 | 31 | 0 |
| 19 | CS | 646 | 0 | 644 | 40 | 0 |
| 20 | AT | 728 | 0 | 798 | 26 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20 | CT | 731 | 0 | 807 | 26 | 0 |
| 21 | AU | 199 | 0 | 208 | 8 | 0 |
| 21 | CU | 199 | 0 | 208 | 9 | 0 |
| 22 | AV | 277 | 0 | 140 | 3 | 0 |
| 22 | CV | 252 | 0 | 130 | 6 | 0 |
| 23 | AW | 1599 | 0 | 808 | 42 | 0 |
| 23 | CW | 1552 | 0 | 772 | 51 | 0 |
| 24 | AX | 1635 | 0 | 817 | 23 | 0 |
| 24 | CX | 1635 | 0 | 817 | 36 | 0 |
| 25 | AY | 1581 | 0 | 805 | 82 | 0 |
| 25 | CY | 1561 | 0 | 796 | 94 | 0 |
| 26 | BA | 60729 | 0 | 30622 | 666 | 0 |
| 26 | DA | 60311 | 0 | 30412 | 876 | 0 |
| 27 | BB | 2573 | 0 | 1306 | 20 | 0 |
| 27 | DB | 2573 | 0 | 1306 | 76 | 0 |
| 28 | BD | 2136 | 0 | 2218 | 42 | 0 |
| 28 | DD | 2142 | 0 | 2229 | 58 | 0 |
| 29 | BE | 1559 | 0 | 1618 | 25 | 0 |
| 29 | DE | 1559 | 0 | 1618 | 39 | 0 |
| 30 | BF | 1584 | 0 | 1625 | 39 | 0 |
| 30 | DF | 1580 | 0 | 1619 | 60 | 0 |
| 31 | BG | 1425 | 0 | 1443 | 38 | 0 |
| 31 | DG | 1424 | 0 | 1434 | 90 | 0 |
| 32 | BH | 1330 | 0 | 1407 | 34 | 0 |
| 32 | DH | 1330 | 0 | 1407 | 44 | 0 |
| 33 | BI | 1085 | 0 | 1114 | 37 | 0 |
| 33 | DI | 1073 | 0 | 1106 | 22 | 0 |
| 34 | BN | 1117 | 0 | 1184 | 23 | 0 |
| 34 | DN | 1117 | 0 | 1184 | 26 | 0 |
| 35 | BO | 933 | 0 | 996 | 25 | 0 |
| 35 | DO | 933 | 0 | 996 | 32 | 0 |
| 36 | BP | 1139 | 0 | 1223 | 41 | 0 |
| 36 | DP | 1135 | 0 | 1212 | 52 | 0 |
| 37 | BQ | 1122 | 0 | 1179 | 28 | 0 |
| 37 | DQ | 1122 | 0 | 1179 | 40 | 0 |
| 38 | BR | 968 | 0 | 1033 | 22 | 0 |
| 38 | DR | 968 | 0 | 1033 | 28 | 0 |
| 39 | BS | 877 | 0 | 938 | 20 | 0 |
| 39 | DS | 870 | 0 | 923 | 33 | 0 |
| 40 | BT | 1091 | 0 | 1151 | 26 | 0 |
| 40 | DT | 1083 | 0 | 1136 | 37 | 0 |
| 41 | BU | 959 | 0 | 1019 | 18 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41 | DU | 959 | 0 | 1018 | 30 | 0 |
| 42 | BV | 771 | 0 | 830 | 13 | 0 |
| 42 | DV | 771 | 0 | 830 | 24 | 0 |
| 43 | BW | 886 | 0 | 940 | 17 | 0 |
| 43 | DW | 886 | 0 | 940 | 13 | 0 |
| 44 | BX | 750 | 0 | 814 | 15 | 0 |
| 44 | DX | 750 | 0 | 814 | 27 | 0 |
| 45 | BY | 806 | 0 | 881 | 27 | 0 |
| 45 | DY | 806 | 0 | 881 | 30 | 0 |
| 46 | BZ | 1349 | 0 | 1355 | 44 | 0 |
| 46 | DZ | 1360 | 0 | 1363 | 70 | 0 |
| 47 | B0 | 653 | 0 | 674 | 13 | 0 |
| 47 | D0 | 653 | 0 | 674 | 22 | 0 |
| 48 | B1 | 755 | 0 | 826 | 16 | 0 |
| 48 | D1 | 755 | 0 | 826 | 18 | 0 |
| 49 | B2 | 588 | 0 | 643 | 11 | 0 |
| 49 | D2 | 588 | 0 | 643 | 14 | 0 |
| 50 | B3 | 469 | 0 | 518 | 6 | 0 |
| 50 | D3 | 464 | 0 | 514 | 13 | 0 |
| 51 | B4 | 558 | 0 | 544 | 37 | 0 |
| 51 | D4 | 532 | 0 | 503 | 25 | 0 |
| 52 | B5 | 455 | 0 | 465 | 14 | 0 |
| 52 | D5 | 455 | 0 | 465 | 13 | 0 |
| 53 | B6 | 453 | 0 | 473 | 13 | 0 |
| 53 | D6 | 449 | 0 | 469 | 12 | 0 |
| 54 | B7 | 418 | 0 | 467 | 10 | 0 |
| 54 | D7 | 418 | 0 | 467 | 13 | 0 |
| 55 | B8 | 517 | 0 | 582 | 17 | 0 |
| 55 | D8 | 517 | 0 | 582 | 15 | 0 |
| 56 | B9 | 307 | 0 | 335 | 7 | 0 |
| 56 | D9 | 307 | 0 | 335 | 11 | 0 |
| 57 | AA | 216 | 0 | 0 | 0 | 0 |
| 57 | AB | 1 | 0 | 0 | 0 | 0 |
| 57 | AE | 1 | 0 | 0 | 0 | 0 |
| 57 | AF | 1 | 0 | 0 | 0 | 0 |
| 57 | AK | 1 | 0 | 0 | 0 | 0 |
| 57 | AL | 2 | 0 | 0 | 0 | 0 |
| 57 | AM | 2 | 0 | 0 | 0 | 0 |
| 57 | AN | 2 | 0 | 0 | 0 | 0 |
| 57 | AT | 1 | 0 | 0 | 0 | 0 |
| 57 | AU | 1 | 0 | 0 | 0 | 0 |
| 57 | AW | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | AX | 15 | 0 | 0 | 0 | 0 |
| 57 | AY | 3 | 0 | 0 | 0 | 0 |
| 57 | B0 | 2 | 0 | 0 | 0 | 0 |
| 57 | B2 | 1 | 0 | 0 | 0 | 0 |
| 57 | B4 | 1 | 0 | 0 | 0 | 0 |
| 57 | B5 | 3 | 0 | 0 | 0 | 0 |
| 57 | B6 | 2 | 0 | 0 | 0 | 0 |
| 57 | B7 | 5 | 0 | 0 | 0 | 0 |
| 57 | B8 | 2 | 0 | 0 | 0 | 0 |
| 57 | B9 | 1 | 0 | 0 | 0 | 0 |
| 57 | BA | 814 | 0 | 0 | 0 | 0 |
| 57 | BB | 23 | 0 | 0 | 0 | 0 |
| 57 | BD | 10 | 0 | 0 | 0 | 0 |
| 57 | BE | 6 | 0 | 0 | 0 | 0 |
| 57 | BF | 11 | 0 | 0 | 0 | 0 |
| 57 | BG | 2 | 0 | 0 | 0 | 0 |
| 57 | BH | 1 | 0 | 0 | 0 | 0 |
| 57 | BN | 3 | 0 | 0 | 0 | 0 |
| 57 | BO | 1 | 0 | 0 | 0 | 0 |
| 57 | BP | 2 | 0 | 0 | 0 | 0 |
| 57 | BQ | 2 | 0 | 0 | 0 | 0 |
| 57 | BR | 2 | 0 | 0 | 0 | 0 |
| 57 | BU | 4 | 0 | 0 | 0 | 0 |
| 57 | BV | 5 | 0 | 0 | 0 | 0 |
| 57 | BW | 4 | 0 | 0 | 0 | 0 |
| 57 | BX | 1 | 0 | 0 | 0 | 0 |
| 57 | BY | 1 | 0 | 0 | 0 | 0 |
| 57 | BZ | 2 | 0 | 0 | 0 | 0 |
| 57 | CA | 169 | 0 | 0 | 0 | 0 |
| 57 | CD | 1 | 0 | 0 | 0 | 0 |
| 57 | CE | 2 | 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 | D0 | 1 | 0 | 0 | 0 | 0 |
| 57 | D3 | 1 | 0 | 0 | 0 | 0 |
| 57 | D8 | 1 | 0 | 0 | 0 | 0 |
| 57 | DA | 664 | 0 | 0 | 0 | 0 |
| 57 | DB | 13 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57 | DD | 4 | 0 | 0 | 0 | 0 |
| 57 | DE | 7 | 0 | 0 | 0 | 0 |
| 57 | DF | 5 | 0 | 0 | 0 | 0 |
| 57 | DG | 1 | 0 | 0 | 0 | 0 |
| 57 | DN | 1 | 0 | 0 | 0 | 0 |
| 57 | DO | 2 | 0 | 0 | 0 | 0 |
| 57 | DP | 2 | 0 | 0 | 0 | 0 |
| 57 | DQ | 3 | 0 | 0 | 0 | 0 |
| 57 | DR | 1 | 0 | 0 | 0 | 0 |
| 57 | DU | 1 | 0 | 0 | 0 | 0 |
| 57 | DV | 1 | 0 | 0 | 0 | 0 |
| 57 | DW | 1 | 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 |
| 61 | AA | 210 | 0 | 0 | 13 | 0 |
| 61 | AD | 1 | 0 | 0 | 0 | 0 |
| 61 | AE | 2 | 0 | 0 | 0 | 0 |
| 61 | AJ | 1 | 0 | 0 | 0 | 0 |
| 61 | AL | 2 | 0 | 0 | 1 | 0 |
| 61 | AM | 2 | 0 | 0 | 0 | 0 |
| 61 | AV | 2 | 0 | 0 | 0 | 0 |
| 61 | AW | 4 | 0 | 0 | 0 | 0 |
| 61 | AX | 4 | 0 | 0 | 0 | 0 |
| 61 | AY | 1 | 0 | 0 | 0 | 0 |
| 61 | B0 | 6 | 0 | 0 | 0 | 0 |
| 61 | B1 | 2 | 0 | 0 | 0 | 0 |
| 61 | B3 | 2 | 0 | 0 | 0 | 0 |
| 61 | B5 | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61 | B6 | 2 | 0 | 0 | 0 | 0 |
| 61 | B7 | 3 | 0 | 0 | 2 | 0 |
| 61 | B8 | 13 | 0 | 0 | 0 | 0 |
| 61 | B9 | 1 | 0 | 0 | 0 | 0 |
| 61 | BA | 1406 | 0 | 0 | 56 | 0 |
| 61 | BB | 37 | 0 | 0 | 1 | 0 |
| 61 | BD | 15 | 0 | 0 | 2 | 0 |
| 61 | BE | 17 | 0 | 0 | 4 | 0 |
| 61 | BF | 11 | 0 | 0 | 0 | 0 |
| 61 | BG | 3 | 0 | 0 | 0 | 0 |
| 61 | BH | 1 | 0 | 0 | 0 | 0 |
| 61 | BI | 1 | 0 | 0 | 0 | 0 |
| 61 | BN | 1 | 0 | 0 | 0 | 0 |
| 61 | BO | 2 | 0 | 0 | 0 | 0 |
| 61 | BP | 13 | 0 | 0 | 0 | 0 |
| 61 | BQ | 4 | 0 | 0 | 0 | 0 |
| 61 | BR | 2 | 0 | 0 | 0 | 0 |
| 61 | BS | 2 | 0 | 0 | 0 | 0 |
| 61 | BT | 2 | 0 | 0 | 0 | 0 |
| 61 | BU | 4 | 0 | 0 | 0 | 0 |
| 61 | BV | 2 | 0 | 0 | 0 | 0 |
| 61 | BW | 3 | 0 | 0 | 1 | 0 |
| 61 | BX | 3 | 0 | 0 | 0 | 0 |
| 61 | BZ | 1 | 0 | 0 | 0 | 0 |
| 61 | CA | 156 | 0 | 0 | 11 | 0 |
| 61 | CE | 2 | 0 | 0 | 0 | 0 |
| 61 | CH | 1 | 0 | 0 | 0 | 0 |
| 61 | CJ | 1 | 0 | 0 | 0 | 0 |
| 61 | CK | 1 | 0 | 0 | 0 | 0 |
| 61 | CL | 1 | 0 | 0 | 1 | 0 |
| 61 | CT | 1 | 0 | 0 | 0 | 0 |
| 61 | CW | 2 | 0 | 0 | 2 | 0 |
| 61 | CX | 2 | 0 | 0 | 0 | 0 |
| 61 | CY | 1 | 0 | 0 | 0 | 0 |
| 61 | D0 | 4 | 0 | 0 | 0 | 0 |
| 61 | D1 | 1 | 0 | 0 | 0 | 0 |
| 61 | D3 | 2 | 0 | 0 | 0 | 0 |
| 61 | D5 | 1 | 0 | 0 | 0 | 0 |
| 61 | D6 | 1 | 0 | 0 | 0 | 0 |
| 61 | D8 | 3 | 0 | 0 | 0 | 0 |
| 61 | DA | 989 | 0 | 0 | 44 | 0 |
| 61 | DB | 9 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | DD | 18 | 0 | 0 | 3 | 0 |
| 61 | DE | 5 | 0 | 0 | 0 | 0 |
| 61 | DF | 4 | 0 | 0 | 0 | 0 |
| 61 | DN | 2 | 0 | 0 | 0 | 0 |
| 61 | DP | 12 | 0 | 0 | 4 | 0 |
| 61 | DQ | 1 | 0 | 0 | 0 | 0 |
| 61 | DT | 4 | 0 | 0 | 0 | 0 |
| 61 | DU | 1 | 0 | 0 | 0 | 0 |
| 61 | DV | 1 | 0 | 0 | 0 | 0 |
| 61 | DW | 1 | 0 | 0 | 0 | 0 |
| 61 | DX | 2 | 0 | 0 | 0 | 0 |
| 61 | DY | 1 | 0 | 0 | 0 | 0 |
| All | All | 297127 | 0 | 196316 | 5502 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 5502 close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 26:DA:2139:C:N4 | 26:DA:2152:G:H1 | 1.46 | 1.14 |
| 1:CA:999:C:N4 | 1:CA:1042:G:H1 | 1.48 | 1.12 |
| 25:AY:49:C:N4 | 25:AY:65:G:H1 | 1.51 | 1.09 |
| 1:CA:985:C:N4 | 1:CA:1220:G:H1 | 1.50 | 1.09 |
| 1:CA:998:G:H1 | 1:CA:1043:C:N4 | 1.51 | 1.09 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 2 | AB | 229/256 (90%) | 208 (91%) | 13 (6%) | 8 (4%) | 6 8 |
| 2 | CB | 229/256 (90%) | 208 (91%) | 14 (6%) | 7 (3%) | 7 10 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3 | AC | 204/239 (85%) | 193 (95%) | 10 (5%) | 1 (0%) | 38 | 67 |
| 3 | CC | 204/239 (85%) | 191 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | AD | 206/209 (99%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 4 | CD | 206/209 (99%) | 200 (97%) | 5 (2%) | 1 (0%) | 38 | 67 |
| 5 | AE | 146/162 (90%) | 142 (97%) | 4 (3%) | 0 | 100 | 100 |
| 5 | CE | 146/162 (90%) | 142 (97%) | 3 (2%) | 1 (1%) | 30 | 58 |
| 6 | AF | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 6 | CF | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 7 | AG | 153/156 (98%) | 149 (97%) | 3 (2%) | 1 (1%) | 30 | 58 |
| 7 | CG | 153/156 (98%) | 149 (97%) | 3 (2%) | 1 (1%) | 30 | 58 |
| 8 | AH | 135/138 (98%) | 133 (98%) | 2 (2%) | 0 | 100 | 100 |
| 8 | CH | 135/138 (98%) | 131 (97%) | 4 (3%) | 0 | 100 | 100 |
| 9 | AI | 125/128 (98%) | 119 (95%) | 5 (4%) | 1 (1%) | 27 | 53 |
| 9 | CI | 125/128 (98%) | 120 (96%) | 4 (3%) | 1 (1%) | 27 | 53 |
| 10 | AJ | 95/105 (90%) | 85 (90%) | 8 (8%) | 2 (2%) | 11 | 19 |
| 10 | CJ | 94/105 (90%) | 84 (89%) | 6 (6%) | 4 (4%) | 4 | 5 |
| 11 | AK | 112/129 (87%) | 107 (96%) | 4 (4%) | 1 (1%) | 25 | 49 |
| 11 | CK | 112/129 (87%) | 107 (96%) | 4 (4%) | 1 (1%) | 25 | 49 |
| 12 | AL | 120/132 (91%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 12 | CL | 120/132 (91%) | 117 (98%) | 2 (2%) | 1 (1%) | 27 | 53 |
| 13 | AM | 121/126 (96%) | 116 (96%) | 4 (3%) | 1 (1%) | 27 | 53 |
| 13 | CM | 120/126 (95%) | 113 (94%) | 4 (3%) | 3 (2%) | 9 | 14 |
| 14 | AN | 58/61 (95%) | 57 (98%) | 1 (2%) | 0 | 100 | 100 |
| 14 | CN | 58/61 (95%) | 57 (98%) | 1 (2%) | 0 | 100 | 100 |
| 15 | AO | 86/89 (97%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | CO | 86/89 (97%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | AP | 80/88 (91%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | CP | 80/88 (91%) | 78 (98%) | 1 (1%) | 1 (1%) | 18 | 35 |
| 17 | AQ | 97/105 (92%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 17 | CQ | 97/105 (92%) | 94 (97%) | 3 (3%) | 0 | 100 | 100 |
| 18 | AR | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 18 | CR | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 19 | AS | 82/93 (88%) | 76 (93%) | 5 (6%) | 1 (1%) | 19 | 39 |
| 19 | CS | 81/93 (87%) | 75 (93%) | 6 (7%) | 0 | 100 | 100 |
| 20 | AT | 94/106 (89%) | 85 (90%) | 4 (4%) | 5 (5%) | 3 | 3 |
| 20 | CT | 94/106 (89%) | 85 (90%) | 4 (4%) | 5 (5%) | 3 | 3 |
| 21 | AU | 21/27 (78%) | 20 (95%) | 1 (5%) | 0 | 100 | 100 |
| 21 | CU | 21/27 (78%) | 21 (100%) | 0 | 0 | 100 | 100 |
| 28 | BD | 273/276 (99%) | 263 (96%) | 9 (3%) | 1 (0%) | 43 | 72 |
| 28 | DD | 273/276 (99%) | 261 (96%) | 10 (4%) | 2 (1%) | 30 | 58 |
| 29 | BE | 202/206 (98%) | 196 (97%) | 5 (2%) | 1 (0%) | 38 | 67 |
| 29 | DE | 202/206 (98%) | 196 (97%) | 5 (2%) | 1 (0%) | 38 | 67 |
| 30 | BF | 201/210 (96%) | 197 (98%) | 3 (2%) | 1 (0%) | 38 | 67 |
| 30 | DF | 201/210 (96%) | 197 (98%) | 3 (2%) | 1 (0%) | 38 | 67 |
| 31 | BG | 179/182 (98%) | 171 (96%) | 7 (4%) | 1 (1%) | 33 | 63 |
| 31 | DG | 179/182 (98%) | 168 (94%) | 8 (4%) | 3 (2%) | 14 | 26 |
| 32 | BH | 172/180 (96%) | 166 (96%) | 6 (4%) | 0 | 100 | 100 |
| 32 | DH | 172/180 (96%) | 166 (96%) | 6 (4%) | 0 | 100 | 100 |
| 33 | BI | 144/148 (97%) | 132 (92%) | 7 (5%) | 5 (4%) | 6 | 8 |
| 33 | DI | 144/148 (97%) | 135 (94%) | 8 (6%) | 1 (1%) | 30 | 58 |
| 34 | BN | 138/140 (99%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 34 | DN | 138/140 (99%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 35 | BO | 120/122 (98%) | 114 (95%) | 6 (5%) | 0 | 100 | 100 |
| 35 | DO | 120/122 (98%) | 115 (96%) | 5 (4%) | 0 | 100 | 100 |
| 36 | BP | 147/150 (98%) | 142 (97%) | 4 (3%) | 1 (1%) | 30 | 58 |
| 36 | DP | 147/150 (98%) | 139 (95%) | 6 (4%) | 2 (1%) | 16 | 32 |
| 37 | BQ | 139/141 (99%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 37 | DQ | 139/141 (99%) | 134 (96%) | 4 (3%) | 1 (1%) | 30 | 58 |
| 38 | BR | 116/118 (98%) | 115 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | DR | 116/118 (98%) | 114 (98%) | 2 (2%) | 0 | 100 | 100 |
| 39 | BS | 108/112 (96%) | 106 (98%) | 2 (2%) | 0 | 100 | 100 |
| 39 | DS | 108/112 (96%) | 107 (99%) | 0 | 1 (1%) | 25 | 49 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 40 | BT | 129/146 (88%) | 123 (95%) | 6 (5%) | 0 | 100 | 100 |
| 40 | DT | 129/146 (88%) | 126 (98%) | 3 (2%) | 0 | 100 | 100 |
| 41 | BU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 41 | DU | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 42 | BV | 99/101 (98%) | 93 (94%) | 5 (5%) | 1 (1%) | 22 | 45 |
| 42 | DV | 99/101 (98%) | 96 (97%) | 2 (2%) | 1 (1%) | 22 | 45 |
| 43 | BW | 110/113 (97%) | 110 (100%) | 0 | 0 | 100 | 100 |
| 43 | DW | 110/113 (97%) | 110 (100%) | 0 | 0 | 100 | 100 |
| 44 | BX | 93/96 (97%) | 91 (98%) | 2 (2%) | 0 | 100 | 100 |
| 44 | DX | 93/96 (97%) | 91 (98%) | 1 (1%) | 1 (1%) | 21 | 42 |
| 45 | BY | 105/110 (96%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 45 | DY | 105/110 (96%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 46 | BZ | 169/206 (82%) | 153 (90%) | 15 (9%) | 1 (1%) | 33 | 63 |
| 46 | DZ | 172/206 (84%) | 159 (92%) | 13 (8%) | 0 | 100 | 100 |
| 47 | B0 | 81/85 (95%) | 81 (100%) | 0 | 0 | 100 | 100 |
| 47 | D0 | 81/85 (95%) | 79 (98%) | 1 (1%) | 1 (1%) | 19 | 39 |
| 48 | B1 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 21 | 42 |
| 48 | D1 | 95/98 (97%) | 92 (97%) | 2 (2%) | 1 (1%) | 21 | 42 |
| 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%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 50 | D3 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 51 | B4 | 67/71 (94%) | 54 (81%) | 9 (13%) | 4 (6%) | 2 | 2 |
| 51 | D4 | 67/71 (94%) | 53 (79%) | 11 (16%) | 3 (4%) | 4 | 4 |
| 52 | B5 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 52 | D5 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | B6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 53 | D6 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 54 | B7 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | D7 | 46/49 (94%) | 45 (98%) | 0 | 1 (2%) | 10 | 18 |
| 55 | B8 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 55 | D8 | 62/65 (95%) | 62 (100%) | 0 | 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 | 11410/12128 (94%) | 10945 (96%) | 381 (3%) | 84 (1%) | 30 | 58 |

5 of 84 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 17 | PHE |
| 2 | AB | 19 | HIS |
| 2 | AB | 231 | GLU |
| 9 | AI | 54 | ASP |
| 10 | AJ | 56 | HIS |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | AB | 192/220 (87%) | 155 (81%) | 37 (19%) | 2 | 3 |
| 2 | CB | 187/220 (85%) | 151 (81%) | 36 (19%) | 2 | 3 |
| 3 | AC | 143/188 (76%) | 127 (89%) | 16 (11%) | 9 | 16 |
| 3 | CC | 141/188 (75%) | 116 (82%) | 25 (18%) | 3 | 4 |
| 4 | AD | 170/181 (94%) | 147 (86%) | 23 (14%) | 6 | 10 |
| 4 | CD | 174/181 (96%) | 147 (84%) | 27 (16%) | 4 | 6 |
| 5 | AE | 113/123 (92%) | 106 (94%) | 7 (6%) | 26 | 49 |
| 5 | CE | 114/123 (93%) | 99 (87%) | 15 (13%) | 6 | 10 |
| 6 | AF | 84/90 (93%) | 74 (88%) | 10 (12%) | 8 | 14 |
| 6 | CF | 86/90 (96%) | 79 (92%) | 7 (8%) | 17 | 32 |
| 7 | AG | 119/127 (94%) | 99 (83%) | 20 (17%) | 3 | 5 |
| 7 | CG | 120/127 (94%) | 106 (88%) | 14 (12%) | 8 | 14 |
| 8 | AH | 114/119 (96%) | 101 (89%) | 13 (11%) | 8 | 15 |
| 8 | CH | 114/119 (96%) | 97 (85%) | 17 (15%) | 4 | 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 9 | AI | 91/99 (92%) | 73 (80%) | 18 (20%) | 2 | 3 |
| 9 | CI | 89/99 (90%) | 69 (78%) | 20 (22%) | 1 | 2 |
| 10 | AJ | 66/92 (72%) | 60 (91%) | 6 (9%) | 14 | 25 |
| 10 | CJ | 69/92 (75%) | 61 (88%) | 8 (12%) | 8 | 14 |
| 11 | AK | 83/99 (84%) | 74 (89%) | 9 (11%) | 9 | 17 |
| 11 | CK | 83/99 (84%) | 72 (87%) | 11 (13%) | 6 | 10 |
| 12 | AL | 97/109 (89%) | 88 (91%) | 9 (9%) | 13 | 24 |
| 12 | CL | 97/109 (89%) | 85 (88%) | 12 (12%) | 7 | 13 |
| 13 | AM | 95/101 (94%) | 81 (85%) | 14 (15%) | 4 | 8 |
| 13 | CM | 92/101 (91%) | 74 (80%) | 18 (20%) | 2 | 3 |
| 14 | AN | 49/50 (98%) | 40 (82%) | 9 (18%) | 2 | 4 |
| 14 | CN | 49/50 (98%) | 37 (76%) | 12 (24%) | 1 | 2 |
| 15 | AO | 78/80 (98%) | 70 (90%) | 8 (10%) | 10 | 19 |
| 15 | CO | 78/80 (98%) | 67 (86%) | 11 (14%) | 5 | 9 |
| 16 | AP | 69/74 (93%) | 58 (84%) | 11 (16%) | 4 | 6 |
| 16 | CP | 68/74 (92%) | 59 (87%) | 9 (13%) | 6 | 10 |
| 17 | AQ | 94/97 (97%) | 87 (93%) | 7 (7%) | 20 | 38 |
| 17 | CQ | 94/97 (97%) | 84 (89%) | 10 (11%) | 10 | 18 |
| 18 | AR | 59/77 (77%) | 50 (85%) | 9 (15%) | 4 | 7 |
| 18 | CR | 59/77 (77%) | 46 (78%) | 13 (22%) | 1 | 2 |
| 19 | AS | 70/80 (88%) | 59 (84%) | 11 (16%) | 4 | 6 |
| 19 | CS | 67/80 (84%) | 54 (81%) | 13 (19%) | 2 | 3 |
| 20 | AT | 70/82 (85%) | 60 (86%) | 10 (14%) | 5 | 8 |
| 20 | CT | 71/82 (87%) | 62 (87%) | 9 (13%) | 6 | 12 |
| 21 | AU | 18/22 (82%) | 15 (83%) | 3 (17%) | 3 | 5 |
| 21 | CU | 18/22 (82%) | 15 (83%) | 3 (17%) | 3 | 5 |
| 28 | BD | 215/218 (99%) | 196 (91%) | 19 (9%) | 14 | 27 |
| 28 | DD | 216/218 (99%) | 200 (93%) | 16 (7%) | 20 | 38 |
| 29 | BE | 164/166 (99%) | 145 (88%) | 19 (12%) | 8 | 14 |
| 29 | DE | 164/166 (99%) | 141 (86%) | 23 (14%) | 5 | 9 |
| 30 | BF | 160/166 (96%) | 142 (89%) | 18 (11%) | 9 | 15 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30 | DF | 159/166 (96%) | 138 (87%) | 21 (13%) | 6 | 10 |
| 31 | BG | 143/156 (92%) | 127 (89%) | 16 (11%) | 9 | 16 |
| 31 | DG | 142/156 (91%) | 119 (84%) | 23 (16%) | 3 | 6 |
| 32 | BH | 144/148 (97%) | 129 (90%) | 15 (10%) | 10 | 18 |
| 32 | DH | 144/148 (97%) | 124 (86%) | 20 (14%) | 5 | 9 |
| 33 | BI | 110/124 (89%) | 88 (80%) | 22 (20%) | 2 | 3 |
| 33 | DI | 107/124 (86%) | 87 (81%) | 20 (19%) | 2 | 3 |
| 34 | BN | 118/119 (99%) | 101 (86%) | 17 (14%) | 5 | 8 |
| 34 | DN | 118/119 (99%) | 101 (86%) | 17 (14%) | 5 | 8 |
| 35 | BO | 100/100 (100%) | 92 (92%) | 8 (8%) | 17 | 33 |
| 35 | DO | 100/100 (100%) | 89 (89%) | 11 (11%) | 9 | 16 |
| 36 | BP | 116/116 (100%) | 104 (90%) | 12 (10%) | 10 | 19 |
| 36 | DP | 115/116 (99%) | 103 (90%) | 12 (10%) | 10 | 18 |
| 37 | BQ | 111/111 (100%) | 95 (86%) | 16 (14%) | 5 | 8 |
| 37 | DQ | 111/111 (100%) | 97 (87%) | 14 (13%) | 7 | 12 |
| 38 | BR | 101/101 (100%) | 83 (82%) | 18 (18%) | 2 | 4 |
| 38 | DR | 101/101 (100%) | 86 (85%) | 15 (15%) | 4 | 7 |
| 39 | BS | 87/88 (99%) | 79 (91%) | 8 (9%) | 13 | 24 |
| 39 | DS | 85/88 (97%) | 74 (87%) | 11 (13%) | 6 | 11 |
| 40 | BT | 115/127 (91%) | 107 (93%) | 8 (7%) | 21 | 41 |
| 40 | DT | 113/127 (89%) | 105 (93%) | 8 (7%) | 21 | 40 |
| 41 | BU | 93/94 (99%) | 86 (92%) | 7 (8%) | 19 | 36 |
| 41 | DU | 93/94 (99%) | 87 (94%) | 6 (6%) | 24 | 46 |
| 42 | BV | 80/82 (98%) | 70 (88%) | 10 (12%) | 7 | 12 |
| 42 | DV | 80/82 (98%) | 67 (84%) | 13 (16%) | 3 | 6 |
| 43 | BW | 90/92 (98%) | 83 (92%) | 7 (8%) | 18 | 34 |
| 43 | DW | 90/92 (98%) | 84 (93%) | 6 (7%) | 23 | 44 |
| 44 | BX | 77/78 (99%) | 72 (94%) | 5 (6%) | 24 | 46 |
| 44 | DX | 77/78 (99%) | 70 (91%) | 7 (9%) | 14 | 25 |
| 45 | BY | 85/91 (93%) | 77 (91%) | 8 (9%) | 13 | 23 |
| 45 | DY | 85/91 (93%) | 78 (92%) | 7 (8%) | 17 | 31 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 46 | BZ | 145/179 (81%) | 128 (88%) | 17 (12%) | 8 | 14 |
| 46 | DZ | 145/179 (81%) | 127 (88%) | 18 (12%) | 7 | 13 |
| 47 | B0 | 65/67 (97%) | 61 (94%) | 4 (6%) | 26 | 49 |
| 47 | D0 | 65/67 (97%) | 59 (91%) | 6 (9%) | 13 | 24 |
| 48 | B1 | 80/83 (96%) | 72 (90%) | 8 (10%) | 11 | 20 |
| 48 | D1 | 80/83 (96%) | 71 (89%) | 9 (11%) | 9 | 15 |
| 49 | B2 | 65/67 (97%) | 59 (91%) | 6 (9%) | 13 | 24 |
| 49 | D2 | 65/67 (97%) | 60 (92%) | 5 (8%) | 18 | 35 |
| 50 | B3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 18 | 34 |
| 50 | D3 | 50/52 (96%) | 47 (94%) | 3 (6%) | 27 | 51 |
| 51 | B4 | 60/63 (95%) | 51 (85%) | 9 (15%) | 4 | 7 |
| 51 | D4 | 53/63 (84%) | 38 (72%) | 15 (28%) | 0 | 1 |
| 52 | B5 | 50/52 (96%) | 46 (92%) | 4 (8%) | 17 | 33 |
| 52 | D5 | 50/52 (96%) | 48 (96%) | 2 (4%) | 42 | 73 |
| 53 | B6 | 51/52 (98%) | 45 (88%) | 6 (12%) | 8 | 14 |
| 53 | D6 | 50/52 (96%) | 47 (94%) | 3 (6%) | 27 | 51 |
| 54 | B7 | 41/42 (98%) | 39 (95%) | 2 (5%) | 35 | 62 |
| 54 | D7 | 41/42 (98%) | 39 (95%) | 2 (5%) | 35 | 62 |
| 55 | B8 | 54/55 (98%) | 50 (93%) | 4 (7%) | 20 | 38 |
| 55 | D8 | 54/55 (98%) | 50 (93%) | 4 (7%) | 20 | 38 |
| 56 | B9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 55 | 83 |
| 56 | D9 | 34/34 (100%) | 33 (97%) | 1 (3%) | 55 | 83 |
| All | All | 9336/10066 (93%) | 8180 (88%) | 1156 (12%) | 7 | 13 |

5 of 1156 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | B4 | 3 | GLU |
| 5 | CE | 79 | GLU |
| 43 | DW | 4 | LYS |
| 53 | B6 | 28 | ARG |
| 3 | CC | 21 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51 | B4 | 46 | GLN |
| 4 | CD | 77 | ASN |
| 42 | DV | 64 | HIS |
| 2 | CB | 16 | HIS |
| 3 | CC | 3 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1494/1521 (98%) | 361 (24%) | 19 (1%) |
| 1 | CA | 1501/1521 (98%) | 370 (24%) | 25 (1%) |
| 22 | AV | 12/24 (50%) | 3 (25%) | 0 |
| 22 | CV | 11/24 (45%) | 3 (27%) | 0 |
| 23 | AW | 70/76 (92%) | 27 (38%) | 2 (2%) |
| 23 | CW | 67/76 (88%) | 26 (38%) | 3 (4%) |
| 24 | AX | 74/77 (96%) | 16 (21%) | 0 |
| 24 | CX | 74/77 (96%) | 23 (31%) | 0 |
| 25 | AY | 71/76 (93%) | 37 (52%) | 3 (4%) |
| 25 | CY | 69/76 (90%) | 36 (52%) | 1 (1%) |
| 26 | BA | 2812/2915 (96%) | 444 (15%) | 36 (1%) |
| 26 | DA | 2791/2915 (95%) | 563 (20%) | 24 (0%) |
| 27 | BB | 119/121 (98%) | 13 (10%) | 0 |
| 27 | DB | 119/121 (98%) | 38 (31%) | 0 |
| All | All | 9284/9620 (96%) | 1960 (21%) | 113 (1%) |

5 of 1960 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 5 | U |
| 1 | AA | 7 | G |
| 1 | AA | 9 | G |
| 1 | AA | 22 | G |
| 1 | AA | 29 | G |

5 of 113 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | BA | 2203 | G |
| 1 | CA | 266 | G |
| 26 | DA | 1653 | G |
| 26 | BA | 2205 | C |
| 26 | BA | 2701 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|-------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 23 | PSU | AW | 32 | 57,23 | 19,21,22 | 1.82 | 4 (21%) | 23,30,33 | 0.99 | 2 (8%) |
| 23 | MIA | AW | 37 | 23 | 29,31,32 | 1.82 | 5 (17%) | 41,44,47 | 1.86 | 7 (17%) |
| 23 | PSU | AW | 39 | 23 | 19,21,22 | 1.81 | 4 (21%) | 23,30,33 | 0.98 | 2 (8%) |
| 23 | 7MG | AW | 46 | 23 | 24,26,27 | 1.97 | 7 (29%) | 34,39,42 | 2.45 | 10 (29%) |
| 23 | 5MU | AW | 54 | 23 | 20,22,23 | 1.67 | 4 (20%) | 25,32,35 | 2.09 | 4 (16%) |
