



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:04 AM UTC

PDB ID : 4V9B / pdb\_00004v9b  
Title : Crystal Structure of the 70S ribosome with tigecycline.  
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.  
Deposited on : 2012-07-18  
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

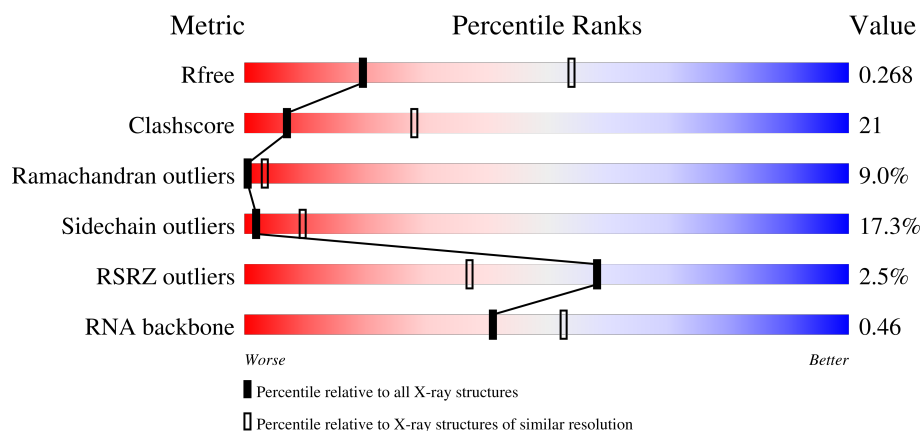
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |
| RNA backbone          | 3983                        | 1022 (3.32-2.88)                                      |

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

| Mol | Chain | Length | Quality of chain                                     |
|-----|-------|--------|------------------------------------------------------|
| 1   | AA    | 1506   | <div> <div>2%</div> <div>37% 48% 15%</div> </div>    |
| 1   | CA    | 1506   | <div> <div>41% 44% 15%</div> </div>                  |
| 2   | AE    | 256    | <div> <div>32% 40% 20% 7%</div> </div>               |
| 2   | CE    | 256    | <div> <div>2%</div> <div>25% 45% 19% 7%</div> </div> |

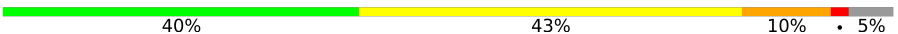
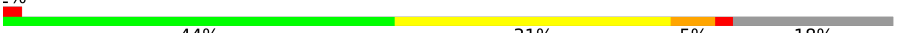
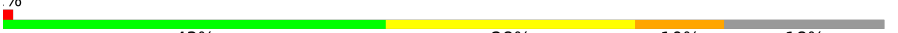
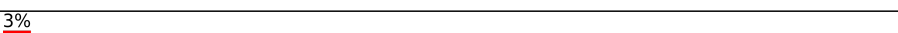
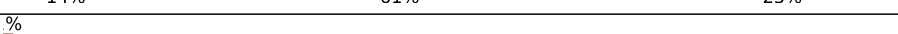
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AF    | 239    |                  |
| 3   | CF    | 239    |                  |
| 4   | AG    | 208    |                  |
| 4   | CG    | 208    |                  |
| 5   | AH    | 162    |                  |
| 5   | CH    | 162    |                  |
| 6   | AI    | 101    |                  |
| 6   | CI    | 101    |                  |
| 7   | AJ    | 156    |                  |
| 7   | CJ    | 156    |                  |
| 8   | AK    | 138    |                  |
| 8   | CK    | 138    |                  |
| 9   | AL    | 128    |                  |
| 9   | CL    | 128    |                  |
| 10  | AM    | 105    |                  |
| 10  | CM    | 105    |                  |
| 11  | AN    | 129    |                  |
| 11  | CN    | 129    |                  |
| 12  | AO    | 128    |                  |
| 12  | CO    | 128    |                  |
| 13  | AP    | 126    |                  |
| 13  | CP    | 126    |                  |
| 14  | AQ    | 61     |                  |
| 14  | CQ    | 61     |                  |
| 15  | AR    | 89     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 15  | CR    | 89     |    |
| 16  | AS    | 88     |    |
| 16  | CS    | 88     |    |
| 17  | AT    | 105    |    |
| 17  | CT    | 105    |    |
| 18  | AU    | 88     |    |
| 18  | CU    | 88     |    |
| 19  | AV    | 93     |    |
| 19  | CV    | 93     |    |
| 20  | AW    | 106    |    |
| 20  | CW    | 106    |    |
| 21  | AX    | 27     |    |
| 21  | CX    | 27     |  |
| 22  | AC    | 77     |  |
| 22  | AD    | 77     |  |
| 22  | CC    | 77     |  |
| 22  | CD    | 77     |  |
| 23  | A1    | 6      |  |
| 23  | C1    | 6      |  |
| 24  | BA    | 2912   |  |
| 24  | DA    | 2912   |  |
| 25  | BB    | 122    |  |
| 25  | DB    | 122    |  |
| 26  | BD    | 276    |  |
| 26  | DD    | 276    |  |

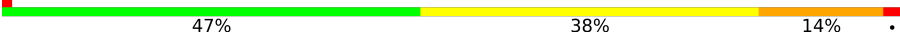
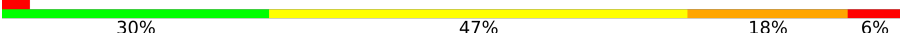
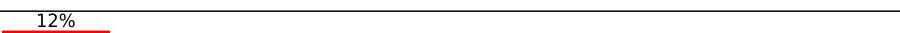
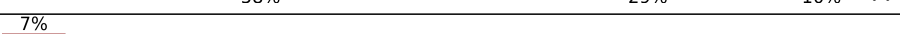
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | BE    | 206    |                  |
| 27  | DE    | 206    |                  |
| 28  | BF    | 210    |                  |
| 28  | DF    | 210    |                  |
| 29  | BG    | 182    |                  |
| 29  | DG    | 182    |                  |
| 30  | BH    | 180    |                  |
| 30  | DH    | 180    |                  |
| 31  | BK    | 148    |                  |
| 31  | DK    | 148    |                  |
| 32  | BM    | 140    |                  |
| 32  | DM    | 140    |                  |
| 33  | BN    | 122    |                  |
| 33  | DN    | 122    |                  |
| 34  | BO    | 150    |                  |
| 34  | DO    | 150    |                  |
| 35  | BP    | 141    |                  |
| 35  | DP    | 141    |                  |
| 36  | B0    | 118    |                  |
| 36  | D0    | 118    |                  |
| 37  | BQ    | 112    |                  |
| 37  | DQ    | 112    |                  |
| 38  | BR    | 146    |                  |
| 38  | DR    | 146    |                  |
| 39  | B1    | 118    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 39  | D1    | 118    |    |
| 40  | B2    | 101    |    |
| 40  | D2    | 101    |    |
| 41  | BS    | 113    |    |
| 41  | DS    | 113    |    |
| 42  | BT    | 96     |    |
| 42  | DT    | 96     |    |
| 43  | BU    | 110    |    |
| 43  | DU    | 110    |    |
| 44  | BV    | 206    |    |
| 44  | DV    | 206    |    |
| 45  | B3    | 85     |    |
| 45  | D3    | 85     |  |
| 46  | BZ    | 98     |  |
| 46  | DZ    | 98     |  |
| 47  | BW    | 72     |  |
| 47  | DW    | 72     |  |
| 48  | BX    | 60     |  |
| 48  | DX    | 60     |  |
| 49  | B4    | 71     |  |
| 49  | D4    | 71     |  |
| 50  | B5    | 60     |  |
| 50  | D5    | 60     |  |
| 51  | B6    | 54     |  |
| 51  | D6    | 54     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | B7    | 49     |                  |
| 52  | D7    | 49     |                  |
| 53  | B8    | 65     |                  |
| 53  | D8    | 65     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | BA    | 3082 | -         | -        | -       | X                |
| 54  | MG   | BA    | 3111 | -         | -        | -       | X                |
| 54  | MG   | BA    | 3166 | -         | -        | -       | X                |
| 54  | MG   | BA    | 3171 | -         | -        | -       | X                |
| 54  | MG   | BA    | 3510 | -         | -        | -       | X                |
| 54  | MG   | BA    | 3566 | -         | -        | -       | X                |
| 54  | MG   | CA    | 1603 | -         | -        | -       | X                |
| 54  | MG   | CA    | 1622 | -         | -        | -       | X                |
| 54  | MG   | CA    | 1681 | -         | -        | -       | X                |
| 54  | MG   | CA    | 1746 | -         | -        | -       | X                |
| 54  | MG   | CA    | 1753 | -         | -        | -       | X                |
| 54  | MG   | CA    | 1779 | -         | -        | -       | X                |
| 54  | MG   | CL    | 201  | -         | -        | -       | X                |
| 54  | MG   | DA    | 3064 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3067 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3085 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3150 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3167 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3258 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3324 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3418 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3453 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3521 | -         | -        | -       | X                |

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 295766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1506     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32369 | 14408 | 5997 | 10459 | 1505 |         |         |       |
| 1   | CA    | 1506     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32372 | 14408 | 5997 | 10461 | 1506 |         |         |       |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AE    | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |
| 2   | CE    | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AF    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1011 | 313 | 280 | 1 |         |         |       |
| 3   | CF    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AH    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |
| 5   | CH    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AM    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CM    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AO    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |
| 12  | CO    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AP    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 928   | 574 | 191 | 161 | 2 |         |         |       |
| 13  | CP    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 577 | 192 | 162 | 2 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |
| 16  | CS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AT    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 17  | CT    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AU    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 591   | 376 | 117 | 98 |         |         |       |
| 18  | CU    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 591   | 376 | 117 | 98 |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AV    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 424 | 124 | 115 | 2 |         |         |       |
| 19  | CV    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 398 | 115 | 109 | 2 |         |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | AX    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |
| 21  | CX    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 22 is a RNA chain called TRNA-FMET.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | AD    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | CC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | CD    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| AC    | 17A     | C        | U      | conflict | GB AP008226.1 |
| AC    | 50      | U        | C      | conflict | GB AP008226.1 |
| AC    | 51      | C        | G      | conflict | GB AP008226.1 |
| AC    | 63      | G        | C      | conflict | GB AP008226.1 |
| AD    | 17A     | C        | U      | conflict | GB AP008226.1 |
| AD    | 50      | U        | C      | conflict | GB AP008226.1 |
| AD    | 51      | C        | G      | conflict | GB AP008226.1 |
| AD    | 63      | G        | C      | conflict | GB AP008226.1 |
| CC    | 17A     | C        | U      | conflict | GB AP008226.1 |
| CC    | 50      | U        | C      | conflict | GB AP008226.1 |
| CC    | 51      | C        | G      | conflict | GB AP008226.1 |
| CC    | 63      | G        | C      | conflict | GB AP008226.1 |
| CD    | 17A     | C        | U      | conflict | GB AP008226.1 |
| CD    | 50      | U        | C      | conflict | GB AP008226.1 |
| CD    | 51      | C        | G      | conflict | GB AP008226.1 |
| CD    | 63      | G        | C      | conflict | GB AP008226.1 |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23  | A1    | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 129   | 58 | 24 | 41 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 23  | C1    | 6        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 129   | 58 | 24 | 41 | 6 |         |         |       |

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 24  | BA    | 2912     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62707 | 27911 | 11722 | 20163 | 2911 |         |         |       |
| 24  | DA    | 2906     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62587 | 27857 | 11709 | 20116 | 2905 |         |         |       |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference     |
|-------|---------|----------|--------|----------------|---------------|
| BA    | 161     | U        | -      | expression tag | GB AP008226.1 |
| BA    | 654A    | A        | G      | conflict       | GB AP008226.1 |
| BA    | 654E    | C        | G      | conflict       | GB AP008226.1 |
| BA    | 654P    | G        | C      | conflict       | GB AP008226.1 |
| BA    | 654T    | A        | C      | conflict       | GB AP008226.1 |
| BA    | 1058    | U        | G      | conflict       | GB AP008226.1 |
| BA    | 1080    | A        | C      | conflict       | GB AP008226.1 |
| DA    | 166     | U        | -      | insertion      | GB AP008226.1 |
| DA    | 654A    | A        | G      | conflict       | GB AP008226.1 |
| DA    | 654E    | C        | G      | conflict       | GB AP008226.1 |
| DA    | 654P    | G        | C      | conflict       | GB AP008226.1 |
| DA    | 654T    | A        | C      | conflict       | GB AP008226.1 |
| DA    | 1058    | U        | G      | conflict       | GB AP008226.1 |
| DA    | 1080    | A        | C      | conflict       | GB AP008226.1 |

- Molecule 25 is a RNA chain called 5S RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 25  | BB    | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |
| 25  | DB    | 122      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2617  | 1166 | 486 | 844 | 121 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | BD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | DD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 27  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28  | BF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |
| 28  | DF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 29  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |
| 30  | DH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 31  | DK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 32  | DM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 33  | DN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 34  | DO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 35  | DP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | B0    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 36  | D0    | 117      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |   |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 37  | BQ    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |
| 37  | DQ    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BR    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 38  | DR    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | B1    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 39  | D1    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | B2    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 40  | D2    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |
| 41  | DS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | BT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | DT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |
| 43  | DU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BV    | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1397  | 892 | 251 | 251 | 3 |         |         |       |
| 44  | DV    | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 911 | 255 | 259 | 3 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | B3    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 607   | 376 | 128 | 102 | 1 |         |         |       |
| 45  | D3    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 613   | 379 | 129 | 104 | 1 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 46  | DZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BW    | 66       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 558   | 346 | 113 | 98  | 1 |         |         |       |
| 47  | DW    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 48  | BX    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 48  | DX    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49  | B4    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 533   | 335 | 96 | 97 | 5 |         |         |       |
| 49  | D4    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 515   | 326 | 93 | 91 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 50  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | B6    | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 389   | 241 | 79 | 65 | 4 |         |         |       |
| 51  | D6    | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 389   | 241 | 79 | 65 | 4 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52  | B7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |
| 52  | D7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms        |          |         |         |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|---------|-------|
| 53  | B8    | 61       | Total<br>488 | C<br>312 | N<br>99 | O<br>75 | S<br>2 | 0       | 0       | 0     |
| 53  | D8    | 61       | Total<br>488 | C<br>312 | N<br>99 | O<br>75 | S<br>2 | 0       | 0       | 0     |

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | AA    | 236      | Total<br>236 | Mg<br>236 | 0       | 0       |
| 54  | AG    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | AH    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | AN    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | AQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | AT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | AC    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 54  | AD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | A1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BA    | 632      | Total<br>632 | Mg<br>632 | 0       | 0       |
| 54  | BB    | 16       | Total<br>16  | Mg<br>16  | 0       | 0       |
| 54  | BD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BE    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | BF    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | BO    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | B0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | BU    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | B3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | B5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B7    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | B8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | CA    | 199      | Total<br>199 | Mg<br>199 | 0       | 0       |
| 54  | CG    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | CL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CS    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CC    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 54  | DA    | 523      | Total<br>523 | Mg<br>523 | 0       | 0       |
| 54  | DB    | 15       | Total<br>15  | Mg<br>15  | 0       | 0       |
| 54  | DE    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | DP    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | DR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | D1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | DU    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | D3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | D5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

*Continued on next page...*

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 54  | D8    | 1        | Total Mg<br>1 1 | 0       | 0       |

- # T1C

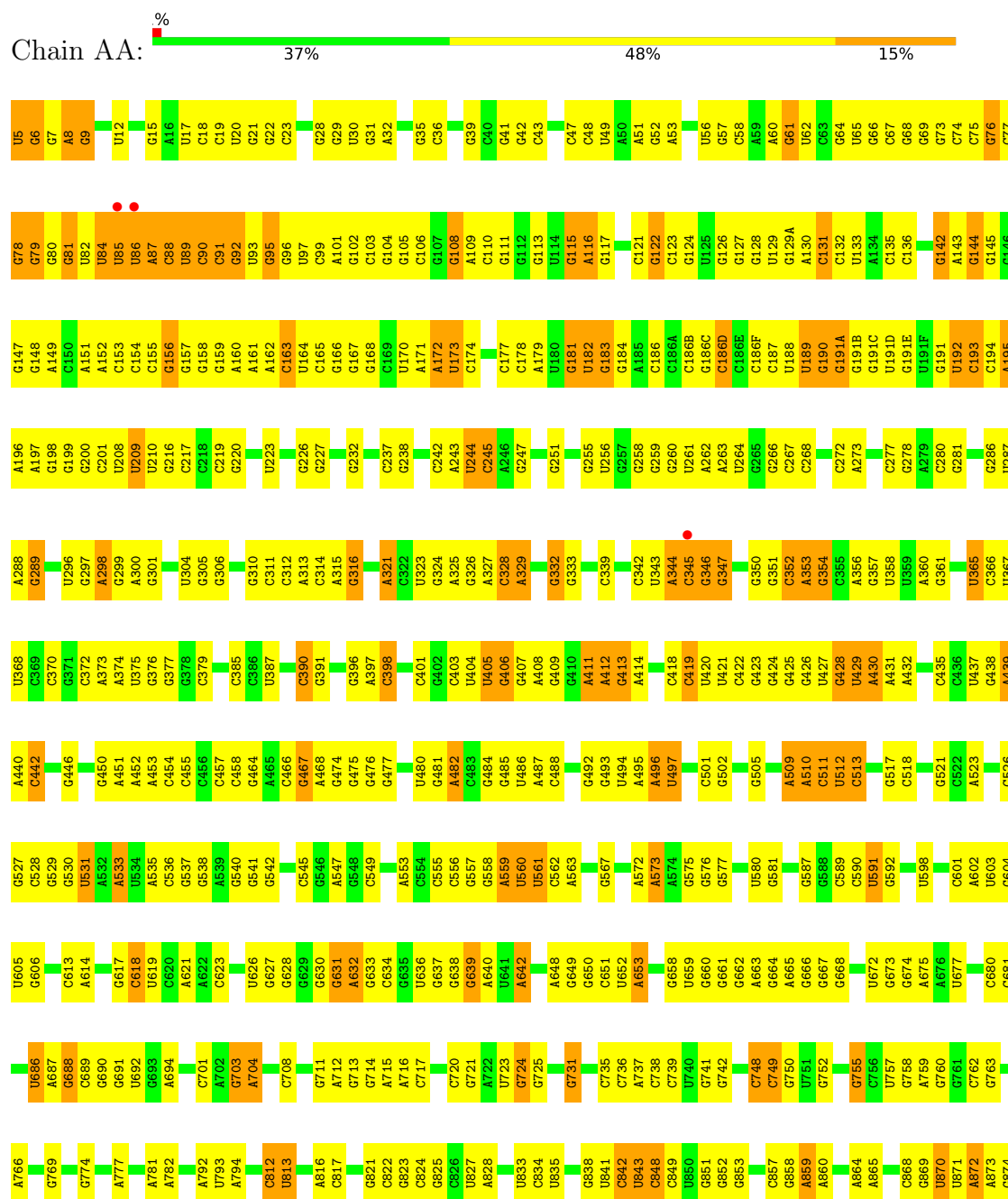
| Mol | Chain | Residues | Atoms       |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 55  | AA    | 1        | Total<br>42 | C<br>29 | N<br>5 | O<br>8 | 0       | 0       |
| 55  | CA    | 1        | Total<br>42 | C<br>29 | N<br>5 | O<br>8 | 0       | 0       |