| 23 | PSU | AW | 55 | 23 | 19,21,22 | 1.89 | 4 (21%) | 23,30,33 | 1.39 | 1 (4%) |
| 23 | F3N | AW | 76 | 23 | 34,36,37 | 1.45 | 4 (11%) | 48,51,54 | 2.02 | 6 (12%) |
| 23 | 4SU | AW | 8 | 23 | 19,21,22 | 1.88 | 4 (21%) | 23,30,33 | 3.02 | 4 (17%) |
| 24 | 5MC | AX | 32 | 24 | 20,22,23 | 1.73 | 4 (20%) | 26,32,35 | 1.46 | 4 (15%) |
| 24 | 5MU | AX | 54 | 24,57 | 20,22,23 | 1.58 | 5 (25%) | 25,32,35 | 2.03 | 4 (16%) |
| 24 | PSU | AX | 55 | 24 | 19,21,22 | 2.01 | 5 (26%) | 23,30,33 | 1.03 | 3 (13%) |
| 24 | 31H | AX | 76 | 24,57 | 32,34,35 | 1.22 | 3 (9%) | 44,47,50 | 2.33 | 11 (25%) |
| 24 | 4SU | AX | 8 | 24 | 19,21,22 | 1.89 | 4 (21%) | 23,30,33 | 33.54 | 2 (8%) |
| 25 | PSU | AY | 32 | 25 | 19,21,22 | 1.78 | 4 (21%) | 23,30,33 | 1.04 | 3 (13%) |
| 25 | MIA | AY | 37 | 25 | 20,24,32 | 1.76 | 5 (25%) | 27,35,47 | 1.92 | 4 (14%) |
| 25 | PSU | AY | 39 | 25 | 19,21,22 | 1.84 | 5 (26%) | 23,30,33 | 1.07 | 2 (8%) |
| 25 | 7MG | AY | 46 | 25 | 24,26,27 | 1.98 | 6 (25%) | 34,39,42 | 2.64 | 12 (35%) |
| 25 | 5MU | AY | 54 | 25 | 20,22,23 | 1.90 | 4 (20%) | 25,32,35 | 2.70 | 5 (20%) |
| 25 | PSU | AY | 55 | 25 | 19,21,22 | 1.90 | 4 (21%) | 23,30,33 | 0.86 | 2 (8%) |
| 25 | 4SU | AY | 8 | 25 | 19,21,22 | 1.70 | 4 (21%) | 23,30,33 | 4.73 | 4 (17%) |
| 23 | PSU | CW | 32 | 23 | 19,21,22 | 1.83 | 4 (21%) | 23,30,33 | 1.21 | 2 (8%) |
| 23 | MIA | CW | 37 | 23 | 20,24,32 | 1.73 | 5 (25%) | 27,35,47 | 1.93 | 4 (14%) |
| 23 | PSU | CW | 39 | 23 | 19,21,22 | 1.95 | 4 (21%) | 23,30,33 | 1.19 | 1 (4%) |
| 23 | 7MG | CW | 46 | 23 | 24,26,27 | 2.05 | 6 (25%) | 34,39,42 | 2.25 | 9 (26%) |
| 23 | 5MU | CW | 54 | 23 | 20,22,23 | 1.65 | 4 (20%) | 25,32,35 | 1.79 | 3 (12%) |
| 23 | PSU | CW | 55 | 23 | 19,21,22 | 1.87 | 4 (21%) | 23,30,33 | 1.29 | 2 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|-------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 23 | F3N | CW | 76 | 23 | 34,36,37 | 1.49 | 4 (11%) | 48,51,54 | 2.08 | 7 (14%) |
| 23 | 4SU | CW | 8 | 23 | 19,21,22 | 1.81 | 4 (21%) | 23,30,33 | 6.41 | 4 (17%) |
| 24 | 5MC | CX | 32 | 24 | 20,22,23 | 1.74 | 4 (20%) | 26,32,35 | 1.55 | 5 (19%) |
| 24 | 5MU | CX | 54 | 24 | 20,22,23 | 1.61 | 4 (20%) | 25,32,35 | 2.30 | 4 (16%) |
| 24 | PSU | CX | 55 | 24 | 19,21,22 | 1.84 | 4 (21%) | 23,30,33 | 0.96 | 2 (8%) |
| 24 | 31H | CX | 76 | 24,57 | 32,34,35 | 1.24 | 3 (9%) | 44,47,50 | 2.62 | 12 (27%) |
| 24 | 4SU | CX | 8 | 24 | 19,21,22 | 1.84 | 4 (21%) | 23,30,33 | 23.31 | 2 (8%) |
| 25 | PSU | CY | 32 | 25 | 19,21,22 | 1.79 | 4 (21%) | 23,30,33 | 1.11 | 2 (8%) |
| 25 | MIA | CY | 37 | 25 | 20,24,32 | 1.79 | 5 (25%) | 27,35,47 | 1.95 | 5 (18%) |
| 25 | PSU | CY | 39 | 25 | 19,21,22 | 2.04 | 5 (26%) | 23,30,33 | 1.55 | 3 (13%) |
| 25 | 7MG | CY | 46 | 25 | 24,26,27 | 2.03 | 8 (33%) | 34,39,42 | 2.61 | 10 (29%) |
| 25 | 5MU | CY | 54 | 25 | 20,22,23 | 1.67 | 4 (20%) | 25,32,35 | 2.03 | 4 (16%) |
| 25 | PSU | CY | 55 | 25 | 19,21,22 | 1.78 | 4 (21%) | 23,30,33 | 1.17 | 2 (8%) |
| 25 | 4SU | CY | 8 | 25 | 19,21,22 | 1.96 | 4 (21%) | 23,30,33 | 4.24 | 4 (17%) |

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 |
|-----|------|-------|-----|-------|---------|------------|---------|
| 23 | PSU | AW | 32 | 57,23 | - | 0/8/25/26 | 0/2/2/2 |
| 23 | MIA | AW | 37 | 23 | - | 0/16/33/34 | 0/3/3/3 |
| 23 | PSU | AW | 39 | 23 | - | 0/8/25/26 | 0/2/2/2 |
| 23 | 7MG | AW | 46 | 23 | - | 1/8/37/38 | 0/3/3/3 |
| 23 | 5MU | AW | 54 | 23 | - | 0/6/25/26 | 0/2/2/2 |
| 23 | PSU | AW | 55 | 23 | - | 0/8/25/26 | 0/2/2/2 |
| 23 | F3N | AW | 76 | 23 | - | 0/20/37/38 | 0/4/4/4 |
| 23 | 4SU | AW | 8 | 23 | - | 0/6/25/26 | 0/2/2/2 |
| 24 | 5MC | AX | 32 | 24 | - | 0/6/25/26 | 0/2/2/2 |
| 24 | 5MU | AX | 54 | 24,57 | - | 0/6/25/26 | 0/2/2/2 |
| 24 | PSU | AX | 55 | 24 | - | 0/8/25/26 | 0/2/2/2 |
| 24 | 31H | AX | 76 | 24,57 | - | 1/23/40/41 | 0/3/3/3 |
| 24 | 4SU | AX | 8 | 24 | - | 0/6/25/26 | 0/2/2/2 |
| 25 | PSU | AY | 32 | 25 | - | 0/8/25/26 | 0/2/2/2 |
| 25 | MIA | AY | 37 | 25 | - | 0/8/25/34 | 0/3/3/3 |
| 25 | PSU | AY | 39 | 25 | - | 0/8/25/26 | 0/2/2/2 |
| 25 | 7MG | AY | 46 | 25 | - | 1/8/37/38 | 0/3/3/3 |
| 25 | 5MU | AY | 54 | 25 | - | 0/6/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|------------|---------|
| 25 | PSU | AY | 55 | 25 | - | 0/8/25/26 | 0/2/2/2 |
| 25 | 4SU | AY | 8 | 25 | - | 0/6/25/26 | 0/2/2/2 |
| 23 | PSU | CW | 32 | 23 | - | 0/8/25/26 | 0/2/2/2 |
| 23 | MIA | CW | 37 | 23 | - | 0/8/25/34 | 0/3/3/3 |
| 23 | PSU | CW | 39 | 23 | - | 0/8/25/26 | 0/2/2/2 |
| 23 | 7MG | CW | 46 | 23 | - | 0/8/37/38 | 0/3/3/3 |
| 23 | 5MU | CW | 54 | 23 | - | 0/6/25/26 | 0/2/2/2 |
| 23 | PSU | CW | 55 | 23 | - | 0/8/25/26 | 0/2/2/2 |
| 23 | F3N | CW | 76 | 23 | - | 0/20/37/38 | 0/4/4/4 |
| 23 | 4SU | CW | 8 | 23 | - | 0/6/25/26 | 0/2/2/2 |
| 24 | 5MC | CX | 32 | 24 | - | 0/6/25/26 | 0/2/2/2 |
| 24 | 5MU | CX | 54 | 24 | - | 0/6/25/26 | 0/2/2/2 |
| 24 | PSU | CX | 55 | 24 | - | 0/8/25/26 | 0/2/2/2 |
| 24 | 31H | CX | 76 | 24,57 | - | 1/23/40/41 | 0/3/3/3 |
| 24 | 4SU | CX | 8 | 24 | - | 0/6/25/26 | 0/2/2/2 |
| 25 | PSU | CY | 32 | 25 | - | 0/8/25/26 | 0/2/2/2 |
| 25 | MIA | CY | 37 | 25 | - | 0/8/25/34 | 0/3/3/3 |
| 25 | PSU | CY | 39 | 25 | - | 0/8/25/26 | 0/2/2/2 |
| 25 | 7MG | CY | 46 | 25 | - | 0/8/37/38 | 0/3/3/3 |
| 25 | 5MU | CY | 54 | 25 | - | 0/6/25/26 | 0/2/2/2 |
| 25 | PSU | CY | 55 | 25 | - | 0/8/25/26 | 0/2/2/2 |
| 25 | 4SU | CY | 8 | 25 | - | 0/6/25/26 | 0/2/2/2 |

The worst 5 of 177 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 23 | AW | 37 | MIA | C2-S10 | -6.26 | 1.70 | 1.75 |
| 23 | CW | 46 | 7MG | C6-C5 | 6.20 | 1.49 | 1.41 |
| 25 | CY | 46 | 7MG | C6-C5 | 5.42 | 1.48 | 1.41 |
| 23 | AW | 46 | 7MG | C6-C5 | 5.33 | 1.48 | 1.41 |
| 24 | AX | 55 | PSU | C5-C1' | -5.20 | 1.47 | 1.52 |

The worst 5 of 179 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 24 | AX | 8 | 4SU | C4-N3-C2 | 160.78 | 128.48 | 121.60 |
| 24 | CX | 8 | 4SU | C4-N3-C2 | 111.46 | 126.37 | 121.60 |
| 23 | CW | 8 | 4SU | C4-N3-C2 | -29.19 | 120.35 | 121.60 |
| 25 | AY | 8 | 4SU | C4-N3-C2 | -21.05 | 120.70 | 121.60 |
| 25 | CY | 8 | 4SU | C4-N3-C2 | -17.66 | 120.85 | 121.60 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 24 | AX | 76 | 31H | OCN-CN-N-CA |
| 24 | CX | 76 | 31H | OCN-CN-N-CA |
| 25 | AY | 46 | 7MG | OP2-P-O5'-C5' |
| 23 | AW | 46 | 7MG | OP2-P-O5'-C5' |

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2063 ligands modelled in this entry, 2061 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 | 501 | 4 | 12,12,12 | 22.24 | 12 (100%) | 0,24,24 | 0.00 | - |
| 58 | SF4 | CD | 501 | 4 | 12,12,12 | 21.71 | 12 (100%) | 0,24,24 | 0.00 | - |

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 | 501 | 4 | - | 0/0/48/48 | 0/6/5/5 |
| 58 | SF4 | CD | 501 | 4 | - | 0/0/48/48 | 0/6/5/5 |

The worst 5 of 24 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 58 | AD | 501 | SF4 | S1-FE2 | -23.30 | 2.17 | 2.33 |
| 58 | AD | 501 | SF4 | S3-FE4 | -22.80 | 2.17 | 2.33 |
| 58 | AD | 501 | SF4 | S4-FE2 | -22.72 | 2.18 | 2.33 |
| 58 | AD | 501 | SF4 | S2-FE4 | -22.43 | 2.18 | 2.33 |
| 58 | AD | 501 | SF4 | S2-FE1 | -22.18 | 2.18 | 2.33 |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 1497/1521 (98%) | 0.08 | 17 (1%) 77 79 | 41, 72, 93, 106 | 0 |
| 1 | CA | 1503/1521 (98%) | 0.17 | 64 (4%) 34 30 | 43, 75, 94, 106 | 0 |
| 2 | AB | 231/256 (90%) | 1.23 | 57 (24%) 1 1 | 68, 82, 89, 95 | 0 |
| 2 | CB | 231/256 (90%) | 2.90 | 131 (56%) 0 0 | 68, 83, 90, 96 | 0 |
| 3 | AC | 206/239 (86%) | 0.81 | 23 (11%) 6 4 | 69, 79, 87, 94 | 0 |
| 3 | CC | 206/239 (86%) | 1.84 | 88 (42%) 1 0 | 70, 82, 90, 94 | 0 |
| 4 | AD | 208/209 (99%) | 0.78 | 32 (15%) 3 2 | 57, 72, 81, 87 | 0 |
| 4 | CD | 208/209 (99%) | 0.68 | 21 (10%) 7 5 | 60, 72, 81, 89 | 0 |
| 5 | AE | 148/162 (91%) | 0.57 | 8 (5%) 25 21 | 58, 71, 81, 85 | 0 |
| 5 | CE | 148/162 (91%) | 0.98 | 17 (11%) 5 4 | 60, 74, 83, 86 | 0 |
| 6 | AF | 100/101 (99%) | 0.21 | 1 (1%) 79 81 | 52, 67, 75, 85 | 0 |
| 6 | CF | 100/101 (99%) | 0.25 | 3 (3%) 48 45 | 57, 71, 81, 85 | 0 |
| 7 | AG | 155/156 (99%) | 0.50 | 13 (8%) 11 8 | 66, 76, 85, 96 | 0 |
| 7 | CG | 155/156 (99%) | 1.31 | 43 (27%) 1 1 | 68, 77, 86, 97 | 0 |
| 8 | AH | 137/138 (99%) | 0.18 | 1 (0%) 84 86 | 62, 72, 79, 83 | 0 |
| 8 | CH | 137/138 (99%) | 1.45 | 38 (27%) 1 1 | 64, 74, 80, 85 | 0 |
| 9 | AI | 127/128 (99%) | 1.86 | 53 (41%) 1 0 | 62, 80, 87, 89 | 0 |
| 9 | CI | 127/128 (99%) | 3.66 | 97 (76%) 0 0 | 69, 82, 89, 91 | 0 |
| 10 | AJ | 97/105 (92%) | 1.63 | 34 (35%) 1 1 | 66, 83, 91, 92 | 0 |
| 10 | CJ | 96/105 (91%) | 2.94 | 63 (65%) 0 0 | 68, 84, 91, 93 | 0 |
| 11 | AK | 114/129 (88%) | 0.92 | 19 (16%) 2 1 | 51, 70, 80, 84 | 0 |
| 11 | CK | 114/129 (88%) | 1.15 | 25 (21%) 1 1 | 52, 72, 81, 85 | 0 |
| 12 | AL | 122/132 (92%) | 0.16 | 3 (2%) 54 52 | 41, 56, 71, 75 | 0 |
| 12 | CL | 122/132 (92%) | 1.13 | 27 (22%) 1 1 | 58, 73, 82, 87 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AM | 123/126 (97%) | 0.57 | 13 (10%) 7 5 | 57, 72, 83, 88 | 0 |
| 13 | CM | 122/126 (96%) | 2.61 | 59 (48%) 1 0 | 69, 85, 92, 97 | 0 |
| 14 | AN | 60/61 (98%) | 0.96 | 9 (15%) 3 2 | 70, 76, 83, 84 | 0 |
| 14 | CN | 60/61 (98%) | 3.39 | 44 (73%) 0 0 | 73, 79, 85, 87 | 0 |
| 15 | AO | 88/89 (98%) | 0.84 | 9 (10%) 7 5 | 54, 68, 79, 83 | 0 |
| 15 | CO | 88/89 (98%) | 1.34 | 21 (23%) 1 1 | 56, 70, 81, 84 | 0 |
| 16 | AP | 82/88 (93%) | 1.81 | 27 (32%) 1 1 | 59, 71, 79, 84 | 0 |
| 16 | CP | 82/88 (93%) | 0.94 | 11 (13%) 4 3 | 59, 70, 79, 83 | 0 |
| 17 | AQ | 99/105 (94%) | 0.58 | 9 (9%) 9 7 | 57, 70, 79, 84 | 0 |
| 17 | CQ | 99/105 (94%) | 0.90 | 13 (13%) 4 3 | 60, 71, 79, 84 | 0 |
| 18 | AR | 68/88 (77%) | 0.93 | 13 (19%) 2 1 | 59, 69, 81, 84 | 0 |
| 18 | CR | 68/88 (77%) | 0.91 | 11 (16%) 2 1 | 58, 70, 81, 85 | 0 |
| 19 | AS | 84/93 (90%) | 0.48 | 8 (9%) 8 6 | 70, 81, 87, 92 | 0 |
| 19 | CS | 83/93 (89%) | 2.44 | 48 (57%) 0 0 | 74, 83, 90, 94 | 0 |
| 20 | AT | 96/106 (90%) | 0.57 | 8 (8%) 11 8 | 59, 71, 80, 83 | 0 |
| 20 | CT | 96/106 (90%) | 0.92 | 15 (15%) 3 2 | 59, 71, 80, 83 | 0 |
| 21 | AU | 23/27 (85%) | 0.84 | 3 (13%) 4 3 | 70, 75, 78, 82 | 0 |
| 21 | CU | 23/27 (85%) | 3.35 | 16 (69%) 0 0 | 71, 78, 81, 82 | 0 |
| 22 | AV | 13/24 (54%) | 1.54 | 4 (30%) 1 1 | 58, 77, 95, 100 | 0 |
| 22 | CV | 12/24 (50%) | 3.21 | 7 (58%) 0 0 | 64, 81, 93, 95 | 0 |
| 23 | AW | 72/76 (94%) | 0.77 | 10 (13%) 4 2 | 66, 95, 102, 105 | 0 |
| 23 | CW | 70/76 (92%) | 2.86 | 50 (71%) 0 0 | 70, 96, 101, 106 | 0 |
| 24 | AX | 75/77 (97%) | 0.04 | 0 100 100 | 42, 71, 90, 96 | 0 |
| 24 | CX | 75/77 (97%) | 0.13 | 2 (2%) 52 49 | 55, 86, 95, 98 | 0 |
| 25 | AY | 73/76 (96%) | 0.45 | 9 (12%) 5 4 | 44, 97, 101, 105 | 0 |
| 25 | CY | 72/76 (94%) | 1.48 | 20 (27%) 1 1 | 48, 98, 102, 103 | 0 |
| 26 | BA | 2819/2915 (96%) | 0.56 | 24 (0%) 81 82 | 23, 43, 87, 106 | 0 |
| 26 | DA | 2800/2915 (96%) | -0.09 | 60 (2%) 60 58 | 27, 48, 90, 108 | 0 |
| 27 | BB | 120/121 (99%) | 0.66 | 0 100 100 | 41, 64, 76, 88 | 0 |
| 27 | DB | 120/121 (99%) | 0.12 | 9 (7%) 14 11 | 48, 70, 80, 91 | 0 |
| 28 | BD | 275/276 (99%) | 0.19 | 3 (1%) 77 79 | 24, 41, 58, 79 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DD | 275/276 (99%) | 0.40 | 15 (5%) 24 20 | 28, 44, 61, 79 | 0 |
| 29 | BE | 204/206 (99%) | 0.59 | 9 (4%) 33 29 | 23, 46, 65, 83 | 0 |
| 29 | DE | 204/206 (99%) | 0.32 | 6 (2%) 49 46 | 26, 50, 67, 84 | 0 |
| 30 | BF | 203/210 (96%) | 0.58 | 6 (2%) 48 45 | 25, 51, 76, 86 | 0 |
| 30 | DF | 203/210 (96%) | 0.75 | 23 (11%) 6 4 | 28, 56, 78, 88 | 0 |
| 31 | BG | 181/182 (99%) | 0.56 | 7 (3%) 37 33 | 55, 72, 83, 93 | 0 |
| 31 | DG | 181/182 (99%) | 2.10 | 84 (46%) 1 0 | 64, 76, 85, 93 | 0 |
| 32 | BH | 174/180 (96%) | 0.53 | 2 (1%) 77 79 | 50, 66, 75, 82 | 0 |
| 32 | DH | 174/180 (96%) | 2.10 | 80 (45%) 1 0 | 56, 71, 79, 83 | 0 |
| 33 | BI | 146/148 (98%) | 0.51 | 12 (8%) 12 9 | 49, 74, 83, 87 | 0 |
| 33 | DI | 146/148 (98%) | 0.32 | 7 (4%) 29 26 | 50, 74, 83, 87 | 0 |
| 34 | BN | 140/140 (100%) | 0.56 | 0 100 100 | 29, 48, 67, 79 | 0 |
| 34 | DN | 140/140 (100%) | 1.17 | 21 (15%) 3 2 | 35, 53, 70, 82 | 0 |
| 35 | BO | 122/122 (100%) | 0.04 | 0 100 100 | 25, 40, 57, 67 | 0 |
| 35 | DO | 122/122 (100%) | 0.27 | 0 100 100 | 44, 58, 74, 79 | 0 |
| 36 | BP | 149/150 (99%) | 0.59 | 6 (4%) 36 32 | 25, 55, 75, 80 | 0 |
| 36 | DP | 149/150 (99%) | 0.85 | 19 (12%) 4 3 | 28, 58, 78, 83 | 0 |
| 37 | BQ | 141/141 (100%) | 0.67 | 5 (3%) 42 38 | 37, 52, 68, 77 | 0 |
| 37 | DQ | 141/141 (100%) | 1.44 | 38 (26%) 1 1 | 41, 58, 72, 79 | 0 |
| 38 | BR | 118/118 (100%) | 0.25 | 0 100 100 | 22, 34, 50, 59 | 0 |
| 38 | DR | 118/118 (100%) | 0.90 | 15 (12%) 4 3 | 38, 53, 64, 75 | 0 |
| 39 | BS | 110/112 (98%) | 0.33 | 2 (1%) 65 64 | 34, 50, 64, 70 | 0 |
| 39 | DS | 110/112 (98%) | 2.83 | 69 (62%) 0 0 | 70, 79, 87, 91 | 0 |
| 40 | BT | 131/146 (89%) | 0.37 | 2 (1%) 70 71 | 38, 51, 73, 82 | 0 |
| 40 | DT | 131/146 (89%) | 0.17 | 2 (1%) 70 71 | 40, 54, 75, 81 | 0 |
| 41 | BU | 116/118 (98%) | 0.34 | 2 (1%) 67 66 | 17, 30, 50, 63 | 0 |
| 41 | DU | 116/118 (98%) | 0.75 | 8 (6%) 17 14 | 40, 59, 79, 85 | 0 |
| 42 | BV | 101/101 (100%) | 0.12 | 1 (0%) 79 81 | 16, 38, 58, 68 | 0 |
| 42 | DV | 101/101 (100%) | 0.91 | 17 (16%) 2 1 | 44, 73, 81, 92 | 0 |
| 43 | BW | 112/113 (99%) | 0.40 | 2 (1%) 65 64 | 22, 30, 49, 83 | 0 |
| 43 | DW | 112/113 (99%) | 1.08 | 18 (16%) 2 1 | 35, 50, 66, 86 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BX | 95/96 (98%) | 0.50 | 0 100 100 | 31, 46, 67, 83 | 0 |
| 44 | DX | 95/96 (98%) | 0.93 | 11 (11%) 5 4 | 36, 50, 68, 83 | 0 |
| 45 | BY | 107/110 (97%) | 0.74 | 11 (10%) 7 5 | 42, 59, 73, 84 | 0 |
| 45 | DY | 107/110 (97%) | 1.50 | 32 (29%) 1 1 | 47, 61, 75, 84 | 0 |
| 46 | BZ | 171/206 (83%) | 1.16 | 35 (20%) 1 1 | 40, 66, 91, 95 | 0 |
| 46 | DZ | 174/206 (84%) | 2.66 | 101 (58%) 0 0 | 69, 85, 94, 101 | 0 |
| 47 | B0 | 83/85 (97%) | 0.88 | 6 (7%) 15 12 | 34, 50, 67, 75 | 0 |
| 47 | D0 | 83/85 (97%) | 1.54 | 22 (26%) 1 1 | 40, 56, 71, 76 | 0 |
| 48 | B1 | 97/98 (98%) | 0.29 | 1 (1%) 79 81 | 31, 49, 72, 76 | 0 |
| 48 | D1 | 97/98 (98%) | 0.59 | 8 (8%) 12 9 | 34, 53, 73, 78 | 0 |
| 49 | B2 | 70/72 (97%) | 0.32 | 1 (1%) 72 72 | 33, 49, 64, 82 | 0 |
| 49 | D2 | 70/72 (97%) | 0.58 | 2 (2%) 49 46 | 58, 69, 78, 82 | 0 |
| 50 | B3 | 59/60 (98%) | 0.08 | 0 100 100 | 24, 37, 63, 74 | 0 |
| 50 | D3 | 59/60 (98%) | 1.24 | 12 (20%) 1 1 | 52, 65, 79, 87 | 0 |
| 51 | B4 | 69/71 (97%) | 0.83 | 13 (18%) 2 1 | 49, 76, 89, 91 | 0 |
| 51 | D4 | 69/71 (97%) | 1.73 | 27 (39%) 1 0 | 74, 89, 95, 99 | 0 |
| 52 | B5 | 59/60 (98%) | 0.14 | 1 (1%) 67 66 | 16, 30, 46, 68 | 0 |
| 52 | D5 | 59/60 (98%) | 0.36 | 1 (1%) 67 66 | 35, 49, 65, 77 | 0 |
| 53 | B6 | 53/54 (98%) | 0.19 | 0 100 100 | 32, 44, 57, 72 | 0 |
| 53 | D6 | 53/54 (98%) | 0.62 | 5 (9%) 9 6 | 49, 64, 74, 79 | 0 |
| 54 | B7 | 48/49 (97%) | 0.50 | 4 (8%) 11 8 | 23, 32, 58, 70 | 0 |
| 54 | D7 | 48/49 (97%) | 1.16 | 6 (12%) 5 3 | 26, 35, 61, 70 | 0 |
| 55 | B8 | 64/65 (98%) | 0.48 | 1 (1%) 68 69 | 34, 42, 50, 65 | 0 |
| 55 | D8 | 64/65 (98%) | 0.61 | 3 (4%) 30 27 | 37, 46, 54, 65 | 0 |
| 56 | B9 | 37/37 (100%) | 1.18 | 6 (16%) 2 1 | 36, 51, 65, 73 | 0 |
| 56 | D9 | 37/37 (100%) | 0.53 | 4 (10%) 6 5 | 43, 55, 68, 76 | 0 |
| All | All | 20927/21748 (96%) | 0.65 | 2204 (10%) 7 5 | 16, 64, 90, 108 | 0 |

The worst 5 of 2204 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | CB | 165 | VAL | 16.5 |
| 13 | CM | 124 | PRO | 15.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13 | CM | 123 | ALA | 13.6 |
| 13 | CM | 122 | LYS | 13.0 |
| 46 | DZ | 171 | ILE | 11.8 |

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

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

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 23 | PSU | AW | 32 | 20/21 | 0.23 | - | 77,84,98,106 | 0 |
| 23 | MIA | AW | 37 | 29/30 | 0.22 | - | 56,65,80,82 | 0 |
| 23 | MIA | CW | 37 | 22/30 | 0.29 | - | 72,86,92,96 | 0 |
| 24 | 31H | AX | 76 | 32/33 | 0.31 | - | 31,57,76,77 | 10 |
| 23 | 7MG | AW | 46 | 24/25 | 0.17 | - | 80,97,112,135 | 0 |
| 25 | 7MG | AY | 46 | 24/25 | 0.20 | - | 80,99,107,116 | 0 |
| 24 | 4SU | CX | 8 | 20/21 | 0.13 | - | 84,92,105,111 | 0 |
| 25 | PSU | CY | 32 | 20/21 | 0.23 | - | 77,91,109,114 | 0 |
| 23 | PSU | CW | 32 | 20/21 | 0.55 | - | 77,86,95,106 | 0 |
| 23 | PSU | AW | 55 | 20/21 | 0.20 | - | 76,88,103,105 | 0 |
| 25 | PSU | CY | 55 | 20/21 | 0.40 | - | 86,100,107,118 | 0 |
| 25 | PSU | AY | 55 | 20/21 | 0.18 | - | 85,96,106,117 | 0 |
| 23 | 5MU | AW | 54 | 21/22 | 0.17 | - | 66,80,87,93 | 0 |
| 24 | 5MC | AX | 32 | 21/22 | 0.16 | - | 50,57,69,76 | 0 |
| 23 | 4SU | AW | 8 | 20/21 | 0.12 | - | 83,89,107,110 | 0 |
| 23 | PSU | AW | 39 | 20/21 | 0.18 | - | 71,82,92,93 | 0 |
| 25 | MIA | AY | 37 | 22/30 | 0.18 | - | 79,89,101,116 | 0 |
| 24 | 5MU | CX | 54 | 21/22 | 0.15 | - | 71,85,94,104 | 0 |
| 24 | 5MC | CX | 32 | 21/22 | 0.16 | - | 63,77,85,87 | 0 |
| 23 | F3N | CW | 76 | 33/34 | 0.45 | - | 53,69,79,80 | 0 |
| 25 | PSU | AY | 32 | 20/21 | 0.21 | - | 76,92,107,110 | 0 |
| 24 | PSU | CX | 55 | 20/21 | 0.12 | - | 81,87,92,97 | 0 |
| 23 | 5MU | CW | 54 | 21/22 | 0.17 | - | 76,87,97,99 | 0 |
| 23 | PSU | CW | 55 | 20/21 | 0.24 | - | 76,90,103,106 | 0 |
| 25 | 4SU | CY | 8 | 20/21 | 0.14 | - | 88,102,112,128 | 0 |
| 23 | F3N | AW | 76 | 33/34 | 0.33 | - | 44,58,72,77 | 0 |
| 24 | PSU | AX | 55 | 20/21 | 0.15 | - | 52,69,77,77 | 0 |
| 25 | 4SU | AY | 8 | 20/21 | 0.12 | - | 83,95,104,129 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 25 | 5MU | CY | 54 | 21/22 | 0.52 | - | 89,99,105,136 | 0 |
| 23 | 4SU | CW | 8 | 20/21 | 0.23 | - | 85,96,117,121 | 0 |
| 25 | PSU | CY | 39 | 20/21 | 0.23 | - | 86,91,104,110 | 0 |
| 25 | MIA | CY | 37 | 22/30 | 0.26 | - | 79,95,102,124 | 0 |
| 25 | 5MU | AY | 54 | 21/22 | 0.15 | - | 81,89,99,128 | 0 |
| 24 | 4SU | AX | 8 | 20/21 | 0.16 | - | 59,69,79,85 | 0 |
| 23 | 7MG | CW | 46 | 24/25 | 0.27 | - | 81,97,101,125 | 0 |
| 25 | 7MG | CY | 46 | 24/25 | 0.21 | - | 87,101,108,135 | 0 |
| 23 | PSU | CW | 39 | 20/21 | 0.41 | - | 76,85,92,95 | 0 |
| 24 | 5MU | AX | 54 | 21/22 | 0.15 | - | 46,72,77,86 | 0 |
| 25 | PSU | AY | 39 | 20/21 | 0.20 | - | 84,90,102,107 | 0 |
| 24 | 31H | CX | 76 | 32/33 | 0.34 | - | 48,68,88,99 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3605 | 1/1 | 0.17 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3126 | 1/1 | 0.22 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3442 | 1/1 | 0.16 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3401 | 1/1 | 0.05 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3487 | 1/1 | 0.11 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1643 | 1/1 | 0.15 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3583 | 1/1 | 0.12 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3007 | 1/1 | 0.10 | - | 30,30,30,30 | 0 |
| 57 | MG | DA | 3207 | 1/1 | 0.12 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3014 | 1/1 | 0.23 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3482 | 1/1 | 0.13 | - | 60,60,60,60 | 0 |
| 57 | MG | AX | 3011 | 1/1 | 0.11 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3688 | 1/1 | 0.25 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3523 | 1/1 | 0.13 | - | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BF | 310 | 1/1 | 0.20 | - | 56,56,56,56 | 0 |
| 57 | MG | AA | 1656 | 1/1 | 0.18 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3016 | 1/1 | 0.26 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3345 | 1/1 | 0.11 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3285 | 1/1 | 0.12 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3552 | 1/1 | 0.12 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3532 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3568 | 1/1 | 0.23 | - | 24,24,24,24 | 0 |
| 57 | MG | DA | 3652 | 1/1 | 0.12 | - | 31,31,31,31 | 0 |
| 57 | MG | CA | 3100 | 1/1 | 0.10 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3296 | 1/1 | 0.08 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3570 | 1/1 | 0.18 | - | 31,31,31,31 | 0 |
| 57 | MG | AA | 1746 | 1/1 | 0.12 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3174 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1672 | 1/1 | 0.19 | - | 45,45,45,45 | 0 |
| 57 | MG | BB | 3005 | 1/1 | 0.21 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3073 | 1/1 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | CA | 3169 | 1/1 | 0.30 | - | 62,62,62,62 | 0 |
| 57 | MG | B9 | 502 | 1/1 | 0.33 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3312 | 1/1 | 0.12 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3586 | 1/1 | 0.09 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3512 | 1/1 | 0.18 | - | 23,23,23,23 | 0 |
| 57 | MG | CA | 3013 | 1/1 | 0.10 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3261 | 1/1 | 0.14 | - | 39,39,39,39 | 0 |
| 57 | MG | CA | 3041 | 1/1 | 0.10 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3603 | 1/1 | 0.25 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3194 | 1/1 | 0.14 | - | 48,48,48,48 | 0 |
| 57 | MG | DW | 3001 | 1/1 | 0.21 | - | 41,41,41,41 | 0 |
| 57 | MG | BV | 203 | 1/1 | 0.18 | - | 23,23,23,23 | 0 |
| 57 | MG | BA | 3679 | 1/1 | 0.18 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1742 | 1/1 | 0.13 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3013 | 1/1 | 0.14 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3007 | 1/1 | 0.17 | - | 21,21,21,21 | 0 |
| 57 | MG | BA | 3290 | 1/1 | 0.17 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3019 | 1/1 | 0.24 | - | 54,54,54,54 | 0 |
| 57 | MG | BB | 3019 | 1/1 | 0.17 | - | 70,70,70,70 | 0 |
| 57 | MG | DA | 3051 | 1/1 | 0.08 | - | 44,44,44,44 | 0 |
| 57 | MG | BR | 5002 | 1/1 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1807 | 1/1 | 0.07 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3425 | 1/1 | 0.22 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3734 | 1/1 | 0.13 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3445 | 1/1 | 0.10 | - | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1654 | 1/1 | 0.23 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3348 | 1/1 | 0.21 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3357 | 1/1 | 0.05 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3757 | 1/1 | 0.28 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3494 | 1/1 | 0.08 | - | 38,38,38,38 | 0 |