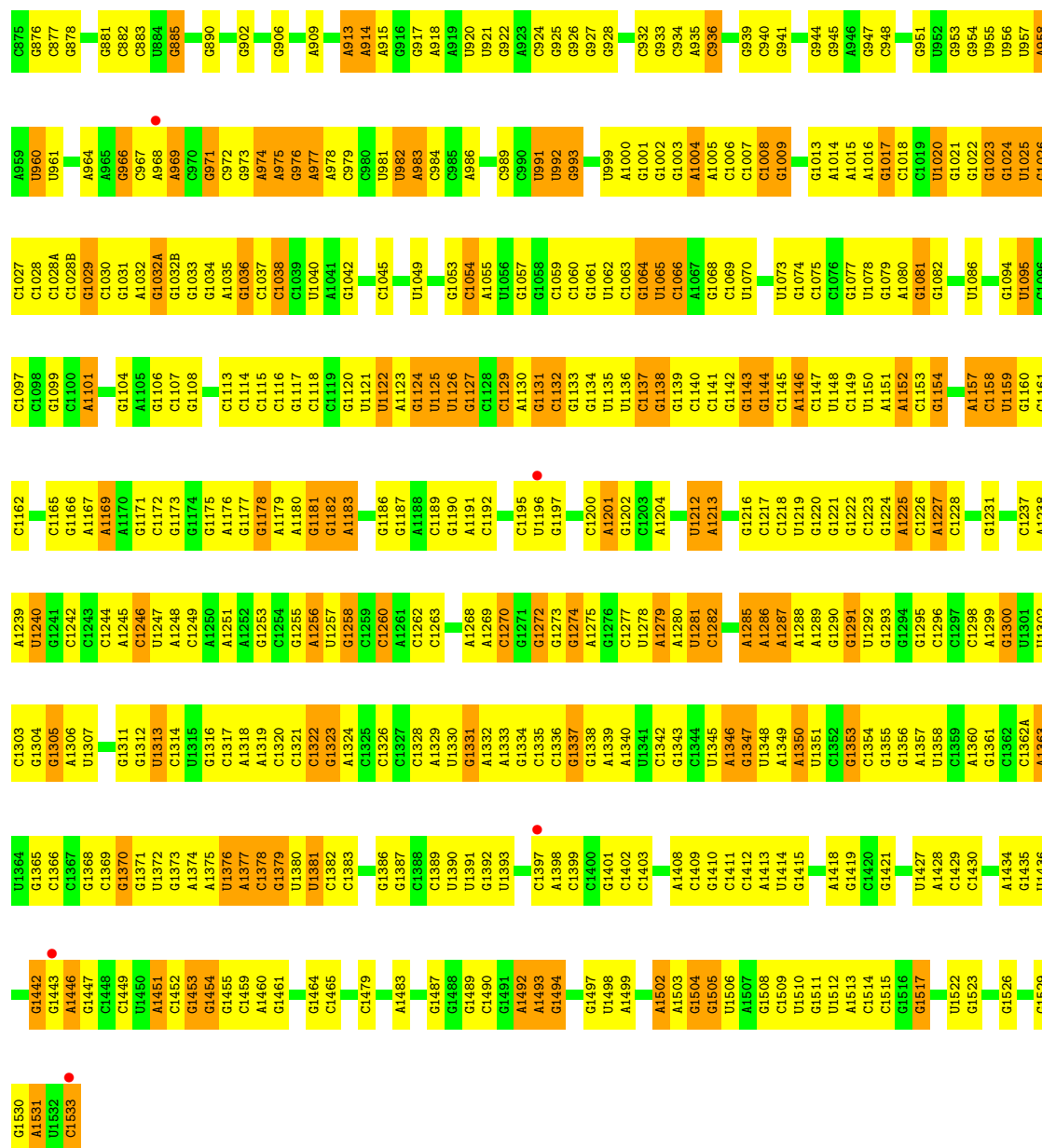
- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 56  | AG    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 56  | AQ    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 56  | CG    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 56  | CQ    | 1        | Total Zn<br>1 1 | 0       | 0       |

### 3 Residue-property plots

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

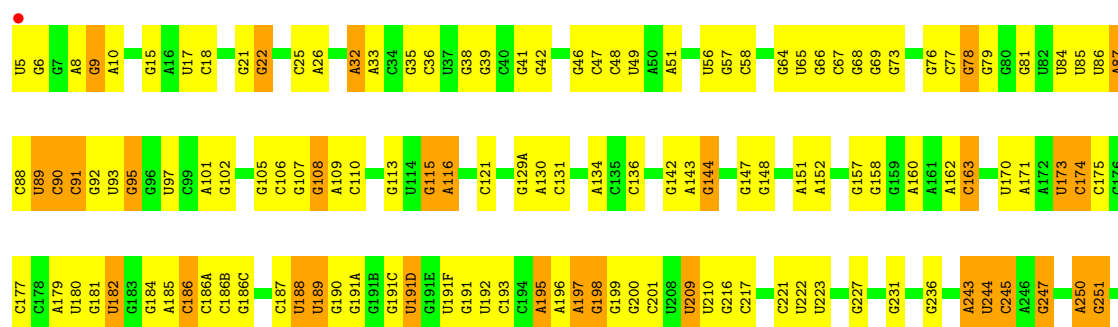
- Molecule 1: 16S ribosomal RNA



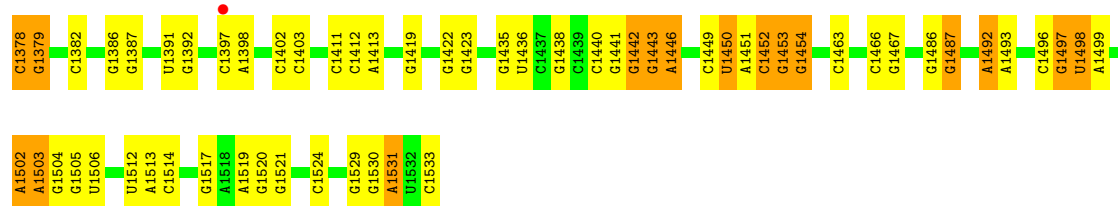


## • Molecule 1: 16S ribosomal RNA

Chain CA:

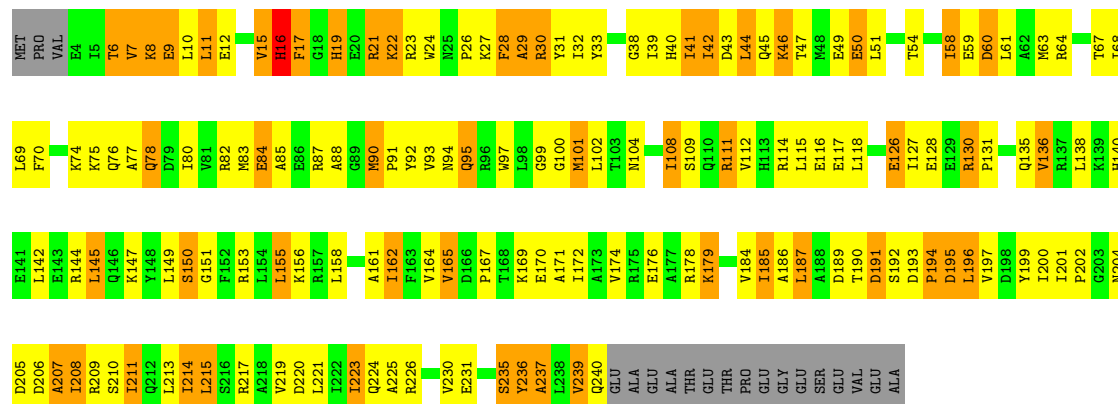






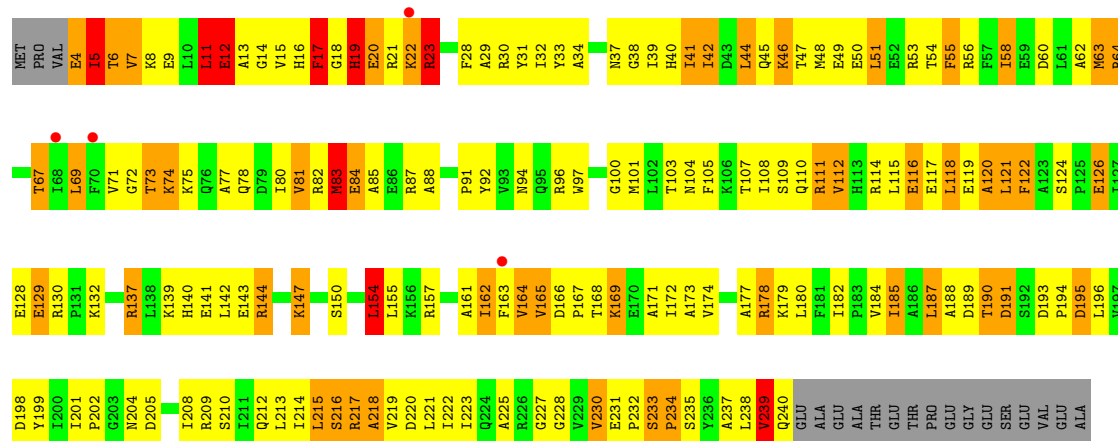
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AE: 32% 40% 20% 7%



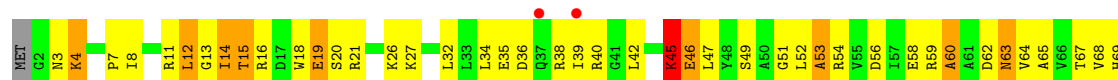
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

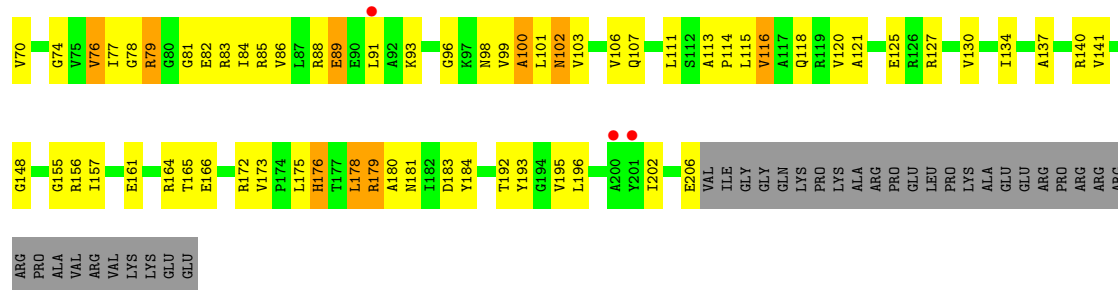
Chain CE: 2% 25% 45% 19% 7%



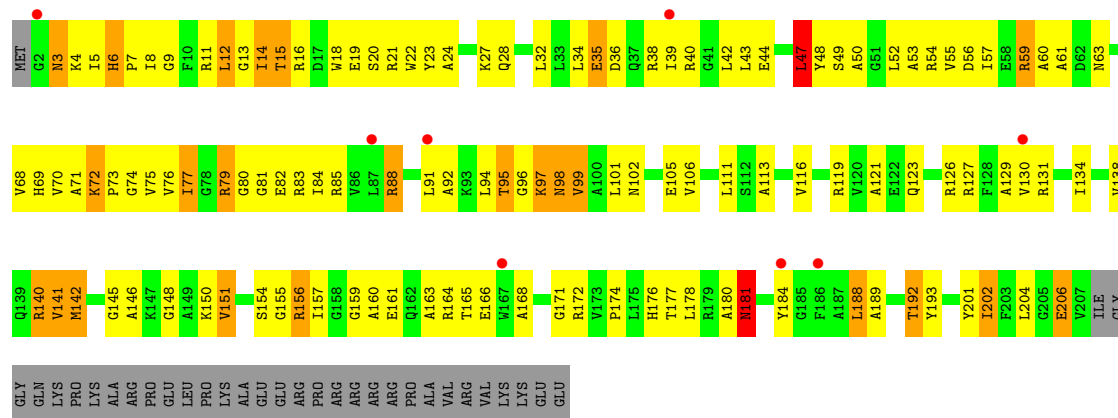
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AF: 2% 41% 37% 8% 14%

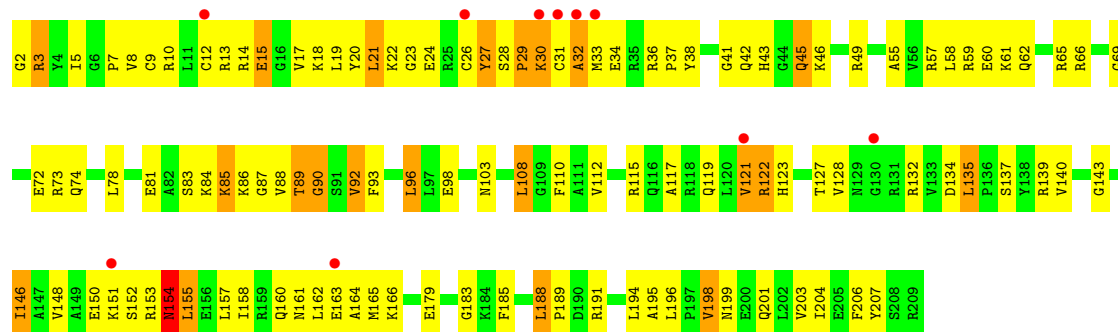




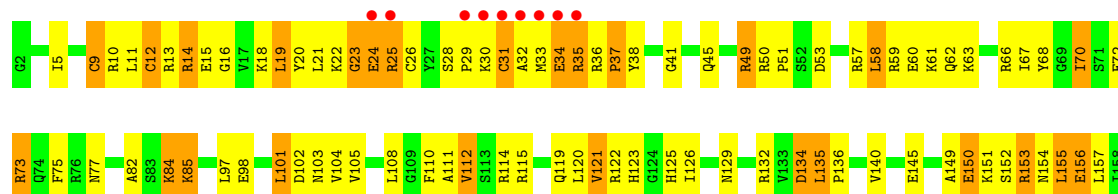
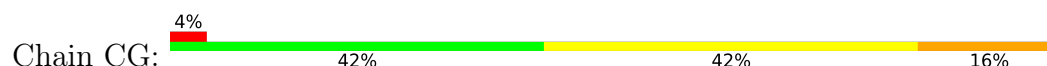
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

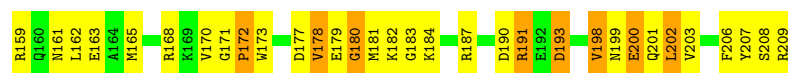


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

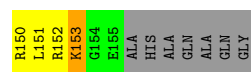
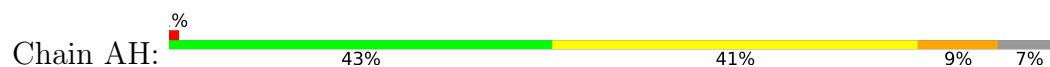


• Molecule 4: 30S RIBOSOMAL PROTEIN S4





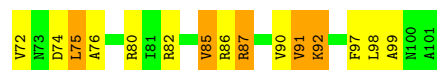
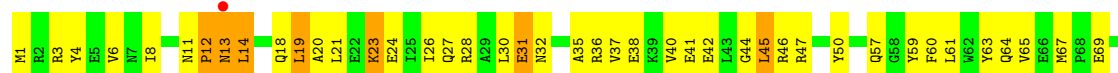
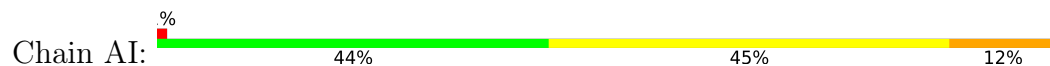
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



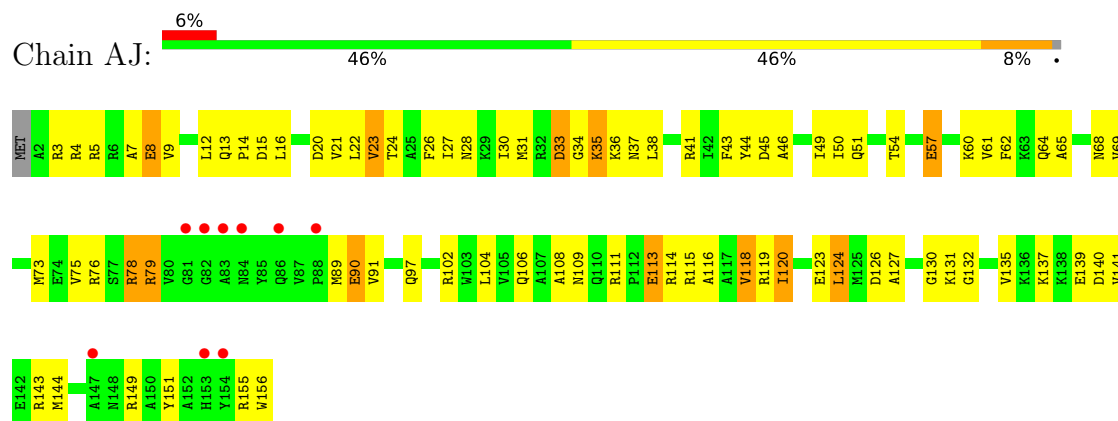
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