| 57 | MG | CA | 3034 | 1/1 | 0.18 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3694 | 1/1 | 0.22 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3783 | 1/1 | 0.13 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3175 | 1/1 | 0.09 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1801 | 1/1 | 0.06 | - | 71,71,71,71 | 0 |
| 57 | MG | AA | 1798 | 1/1 | 0.12 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3213 | 1/1 | 0.21 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3291 | 1/1 | 0.13 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3747 | 1/1 | 0.22 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3323 | 1/1 | 0.18 | - | 57,57,57,57 | 0 |
| 57 | MG | AA | 1731 | 1/1 | 0.13 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3350 | 1/1 | 0.15 | - | 31,31,31,31 | 0 |
| 57 | MG | DA | 3252 | 1/1 | 0.09 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3057 | 1/1 | 0.16 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3278 | 1/1 | 0.07 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3071 | 1/1 | 0.20 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3551 | 1/1 | 0.16 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3074 | 1/1 | 0.04 | - | 59,59,59,59 | 0 |
| 57 | MG | BB | 3021 | 1/1 | 0.20 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3574 | 1/1 | 0.06 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3356 | 1/1 | 0.20 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3225 | 1/1 | 0.12 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3583 | 1/1 | 0.16 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3063 | 1/1 | 0.21 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1697 | 1/1 | 0.11 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1757 | 1/1 | 0.25 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3529 | 1/1 | 0.23 | - | 24,24,24,24 | 0 |
| 57 | MG | BA | 3183 | 1/1 | 0.58 | - | 49,49,49,49 | 0 |
| 57 | MG | BB | 3008 | 1/1 | 0.29 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3123 | 1/1 | 0.09 | - | 43,43,43,43 | 0 |
| 57 | MG | CK | 5001 | 1/1 | 0.11 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3206 | 1/1 | 0.13 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3760 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3358 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3096 | 1/1 | 0.15 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3571 | 1/1 | 0.29 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3173 | 1/1 | 0.22 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59 | ZN | B6 | 102 | 1/1 | 0.23 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1815 | 1/1 | 0.12 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3027 | 1/1 | 0.37 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3032 | 1/1 | 0.20 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3361 | 1/1 | 0.08 | - | 33,33,33,33 | 0 |
| 57 | MG | AA | 1710 | 1/1 | 0.13 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3547 | 1/1 | 0.14 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1795 | 1/1 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | AU | 101 | 1/1 | 0.09 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3588 | 1/1 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3054 | 1/1 | 0.19 | - | 30,30,30,30 | 0 |
| 57 | MG | DN | 5001 | 1/1 | 0.11 | - | 63,63,63,63 | 0 |
| 57 | MG | AA | 1639 | 1/1 | 0.06 | - | 54,54,54,54 | 0 |
| 57 | MG | AA | 1677 | 1/1 | 0.22 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3593 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | DR | 3001 | 1/1 | 0.15 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3527 | 1/1 | 0.13 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3304 | 1/1 | 0.15 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3219 | 1/1 | 0.49 | - | 58,58,58,58 | 0 |
| 57 | MG | AA | 1606 | 1/1 | 0.12 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3314 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | BZ | 302 | 1/1 | 0.11 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3419 | 1/1 | 0.09 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3573 | 1/1 | 0.06 | - | 61,61,61,61 | 0 |
| 57 | MG | B0 | 3002 | 1/1 | 0.18 | - | 63,63,63,63 | 0 |
| 57 | MG | BF | 303 | 1/1 | 0.21 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3117 | 1/1 | 0.06 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3791 | 1/1 | 0.33 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3431 | 1/1 | 0.26 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3383 | 1/1 | 0.14 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3558 | 1/1 | 0.13 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3010 | 1/1 | 0.06 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3040 | 1/1 | 0.11 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3811 | 1/1 | 0.20 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3714 | 1/1 | 0.09 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3049 | 1/1 | 0.16 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3669 | 1/1 | 0.19 | - | 28,28,28,28 | 0 |
| 57 | MG | BF | 309 | 1/1 | 0.21 | - | 31,31,31,31 | 0 |
| 57 | MG | DA | 3232 | 1/1 | 0.17 | - | 56,56,56,56 | 0 |
| 57 | MG | DB | 3010 | 1/1 | 0.08 | - | 75,75,75,75 | 0 |
| 57 | MG | DA | 3366 | 1/1 | 0.10 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3061 | 1/1 | 0.24 | - | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3101 | 1/1 | 0.22 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3335 | 1/1 | 0.19 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3627 | 1/1 | 0.15 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3134 | 1/1 | 0.18 | - | 40,40,40,40 | 0 |
| 57 | MG | AA | 1716 | 1/1 | 0.15 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3103 | 1/1 | 0.17 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3424 | 1/1 | 0.25 | - | 31,31,31,31 | 0 |
| 57 | MG | AA | 1651 | 1/1 | 0.24 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3609 | 1/1 | 0.17 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3030 | 1/1 | 0.11 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3042 | 1/1 | 0.08 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3261 | 1/1 | 0.14 | - | 18,18,18,18 | 0 |
| 57 | MG | BA | 3463 | 1/1 | 0.24 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3191 | 1/1 | 0.16 | - | 40,40,40,40 | 0 |
| 57 | MG | CA | 3139 | 1/1 | 0.33 | - | 81,81,81,81 | 0 |
| 57 | MG | CA | 3114 | 1/1 | 0.12 | - | 71,71,71,71 | 0 |
| 57 | MG | AA | 1814 | 1/1 | 0.18 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3346 | 1/1 | 0.07 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3464 | 1/1 | 0.28 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3039 | 1/1 | 0.11 | - | 38,38,38,38 | 0 |
| 57 | MG | B6 | 103 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3203 | 1/1 | 0.14 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1741 | 1/1 | 0.12 | - | 86,86,86,86 | 0 |
| 57 | MG | DA | 3381 | 1/1 | 0.10 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3288 | 1/1 | 0.16 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3170 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3560 | 1/1 | 0.15 | - | 60,60,60,60 | 0 |
| 57 | MG | CA | 3002 | 1/1 | 0.17 | - | 77,77,77,77 | 0 |
| 57 | MG | DA | 3512 | 1/1 | 0.11 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3539 | 1/1 | 0.08 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3042 | 1/1 | 0.27 | - | 49,49,49,49 | 0 |
| 57 | MG | BD | 3008 | 1/1 | 0.27 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3662 | 1/1 | 0.19 | - | 50,50,50,50 | 0 |
| 59 | ZN | B4 | 501 | 1/1 | 0.09 | - | 118,118,118,118 | 0 |
| 57 | MG | DA | 3558 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3159 | 1/1 | 0.13 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3370 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3410 | 1/1 | 0.20 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3623 | 1/1 | 0.12 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1684 | 1/1 | 0.11 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3788 | 1/1 | 0.18 | - | 44,44,44,44 | 0 |
| 57 | MG | AA | 1721 | 1/1 | 0.14 | - | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1806 | 1/1 | 0.16 | - | 74,74,74,74 | 0 |
| 59 | ZN | AN | 501 | 1/1 | 0.16 | - | 77,77,77,77 | 0 |
| 57 | MG | BA | 3034 | 1/1 | 0.17 | - | 35,35,35,35 | 0 |
| 57 | MG | AA | 1601 | 1/1 | 0.14 | - | 81,81,81,81 | 0 |
| 57 | MG | DO | 201 | 1/1 | 0.08 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3680 | 1/1 | 0.31 | - | 42,42,42,42 | 0 |
| 57 | MG | CA | 3039 | 1/1 | 0.09 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3288 | 1/1 | 0.14 | - | 39,39,39,39 | 0 |
| 57 | MG | AL | 201 | 1/1 | 0.11 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3629 | 1/1 | 0.12 | - | 57,57,57,57 | 0 |
| 57 | MG | AN | 503 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3298 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3636 | 1/1 | 0.13 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3109 | 1/1 | 0.08 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3545 | 1/1 | 0.18 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3270 | 1/1 | 0.22 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3599 | 1/1 | 0.09 | - | 48,48,48,48 | 0 |
| 57 | MG | BG | 202 | 1/1 | 0.13 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3340 | 1/1 | 0.15 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3119 | 1/1 | 0.09 | - | 46,46,46,46 | 0 |
| 57 | MG | CA | 3113 | 1/1 | 0.13 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1767 | 1/1 | 0.09 | - | 67,67,67,67 | 0 |
| 57 | MG | AA | 1788 | 1/1 | 0.06 | - | 75,75,75,75 | 0 |
| 57 | MG | BA | 3589 | 1/1 | 0.20 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3465 | 1/1 | 0.17 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3272 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3032 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3130 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 59 | ZN | BY | 501 | 1/1 | 0.16 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3468 | 1/1 | 0.15 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1754 | 1/1 | 0.16 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3291 | 1/1 | 0.25 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3480 | 1/1 | 0.11 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3447 | 1/1 | 0.24 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3239 | 1/1 | 0.10 | - | 49,49,49,49 | 0 |
| 57 | MG | DB | 3004 | 1/1 | 0.20 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3347 | 1/1 | 0.16 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3229 | 1/1 | 0.20 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3095 | 1/1 | 0.10 | - | 71,71,71,71 | 0 |
| 57 | MG | DA | 3146 | 1/1 | 0.06 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3417 | 1/1 | 0.21 | - | 24,24,24,24 | 0 |
| 57 | MG | BA | 3384 | 1/1 | 0.10 | - | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3571 | 1/1 | 0.22 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3794 | 1/1 | 0.11 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3211 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3656 | 1/1 | 0.12 | - | 45,45,45,45 | 0 |
| 57 | MG | CA | 3166 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1706 | 1/1 | 0.18 | - | 60,60,60,60 | 0 |
| 57 | MG | CA | 3036 | 1/1 | 0.17 | - | 73,73,73,73 | 0 |
| 57 | MG | DA | 3229 | 1/1 | 0.12 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3388 | 1/1 | 0.22 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3467 | 1/1 | 0.23 | - | 52,52,52,52 | 0 |
| 57 | MG | DE | 3004 | 1/1 | 0.15 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3276 | 1/1 | 0.49 | - | 44,44,44,44 | 0 |
| 57 | MG | CA | 3054 | 1/1 | 0.32 | - | 69,69,69,69 | 0 |
| 57 | MG | DB | 3002 | 1/1 | 0.26 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3233 | 1/1 | 0.14 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3576 | 1/1 | 0.20 | - | 30,30,30,30 | 0 |
| 57 | MG | BA | 3079 | 1/1 | 0.30 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3487 | 1/1 | 0.11 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3224 | 1/1 | 0.24 | - | 59,59,59,59 | 0 |
| 57 | MG | DG | 3001 | 1/1 | 0.09 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3514 | 1/1 | 0.13 | - | 47,47,47,47 | 0 |
| 57 | MG | CA | 3031 | 1/1 | 0.10 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3155 | 1/1 | 0.17 | - | 40,40,40,40 | 0 |
| 57 | MG | BB | 3009 | 1/1 | 0.07 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3456 | 1/1 | 0.24 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3502 | 1/1 | 0.16 | - | 30,30,30,30 | 0 |
| 57 | MG | AA | 1653 | 1/1 | 0.21 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3548 | 1/1 | 0.15 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3302 | 1/1 | 0.18 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3813 | 1/1 | 0.19 | - | 29,29,29,29 | 0 |
| 57 | MG | CA | 3052 | 1/1 | 0.09 | - | 71,71,71,71 | 0 |
| 57 | MG | BA | 3452 | 1/1 | 0.11 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3264 | 1/1 | 0.16 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3066 | 1/1 | 0.08 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3561 | 1/1 | 0.11 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3194 | 1/1 | 0.19 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3370 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3069 | 1/1 | 0.24 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3510 | 1/1 | 0.23 | - | 64,64,64,64 | 0 |
| 59 | ZN | DY | 501 | 1/1 | 0.11 | - | 90,90,90,90 | 0 |
| 57 | MG | DA | 3579 | 1/1 | 0.14 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3102 | 1/1 | 0.24 | - | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3050 | 1/1 | 0.21 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3727 | 1/1 | 0.22 | - | 53,53,53,53 | 0 |
| 57 | MG | DB | 3003 | 1/1 | 0.09 | - | 78,78,78,78 | 0 |
| 57 | MG | BA | 3199 | 1/1 | 0.27 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3092 | 1/1 | 0.12 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3435 | 1/1 | 0.11 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3310 | 1/1 | 0.20 | - | 26,26,26,26 | 0 |
| 57 | MG | BA | 3204 | 1/1 | 0.26 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3075 | 1/1 | 0.07 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3400 | 1/1 | 0.23 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3185 | 1/1 | 0.12 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3212 | 1/1 | 0.20 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3768 | 1/1 | 0.09 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3133 | 1/1 | 0.25 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3036 | 1/1 | 0.10 | - | 56,56,56,56 | 0 |
| 59 | ZN | D5 | 501 | 1/1 | 0.17 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3657 | 1/1 | 0.10 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3022 | 1/1 | 0.10 | - | 25,25,25,25 | 0 |
| 57 | MG | DA | 3642 | 1/1 | 0.13 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3500 | 1/1 | 0.16 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3486 | 1/1 | 0.25 | - | 57,57,57,57 | 0 |
| 57 | MG | BQ | 3001 | 1/1 | 0.19 | - | 37,37,37,37 | 0 |
| 57 | MG | BD | 3005 | 1/1 | 0.19 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3331 | 1/1 | 0.17 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3422 | 1/1 | 0.26 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3336 | 1/1 | 0.12 | - | 20,20,20,20 | 0 |
| 57 | MG | BA | 3230 | 1/1 | 0.22 | - | 58,58,58,58 | 0 |
| 57 | MG | DQ | 3003 | 1/1 | 0.66 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3365 | 1/1 | 0.13 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3144 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3437 | 1/1 | 0.21 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3597 | 1/1 | 0.20 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3107 | 1/1 | 0.08 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3002 | 1/1 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3585 | 1/1 | 0.30 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3564 | 1/1 | 0.08 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3004 | 1/1 | 0.14 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1712 | 1/1 | 0.13 | - | 69,69,69,69 | 0 |
| 57 | MG | CA | 3046 | 1/1 | 0.17 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3611 | 1/1 | 0.16 | - | 59,59,59,59 | 0 |
| 57 | MG | CA | 3135 | 1/1 | 0.09 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3009 | 1/1 | 0.13 | - | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3325 | 1/1 | 0.13 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1714 | 1/1 | 0.16 | - | 56,56,56,56 | 0 |
| 57 | MG | DB | 3005 | 1/1 | 0.14 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3451 | 1/1 | 0.07 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3538 | 1/1 | 0.14 | - | 68,68,68,68 | 0 |
| 57 | MG | CA | 3120 | 1/1 | 0.10 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3383 | 1/1 | 0.13 | - | 28,28,28,28 | 0 |
| 57 | MG | CA | 3020 | 1/1 | 0.15 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3227 | 1/1 | 0.14 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3397 | 1/1 | 0.12 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3212 | 1/1 | 0.21 | - | 57,57,57,57 | 0 |
| 57 | MG | AA | 1657 | 1/1 | 0.09 | - | 64,64,64,64 | 0 |
| 57 | MG | AA | 1621 | 1/1 | 0.11 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3446 | 1/1 | 0.08 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3258 | 1/1 | 0.45 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3041 | 1/1 | 0.28 | - | 60,60,60,60 | 0 |
| 57 | MG | B7 | 105 | 1/1 | 0.21 | - | 28,28,28,28 | 0 |
| 57 | MG | DA | 3242 | 1/1 | 0.07 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3277 | 1/1 | 0.50 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3519 | 1/1 | 0.16 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3218 | 1/1 | 0.11 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1709 | 1/1 | 0.22 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1664 | 1/1 | 0.17 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3806 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | CA | 3115 | 1/1 | 0.19 | - | 82,82,82,82 | 0 |
| 57 | MG | BP | 3002 | 1/1 | 0.15 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3414 | 1/1 | 0.14 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3582 | 1/1 | 0.04 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3106 | 1/1 | 0.24 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3298 | 1/1 | 0.13 | - | 27,27,27,27 | 0 |
| 57 | MG | CA | 3028 | 1/1 | 0.25 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3379 | 1/1 | 0.14 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3008 | 1/1 | 0.08 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1816 | 1/1 | 0.21 | - | 59,59,59,59 | 0 |
| 57 | MG | B7 | 103 | 1/1 | 0.31 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3171 | 1/1 | 0.13 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3491 | 1/1 | 0.22 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3323 | 1/1 | 0.20 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3614 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3640 | 1/1 | 0.08 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3349 | 1/1 | 0.14 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3468 | 1/1 | 0.17 | - | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3369 | 1/1 | 0.13 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3374 | 1/1 | 0.18 | - | 62,62,62,62 | 0 |
| 57 | MG | CA | 3025 | 1/1 | 0.16 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1792 | 1/1 | 0.07 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3472 | 1/1 | 0.19 | - | 24,24,24,24 | 0 |
| 57 | MG | BA | 3536 | 1/1 | 0.11 | - | 32,32,32,32 | 0 |
| 57 | MG | DA | 3329 | 1/1 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3555 | 1/1 | 0.17 | - | 46,46,46,46 | 0 |
| 57 | MG | AA | 1612 | 1/1 | 0.15 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3215 | 1/1 | 0.19 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3306 | 1/1 | 0.25 | - | 65,65,65,65 | 0 |
| 57 | MG | D0 | 101 | 1/1 | 0.15 | - | 71,71,71,71 | 0 |
| 57 | MG | DA | 3067 | 1/1 | 0.12 | - | 63,63,63,63 | 0 |
| 57 | MG | AA | 1802 | 1/1 | 0.06 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3327 | 1/1 | 0.17 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3201 | 1/1 | 0.11 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3235 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3646 | 1/1 | 0.12 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3615 | 1/1 | 0.05 | - | 62,62,62,62 | 0 |
| 57 | MG | AT | 3001 | 1/1 | 0.11 | - | 63,63,63,63 | 0 |
| 57 | MG | CA | 3014 | 1/1 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3251 | 1/1 | 0.11 | - | 40,40,40,40 | 0 |
| 57 | MG | AA | 1689 | 1/1 | 0.19 | - | 71,71,71,71 | 0 |
| 57 | MG | DA | 3098 | 1/1 | 0.05 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3718 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | CA | 3105 | 1/1 | 0.05 | - | 75,75,75,75 | 0 |
| 57 | MG | AA | 1770 | 1/1 | 0.15 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3049 | 1/1 | 0.06 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3276 | 1/1 | 0.15 | - | 28,28,28,28 | 0 |
| 57 | MG | AA | 1618 | 1/1 | 0.17 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3303 | 1/1 | 0.23 | - | 26,26,26,26 | 0 |
| 57 | MG | AA | 1607 | 1/1 | 0.12 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3071 | 1/1 | 0.27 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3070 | 1/1 | 0.20 | - | 41,41,41,41 | 0 |
| 57 | MG | BB | 3002 | 1/1 | 0.26 | - | 55,55,55,55 | 0 |
| 57 | MG | BB | 3007 | 1/1 | 0.14 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1698 | 1/1 | 0.16 | - | 58,58,58,58 | 0 |
| 57 | MG | AA | 1702 | 1/1 | 0.25 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3021 | 1/1 | 0.16 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3569 | 1/1 | 0.20 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3502 | 1/1 | 0.23 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3168 | 1/1 | 0.13 | - | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CA | 3001 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3161 | 1/1 | 0.18 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3299 | 1/1 | 0.09 | - | 46,46,46,46 | 0 |
| 57 | MG | AX | 3008 | 1/1 | 0.14 | - | 76,76,76,76 | 0 |
| 57 | MG | AA | 1615 | 1/1 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3128 | 1/1 | 0.13 | - | 42,42,42,42 | 0 |
| 57 | MG | AX | 3003 | 1/1 | 0.20 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3125 | 1/1 | 0.22 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3466 | 1/1 | 0.12 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3147 | 1/1 | 0.10 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3662 | 1/1 | 0.20 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3436 | 1/1 | 0.11 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3666 | 1/1 | 0.18 | - | 74,74,74,74 | 0 |
| 57 | MG | CA | 3008 | 1/1 | 0.27 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3218 | 1/1 | 0.09 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3284 | 1/1 | 0.08 | - | 57,57,57,57 | 0 |
| 57 | MG | AA | 1634 | 1/1 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3250 | 1/1 | 0.15 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3280 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3279 | 1/1 | 0.23 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3273 | 1/1 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3405 | 1/1 | 0.06 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3726 | 1/1 | 0.17 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3245 | 1/1 | 0.24 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3192 | 1/1 | 0.27 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3047 | 1/1 | 0.12 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3378 | 1/1 | 0.10 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3224 | 1/1 | 0.08 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3130 | 1/1 | 0.43 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3779 | 1/1 | 0.16 | - | 17,17,17,17 | 0 |
| 57 | MG | CA | 3029 | 1/1 | 0.09 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3691 | 1/1 | 0.06 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3110 | 1/1 | 0.06 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3809 | 1/1 | 0.41 | - | 61,61,61,61 | 0 |
| 57 | MG | CA | 3058 | 1/1 | 0.10 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3515 | 1/1 | 0.14 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3575 | 1/1 | 0.12 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3077 | 1/1 | 0.17 | - | 15,15,15,15 | 0 |
| 57 | MG | BA | 3485 | 1/1 | 0.23 | - | 26,26,26,26 | 0 |
| 57 | MG | AA | 1810 | 1/1 | 0.06 | - | 86,86,86,86 | 0 |
| 57 | MG | AA | 1661 | 1/1 | 0.32 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3104 | 1/1 | 0.18 | - | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3371 | 1/1 | 0.14 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3785 | 1/1 | 0.15 | - | 56,56,56,56 | 0 |
| 57 | MG | B7 | 102 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3659 | 1/1 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3501 | 1/1 | 0.11 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3125 | 1/1 | 0.13 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3062 | 1/1 | 0.06 | - | 53,53,53,53 | 0 |
| 57 | MG | BV | 201 | 1/1 | 0.39 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3058 | 1/1 | 0.26 | - | 54,54,54,54 | 0 |
| 57 | MG | AA | 1715 | 1/1 | 0.18 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3594 | 1/1 | 0.13 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3496 | 1/1 | 0.11 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3135 | 1/1 | 0.33 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3621 | 1/1 | 0.54 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3801 | 1/1 | 0.17 | - | 71,71,71,71 | 0 |
| 57 | MG | AA | 1803 | 1/1 | 0.10 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3631 | 1/1 | 0.25 | - | 46,46,46,46 | 0 |
| 57 | MG | CA | 3064 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3051 | 1/1 | 0.18 | - | 37,37,37,37 | 0 |
| 57 | MG | AA | 1663 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1718 | 1/1 | 0.09 | - | 66,66,66,66 | 0 |
| 57 | MG | CA | 3145 | 1/1 | 0.07 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3360 | 1/1 | 0.21 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3001 | 1/1 | 0.15 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3304 | 1/1 | 0.15 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3777 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3146 | 1/1 | 0.15 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1733 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3573 | 1/1 | 0.22 | - | 41,41,41,41 | 0 |
| 57 | MG | CA | 3033 | 1/1 | 0.05 | - | 54,54,54,54 | 0 |
| 57 | MG | BB | 3014 | 1/1 | 0.12 | - | 67,67,67,67 | 0 |
| 57 | MG | BW | 3002 | 1/1 | 0.12 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3313 | 1/1 | 0.11 | - | 39,39,39,39 | 0 |
| 57 | MG | AA | 1738 | 1/1 | 0.39 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3613 | 1/1 | 0.10 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3690 | 1/1 | 0.10 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3223 | 1/1 | 0.14 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3392 | 1/1 | 0.16 | - | 53,53,53,53 | 0 |
| 57 | MG | CA | 3153 | 1/1 | 0.10 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3597 | 1/1 | 0.11 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3248 | 1/1 | 0.12 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3674 | 1/1 | 0.38 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BE | 303 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3630 | 1/1 | 0.13 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3008 | 1/1 | 0.11 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3306 | 1/1 | 0.13 | - | 15,15,15,15 | 0 |
| 57 | MG | CA | 3004 | 1/1 | 0.07 | - | 69,69,69,69 | 0 |
| 57 | MG | AA | 1687 | 1/1 | 0.22 | - | 46,46,46,46 | 0 |
| 57 | MG | CA | 3086 | 1/1 | 0.18 | - | 93,93,93,93 | 0 |
| 57 | MG | BA | 3423 | 1/1 | 0.14 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3256 | 1/1 | 0.12 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3351 | 1/1 | 0.16 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3232 | 1/1 | 0.20 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3148 | 1/1 | 0.21 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3321 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3484 | 1/1 | 0.10 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3023 | 1/1 | 0.12 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3711 | 1/1 | 0.18 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3052 | 1/1 | 0.07 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3602 | 1/1 | 0.24 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3634 | 1/1 | 0.13 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3256 | 1/1 | 0.36 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3171 | 1/1 | 0.45 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3648 | 1/1 | 0.20 | - | 58,58,58,58 | 0 |
| 57 | MG | CA | 3161 | 1/1 | 0.12 | - | 76,76,76,76 | 0 |
| 57 | MG | BA | 3741 | 1/1 | 0.10 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3206 | 1/1 | 0.06 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3460 | 1/1 | 0.10 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1692 | 1/1 | 0.12 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3255 | 1/1 | 0.20 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3260 | 1/1 | 0.11 | - | 19,19,19,19 | 0 |
| 57 | MG | BA | 3775 | 1/1 | 0.28 | - | 39,39,39,39 | 0 |
| 57 | MG | CA | 3158 | 1/1 | 0.16 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3116 | 1/1 | 0.23 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3746 | 1/1 | 0.11 | - | 78,78,78,78 | 0 |
| 57 | MG | BA | 3608 | 1/1 | 0.25 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3759 | 1/1 | 0.11 | - | 70,70,70,70 | 0 |
| 57 | MG | DA | 3457 | 1/1 | 0.14 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3624 | 1/1 | 0.45 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3368 | 1/1 | 0.08 | - | 67,67,67,67 | 0 |
| 57 | MG | AA | 1809 | 1/1 | 0.16 | - | 42,42,42,42 | 0 |
| 57 | MG | BE | 306 | 1/1 | 0.07 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3405 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3113 | 1/1 | 0.09 | - | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3149 | 1/1 | 0.08 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3664 | 1/1 | 0.20 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3188 | 1/1 | 0.23 | - | 35,35,35,35 | 0 |
| 57 | MG | AA | 1673 | 1/1 | 0.11 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3246 | 1/1 | 0.05 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3332 | 1/1 | 0.15 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3338 | 1/1 | 0.08 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3542 | 1/1 | 0.26 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3412 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1793 | 1/1 | 0.15 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3792 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3739 | 1/1 | 0.07 | - | 21,21,21,21 | 0 |
| 57 | MG | AA | 1679 | 1/1 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3324 | 1/1 | 0.16 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3141 | 1/1 | 0.10 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3426 | 1/1 | 0.14 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3616 | 1/1 | 0.16 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3119 | 1/1 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3467 | 1/1 | 0.10 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3347 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 57 | MG | CA | 3121 | 1/1 | 0.07 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3477 | 1/1 | 0.08 | - | 53,53,53,53 | 0 |
| 57 | MG | CA | 3123 | 1/1 | 0.24 | - | 61,61,61,61 | 0 |
| 57 | MG | AA | 1691 | 1/1 | 0.27 | - | 62,62,62,62 | 0 |
| 57 | MG | CA | 3048 | 1/1 | 0.12 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3167 | 1/1 | 0.20 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3012 | 1/1 | 0.20 | - | 25,25,25,25 | 0 |
| 57 | MG | DA | 3515 | 1/1 | 0.09 | - | 55,55,55,55 | 0 |
| 57 | MG | BF | 301 | 1/1 | 0.29 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3447 | 1/1 | 0.15 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3065 | 1/1 | 0.12 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3309 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3004 | 1/1 | 0.16 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3034 | 1/1 | 0.09 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3564 | 1/1 | 0.25 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1640 | 1/1 | 0.17 | - | 54,54,54,54 | 0 |
| 57 | MG | CA | 3061 | 1/1 | 0.16 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3168 | 1/1 | 0.25 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3647 | 1/1 | 0.10 | - | 53,53,53,53 | 0 |
| 57 | MG | DB | 3011 | 1/1 | 0.19 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3645 | 1/1 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3765 | 1/1 | 0.21 | - | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3579 | 1/1 | 0.09 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3239 | 1/1 | 0.21 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3432 | 1/1 | 0.17 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3543 | 1/1 | 0.25 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1680 | 1/1 | 0.14 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3111 | 1/1 | 0.19 | - | 72,72,72,72 | 0 |
| 57 | MG | AA | 1628 | 1/1 | 0.10 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3430 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1769 | 1/1 | 0.19 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3503 | 1/1 | 0.25 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3482 | 1/1 | 0.10 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3715 | 1/1 | 0.19 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3732 | 1/1 | 0.22 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3198 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3557 | 1/1 | 0.14 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3134 | 1/1 | 0.19 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3401 | 1/1 | 0.22 | - | 26,26,26,26 | 0 |
| 57 | MG | BA | 3255 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3053 | 1/1 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1608 | 1/1 | 0.13 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3389 | 1/1 | 0.13 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3193 | 1/1 | 0.10 | - | 47,47,47,47 | 0 |
| 57 | MG | CE | 201 | 1/1 | 0.15 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3808 | 1/1 | 0.13 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3040 | 1/1 | 0.21 | - | 33,33,33,33 | 0 |
| 57 | MG | AA | 1804 | 1/1 | 0.12 | - | 70,70,70,70 | 0 |
| 57 | MG | DB | 3001 | 1/1 | 0.15 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3766 | 1/1 | 0.11 | - | 47,47,47,47 | 0 |
| 57 | MG | DF | 305 | 1/1 | 0.45 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3514 | 1/1 | 0.16 | - | 43,43,43,43 | 0 |
| 57 | MG | CX | 3001 | 1/1 | 0.11 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3322 | 1/1 | 0.14 | - | 42,42,42,42 | 0 |
| 59 | ZN | D6 | 501 | 1/1 | 0.17 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3159 | 1/1 | 0.10 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3505 | 1/1 | 0.17 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3089 | 1/1 | 0.11 | - | 52,52,52,52 | 0 |
| 57 | MG | AY | 3001 | 1/1 | 0.30 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3509 | 1/1 | 0.07 | - | 49,49,49,49 | 0 |
| 57 | MG | AX | 3015 | 1/1 | 0.24 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3616 | 1/1 | 0.18 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3546 | 1/1 | 0.11 | - | 68,68,68,68 | 0 |
| 57 | MG | DU | 201 | 1/1 | 0.70 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3649 | 1/1 | 0.14 | - | 71,71,71,71 | 0 |
| 57 | MG | BA | 3645 | 1/1 | 0.18 | - | 47,47,47,47 | 0 |
| 57 | MG | CA | 3168 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3154 | 1/1 | 0.06 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3371 | 1/1 | 0.07 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3148 | 1/1 | 0.34 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3474 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3082 | 1/1 | 0.14 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3029 | 1/1 | 0.21 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3260 | 1/1 | 0.14 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3586 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | DD | 301 | 1/1 | 0.31 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3736 | 1/1 | 0.14 | - | 22,22,22,22 | 0 |
| 57 | MG | BA | 3053 | 1/1 | 0.22 | - | 23,23,23,23 | 0 |
| 57 | MG | BA | 3451 | 1/1 | 0.20 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3301 | 1/1 | 0.10 | - | 63,63,63,63 | 0 |
| 57 | MG | CA | 3092 | 1/1 | 0.21 | - | 51,51,51,51 | 0 |
| 57 | MG | BO | 5001 | 1/1 | 0.13 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3547 | 1/1 | 0.06 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3043 | 1/1 | 0.18 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3572 | 1/1 | 0.23 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3627 | 1/1 | 0.18 | - | 57,57,57,57 | 0 |
| 57 | MG | CA | 3081 | 1/1 | 0.15 | - | 44,44,44,44 | 0 |
| 57 | MG | CA | 3015 | 1/1 | 0.10 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3458 | 1/1 | 0.18 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3144 | 1/1 | 0.22 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3417 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3406 | 1/1 | 0.10 | - | 56,56,56,56 | 0 |
| 57 | MG | CA | 3099 | 1/1 | 0.10 | - | 64,64,64,64 | 0 |
| 57 | MG | BQ | 3002 | 1/1 | 0.21 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3123 | 1/1 | 0.09 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3316 | 1/1 | 0.22 | - | 57,57,57,57 | 0 |
| 57 | MG | AA | 1768 | 1/1 | 0.10 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1670 | 1/1 | 0.14 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3099 | 1/1 | 0.22 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3441 | 1/1 | 0.18 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3422 | 1/1 | 0.15 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3420 | 1/1 | 0.10 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3162 | 1/1 | 0.15 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3607 | 1/1 | 0.14 | - | 36,36,36,36 | 0 |
| 57 | MG | BF | 306 | 1/1 | 0.27 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3062 | 1/1 | 0.14 | - | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3460 | 1/1 | 0.15 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3002 | 1/1 | 0.21 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3710 | 1/1 | 0.69 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3037 | 1/1 | 0.25 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3010 | 1/1 | 0.07 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3167 | 1/1 | 0.08 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1739 | 1/1 | 0.17 | - | 72,72,72,72 | 0 |
| 57 | MG | CA | 3035 | 1/1 | 0.08 | - | 53,53,53,53 | 0 |
| 57 | MG | BB | 3012 | 1/1 | 0.18 | - | 56,56,56,56 | 0 |
| 57 | MG | AK | 3101 | 1/1 | 0.09 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3181 | 1/1 | 0.09 | - | 49,49,49,49 | 0 |
| 57 | MG | BY | 502 | 1/1 | 0.17 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3549 | 1/1 | 0.13 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3595 | 1/1 | 0.12 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3122 | 1/1 | 0.12 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3176 | 1/1 | 0.21 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3498 | 1/1 | 0.17 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1787 | 1/1 | 0.13 | - | 49,49,49,49 | 0 |
| 57 | MG | B5 | 102 | 1/1 | 0.24 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3140 | 1/1 | 0.08 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3439 | 1/1 | 0.17 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3611 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1671 | 1/1 | 0.10 | - | 60,60,60,60 | 0 |
| 57 | MG | B7 | 101 | 1/1 | 0.09 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3394 | 1/1 | 0.05 | - | 60,60,60,60 | 0 |
| 57 | MG | AA | 1629 | 1/1 | 0.29 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3032 | 1/1 | 0.22 | - | 33,33,33,33 | 0 |
| 57 | MG | CA | 3164 | 1/1 | 0.22 | - | 76,76,76,76 | 0 |
| 57 | MG | DA | 3282 | 1/1 | 0.10 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3271 | 1/1 | 0.14 | - | 60,60,60,60 | 0 |
| 57 | MG | AA | 1622 | 1/1 | 0.17 | - | 69,69,69,69 | 0 |
| 57 | MG | AA | 1647 | 1/1 | 0.23 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3635 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3114 | 1/1 | 0.20 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3139 | 1/1 | 0.14 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3307 | 1/1 | 0.17 | - | 28,28,28,28 | 0 |
| 57 | MG | AA | 1620 | 1/1 | 0.09 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3554 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3640 | 1/1 | 0.17 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3158 | 1/1 | 0.33 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3196 | 1/1 | 0.13 | - | 54,54,54,54 | 0 |
| 57 | MG | CA | 3098 | 1/1 | 0.15 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3493 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3042 | 1/1 | 0.09 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3281 | 1/1 | 0.19 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3496 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3164 | 1/1 | 0.21 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3614 | 1/1 | 0.17 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3341 | 1/1 | 0.12 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3488 | 1/1 | 0.09 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3362 | 1/1 | 0.19 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3409 | 1/1 | 0.21 | - | 22,22,22,22 | 0 |
| 57 | MG | DA | 3497 | 1/1 | 0.13 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3267 | 1/1 | 0.10 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3653 | 1/1 | 0.19 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3560 | 1/1 | 0.12 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3247 | 1/1 | 0.16 | - | 29,29,29,29 | 0 |
| 57 | MG | BE | 305 | 1/1 | 0.23 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3265 | 1/1 | 0.13 | - | 57,57,57,57 | 0 |
| 57 | MG | CA | 3137 | 1/1 | 0.14 | - | 78,78,78,78 | 0 |
| 57 | MG | BA | 3584 | 1/1 | 0.09 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1603 | 1/1 | 0.10 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3620 | 1/1 | 0.09 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3490 | 1/1 | 0.11 | - | 33,33,33,33 | 0 |
| 57 | MG | CA | 3019 | 1/1 | 0.13 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3400 | 1/1 | 0.14 | - | 62,62,62,62 | 0 |
| 57 | MG | CA | 3069 | 1/1 | 0.17 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3498 | 1/1 | 0.17 | - | 35,35,35,35 | 0 |
| 57 | MG | AX | 3012 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3052 | 1/1 | 0.24 | - | 50,50,50,50 | 0 |
| 57 | MG | BZ | 301 | 1/1 | 0.15 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3393 | 1/1 | 0.16 | - | 37,37,37,37 | 0 |
| 57 | MG | AA | 1775 | 1/1 | 0.11 | - | 73,73,73,73 | 0 |
| 57 | MG | DA | 3399 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3070 | 1/1 | 0.14 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3121 | 1/1 | 0.09 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3598 | 1/1 | 0.12 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3064 | 1/1 | 0.10 | - | 46,46,46,46 | 0 |
| 57 | MG | BB | 3013 | 1/1 | 0.18 | - | 39,39,39,39 | 0 |
| 57 | MG | BE | 302 | 1/1 | 0.17 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3388 | 1/1 | 0.19 | - | 25,25,25,25 | 0 |