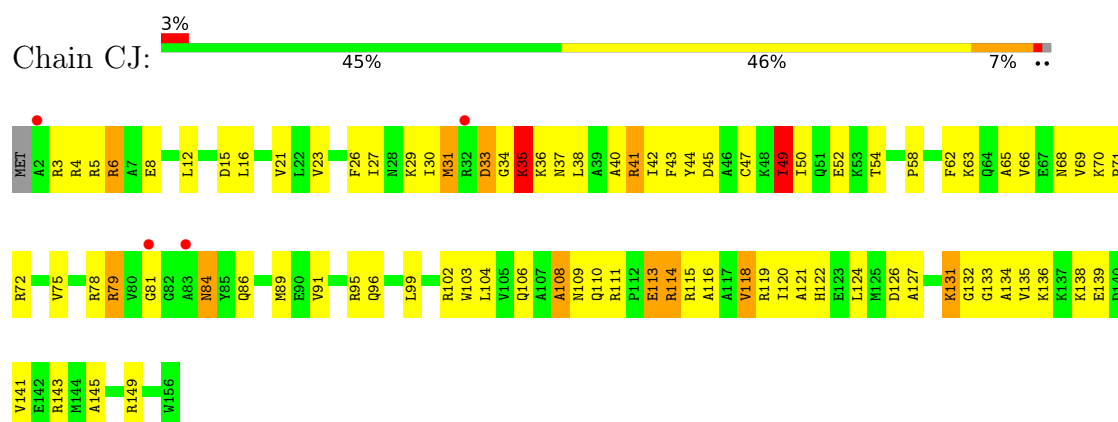
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



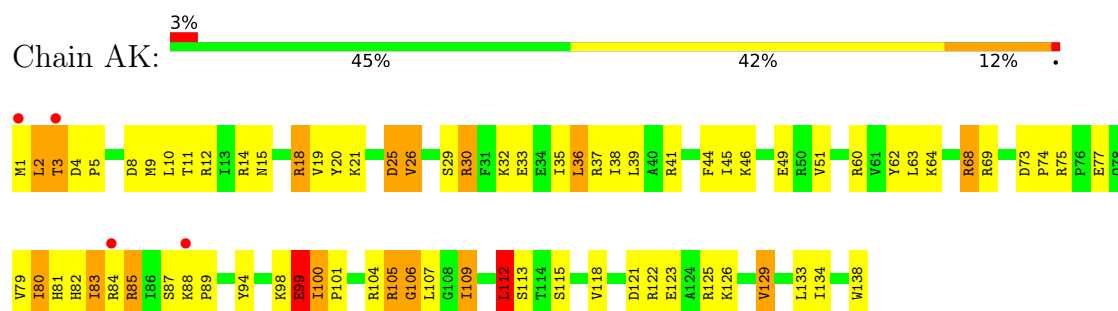
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



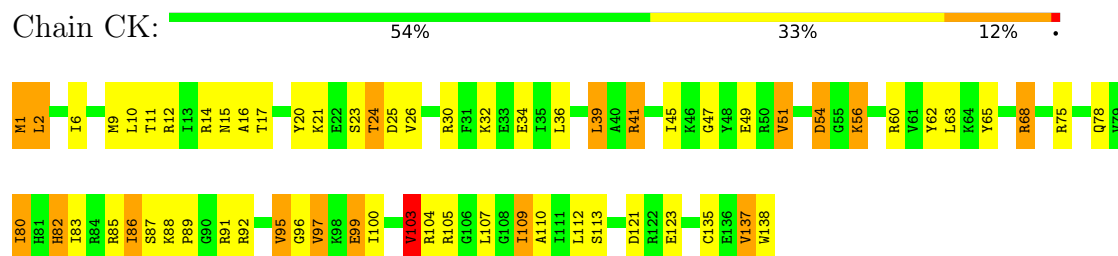
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



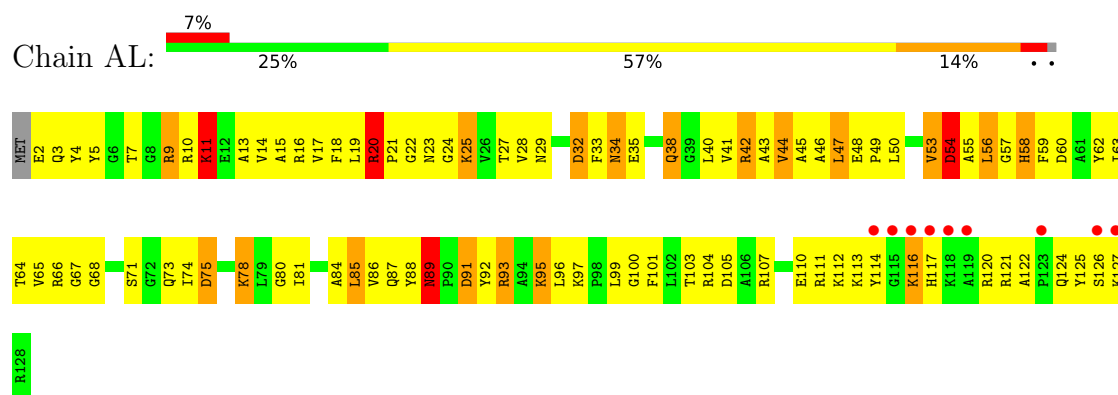
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



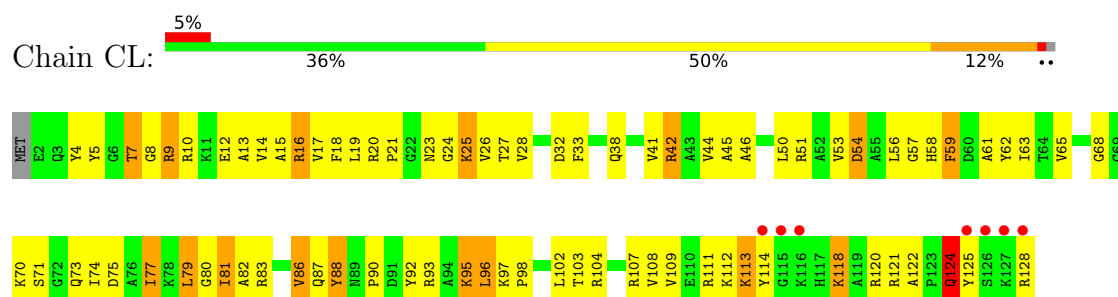
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



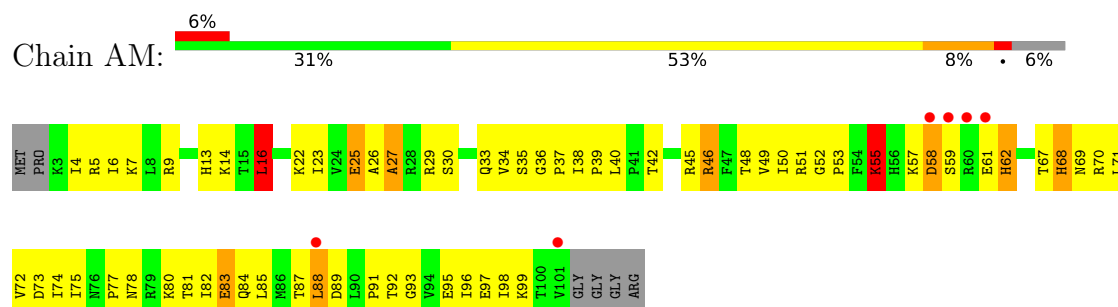
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



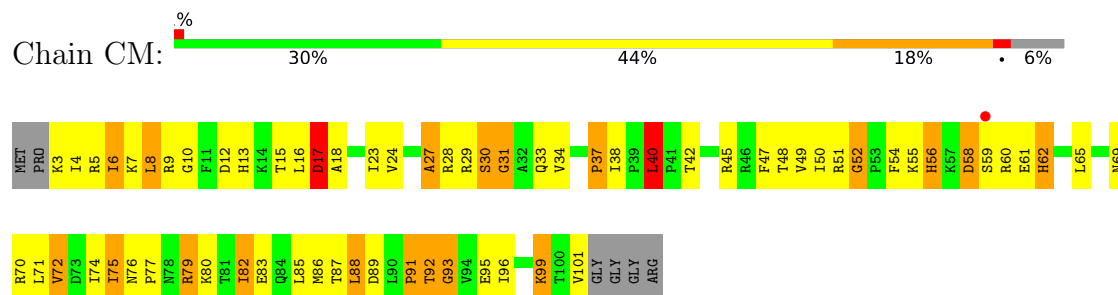
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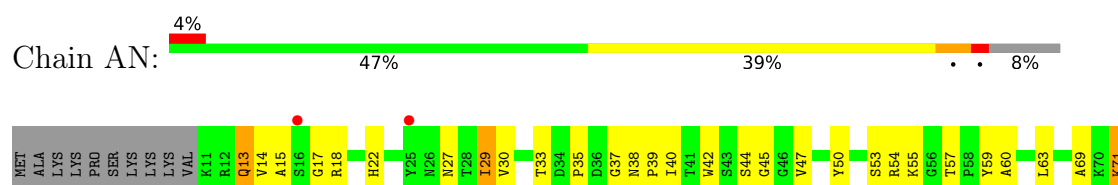
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