| 57 | MG | CA | 3044 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3266 | 1/1 | 0.16 | - | 44,44,44,44 | 0 |
| 57 | MG | DE | 3005 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3197 | 1/1 | 0.19 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3553 | 1/1 | 0.14 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3782 | 1/1 | 0.12 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3022 | 1/1 | 0.38 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3105 | 1/1 | 0.18 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1637 | 1/1 | 0.07 | - | 61,61,61,61 | 0 |
| 57 | MG | AX | 3006 | 1/1 | 0.13 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3479 | 1/1 | 0.13 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3427 | 1/1 | 0.14 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3231 | 1/1 | 0.13 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3278 | 1/1 | 0.91 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3572 | 1/1 | 0.14 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3531 | 1/1 | 0.06 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3211 | 1/1 | 0.17 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3289 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | AA | 1681 | 1/1 | 0.09 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3470 | 1/1 | 0.05 | - | 61,61,61,61 | 0 |
| 57 | MG | BV | 204 | 1/1 | 0.22 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3097 | 1/1 | 0.15 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3656 | 1/1 | 0.33 | - | 41,41,41,41 | 0 |
| 57 | MG | CA | 3043 | 1/1 | 0.13 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3738 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1704 | 1/1 | 0.10 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3709 | 1/1 | 0.34 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3802 | 1/1 | 0.15 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3453 | 1/1 | 0.13 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3036 | 1/1 | 0.12 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3549 | 1/1 | 0.18 | - | 49,49,49,49 | 0 |
| 57 | MG | AA | 1703 | 1/1 | 0.28 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3501 | 1/1 | 0.10 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3587 | 1/1 | 0.11 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3142 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3448 | 1/1 | 0.10 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3326 | 1/1 | 0.12 | - | 24,24,24,24 | 0 |
| 57 | MG | DA | 3395 | 1/1 | 0.14 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3124 | 1/1 | 0.19 | - | 57,57,57,57 | 0 |
| 57 | MG | CA | 3030 | 1/1 | 0.08 | - | 74,74,74,74 | 0 |
| 57 | MG | AA | 1611 | 1/1 | 0.11 | - | 20,20,20,20 | 0 |
| 57 | MG | AA | 1722 | 1/1 | 0.16 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3577 | 1/1 | 0.06 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3414 | 1/1 | 0.12 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3396 | 1/1 | 0.21 | - | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3264 | 1/1 | 0.12 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3152 | 1/1 | 0.21 | - | 23,23,23,23 | 0 |
| 57 | MG | AA | 1645 | 1/1 | 0.12 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3689 | 1/1 | 0.15 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3380 | 1/1 | 0.06 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3237 | 1/1 | 0.10 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3015 | 1/1 | 0.17 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3191 | 1/1 | 0.27 | - | 54,54,54,54 | 0 |
| 57 | MG | CA | 3079 | 1/1 | 0.11 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3589 | 1/1 | 0.06 | - | 29,29,29,29 | 0 |
| 57 | MG | BA | 3196 | 1/1 | 0.21 | - | 56,56,56,56 | 0 |
| 57 | MG | AA | 1808 | 1/1 | 0.12 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3683 | 1/1 | 0.32 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3626 | 1/1 | 0.08 | - | 81,81,81,81 | 0 |
| 57 | MG | CA | 3085 | 1/1 | 0.11 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3294 | 1/1 | 0.08 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3193 | 1/1 | 0.11 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3062 | 1/1 | 0.22 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3324 | 1/1 | 0.08 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3282 | 1/1 | 0.16 | - | 57,57,57,57 | 0 |
| 57 | MG | DQ | 3001 | 1/1 | 0.06 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3209 | 1/1 | 0.13 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3097 | 1/1 | 0.06 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3577 | 1/1 | 0.19 | - | 58,58,58,58 | 0 |
| 57 | MG | CA | 3071 | 1/1 | 0.12 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3667 | 1/1 | 0.19 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3651 | 1/1 | 0.13 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3795 | 1/1 | 0.18 | - | 19,19,19,19 | 0 |
| 57 | MG | DA | 3506 | 1/1 | 0.11 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3391 | 1/1 | 0.14 | - | 41,41,41,41 | 0 |
| 59 | ZN | D9 | 501 | 1/1 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3733 | 1/1 | 0.14 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3273 | 1/1 | 0.15 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1772 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3393 | 1/1 | 0.18 | - | 23,23,23,23 | 0 |
| 57 | MG | BA | 3504 | 1/1 | 0.21 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3731 | 1/1 | 0.12 | - | 32,32,32,32 | 0 |
| 57 | MG | CW | 3001 | 1/1 | 0.23 | - | 66,66,66,66 | 0 |
| 57 | MG | CA | 3091 | 1/1 | 0.15 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3233 | 1/1 | 0.23 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3649 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | BD | 3007 | 1/1 | 0.29 | - | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3319 | 1/1 | 0.21 | - | 23,23,23,23 | 0 |
| 57 | MG | BA | 3309 | 1/1 | 0.15 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3761 | 1/1 | 0.07 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3789 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3375 | 1/1 | 0.09 | - | 57,57,57,57 | 0 |
| 57 | MG | AA | 1655 | 1/1 | 0.10 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3505 | 1/1 | 0.07 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3149 | 1/1 | 0.14 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3271 | 1/1 | 0.14 | - | 30,30,30,30 | 0 |
| 57 | MG | BA | 3085 | 1/1 | 0.24 | - | 31,31,31,31 | 0 |
| 57 | MG | AA | 1652 | 1/1 | 0.13 | - | 62,62,62,62 | 0 |
| 57 | MG | AA | 1707 | 1/1 | 0.10 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3798 | 1/1 | 0.24 | - | 22,22,22,22 | 0 |
| 57 | MG | BA | 3314 | 1/1 | 0.16 | - | 39,39,39,39 | 0 |
| 57 | MG | AA | 1719 | 1/1 | 0.15 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3198 | 1/1 | 0.11 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3099 | 1/1 | 0.18 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3312 | 1/1 | 0.14 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3382 | 1/1 | 0.10 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3568 | 1/1 | 0.12 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3118 | 1/1 | 0.22 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3657 | 1/1 | 0.39 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3485 | 1/1 | 0.10 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3684 | 1/1 | 0.17 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3699 | 1/1 | 0.19 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3650 | 1/1 | 0.11 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3578 | 1/1 | 0.12 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3522 | 1/1 | 0.16 | - | 44,44,44,44 | 0 |
| 57 | MG | CA | 3141 | 1/1 | 0.12 | - | 62,62,62,62 | 0 |
| 57 | MG | CA | 3126 | 1/1 | 0.07 | - | 45,45,45,45 | 0 |
| 57 | MG | CE | 202 | 1/1 | 0.22 | - | 95,95,95,95 | 0 |
| 57 | MG | BA | 3127 | 1/1 | 0.22 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3327 | 1/1 | 0.15 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3102 | 1/1 | 0.28 | - | 40,40,40,40 | 0 |
| 57 | MG | BV | 205 | 1/1 | 0.07 | - | 34,34,34,34 | 0 |
| 57 | MG | CA | 3037 | 1/1 | 0.20 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3803 | 1/1 | 0.27 | - | 55,55,55,55 | 0 |
| 57 | MG | BB | 3011 | 1/1 | 0.19 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3668 | 1/1 | 0.16 | - | 75,75,75,75 | 0 |
| 57 | MG | DA | 3461 | 1/1 | 0.12 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3363 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3580 | 1/1 | 0.11 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3138 | 1/1 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1688 | 1/1 | 0.14 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3530 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3277 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1676 | 1/1 | 0.14 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3415 | 1/1 | 0.21 | - | 35,35,35,35 | 0 |
| 57 | MG | CA | 3060 | 1/1 | 0.10 | - | 71,71,71,71 | 0 |
| 57 | MG | BH | 201 | 1/1 | 0.23 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3693 | 1/1 | 0.15 | - | 77,77,77,77 | 0 |
| 57 | MG | BA | 3544 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3378 | 1/1 | 0.23 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3520 | 1/1 | 0.10 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3431 | 1/1 | 0.17 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3623 | 1/1 | 0.17 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3527 | 1/1 | 0.16 | - | 24,24,24,24 | 0 |
| 57 | MG | BA | 3221 | 1/1 | 0.14 | - | 29,29,29,29 | 0 |
| 57 | MG | DA | 3522 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | AA | 1636 | 1/1 | 0.22 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3069 | 1/1 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3774 | 1/1 | 0.28 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3152 | 1/1 | 0.20 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3101 | 1/1 | 0.19 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3359 | 1/1 | 0.14 | - | 40,40,40,40 | 0 |
| 59 | ZN | B5 | 103 | 1/1 | 0.18 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3503 | 1/1 | 0.08 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3080 | 1/1 | 0.11 | - | 31,31,31,31 | 0 |
| 57 | MG | AA | 1699 | 1/1 | 0.23 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3195 | 1/1 | 0.09 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3086 | 1/1 | 0.29 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3639 | 1/1 | 0.15 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3377 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | CA | 3165 | 1/1 | 0.07 | - | 42,42,42,42 | 0 |
| 57 | MG | AA | 1659 | 1/1 | 0.15 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3618 | 1/1 | 0.09 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3369 | 1/1 | 0.22 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3389 | 1/1 | 0.18 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3576 | 1/1 | 0.12 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3778 | 1/1 | 0.07 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3793 | 1/1 | 0.16 | - | 11,11,11,11 | 0 |
| 57 | MG | DA | 3142 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3366 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3321 | 1/1 | 0.16 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3285 | 1/1 | 0.13 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3334 | 1/1 | 0.19 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3454 | 1/1 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3236 | 1/1 | 0.18 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3009 | 1/1 | 0.14 | - | 73,73,73,73 | 0 |
| 57 | MG | DA | 3297 | 1/1 | 0.16 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3005 | 1/1 | 0.15 | - | 73,73,73,73 | 0 |
| 57 | MG | BA | 3373 | 1/1 | 0.18 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3499 | 1/1 | 0.15 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3584 | 1/1 | 0.05 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3469 | 1/1 | 0.13 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3041 | 1/1 | 0.18 | - | 63,63,63,63 | 0 |
| 57 | MG | BU | 201 | 1/1 | 0.44 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1760 | 1/1 | 0.15 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3525 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3214 | 1/1 | 0.36 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3599 | 1/1 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | CA | 3068 | 1/1 | 0.12 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3471 | 1/1 | 0.15 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3541 | 1/1 | 0.08 | - | 59,59,59,59 | 0 |
| 57 | MG | AA | 1690 | 1/1 | 0.38 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3054 | 1/1 | 0.06 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3550 | 1/1 | 0.04 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3352 | 1/1 | 0.17 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3585 | 1/1 | 0.15 | - | 29,29,29,29 | 0 |
| 57 | MG | BA | 3486 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3352 | 1/1 | 0.10 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3458 | 1/1 | 0.09 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3407 | 1/1 | 0.09 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3418 | 1/1 | 0.07 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1667 | 1/1 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3376 | 1/1 | 0.18 | - | 29,29,29,29 | 0 |
| 57 | MG | DA | 3484 | 1/1 | 0.05 | - | 46,46,46,46 | 0 |
| 57 | MG | CA | 3053 | 1/1 | 0.09 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3234 | 1/1 | 0.10 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3354 | 1/1 | 0.07 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3283 | 1/1 | 0.06 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3262 | 1/1 | 0.32 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3474 | 1/1 | 0.21 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3129 | 1/1 | 0.14 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3663 | 1/1 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3177 | 1/1 | 0.29 | - | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3567 | 1/1 | 0.24 | - | 44,44,44,44 | 0 |
| 57 | MG | AA | 1613 | 1/1 | 0.14 | - | 75,75,75,75 | 0 |
| 57 | MG | DA | 3061 | 1/1 | 0.17 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3120 | 1/1 | 0.29 | - | 45,45,45,45 | 0 |
| 57 | MG | AX | 3010 | 1/1 | 0.41 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3686 | 1/1 | 0.15 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3472 | 1/1 | 0.11 | - | 25,25,25,25 | 0 |
| 57 | MG | DA | 3631 | 1/1 | 0.11 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3269 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1786 | 1/1 | 0.11 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3354 | 1/1 | 0.10 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1609 | 1/1 | 0.09 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3104 | 1/1 | 0.09 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3157 | 1/1 | 0.11 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3228 | 1/1 | 0.09 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3453 | 1/1 | 0.23 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1648 | 1/1 | 0.15 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3339 | 1/1 | 0.24 | - | 52,52,52,52 | 0 |
| 57 | MG | BE | 301 | 1/1 | 0.17 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3166 | 1/1 | 0.15 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3068 | 1/1 | 0.16 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3619 | 1/1 | 0.11 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3243 | 1/1 | 0.68 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3596 | 1/1 | 0.15 | - | 59,59,59,59 | 0 |
| 57 | MG | DB | 3006 | 1/1 | 0.10 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3381 | 1/1 | 0.09 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3326 | 1/1 | 0.08 | - | 46,46,46,46 | 0 |
| 57 | MG | CA | 3102 | 1/1 | 0.12 | - | 71,71,71,71 | 0 |
| 57 | MG | AA | 1642 | 1/1 | 0.23 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3204 | 1/1 | 0.26 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3317 | 1/1 | 0.18 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3244 | 1/1 | 0.24 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1668 | 1/1 | 0.08 | - | 63,63,63,63 | 0 |
| 57 | MG | CA | 3133 | 1/1 | 0.19 | - | 82,82,82,82 | 0 |
| 57 | MG | BA | 3432 | 1/1 | 0.20 | - | 32,32,32,32 | 0 |
| 57 | MG | BA | 3542 | 1/1 | 0.17 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3005 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | CA | 3093 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 57 | MG | CA | 3108 | 1/1 | 0.08 | - | 72,72,72,72 | 0 |
| 57 | MG | DA | 3390 | 1/1 | 0.08 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3010 | 1/1 | 0.18 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3459 | 1/1 | 0.13 | - | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3274 | 1/1 | 0.18 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3740 | 1/1 | 0.20 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1602 | 1/1 | 0.08 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3429 | 1/1 | 0.25 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3551 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3035 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3289 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3020 | 1/1 | 0.08 | - | 26,26,26,26 | 0 |
| 57 | MG | BA | 3339 | 1/1 | 0.17 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3622 | 1/1 | 0.18 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3209 | 1/1 | 0.17 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3265 | 1/1 | 0.24 | - | 72,72,72,72 | 0 |
| 57 | MG | BA | 3435 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3600 | 1/1 | 0.12 | - | 72,72,72,72 | 0 |
| 57 | MG | BA | 3756 | 1/1 | 0.15 | - | 18,18,18,18 | 0 |
| 57 | MG | DA | 3112 | 1/1 | 0.14 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3720 | 1/1 | 0.13 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3330 | 1/1 | 0.15 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3013 | 1/1 | 0.09 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3729 | 1/1 | 0.12 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3489 | 1/1 | 0.07 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3723 | 1/1 | 0.17 | - | 30,30,30,30 | 0 |
| 57 | MG | AA | 1732 | 1/1 | 0.22 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3428 | 1/1 | 0.10 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3641 | 1/1 | 0.14 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3015 | 1/1 | 0.19 | - | 60,60,60,60 | 0 |
| 57 | MG | DB | 3009 | 1/1 | 0.13 | - | 58,58,58,58 | 0 |
| 57 | MG | AA | 1614 | 1/1 | 0.13 | - | 75,75,75,75 | 0 |
| 57 | MG | DA | 3281 | 1/1 | 0.13 | - | 36,36,36,36 | 0 |
| 57 | MG | BU | 202 | 1/1 | 0.22 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3480 | 1/1 | 0.16 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3180 | 1/1 | 0.15 | - | 48,48,48,48 | 0 |
| 57 | MG | B8 | 5001 | 1/1 | 0.15 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3548 | 1/1 | 0.10 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3408 | 1/1 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3622 | 1/1 | 0.07 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3025 | 1/1 | 0.51 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3322 | 1/1 | 0.15 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3219 | 1/1 | 0.15 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3058 | 1/1 | 0.07 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3428 | 1/1 | 0.16 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3156 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3205 | 1/1 | 0.34 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3047 | 1/1 | 0.18 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1780 | 1/1 | 0.13 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3109 | 1/1 | 0.09 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3259 | 1/1 | 0.18 | - | 25,25,25,25 | 0 |
| 57 | MG | BA | 3267 | 1/1 | 0.23 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3531 | 1/1 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3677 | 1/1 | 0.10 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3613 | 1/1 | 0.20 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3654 | 1/1 | 0.09 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3303 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3719 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3083 | 1/1 | 0.24 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3384 | 1/1 | 0.08 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3598 | 1/1 | 0.07 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3166 | 1/1 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | CA | 3021 | 1/1 | 0.07 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3385 | 1/1 | 0.19 | - | 30,30,30,30 | 0 |
| 57 | MG | BA | 3530 | 1/1 | 0.23 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3087 | 1/1 | 0.20 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1784 | 1/1 | 0.28 | - | 72,72,72,72 | 0 |
| 57 | MG | DA | 3139 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | AA | 1728 | 1/1 | 0.21 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3174 | 1/1 | 0.46 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3587 | 1/1 | 0.12 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3566 | 1/1 | 0.18 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3025 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1783 | 1/1 | 0.12 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3620 | 1/1 | 0.07 | - | 29,29,29,29 | 0 |
| 57 | MG | BA | 3121 | 1/1 | 0.26 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3238 | 1/1 | 0.13 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3157 | 1/1 | 0.14 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3186 | 1/1 | 0.12 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3145 | 1/1 | 0.19 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3301 | 1/1 | 0.14 | - | 62,62,62,62 | 0 |
| 57 | MG | BB | 3020 | 1/1 | 0.15 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1725 | 1/1 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | BB | 3016 | 1/1 | 0.16 | - | 34,34,34,34 | 0 |
| 57 | MG | CA | 3007 | 1/1 | 0.14 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3110 | 1/1 | 0.18 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3037 | 1/1 | 0.08 | - | 26,26,26,26 | 0 |
| 57 | MG | DA | 3403 | 1/1 | 0.05 | - | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3651 | 1/1 | 0.13 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3241 | 1/1 | 0.15 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3479 | 1/1 | 0.12 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3643 | 1/1 | 0.07 | - | 54,54,54,54 | 0 |
| 57 | MG | AA | 1796 | 1/1 | 0.09 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3403 | 1/1 | 0.25 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3017 | 1/1 | 0.10 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3404 | 1/1 | 0.32 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3603 | 1/1 | 0.06 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3066 | 1/1 | 0.09 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3722 | 1/1 | 0.15 | - | 64,64,64,64 | 0 |
| 57 | MG | CA | 3022 | 1/1 | 0.18 | - | 76,76,76,76 | 0 |
| 57 | MG | BA | 3563 | 1/1 | 0.12 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3315 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3635 | 1/1 | 0.09 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3637 | 1/1 | 0.14 | - | 72,72,72,72 | 0 |
| 57 | MG | BA | 3311 | 1/1 | 0.18 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3127 | 1/1 | 0.07 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3392 | 1/1 | 0.16 | - | 26,26,26,26 | 0 |
| 57 | MG | BA | 3413 | 1/1 | 0.14 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3046 | 1/1 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | CA | 3055 | 1/1 | 0.08 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3569 | 1/1 | 0.15 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3292 | 1/1 | 0.23 | - | 26,26,26,26 | 0 |
| 57 | MG | DA | 3005 | 1/1 | 0.15 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3208 | 1/1 | 0.15 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3661 | 1/1 | 0.24 | - | 25,25,25,25 | 0 |
| 57 | MG | BA | 3215 | 1/1 | 0.43 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3132 | 1/1 | 0.10 | - | 43,43,43,43 | 0 |
| 57 | MG | BP | 3001 | 1/1 | 0.13 | - | 34,34,34,34 | 0 |
| 57 | MG | CA | 3138 | 1/1 | 0.10 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3074 | 1/1 | 0.18 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3016 | 1/1 | 0.08 | - | 66,66,66,66 | 0 |
| 57 | MG | AX | 3002 | 1/1 | 0.31 | - | 71,71,71,71 | 0 |
| 57 | MG | AA | 1735 | 1/1 | 0.11 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3227 | 1/1 | 0.17 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3653 | 1/1 | 0.13 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3705 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3084 | 1/1 | 0.18 | - | 44,44,44,44 | 0 |
| 57 | MG | AA | 1626 | 1/1 | 0.23 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3670 | 1/1 | 0.13 | - | 54,54,54,54 | 0 |
| 57 | MG | AA | 1778 | 1/1 | 0.07 | - | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CA | 3167 | 1/1 | 0.23 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3192 | 1/1 | 0.15 | - | 19,19,19,19 | 0 |
| 57 | MG | BA | 3238 | 1/1 | 0.37 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3317 | 1/1 | 0.09 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3338 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1736 | 1/1 | 0.06 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3625 | 1/1 | 0.10 | - | 33,33,33,33 | 0 |
| 57 | MG | AA | 1638 | 1/1 | 0.22 | - | 60,60,60,60 | 0 |
| 57 | MG | BD | 3002 | 1/1 | 0.15 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3799 | 1/1 | 0.20 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3183 | 1/1 | 0.12 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3287 | 1/1 | 0.19 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3076 | 1/1 | 0.08 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3415 | 1/1 | 0.16 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3343 | 1/1 | 0.14 | - | 34,34,34,34 | 0 |
| 57 | MG | CA | 3128 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3336 | 1/1 | 0.08 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3178 | 1/1 | 0.12 | - | 32,32,32,32 | 0 |
| 57 | MG | AA | 1700 | 1/1 | 0.06 | - | 71,71,71,71 | 0 |
| 57 | MG | DA | 3122 | 1/1 | 0.29 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3095 | 1/1 | 0.17 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3113 | 1/1 | 0.11 | - | 50,50,50,50 | 0 |
| 57 | MG | CA | 3050 | 1/1 | 0.13 | - | 73,73,73,73 | 0 |
| 57 | MG | B5 | 101 | 1/1 | 0.32 | - | 30,30,30,30 | 0 |
| 57 | MG | AA | 1790 | 1/1 | 0.08 | - | 81,81,81,81 | 0 |
| 57 | MG | DA | 3446 | 1/1 | 0.12 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3202 | 1/1 | 0.31 | - | 62,62,62,62 | 0 |
| 57 | MG | CT | 3001 | 1/1 | 0.11 | - | 60,60,60,60 | 0 |
| 57 | MG | DP | 201 | 1/1 | 0.27 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3672 | 1/1 | 0.20 | - | 44,44,44,44 | 0 |
| 57 | MG | BF | 311 | 1/1 | 0.11 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1675 | 1/1 | 0.20 | - | 61,61,61,61 | 0 |
| 57 | MG | AA | 1708 | 1/1 | 0.14 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3660 | 1/1 | 0.56 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3786 | 1/1 | 0.15 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3011 | 1/1 | 0.12 | - | 30,30,30,30 | 0 |
| 57 | MG | DA | 3426 | 1/1 | 0.09 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3136 | 1/1 | 0.13 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3084 | 1/1 | 0.07 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3280 | 1/1 | 0.16 | - | 25,25,25,25 | 0 |
| 57 | MG | DA | 3068 | 1/1 | 0.14 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1794 | 1/1 | 0.15 | - | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3535 | 1/1 | 0.17 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3024 | 1/1 | 0.52 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3489 | 1/1 | 0.21 | - | 50,50,50,50 | 0 |
| 57 | MG | AE | 3001 | 1/1 | 0.07 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3604 | 1/1 | 0.17 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3088 | 1/1 | 0.30 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3465 | 1/1 | 0.06 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3152 | 1/1 | 0.07 | - | 71,71,71,71 | 0 |
| 57 | MG | DA | 3205 | 1/1 | 0.18 | - | 62,62,62,62 | 0 |
| 57 | MG | AA | 1616 | 1/1 | 0.11 | - | 73,73,73,73 | 0 |
| 57 | MG | BA | 3108 | 1/1 | 0.17 | - | 42,42,42,42 | 0 |
| 57 | MG | CA | 3107 | 1/1 | 0.10 | - | 68,68,68,68 | 0 |
| 57 | MG | DE | 3003 | 1/1 | 0.06 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3293 | 1/1 | 0.08 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3199 | 1/1 | 0.22 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3165 | 1/1 | 0.19 | - | 55,55,55,55 | 0 |
| 57 | MG | BV | 202 | 1/1 | 0.39 | - | 32,32,32,32 | 0 |
| 57 | MG | BA | 3394 | 1/1 | 0.27 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3416 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1730 | 1/1 | 0.22 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3014 | 1/1 | 0.10 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3590 | 1/1 | 0.14 | - | 33,33,33,33 | 0 |
| 57 | MG | B5 | 104 | 1/1 | 0.08 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3601 | 1/1 | 0.40 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3305 | 1/1 | 0.13 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3526 | 1/1 | 0.20 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3073 | 1/1 | 0.12 | - | 32,32,32,32 | 0 |
| 57 | MG | CA | 3150 | 1/1 | 0.12 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3376 | 1/1 | 0.14 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3293 | 1/1 | 0.14 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3316 | 1/1 | 0.15 | - | 54,54,54,54 | 0 |
| 57 | MG | BB | 3015 | 1/1 | 0.21 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3555 | 1/1 | 0.15 | - | 50,50,50,50 | 0 |
| 57 | MG | DF | 301 | 1/1 | 0.22 | - | 48,48,48,48 | 0 |
| 57 | MG | AA | 1705 | 1/1 | 0.20 | - | 70,70,70,70 | 0 |
| 57 | MG | CA | 3127 | 1/1 | 0.08 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3257 | 1/1 | 0.23 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3495 | 1/1 | 0.15 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3721 | 1/1 | 0.10 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3082 | 1/1 | 0.08 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3658 | 1/1 | 0.12 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3397 | 1/1 | 0.14 | - | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3320 | 1/1 | 0.16 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3618 | 1/1 | 0.14 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3044 | 1/1 | 0.08 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3742 | 1/1 | 0.20 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3310 | 1/1 | 0.14 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3546 | 1/1 | 0.08 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3087 | 1/1 | 0.47 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3796 | 1/1 | 0.18 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3675 | 1/1 | 0.22 | - | 56,56,56,56 | 0 |
| 57 | MG | BU | 204 | 1/1 | 0.34 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3364 | 1/1 | 0.10 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3039 | 1/1 | 0.19 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3208 | 1/1 | 0.07 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3462 | 1/1 | 0.21 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3737 | 1/1 | 0.14 | - | 34,34,34,34 | 0 |
| 57 | MG | B2 | 3001 | 1/1 | 0.27 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3351 | 1/1 | 0.17 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3469 | 1/1 | 0.07 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3150 | 1/1 | 0.14 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3386 | 1/1 | 0.13 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3455 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3643 | 1/1 | 0.09 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3080 | 1/1 | 0.09 | - | 49,49,49,49 | 0 |
| 57 | MG | BE | 304 | 1/1 | 0.19 | - | 23,23,23,23 | 0 |
| 57 | MG | AA | 1695 | 1/1 | 0.16 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3222 | 1/1 | 0.15 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3319 | 1/1 | 0.13 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3103 | 1/1 | 0.29 | - | 63,63,63,63 | 0 |
| 57 | MG | DE | 3001 | 1/1 | 0.47 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3763 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | BF | 308 | 1/1 | 0.06 | - | 43,43,43,43 | 0 |
| 57 | MG | CA | 3129 | 1/1 | 0.09 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3434 | 1/1 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3028 | 1/1 | 0.09 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3762 | 1/1 | 0.15 | - | 20,20,20,20 | 0 |
| 57 | MG | BA | 3521 | 1/1 | 0.17 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3079 | 1/1 | 0.10 | - | 72,72,72,72 | 0 |
| 57 | MG | DA | 3249 | 1/1 | 0.13 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3443 | 1/1 | 0.15 | - | 51,51,51,51 | 0 |
| 57 | MG | AA | 1605 | 1/1 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | BB | 3022 | 1/1 | 0.16 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3341 | 1/1 | 0.19 | - | 18,18,18,18 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3562 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3638 | 1/1 | 0.16 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3254 | 1/1 | 0.15 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3257 | 1/1 | 0.20 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3406 | 1/1 | 0.17 | - | 70,70,70,70 | 0 |
| 57 | MG | BA | 3421 | 1/1 | 0.13 | - | 62,62,62,62 | 0 |
| 57 | MG | DY | 502 | 1/1 | 0.09 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3136 | 1/1 | 0.53 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3344 | 1/1 | 0.13 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3475 | 1/1 | 0.17 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3708 | 1/1 | 0.22 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3655 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3270 | 1/1 | 0.15 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3172 | 1/1 | 0.13 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3517 | 1/1 | 0.21 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3033 | 1/1 | 0.68 | - | 68,68,68,68 | 0 |
| 57 | MG | DD | 304 | 1/1 | 0.06 | - | 36,36,36,36 | 0 |
| 57 | MG | CA | 3148 | 1/1 | 0.11 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3664 | 1/1 | 0.08 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3644 | 1/1 | 0.11 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3367 | 1/1 | 0.19 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3142 | 1/1 | 0.23 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3703 | 1/1 | 0.31 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3066 | 1/1 | 0.22 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3507 | 1/1 | 0.25 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3396 | 1/1 | 0.16 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3157 | 1/1 | 0.14 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3165 | 1/1 | 0.25 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3138 | 1/1 | 0.16 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3540 | 1/1 | 0.15 | - | 31,31,31,31 | 0 |
| 57 | MG | DA | 3081 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3217 | 1/1 | 0.07 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3145 | 1/1 | 0.31 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3055 | 1/1 | 0.12 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3478 | 1/1 | 0.10 | - | 54,54,54,54 | 0 |
| 57 | MG | DB | 3012 | 1/1 | 0.21 | - | 66,66,66,66 | 0 |
| 57 | MG | BX | 3001 | 1/1 | 0.31 | - | 44,44,44,44 | 0 |
| 57 | MG | AA | 1799 | 1/1 | 0.09 | - | 78,78,78,78 | 0 |
| 57 | MG | BA | 3707 | 1/1 | 0.19 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3463 | 1/1 | 0.17 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3084 | 1/1 | 0.14 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3540 | 1/1 | 0.06 | - | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1610 | 1/1 | 0.14 | - | 81,81,81,81 | 0 |
| 57 | MG | BA | 3287 | 1/1 | 0.14 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3508 | 1/1 | 0.20 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3177 | 1/1 | 0.09 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3606 | 1/1 | 0.11 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3495 | 1/1 | 0.08 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3045 | 1/1 | 0.17 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3170 | 1/1 | 0.20 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3535 | 1/1 | 0.18 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3700 | 1/1 | 0.24 | - | 36,36,36,36 | 0 |
| 57 | MG | BB | 3018 | 1/1 | 0.05 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3221 | 1/1 | 0.06 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3361 | 1/1 | 0.08 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3612 | 1/1 | 0.06 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3449 | 1/1 | 0.19 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3439 | 1/1 | 0.10 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3150 | 1/1 | 0.11 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1646 | 1/1 | 0.12 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3753 | 1/1 | 0.22 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3423 | 1/1 | 0.20 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3248 | 1/1 | 0.24 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3459 | 1/1 | 0.12 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3628 | 1/1 | 0.21 | - | 77,77,77,77 | 0 |
| 57 | MG | AA | 1734 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1696 | 1/1 | 0.11 | - | 83,83,83,83 | 0 |
| 57 | MG | DA | 3038 | 1/1 | 0.13 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3619 | 1/1 | 0.14 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3412 | 1/1 | 0.13 | - | 30,30,30,30 | 0 |
| 57 | MG | BA | 3185 | 1/1 | 0.11 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3517 | 1/1 | 0.08 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3016 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3660 | 1/1 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3563 | 1/1 | 0.09 | - | 70,70,70,70 | 0 |
| 57 | MG | AA | 1711 | 1/1 | 0.11 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3210 | 1/1 | 0.14 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3647 | 1/1 | 0.08 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3133 | 1/1 | 0.20 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3026 | 1/1 | 0.47 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3625 | 1/1 | 0.09 | - | 60,60,60,60 | 0 |
| 57 | MG | AA | 1623 | 1/1 | 0.19 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3373 | 1/1 | 0.07 | - | 31,31,31,31 | 0 |
| 57 | MG | DA | 3131 | 1/1 | 0.41 | - | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3481 | 1/1 | 0.08 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3173 | 1/1 | 0.26 | - | 32,32,32,32 | 0 |
| 57 | MG | BU | 203 | 1/1 | 0.31 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3592 | 1/1 | 0.11 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3500 | 1/1 | 0.28 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3539 | 1/1 | 0.12 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3164 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3200 | 1/1 | 0.12 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1665 | 1/1 | 0.08 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3295 | 1/1 | 0.22 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3491 | 1/1 | 0.20 | - | 56,56,56,56 | 0 |
| 57 | MG | AA | 1781 | 1/1 | 0.11 | - | 59,59,59,59 | 0 |
| 57 | MG | BG | 201 | 1/1 | 0.12 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3213 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3537 | 1/1 | 0.07 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3673 | 1/1 | 0.23 | - | 61,61,61,61 | 0 |
| 57 | MG | CA | 3067 | 1/1 | 0.13 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3243 | 1/1 | 0.13 | - | 48,48,48,48 | 0 |
| 57 | MG | BW | 3004 | 1/1 | 0.16 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3153 | 1/1 | 0.17 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3169 | 1/1 | 0.28 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3638 | 1/1 | 0.15 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3275 | 1/1 | 0.14 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3758 | 1/1 | 0.14 | - | 41,41,41,41 | 0 |
| 57 | MG | AX | 3016 | 1/1 | 0.53 | - | 86,86,86,86 | 0 |
| 57 | MG | AA | 1765 | 1/1 | 0.10 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3162 | 1/1 | 0.26 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3089 | 1/1 | 0.11 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3800 | 1/1 | 0.16 | - | 29,29,29,29 | 0 |
| 57 | MG | AX | 3014 | 1/1 | 0.20 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3518 | 1/1 | 0.09 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3160 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3263 | 1/1 | 0.11 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1756 | 1/1 | 0.30 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3543 | 1/1 | 0.14 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3717 | 1/1 | 0.13 | - | 72,72,72,72 | 0 |
| 57 | MG | BA | 3402 | 1/1 | 0.14 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3557 | 1/1 | 0.10 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3328 | 1/1 | 0.19 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3440 | 1/1 | 0.10 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3648 | 1/1 | 0.06 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3231 | 1/1 | 0.14 | - | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3659 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3594 | 1/1 | 0.09 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3450 | 1/1 | 0.28 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3642 | 1/1 | 0.26 | - | 64,64,64,64 | 0 |
| 57 | MG | BD | 3010 | 1/1 | 0.14 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3056 | 1/1 | 0.40 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3784 | 1/1 | 0.14 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3163 | 1/1 | 0.15 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3391 | 1/1 | 0.10 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3258 | 1/1 | 0.13 | - | 45,45,45,45 | 0 |
| 57 | MG | DF | 304 | 1/1 | 0.05 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3120 | 1/1 | 0.27 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3078 | 1/1 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1776 | 1/1 | 0.15 | - | 73,73,73,73 | 0 |
| 57 | MG | AA | 1743 | 1/1 | 0.16 | - | 66,66,66,66 | 0 |
| 57 | MG | AA | 1753 | 1/1 | 0.20 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3604 | 1/1 | 0.15 | - | 61,61,61,61 | 0 |
| 57 | MG | CA | 3130 | 1/1 | 0.24 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3448 | 1/1 | 0.14 | - | 17,17,17,17 | 0 |
| 57 | MG | DA | 3266 | 1/1 | 0.09 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3187 | 1/1 | 0.20 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3443 | 1/1 | 0.17 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3292 | 1/1 | 0.09 | - | 29,29,29,29 | 0 |
| 57 | MG | BA | 3355 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 57 | MG | DQ | 3002 | 1/1 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3358 | 1/1 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3040 | 1/1 | 0.11 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3117 | 1/1 | 0.42 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3438 | 1/1 | 0.17 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3524 | 1/1 | 0.19 | - | 33,33,33,33 | 0 |