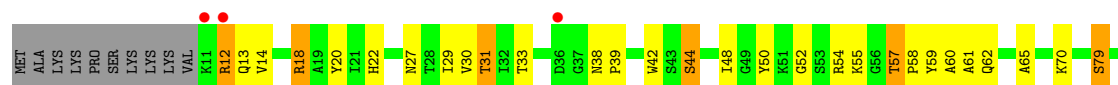


• Molecule 11: 30S RIBOSOMAL PROTEIN S11





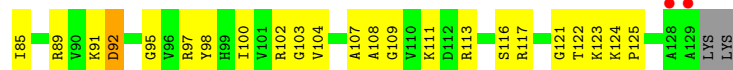
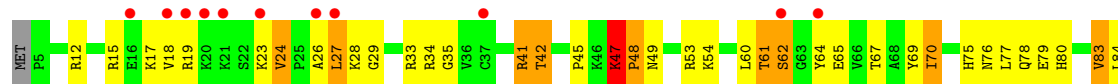
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



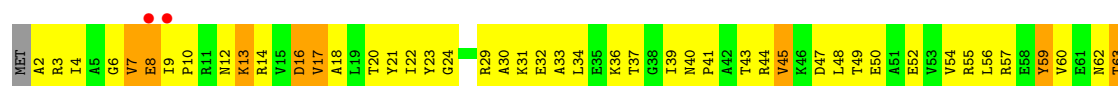
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

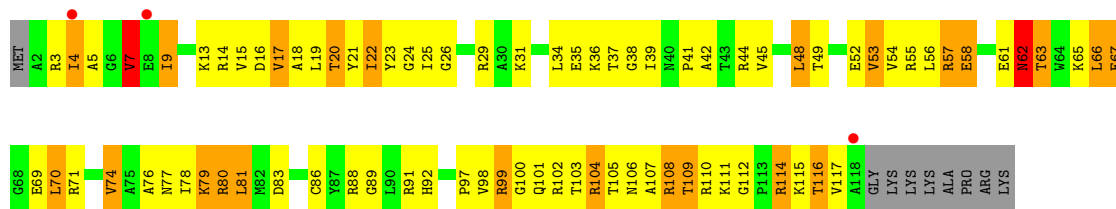


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

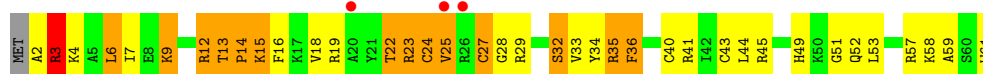


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

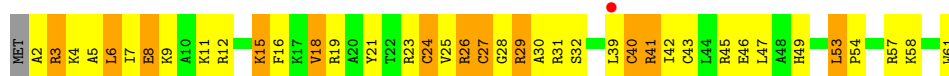
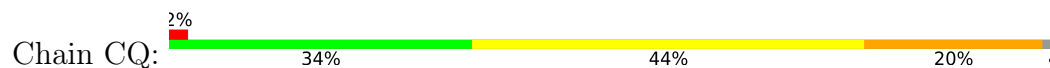




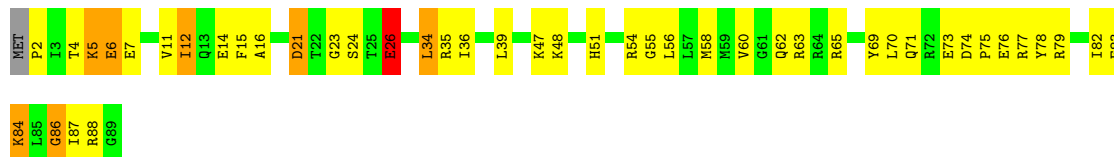
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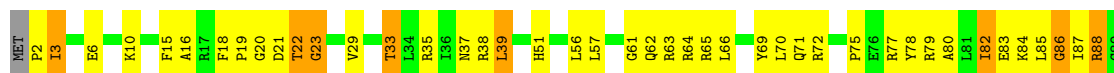
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

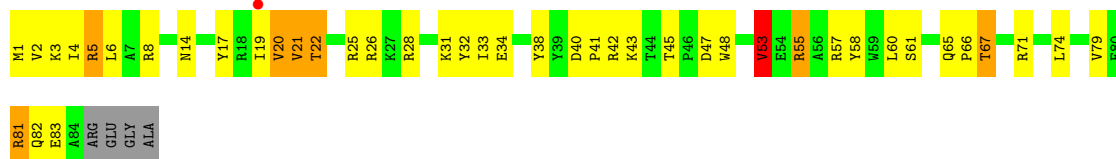


• Molecule 16: 30S RIBOSOMAL PROTEIN S16



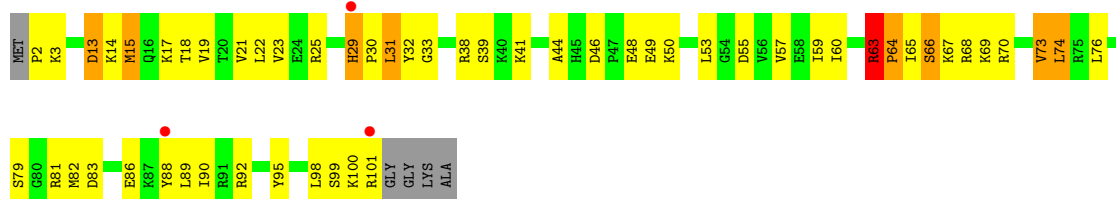
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS:  47% 40% 8% 5%



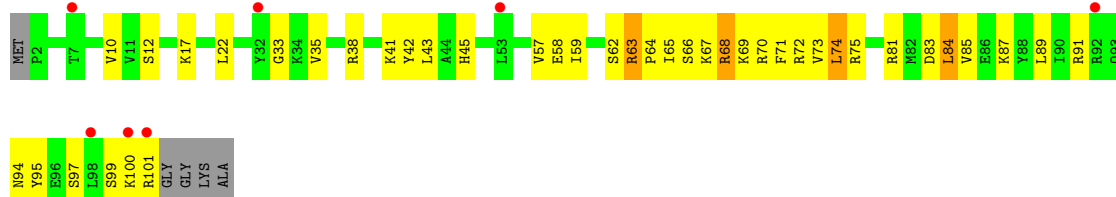
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT:  43% 44% 8% 5%



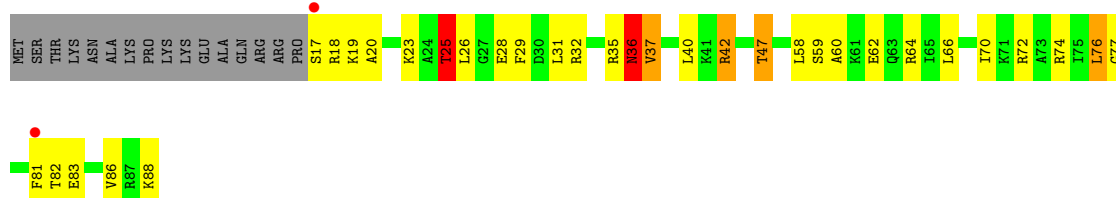
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT:  56% 35% 7% 5%



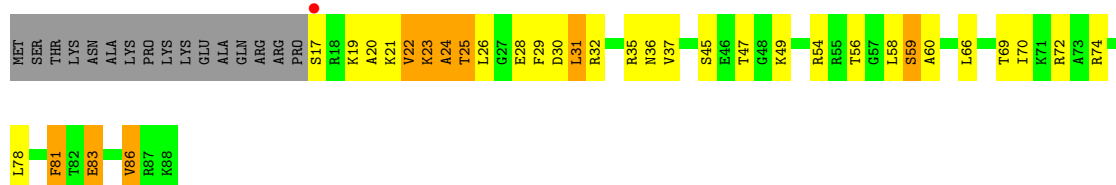
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU:  44% 31% 5% 18%

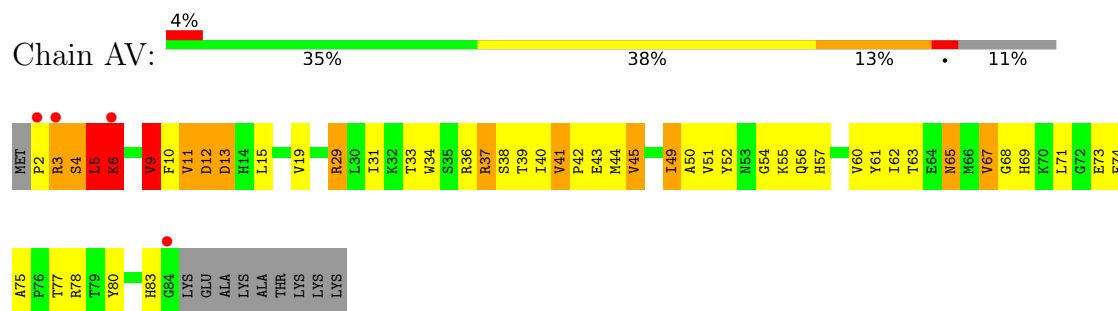


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

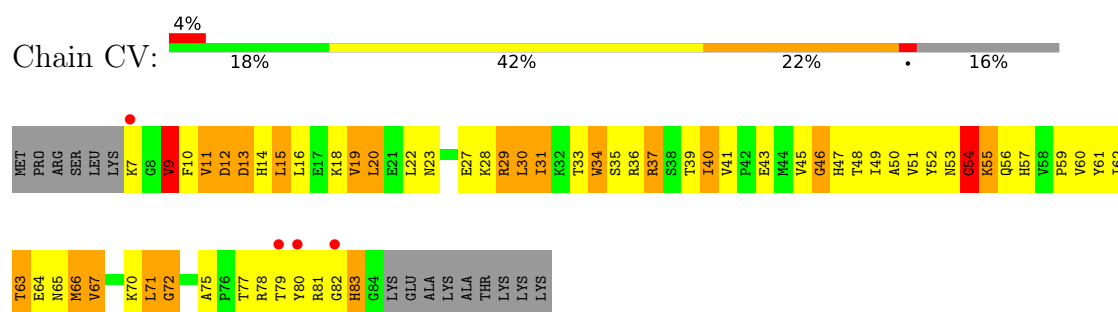
Chain CU:  43% 28% 10% 18%



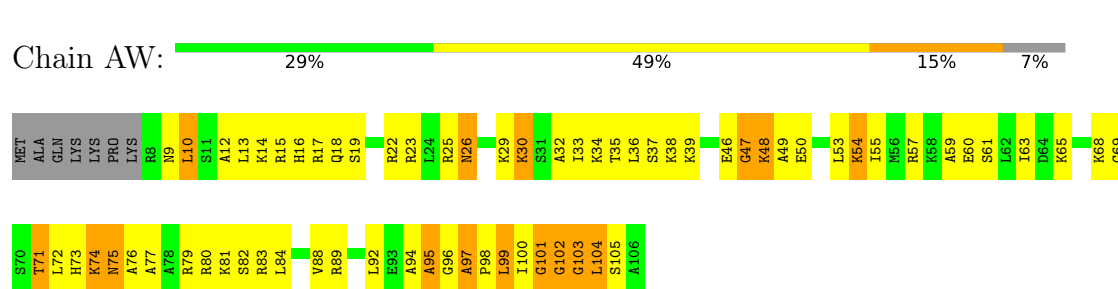
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



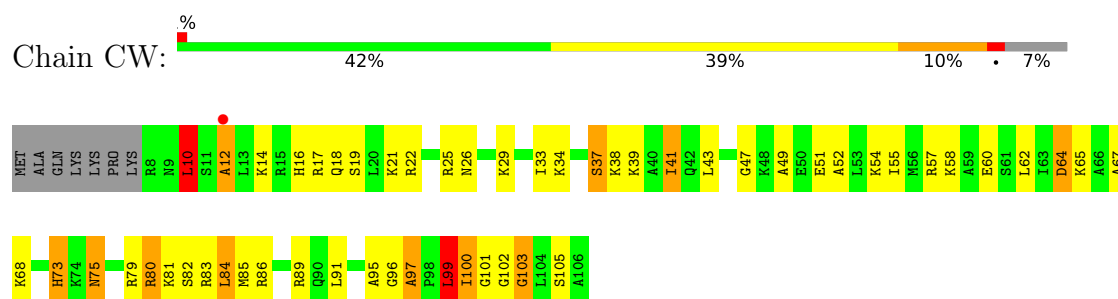
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



- Molecule 20: 30S RIBOSOMAL PROTEIN S20



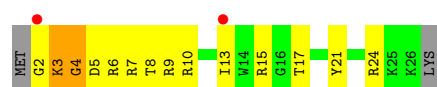
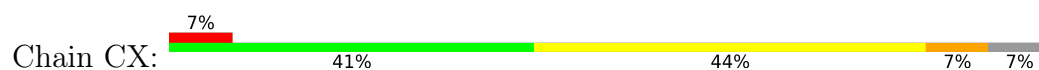
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



- Molecule 21: 30S RIBOSOMAL PROTEIN THX



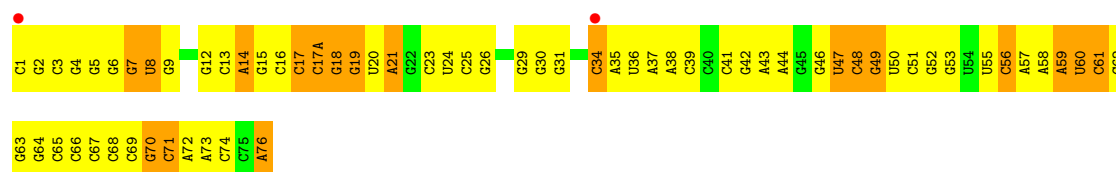
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