| 57 | MG | CA | 3124 | 1/1 | 0.20 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3634 | 1/1 | 0.13 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3176 | 1/1 | 0.24 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3355 | 1/1 | 0.09 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1727 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3600 | 1/1 | 0.23 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3272 | 1/1 | 0.20 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3023 | 1/1 | 0.11 | - | 58,58,58,58 | 0 |
| 57 | MG | AA | 1662 | 1/1 | 0.12 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3246 | 1/1 | 0.26 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1650 | 1/1 | 0.12 | - | 74,74,74,74 | 0 |
| 57 | MG | AA | 1777 | 1/1 | 0.07 | - | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | B4 | 502 | 1/1 | 0.21 | - | 70,70,70,70 | 0 |
| 57 | MG | CA | 3109 | 1/1 | 0.19 | - | 74,74,74,74 | 0 |
| 57 | MG | CA | 3070 | 1/1 | 0.10 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3650 | 1/1 | 0.16 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3725 | 1/1 | 0.15 | - | 31,31,31,31 | 0 |
| 57 | MG | AA | 1762 | 1/1 | 0.16 | - | 66,66,66,66 | 0 |
| 57 | MG | AA | 1813 | 1/1 | 0.18 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3161 | 1/1 | 0.28 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3308 | 1/1 | 0.19 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3493 | 1/1 | 0.17 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3612 | 1/1 | 0.09 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3320 | 1/1 | 0.13 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3290 | 1/1 | 0.10 | - | 33,33,33,33 | 0 |
| 57 | MG | AA | 1604 | 1/1 | 0.11 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3521 | 1/1 | 0.06 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3210 | 1/1 | 0.06 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3178 | 1/1 | 0.12 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3179 | 1/1 | 0.20 | - | 43,43,43,43 | 0 |
| 57 | MG | AA | 1644 | 1/1 | 0.13 | - | 56,56,56,56 | 0 |
| 57 | MG | AA | 1641 | 1/1 | 0.14 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1751 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3445 | 1/1 | 0.18 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3203 | 1/1 | 0.27 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3240 | 1/1 | 0.13 | - | 53,53,53,53 | 0 |
| 57 | MG | CA | 3147 | 1/1 | 0.06 | - | 70,70,70,70 | 0 |
| 57 | MG | BA | 3263 | 1/1 | 0.26 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3003 | 1/1 | 0.20 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3295 | 1/1 | 0.23 | - | 23,23,23,23 | 0 |
| 57 | MG | DA | 3644 | 1/1 | 0.20 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3343 | 1/1 | 0.19 | - | 54,54,54,54 | 0 |
| 57 | MG | CA | 3090 | 1/1 | 0.16 | - | 76,76,76,76 | 0 |
| 57 | MG | DA | 3601 | 1/1 | 0.09 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3735 | 1/1 | 0.18 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3509 | 1/1 | 0.20 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3085 | 1/1 | 0.15 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3749 | 1/1 | 0.07 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3163 | 1/1 | 0.14 | - | 62,62,62,62 | 0 |
| 57 | MG | CA | 3077 | 1/1 | 0.18 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3529 | 1/1 | 0.05 | - | 76,76,76,76 | 0 |
| 57 | MG | DA | 3593 | 1/1 | 0.08 | - | 60,60,60,60 | 0 |
| 59 | ZN | CN | 501 | 1/1 | 0.06 | - | 100,100,100,100 | 0 |
| 57 | MG | CA | 3075 | 1/1 | 0.17 | - | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1789 | 1/1 | 0.12 | - | 60,60,60,60 | 0 |
| 57 | MG | CA | 3017 | 1/1 | 0.14 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3407 | 1/1 | 0.15 | - | 32,32,32,32 | 0 |
| 57 | MG | BA | 3186 | 1/1 | 0.17 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3236 | 1/1 | 0.08 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3153 | 1/1 | 0.11 | - | 45,45,45,45 | 0 |
| 59 | ZN | B9 | 501 | 1/1 | 0.20 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3395 | 1/1 | 0.17 | - | 30,30,30,30 | 0 |
| 57 | MG | DA | 3478 | 1/1 | 0.14 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3226 | 1/1 | 0.17 | - | 25,25,25,25 | 0 |
| 57 | MG | DA | 3190 | 1/1 | 0.14 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3090 | 1/1 | 0.26 | - | 50,50,50,50 | 0 |
| 57 | MG | AF | 3001 | 1/1 | 0.13 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3348 | 1/1 | 0.14 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3019 | 1/1 | 0.07 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3552 | 1/1 | 0.16 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3296 | 1/1 | 0.14 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3433 | 1/1 | 0.17 | - | 59,59,59,59 | 0 |
| 57 | MG | AA | 1625 | 1/1 | 0.21 | - | 73,73,73,73 | 0 |
| 57 | MG | DA | 3544 | 1/1 | 0.15 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3641 | 1/1 | 0.08 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3346 | 1/1 | 0.12 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3158 | 1/1 | 0.16 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3063 | 1/1 | 0.25 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3626 | 1/1 | 0.11 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3106 | 1/1 | 0.15 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3365 | 1/1 | 0.12 | - | 19,19,19,19 | 0 |
| 57 | MG | CA | 3104 | 1/1 | 0.18 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3353 | 1/1 | 0.10 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3334 | 1/1 | 0.22 | - | 57,57,57,57 | 0 |
| 57 | MG | AA | 1720 | 1/1 | 0.13 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3093 | 1/1 | 0.21 | - | 41,41,41,41 | 0 |
| 57 | MG | BD | 3006 | 1/1 | 0.07 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3387 | 1/1 | 0.07 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3421 | 1/1 | 0.11 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3562 | 1/1 | 0.10 | - | 31,31,31,31 | 0 |
| 57 | MG | DA | 3654 | 1/1 | 0.16 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3413 | 1/1 | 0.19 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3632 | 1/1 | 0.12 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1724 | 1/1 | 0.15 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3526 | 1/1 | 0.09 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3697 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3253 | 1/1 | 0.10 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3812 | 1/1 | 0.17 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3536 | 1/1 | 0.07 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1737 | 1/1 | 0.11 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3702 | 1/1 | 0.11 | - | 39,39,39,39 | 0 |
| 57 | MG | BF | 302 | 1/1 | 0.24 | - | 30,30,30,30 | 0 |
| 57 | MG | DA | 3126 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3455 | 1/1 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | AA | 1631 | 1/1 | 0.12 | - | 64,64,64,64 | 0 |
| 57 | MG | AA | 1771 | 1/1 | 0.18 | - | 75,75,75,75 | 0 |
| 57 | MG | DA | 3018 | 1/1 | 0.07 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3772 | 1/1 | 0.10 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3570 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3676 | 1/1 | 0.15 | - | 70,70,70,70 | 0 |
| 57 | MG | BA | 3561 | 1/1 | 0.26 | - | 34,34,34,34 | 0 |
| 57 | MG | CA | 3122 | 1/1 | 0.11 | - | 69,69,69,69 | 0 |
| 57 | MG | DA | 3080 | 1/1 | 0.07 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3187 | 1/1 | 0.15 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3475 | 1/1 | 0.07 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3163 | 1/1 | 0.31 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3524 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3181 | 1/1 | 0.07 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3375 | 1/1 | 0.20 | - | 39,39,39,39 | 0 |
| 57 | MG | DB | 3007 | 1/1 | 0.12 | - | 67,67,67,67 | 0 |
| 57 | MG | AA | 1805 | 1/1 | 0.07 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3559 | 1/1 | 0.12 | - | 67,67,67,67 | 0 |
| 57 | MG | DA | 3241 | 1/1 | 0.09 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3095 | 1/1 | 0.13 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3048 | 1/1 | 0.16 | - | 29,29,29,29 | 0 |
| 57 | MG | DA | 3093 | 1/1 | 0.17 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3201 | 1/1 | 0.09 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3410 | 1/1 | 0.13 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3559 | 1/1 | 0.20 | - | 26,26,26,26 | 0 |
| 57 | MG | BA | 3078 | 1/1 | 0.28 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3692 | 1/1 | 0.10 | - | 58,58,58,58 | 0 |
| 57 | MG | AA | 1666 | 1/1 | 0.31 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3379 | 1/1 | 0.18 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3140 | 1/1 | 0.09 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3532 | 1/1 | 0.11 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3024 | 1/1 | 0.16 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3687 | 1/1 | 0.16 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3554 | 1/1 | 0.08 | - | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3363 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3610 | 1/1 | 0.10 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3473 | 1/1 | 0.18 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3088 | 1/1 | 0.21 | - | 43,43,43,43 | 0 |
| 57 | MG | CX | 3002 | 1/1 | 0.10 | - | 67,67,67,67 | 0 |
| 57 | MG | CA | 3003 | 1/1 | 0.13 | - | 58,58,58,58 | 0 |
| 57 | MG | AA | 1726 | 1/1 | 0.11 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3235 | 1/1 | 0.15 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3156 | 1/1 | 0.15 | - | 35,35,35,35 | 0 |
| 57 | MG | AA | 1740 | 1/1 | 0.13 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3105 | 1/1 | 0.11 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3050 | 1/1 | 0.14 | - | 32,32,32,32 | 0 |
| 57 | MG | CA | 3082 | 1/1 | 0.10 | - | 66,66,66,66 | 0 |
| 57 | MG | DF | 302 | 1/1 | 0.15 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3367 | 1/1 | 0.22 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3090 | 1/1 | 0.23 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3360 | 1/1 | 0.10 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3810 | 1/1 | 0.16 | - | 35,35,35,35 | 0 |
| 57 | MG | AA | 1774 | 1/1 | 0.17 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3268 | 1/1 | 0.09 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3429 | 1/1 | 0.17 | - | 36,36,36,36 | 0 |
| 57 | MG | AN | 502 | 1/1 | 0.23 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3545 | 1/1 | 0.11 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3508 | 1/1 | 0.19 | - | 20,20,20,20 | 0 |
| 57 | MG | DO | 202 | 1/1 | 0.09 | - | 60,60,60,60 | 0 |
| 57 | MG | AA | 1633 | 1/1 | 0.29 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3332 | 1/1 | 0.07 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3275 | 1/1 | 0.19 | - | 65,65,65,65 | 0 |
| 57 | MG | AB | 3001 | 1/1 | 0.11 | - | 77,77,77,77 | 0 |
| 57 | MG | BA | 3682 | 1/1 | 0.08 | - | 60,60,60,60 | 0 |
| 57 | MG | AX | 3013 | 1/1 | 0.17 | - | 70,70,70,70 | 0 |
| 57 | MG | AA | 1758 | 1/1 | 0.06 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3333 | 1/1 | 0.16 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3773 | 1/1 | 0.16 | - | 32,32,32,32 | 0 |
| 57 | MG | AY | 3003 | 1/1 | 0.06 | - | 79,79,79,79 | 0 |
| 57 | MG | DA | 3331 | 1/1 | 0.15 | - | 47,47,47,47 | 0 |
| 57 | MG | CA | 3088 | 1/1 | 0.12 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3637 | 1/1 | 0.16 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3399 | 1/1 | 0.17 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3098 | 1/1 | 0.16 | - | 23,23,23,23 | 0 |
| 57 | MG | BB | 3017 | 1/1 | 0.16 | - | 81,81,81,81 | 0 |
| 57 | MG | DA | 3494 | 1/1 | 0.18 | - | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1658 | 1/1 | 0.11 | - | 64,64,64,64 | 0 |
| 57 | MG | BD | 3003 | 1/1 | 0.24 | - | 37,37,37,37 | 0 |
| 57 | MG | BB | 3006 | 1/1 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3424 | 1/1 | 0.16 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3345 | 1/1 | 0.17 | - | 51,51,51,51 | 0 |
| 57 | MG | BN | 3003 | 1/1 | 0.13 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3003 | 1/1 | 0.13 | - | 33,33,33,33 | 0 |
| 57 | MG | CA | 3149 | 1/1 | 0.10 | - | 54,54,54,54 | 0 |
| 57 | MG | CA | 3110 | 1/1 | 0.10 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3797 | 1/1 | 0.23 | - | 51,51,51,51 | 0 |
| 57 | MG | AA | 1745 | 1/1 | 0.17 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3100 | 1/1 | 0.06 | - | 47,47,47,47 | 0 |
| 57 | MG | AX | 3009 | 1/1 | 0.35 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3440 | 1/1 | 0.16 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3636 | 1/1 | 0.11 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3143 | 1/1 | 0.08 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3430 | 1/1 | 0.20 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3470 | 1/1 | 0.11 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3182 | 1/1 | 0.56 | - | 52,52,52,52 | 0 |
| 57 | MG | CA | 3059 | 1/1 | 0.17 | - | 75,75,75,75 | 0 |
| 57 | MG | DE | 3006 | 1/1 | 0.15 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3311 | 1/1 | 0.12 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3646 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3754 | 1/1 | 0.11 | - | 42,42,42,42 | 0 |
| 57 | MG | AA | 1682 | 1/1 | 0.21 | - | 59,59,59,59 | 0 |
| 57 | MG | AA | 1635 | 1/1 | 0.11 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3313 | 1/1 | 0.18 | - | 38,38,38,38 | 0 |
| 57 | MG | CA | 3146 | 1/1 | 0.14 | - | 72,72,72,72 | 0 |
| 57 | MG | AX | 3004 | 1/1 | 0.15 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3094 | 1/1 | 0.06 | - | 39,39,39,39 | 0 |
| 57 | MG | DE | 3002 | 1/1 | 0.10 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3716 | 1/1 | 0.25 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3151 | 1/1 | 0.10 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3115 | 1/1 | 0.16 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3411 | 1/1 | 0.18 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3330 | 1/1 | 0.16 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3566 | 1/1 | 0.22 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3374 | 1/1 | 0.18 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3372 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 57 | MG | DB | 3008 | 1/1 | 0.20 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3329 | 1/1 | 0.10 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3035 | 1/1 | 0.13 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3141 | 1/1 | 0.28 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3752 | 1/1 | 0.09 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3111 | 1/1 | 0.34 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3449 | 1/1 | 0.10 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3001 | 1/1 | 0.11 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3590 | 1/1 | 0.21 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3513 | 1/1 | 0.30 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3608 | 1/1 | 0.06 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3466 | 1/1 | 0.08 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3132 | 1/1 | 0.11 | - | 64,64,64,64 | 0 |
| 57 | MG | AA | 1660 | 1/1 | 0.19 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3184 | 1/1 | 0.10 | - | 42,42,42,42 | 0 |
| 57 | MG | CA | 3112 | 1/1 | 0.08 | - | 72,72,72,72 | 0 |
| 57 | MG | CA | 3078 | 1/1 | 0.17 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3764 | 1/1 | 0.12 | - | 66,66,66,66 | 0 |
| 57 | MG | AA | 1797 | 1/1 | 0.13 | - | 59,59,59,59 | 0 |
| 57 | MG | AA | 1678 | 1/1 | 0.22 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3681 | 1/1 | 0.15 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3160 | 1/1 | 0.31 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3380 | 1/1 | 0.12 | - | 40,40,40,40 | 0 |
| 57 | MG | CA | 3023 | 1/1 | 0.09 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3043 | 1/1 | 0.13 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3565 | 1/1 | 0.05 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3064 | 1/1 | 0.21 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1701 | 1/1 | 0.22 | - | 73,73,73,73 | 0 |
| 57 | MG | CA | 3083 | 1/1 | 0.12 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3411 | 1/1 | 0.17 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3128 | 1/1 | 0.24 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3072 | 1/1 | 0.12 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3283 | 1/1 | 0.31 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3518 | 1/1 | 0.19 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3523 | 1/1 | 0.19 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1694 | 1/1 | 0.06 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3805 | 1/1 | 0.11 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3457 | 1/1 | 0.17 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3724 | 1/1 | 0.14 | - | 20,20,20,20 | 0 |
| 57 | MG | BA | 3511 | 1/1 | 0.12 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3055 | 1/1 | 0.22 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3274 | 1/1 | 0.27 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3031 | 1/1 | 0.22 | - | 36,36,36,36 | 0 |
| 57 | MG | BR | 5001 | 1/1 | 0.11 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1782 | 1/1 | 0.11 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3143 | 1/1 | 0.10 | - | 62,62,62,62 | 0 |
| 57 | MG | AA | 1683 | 1/1 | 0.16 | - | 62,62,62,62 | 0 |
| 57 | MG | B0 | 3001 | 1/1 | 0.30 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3652 | 1/1 | 0.08 | - | 58,58,58,58 | 0 |
| 57 | MG | CA | 3056 | 1/1 | 0.08 | - | 64,64,64,64 | 0 |
| 57 | MG | CA | 3065 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3009 | 1/1 | 0.13 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3077 | 1/1 | 0.09 | - | 38,38,38,38 | 0 |
| 57 | MG | BD | 3004 | 1/1 | 0.32 | - | 28,28,28,28 | 0 |
| 57 | MG | B7 | 104 | 1/1 | 0.19 | - | 62,62,62,62 | 0 |
| 57 | MG | BB | 3010 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3427 | 1/1 | 0.15 | - | 47,47,47,47 | 0 |
| 57 | MG | AA | 1669 | 1/1 | 0.17 | - | 69,69,69,69 | 0 |
| 57 | MG | AA | 1752 | 1/1 | 0.13 | - | 48,48,48,48 | 0 |
| 58 | SF4 | AD | 501 | 8/8 | 0.17 | - | 59,68,73,79 | 0 |
| 57 | MG | BA | 3169 | 1/1 | 0.14 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3096 | 1/1 | 0.08 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3377 | 1/1 | 0.19 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3606 | 1/1 | 0.17 | - | 74,74,74,74 | 0 |
| 57 | MG | AA | 1729 | 1/1 | 0.13 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3581 | 1/1 | 0.11 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3698 | 1/1 | 0.09 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3151 | 1/1 | 0.14 | - | 36,36,36,36 | 0 |
| 57 | MG | CA | 3049 | 1/1 | 0.26 | - | 65,65,65,65 | 0 |
| 57 | MG | BA | 3092 | 1/1 | 0.28 | - | 40,40,40,40 | 0 |
| 57 | MG | AA | 1630 | 1/1 | 0.09 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3704 | 1/1 | 0.21 | - | 26,26,26,26 | 0 |
| 57 | MG | BF | 304 | 1/1 | 0.40 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3390 | 1/1 | 0.07 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3537 | 1/1 | 0.07 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3344 | 1/1 | 0.09 | - | 71,71,71,71 | 0 |
| 57 | MG | BA | 3172 | 1/1 | 0.32 | - | 40,40,40,40 | 0 |
| 57 | MG | AA | 1749 | 1/1 | 0.17 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3220 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3006 | 1/1 | 0.41 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3456 | 1/1 | 0.27 | - | 37,37,37,37 | 0 |
| 58 | SF4 | CD | 501 | 8/8 | 0.16 | - | 64,67,74,91 | 0 |
| 57 | MG | AA | 1785 | 1/1 | 0.12 | - | 72,72,72,72 | 0 |
| 57 | MG | BA | 3268 | 1/1 | 0.17 | - | 54,54,54,54 | 0 |
| 57 | MG | CA | 3119 | 1/1 | 0.10 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3713 | 1/1 | 0.26 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3190 | 1/1 | 0.27 | - | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3444 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3337 | 1/1 | 0.06 | - | 48,48,48,48 | 0 |
| 57 | MG | AA | 1617 | 1/1 | 0.11 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3335 | 1/1 | 0.11 | - | 40,40,40,40 | 0 |
| 57 | MG | AA | 1773 | 1/1 | 0.09 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3059 | 1/1 | 0.06 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3188 | 1/1 | 0.16 | - | 32,32,32,32 | 0 |
| 57 | MG | DA | 3108 | 1/1 | 0.09 | - | 50,50,50,50 | 0 |
| 57 | MG | CA | 3089 | 1/1 | 0.21 | - | 74,74,74,74 | 0 |
| 57 | MG | DA | 3137 | 1/1 | 0.15 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3450 | 1/1 | 0.06 | - | 50,50,50,50 | 0 |
| 57 | MG | BB | 3001 | 1/1 | 0.27 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3556 | 1/1 | 0.08 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3525 | 1/1 | 0.10 | - | 28,28,28,28 | 0 |
| 57 | MG | DA | 3116 | 1/1 | 0.13 | - | 53,53,53,53 | 0 |
| 57 | MG | CA | 3117 | 1/1 | 0.07 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3318 | 1/1 | 0.14 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3528 | 1/1 | 0.18 | - | 36,36,36,36 | 0 |
| 57 | MG | AM | 3002 | 1/1 | 0.09 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3252 | 1/1 | 0.17 | - | 36,36,36,36 | 0 |
| 57 | MG | B8 | 5002 | 1/1 | 0.23 | - | 53,53,53,53 | 0 |
| 57 | MG | AA | 1755 | 1/1 | 0.09 | - | 80,80,80,80 | 0 |
| 57 | MG | CA | 3006 | 1/1 | 0.07 | - | 68,68,68,68 | 0 |
| 57 | MG | CA | 3045 | 1/1 | 0.21 | - | 62,62,62,62 | 0 |
| 57 | MG | BN | 3002 | 1/1 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3024 | 1/1 | 0.11 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3408 | 1/1 | 0.20 | - | 51,51,51,51 | 0 |
| 57 | MG | DD | 302 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3074 | 1/1 | 0.11 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3249 | 1/1 | 0.18 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3234 | 1/1 | 0.10 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3398 | 1/1 | 0.20 | - | 32,32,32,32 | 0 |
| 57 | MG | CA | 3026 | 1/1 | 0.13 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3621 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3045 | 1/1 | 0.10 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3223 | 1/1 | 0.15 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3294 | 1/1 | 0.13 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3728 | 1/1 | 0.13 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3454 | 1/1 | 0.15 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3755 | 1/1 | 0.18 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3804 | 1/1 | 0.14 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3628 | 1/1 | 0.24 | - | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3189 | 1/1 | 0.16 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3473 | 1/1 | 0.18 | - | 28,28,28,28 | 0 |
| 57 | MG | BA | 3359 | 1/1 | 0.06 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3661 | 1/1 | 0.08 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3350 | 1/1 | 0.07 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3325 | 1/1 | 0.19 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3617 | 1/1 | 0.21 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3012 | 1/1 | 0.08 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3574 | 1/1 | 0.16 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3091 | 1/1 | 0.34 | - | 42,42,42,42 | 0 |
| 57 | MG | DD | 303 | 1/1 | 0.32 | - | 51,51,51,51 | 0 |
| 57 | MG | DA | 3179 | 1/1 | 0.05 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3665 | 1/1 | 0.14 | - | 42,42,42,42 | 0 |
| 57 | MG | BF | 305 | 1/1 | 0.20 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3021 | 1/1 | 0.08 | - | 43,43,43,43 | 0 |
| 57 | MG | B6 | 101 | 1/1 | 0.19 | - | 60,60,60,60 | 0 |
| 57 | MG | CA | 3134 | 1/1 | 0.14 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3357 | 1/1 | 0.12 | - | 33,33,33,33 | 0 |
| 57 | MG | DA | 3111 | 1/1 | 0.10 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3678 | 1/1 | 0.10 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3200 | 1/1 | 0.16 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3730 | 1/1 | 0.17 | - | 68,68,68,68 | 0 |
| 57 | MG | BA | 3595 | 1/1 | 0.08 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3242 | 1/1 | 0.68 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1811 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3151 | 1/1 | 0.08 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3387 | 1/1 | 0.18 | - | 29,29,29,29 | 0 |
| 57 | MG | BA | 3520 | 1/1 | 0.23 | - | 29,29,29,29 | 0 |
| 57 | MG | DP | 202 | 1/1 | 0.08 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3685 | 1/1 | 0.22 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3072 | 1/1 | 0.24 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3318 | 1/1 | 0.10 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1744 | 1/1 | 0.15 | - | 44,44,44,44 | 0 |
| 57 | MG | CA | 3038 | 1/1 | 0.10 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3776 | 1/1 | 0.16 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3124 | 1/1 | 0.16 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3220 | 1/1 | 0.22 | - | 50,50,50,50 | 0 |
| 57 | MG | AA | 1748 | 1/1 | 0.17 | - | 64,64,64,64 | 0 |
| 57 | MG | CA | 3144 | 1/1 | 0.10 | - | 82,82,82,82 | 0 |
| 57 | MG | AA | 1624 | 1/1 | 0.23 | - | 66,66,66,66 | 0 |
| 57 | MG | BB | 3023 | 1/1 | 0.13 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3507 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | AA | 1693 | 1/1 | 0.22 | - | 76,76,76,76 | 0 |
| 57 | MG | BA | 3701 | 1/1 | 0.28 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3060 | 1/1 | 0.16 | - | 51,51,51,51 | 0 |
| 57 | MG | AA | 1649 | 1/1 | 0.13 | - | 28,28,28,28 | 0 |
| 57 | MG | CA | 3154 | 1/1 | 0.13 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3056 | 1/1 | 0.10 | - | 49,49,49,49 | 0 |
| 57 | MG | AM | 3001 | 1/1 | 0.10 | - | 66,66,66,66 | 0 |
| 57 | MG | AA | 1619 | 1/1 | 0.08 | - | 64,64,64,64 | 0 |
| 57 | MG | CA | 3027 | 1/1 | 0.10 | - | 65,65,65,65 | 0 |
| 57 | MG | BB | 3003 | 1/1 | 0.13 | - | 30,30,30,30 | 0 |
| 57 | MG | CA | 3156 | 1/1 | 0.06 | - | 59,59,59,59 | 0 |
| 57 | MG | DA | 3029 | 1/1 | 0.46 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3129 | 1/1 | 0.15 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3418 | 1/1 | 0.19 | - | 38,38,38,38 | 0 |
| 57 | MG | CA | 3072 | 1/1 | 0.18 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3244 | 1/1 | 0.23 | - | 31,31,31,31 | 0 |
| 57 | MG | DA | 3063 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3226 | 1/1 | 0.18 | - | 57,57,57,57 | 0 |
| 57 | MG | CA | 3103 | 1/1 | 0.12 | - | 73,73,73,73 | 0 |
| 57 | MG | DA | 3214 | 1/1 | 0.07 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3337 | 1/1 | 0.23 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3671 | 1/1 | 0.16 | - | 24,24,24,24 | 0 |
| 57 | MG | DA | 3476 | 1/1 | 0.07 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3031 | 1/1 | 0.08 | - | 42,42,42,42 | 0 |
| 57 | MG | D3 | 3001 | 1/1 | 0.34 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3477 | 1/1 | 0.13 | - | 68,68,68,68 | 0 |
| 57 | MG | AA | 1800 | 1/1 | 0.12 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3624 | 1/1 | 0.11 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3254 | 1/1 | 0.10 | - | 33,33,33,33 | 0 |
| 57 | MG | CA | 3076 | 1/1 | 0.17 | - | 77,77,77,77 | 0 |
| 60 | K | AX | 3001 | 1/1 | 0.11 | - | 77,77,77,77 | 0 |
| 57 | MG | DA | 3382 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3499 | 1/1 | 0.17 | - | 52,52,52,52 | 0 |
| 59 | ZN | D4 | 501 | 1/1 | 0.10 | - | 162,162,162,162 | 0 |
| 57 | MG | DB | 3013 | 1/1 | 0.09 | - | 66,66,66,66 | 0 |
| 57 | MG | CA | 3143 | 1/1 | 0.15 | - | 74,74,74,74 | 0 |
| 57 | MG | BA | 3253 | 1/1 | 0.20 | - | 31,31,31,31 | 0 |
| 57 | MG | AX | 3005 | 1/1 | 0.10 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3006 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3610 | 1/1 | 0.06 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3452 | 1/1 | 0.09 | - | 45,45,45,45 | 0 |
| 57 | MG | BW | 3003 | 1/1 | 0.13 | - | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3018 | 1/1 | 0.36 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3385 | 1/1 | 0.06 | - | 60,60,60,60 | 0 |
| 57 | MG | AX | 3007 | 1/1 | 0.30 | - | 68,68,68,68 | 0 |
| 57 | MG | DA | 3437 | 1/1 | 0.23 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3222 | 1/1 | 0.15 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3240 | 1/1 | 0.06 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3745 | 1/1 | 0.27 | - | 61,61,61,61 | 0 |
| 57 | MG | CA | 3106 | 1/1 | 0.10 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3639 | 1/1 | 0.14 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3057 | 1/1 | 0.15 | - | 84,84,84,84 | 0 |
| 57 | MG | BA | 3771 | 1/1 | 0.10 | - | 41,41,41,41 | 0 |
| 57 | MG | AA | 1747 | 1/1 | 0.17 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3216 | 1/1 | 0.15 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3362 | 1/1 | 0.20 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3488 | 1/1 | 0.12 | - | 20,20,20,20 | 0 |
| 57 | MG | BA | 3420 | 1/1 | 0.17 | - | 25,25,25,25 | 0 |
| 57 | MG | CA | 3140 | 1/1 | 0.15 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3630 | 1/1 | 0.23 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3534 | 1/1 | 0.07 | - | 46,46,46,46 | 0 |
| 57 | MG | AA | 1766 | 1/1 | 0.13 | - | 71,71,71,71 | 0 |
| 57 | MG | BA | 3100 | 1/1 | 0.22 | - | 61,61,61,61 | 0 |
| 57 | MG | AA | 1761 | 1/1 | 0.21 | - | 70,70,70,70 | 0 |
| 57 | MG | DA | 3633 | 1/1 | 0.14 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3696 | 1/1 | 0.10 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3118 | 1/1 | 0.11 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3067 | 1/1 | 0.21 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3602 | 1/1 | 0.07 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3372 | 1/1 | 0.09 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3342 | 1/1 | 0.28 | - | 67,67,67,67 | 0 |
| 57 | MG | AA | 1632 | 1/1 | 0.10 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3107 | 1/1 | 0.23 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3340 | 1/1 | 0.13 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3464 | 1/1 | 0.05 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3419 | 1/1 | 0.16 | - | 25,25,25,25 | 0 |
| 57 | MG | DA | 3342 | 1/1 | 0.15 | - | 53,53,53,53 | 0 |
| 57 | MG | AW | 3002 | 1/1 | 0.09 | - | 79,79,79,79 | 0 |
| 57 | MG | BA | 3787 | 1/1 | 0.11 | - | 45,45,45,45 | 0 |
| 57 | MG | DA | 3471 | 1/1 | 0.34 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3011 | 1/1 | 0.07 | - | 35,35,35,35 | 0 |
| 57 | MG | BA | 3617 | 1/1 | 0.07 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3300 | 1/1 | 0.10 | - | 38,38,38,38 | 0 |
| 57 | MG | DA | 3086 | 1/1 | 0.11 | - | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3504 | 1/1 | 0.13 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3333 | 1/1 | 0.15 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3663 | 1/1 | 0.15 | - | 73,73,73,73 | 0 |
| 57 | MG | DA | 3279 | 1/1 | 0.10 | - | 36,36,36,36 | 0 |
| 57 | MG | CA | 3051 | 1/1 | 0.12 | - | 77,77,77,77 | 0 |
| 57 | MG | BA | 3615 | 1/1 | 0.12 | - | 71,71,71,71 | 0 |
| 57 | MG | DA | 3184 | 1/1 | 0.09 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3038 | 1/1 | 0.20 | - | 20,20,20,20 | 0 |
| 57 | MG | AW | 3001 | 1/1 | 0.10 | - | 59,59,59,59 | 0 |
| 57 | MG | AA | 1791 | 1/1 | 0.07 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3706 | 1/1 | 0.16 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3083 | 1/1 | 0.16 | - | 41,41,41,41 | 0 |
| 57 | MG | BF | 307 | 1/1 | 0.09 | - | 34,34,34,34 | 0 |
| 57 | MG | BA | 3743 | 1/1 | 0.59 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3492 | 1/1 | 0.05 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3160 | 1/1 | 0.08 | - | 73,73,73,73 | 0 |
| 57 | MG | BA | 3308 | 1/1 | 0.17 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3195 | 1/1 | 0.14 | - | 36,36,36,36 | 0 |
| 57 | MG | AA | 1763 | 1/1 | 0.05 | - | 79,79,79,79 | 0 |
| 57 | MG | BA | 3017 | 1/1 | 0.27 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3057 | 1/1 | 0.15 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3364 | 1/1 | 0.14 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3425 | 1/1 | 0.15 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3302 | 1/1 | 0.13 | - | 49,49,49,49 | 0 |
| 57 | MG | DA | 3404 | 1/1 | 0.08 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3305 | 1/1 | 0.11 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3250 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | CF | 3001 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3300 | 1/1 | 0.14 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3483 | 1/1 | 0.06 | - | 53,53,53,53 | 0 |
| 57 | MG | BW | 3001 | 1/1 | 0.25 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3386 | 1/1 | 0.07 | - | 44,44,44,44 | 0 |
| 57 | MG | DA | 3481 | 1/1 | 0.10 | - | 40,40,40,40 | 0 |
| 57 | MG | DA | 3605 | 1/1 | 0.08 | - | 45,45,45,45 | 0 |
| 57 | MG | BA | 3094 | 1/1 | 0.17 | - | 52,52,52,52 | 0 |
| 57 | MG | AA | 1750 | 1/1 | 0.13 | - | 49,49,49,49 | 0 |
| 57 | MG | BA | 3175 | 1/1 | 0.25 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3075 | 1/1 | 0.12 | - | 24,24,24,24 | 0 |
| 57 | MG | DA | 3538 | 1/1 | 0.09 | - | 60,60,60,60 | 0 |
| 57 | MG | AA | 1713 | 1/1 | 0.11 | - | 67,67,67,67 | 0 |
| 57 | MG | BA | 3251 | 1/1 | 0.29 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3751 | 1/1 | 0.21 | - | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3020 | 1/1 | 0.15 | - | 25,25,25,25 | 0 |
| 57 | MG | CA | 3155 | 1/1 | 0.12 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3091 | 1/1 | 0.22 | - | 54,54,54,54 | 0 |
| 57 | MG | DF | 303 | 1/1 | 0.29 | - | 42,42,42,42 | 0 |
| 57 | MG | BD | 3009 | 1/1 | 0.13 | - | 37,37,37,37 | 0 |
| 57 | MG | DA | 3048 | 1/1 | 0.07 | - | 59,59,59,59 | 0 |
| 57 | MG | CA | 3097 | 1/1 | 0.22 | - | 60,60,60,60 | 0 |
| 57 | MG | AA | 1717 | 1/1 | 0.14 | - | 75,75,75,75 | 0 |
| 57 | MG | BA | 3575 | 1/1 | 0.13 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3245 | 1/1 | 0.07 | - | 58,58,58,58 | 0 |
| 57 | MG | CA | 3162 | 1/1 | 0.08 | - | 79,79,79,79 | 0 |
| 57 | MG | DA | 3115 | 1/1 | 0.21 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3516 | 1/1 | 0.19 | - | 67,67,67,67 | 0 |
| 57 | MG | CA | 3131 | 1/1 | 0.17 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3299 | 1/1 | 0.18 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3609 | 1/1 | 0.19 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3189 | 1/1 | 0.15 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3462 | 1/1 | 0.09 | - | 53,53,53,53 | 0 |
| 57 | MG | DA | 3356 | 1/1 | 0.16 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3712 | 1/1 | 0.22 | - | 51,51,51,51 | 0 |
| 57 | MG | BA | 3506 | 1/1 | 0.18 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3328 | 1/1 | 0.16 | - | 27,27,27,27 | 0 |
| 57 | MG | BA | 3131 | 1/1 | 0.22 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3695 | 1/1 | 0.10 | - | 40,40,40,40 | 0 |
| 57 | MG | BA | 3591 | 1/1 | 0.39 | - | 41,41,41,41 | 0 |
| 57 | MG | DA | 3307 | 1/1 | 0.09 | - | 51,51,51,51 | 0 |
| 57 | MG | AA | 1779 | 1/1 | 0.11 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3315 | 1/1 | 0.12 | - | 40,40,40,40 | 0 |
| 57 | MG | AA | 1685 | 1/1 | 0.18 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3490 | 1/1 | 0.14 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3444 | 1/1 | 0.18 | - | 44,44,44,44 | 0 |
| 57 | MG | AA | 1674 | 1/1 | 0.14 | - | 58,58,58,58 | 0 |
| 57 | MG | AL | 202 | 1/1 | 0.23 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3225 | 1/1 | 0.08 | - | 55,55,55,55 | 0 |
| 57 | MG | CA | 3047 | 1/1 | 0.12 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3658 | 1/1 | 0.43 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3578 | 1/1 | 0.30 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3135 | 1/1 | 0.28 | - | 63,63,63,63 | 0 |
| 57 | MG | DA | 3228 | 1/1 | 0.13 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3065 | 1/1 | 0.25 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3629 | 1/1 | 0.19 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3269 | 1/1 | 0.17 | - | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | BA | 3461 | 1/1 | 0.07 | - | 45,45,45,45 | 0 |
| 57 | MG | AA | 1759 | 1/1 | 0.16 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3416 | 1/1 | 0.28 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3112 | 1/1 | 0.24 | - | 41,41,41,41 | 0 |
| 57 | MG | BA | 3582 | 1/1 | 0.11 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3059 | 1/1 | 0.11 | - | 36,36,36,36 | 0 |
| 57 | MG | AA | 1764 | 1/1 | 0.06 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3409 | 1/1 | 0.09 | - | 54,54,54,54 | 0 |
| 57 | MG | BA | 3368 | 1/1 | 0.25 | - | 32,32,32,32 | 0 |
| 57 | MG | DA | 3511 | 1/1 | 0.09 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3533 | 1/1 | 0.18 | - | 23,23,23,23 | 0 |
| 57 | MG | BA | 3565 | 1/1 | 0.14 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3744 | 1/1 | 0.15 | - | 55,55,55,55 | 0 |
| 57 | MG | BA | 3180 | 1/1 | 0.24 | - | 46,46,46,46 | 0 |
| 57 | MG | BA | 3633 | 1/1 | 0.16 | - | 57,57,57,57 | 0 |
| 57 | MG | DA | 3513 | 1/1 | 0.15 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3567 | 1/1 | 0.23 | - | 32,32,32,32 | 0 |
| 57 | MG | BA | 3044 | 1/1 | 0.30 | - | 43,43,43,43 | 0 |
| 57 | MG | BA | 3770 | 1/1 | 0.43 | - | 49,49,49,49 | 0 |
| 57 | MG | CA | 3125 | 1/1 | 0.21 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3438 | 1/1 | 0.06 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3247 | 1/1 | 0.09 | - | 49,49,49,49 | 0 |
| 57 | MG | AY | 3002 | 1/1 | 0.36 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3147 | 1/1 | 0.16 | - | 36,36,36,36 | 0 |
| 57 | MG | BA | 3632 | 1/1 | 0.26 | - | 55,55,55,55 | 0 |
| 57 | MG | AA | 1627 | 1/1 | 0.09 | - | 54,54,54,54 | 0 |
| 57 | MG | DA | 3581 | 1/1 | 0.05 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3137 | 1/1 | 0.23 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3073 | 1/1 | 0.05 | - | 33,33,33,33 | 0 |
| 57 | MG | BA | 3748 | 1/1 | 0.08 | - | 61,61,61,61 | 0 |
| 57 | MG | DA | 3519 | 1/1 | 0.14 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3434 | 1/1 | 0.08 | - | 19,19,19,19 | 0 |
| 57 | MG | AA | 1686 | 1/1 | 0.16 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3767 | 1/1 | 0.32 | - | 45,45,45,45 | 0 |
| 57 | MG | BD | 3001 | 1/1 | 0.10 | - | 34,34,34,34 | 0 |
| 57 | MG | CA | 3159 | 1/1 | 0.12 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3286 | 1/1 | 0.12 | - | 55,55,55,55 | 0 |
| 57 | MG | DA | 3259 | 1/1 | 0.09 | - | 42,42,42,42 | 0 |
| 57 | MG | BA | 3592 | 1/1 | 0.07 | - | 65,65,65,65 | 0 |
| 57 | MG | CD | 502 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |
| 57 | MG | BA | 3433 | 1/1 | 0.22 | - | 27,27,27,27 | 0 |
| 57 | MG | DA | 3155 | 1/1 | 0.19 | - | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | DA | 3060 | 1/1 | 0.22 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3483 | 1/1 | 0.12 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3030 | 1/1 | 0.20 | - | 39,39,39,39 | 0 |
| 57 | MG | DA | 3217 | 1/1 | 0.15 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3541 | 1/1 | 0.19 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3442 | 1/1 | 0.19 | - | 65,65,65,65 | 0 |
| 57 | MG | AA | 1723 | 1/1 | 0.13 | - | 63,63,63,63 | 0 |
| 57 | MG | BA | 3081 | 1/1 | 0.20 | - | 48,48,48,48 | 0 |
| 57 | MG | DA | 3553 | 1/1 | 0.06 | - | 72,72,72,72 | 0 |
| 57 | MG | DA | 3114 | 1/1 | 0.10 | - | 51,51,51,51 | 0 |
| 57 | MG | CA | 3118 | 1/1 | 0.14 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3790 | 1/1 | 0.72 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3750 | 1/1 | 0.18 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3230 | 1/1 | 0.09 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3436 | 1/1 | 0.11 | - | 35,35,35,35 | 0 |
| 57 | MG | DA | 3402 | 1/1 | 0.07 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3028 | 1/1 | 0.18 | - | 37,37,37,37 | 0 |
| 57 | MG | BA | 3349 | 1/1 | 0.17 | - | 34,34,34,34 | 0 |
| 57 | MG | DA | 3046 | 1/1 | 0.13 | - | 56,56,56,56 | 0 |
| 57 | MG | BB | 3004 | 1/1 | 0.18 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3096 | 1/1 | 0.14 | - | 60,60,60,60 | 0 |
| 57 | MG | DA | 3284 | 1/1 | 0.10 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3197 | 1/1 | 0.21 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3216 | 1/1 | 0.27 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3814 | 1/1 | 0.21 | - | 39,39,39,39 | 0 |
| 57 | MG | BA | 3026 | 1/1 | 0.25 | - | 60,60,60,60 | 0 |
| 57 | MG | BA | 3237 | 1/1 | 0.13 | - | 44,44,44,44 | 0 |
| 57 | MG | DE | 3007 | 1/1 | 0.08 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3154 | 1/1 | 0.18 | - | 52,52,52,52 | 0 |
| 57 | MG | BA | 3510 | 1/1 | 0.18 | - | 45,45,45,45 | 0 |
| 57 | MG | BN | 3001 | 1/1 | 0.15 | - | 48,48,48,48 | 0 |
| 57 | MG | BA | 3534 | 1/1 | 0.23 | - | 26,26,26,26 | 0 |
| 57 | MG | CA | 3087 | 1/1 | 0.07 | - | 57,57,57,57 | 0 |
| 57 | MG | BA | 3780 | 1/1 | 0.08 | - | 42,42,42,42 | 0 |
| 57 | MG | D8 | 5001 | 1/1 | 0.18 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3202 | 1/1 | 0.09 | - | 62,62,62,62 | 0 |
| 57 | MG | BA | 3076 | 1/1 | 0.22 | - | 42,42,42,42 | 0 |
| 57 | MG | DA | 3441 | 1/1 | 0.19 | - | 58,58,58,58 | 0 |
| 57 | MG | BA | 3297 | 1/1 | 0.22 | - | 42,42,42,42 | 0 |
| 57 | MG | DV | 201 | 1/1 | 0.78 | - | 58,58,58,58 | 0 |
| 57 | MG | DA | 3655 | 1/1 | 0.14 | - | 38,38,38,38 | 0 |
| 57 | MG | CA | 3136 | 1/1 | 0.14 | - | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | CA | 3094 | 1/1 | 0.08 | - | 61,61,61,61 | 0 |
| 57 | MG | BA | 3550 | 1/1 | 0.15 | - | 50,50,50,50 | 0 |
| 57 | MG | CA | 3011 | 1/1 | 0.23 | - | 66,66,66,66 | 0 |
| 57 | MG | DA | 3607 | 1/1 | 0.09 | - | 64,64,64,64 | 0 |
| 57 | MG | DA | 3398 | 1/1 | 0.07 | - | 40,40,40,40 | 0 |
| 57 | MG | CA | 3018 | 1/1 | 0.11 | - | 63,63,63,63 | 0 |
| 57 | MG | CA | 3012 | 1/1 | 0.25 | - | 64,64,64,64 | 0 |
| 57 | MG | BA | 3476 | 1/1 | 0.14 | - | 48,48,48,48 | 0 |
| 57 | MG | CA | 3116 | 1/1 | 0.18 | - | 57,57,57,57 | 0 |
| 57 | MG | CA | 3101 | 1/1 | 0.09 | - | 65,65,65,65 | 0 |
| 57 | MG | DA | 3182 | 1/1 | 0.20 | - | 52,52,52,52 | 0 |
| 57 | MG | DA | 3528 | 1/1 | 0.14 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3533 | 1/1 | 0.16 | - | 56,56,56,56 | 0 |
| 57 | MG | BA | 3132 | 1/1 | 0.10 | - | 50,50,50,50 | 0 |
| 57 | MG | BA | 3769 | 1/1 | 0.17 | - | 47,47,47,47 | 0 |
| 57 | MG | DA | 3596 | 1/1 | 0.29 | - | 69,69,69,69 | 0 |
| 57 | MG | BA | 3207 | 1/1 | 0.21 | - | 36,36,36,36 | 0 |
| 57 | MG | DA | 3353 | 1/1 | 0.12 | - | 47,47,47,47 | 0 |
| 57 | MG | BA | 3286 | 1/1 | 0.14 | - | 44,44,44,44 | 0 |
| 57 | MG | BA | 3781 | 1/1 | 0.15 | - | 56,56,56,56 | 0 |
| 57 | MG | DA | 3027 | 1/1 | 0.46 | - | 43,43,43,43 | 0 |
| 57 | MG | DA | 3591 | 1/1 | 0.07 | - | 66,66,66,66 | 0 |
| 57 | MG | BA | 3033 | 1/1 | 0.47 | - | 31,31,31,31 | 0 |
| 57 | MG | BA | 3556 | 1/1 | 0.09 | - | 46,46,46,46 | 0 |
| 57 | MG | AA | 1812 | 1/1 | 0.13 | - | 63,63,63,63 | 0 |
| 57 | MG | CJ | 5001 | 1/1 | 0.12 | - | 77,77,77,77 | 0 |
| 57 | MG | BA | 3516 | 1/1 | 0.23 | - | 46,46,46,46 | 0 |
| 57 | MG | DA | 3588 | 1/1 | 0.18 | - | 59,59,59,59 | 0 |
| 57 | MG | BA | 3492 | 1/1 | 0.06 | - | 38,38,38,38 | 0 |
| 57 | MG | BA | 3497 | 1/1 | 0.16 | - | 50,50,50,50 | 0 |
| 57 | MG | DA | 3580 | 1/1 | 0.20 | - | 62,62,62,62 | 0 |
| 57 | MG | DA | 3262 | 1/1 | 0.09 | - | 20,20,20,20 | 0 |
| 57 | MG | BA | 3807 | 1/1 | 0.20 | - | 66,66,66,66 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.