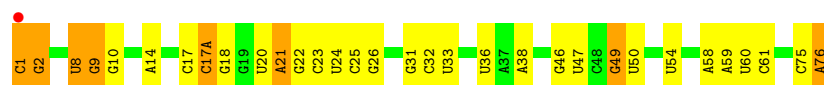
• Molecule 22: TRNA-FMET



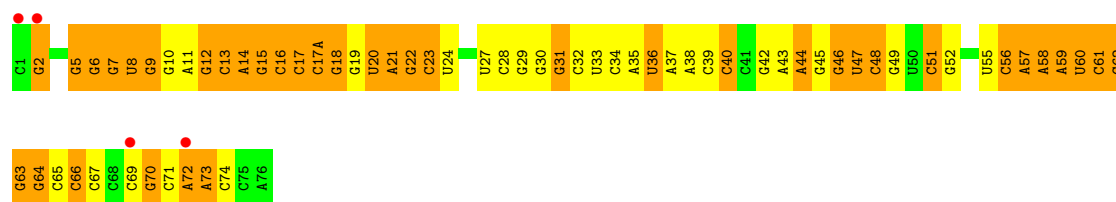
• Molecule 22: TRNA-FMET



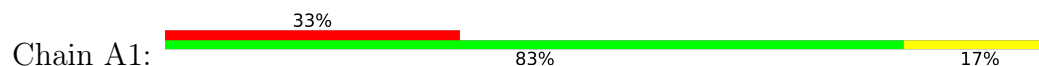
• Molecule 22: TRNA-FMET



• Molecule 22: TRNA-FMET



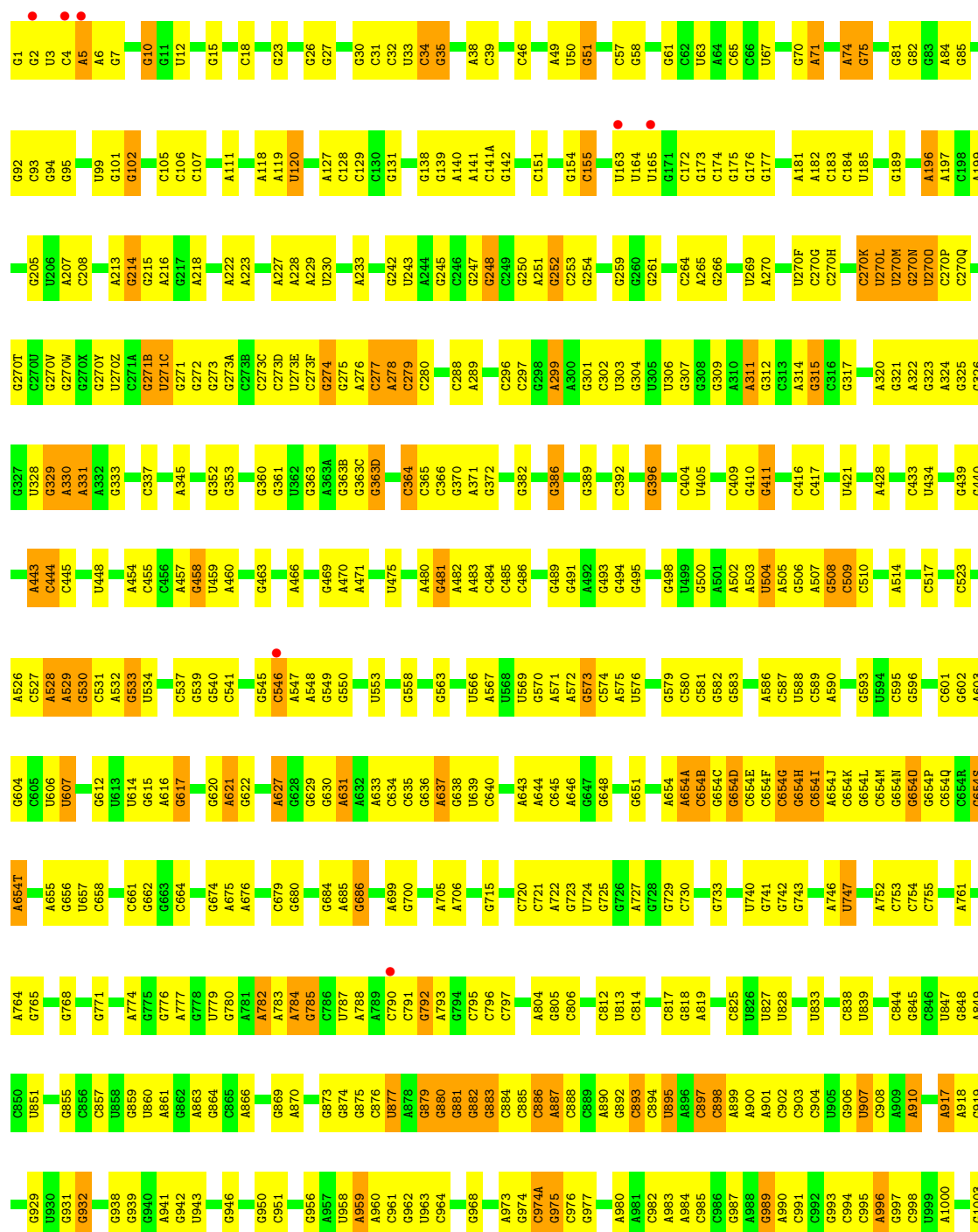
• Molecule 23: MRNA



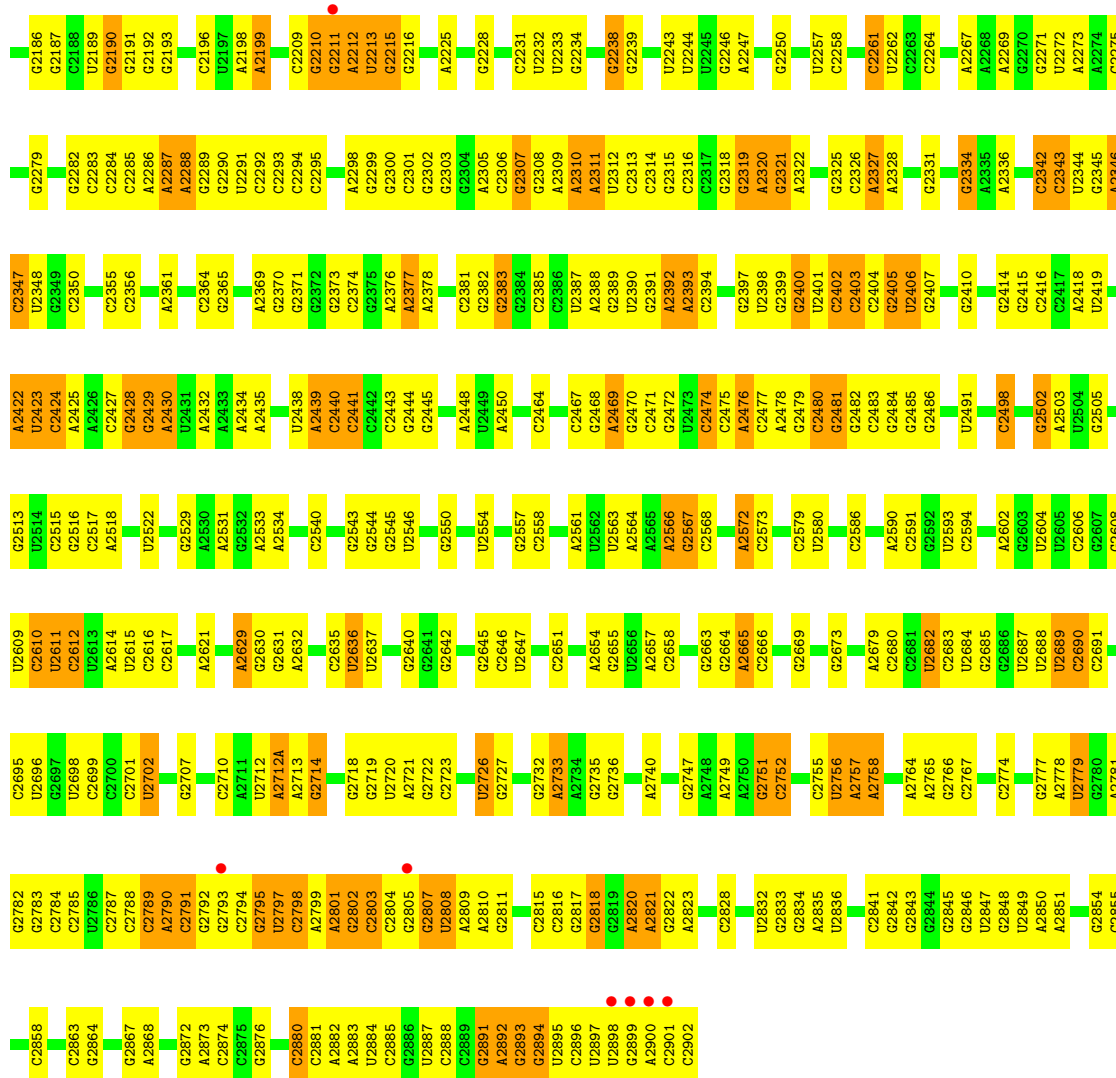
• Molecule 23: MRNA



Chain BA: 

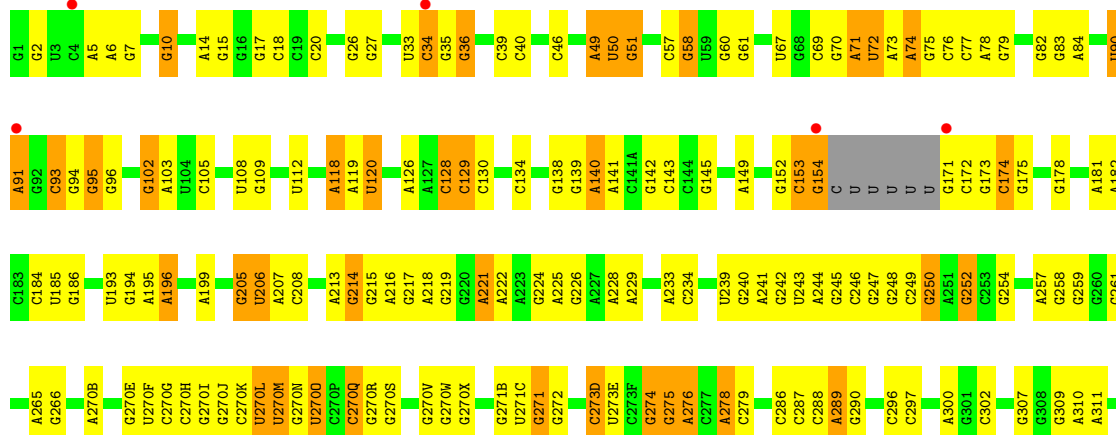


|       |       |       |       |        |       |        |       |        |       |       |       |
|-------|-------|-------|-------|--------|-------|--------|-------|--------|-------|-------|-------|
| U1212 | C2039 | A1938 | U1699 | A1545A | U1479 | C1404  | C1314 | A1214  | U1143 | A1070 | C1004 |
| G2123 | C2040 | U1939 | C1640 | C1946  | G1479 | U1405  | C1315 | G1215  | U1142 | G1071 | C1005 |
| G2124 | U2041 | U1940 | G1645 | C1547  | U1480 | C1406  | C1480 | G1216  | U1316 | C1072 | C1006 |
| A2042 | C2043 | G1753 | G1646 | C1551  | U1482 | C1407  | A1317 | G1217  | A1143 | A1073 | C1007 |
| G2048 | G1949 | C1754 | G1647 | C1552  | G1483 | C1408  | A1322 | C1218  | A1148 | G1074 | C1008 |
| A2051 | U1950 | U1951 | C1648 | A1553  | A1486 | C1409  | U1923 | A1220  | G1149 | C1075 | A1009 |
| G2052 | A1952 | G1756 | G1649 | A1554  | G1487 | G1410  | G1324 | C1221  | G1150 | C1076 | A1010 |
| G2053 | U1955 | U1757 | A1652 | C1557  | A1490 | G1411  | G1328 | C1222  | G1151 | A1077 | G1011 |
| A2054 | C1958 | A1762 | G1653 | A1558  | A1491 | G1414  | U1329 | G1223  | G1152 | U1078 | G1012 |
| G2055 | G1963 | G1763 | A1654 | G1559  | G1492 | G1415  | A1330 | G1224  | C1152 | C1079 | C1013 |
| G2056 | U1964 | G1765 | C1656 | G1560  | C1493 | G1416  | A1331 | G1225  | C1153 | A1080 | U1014 |
| A2060 | G1967 | U1766 | C1657 | A1566  | A1496 | G1417  | G1332 | A1227  | G1154 | U1081 | G1015 |
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### • Molecule 24: 23S ribosomal RNA

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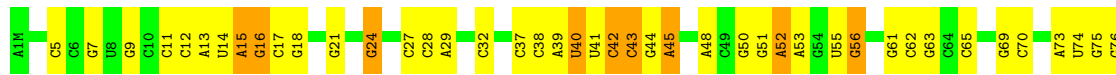


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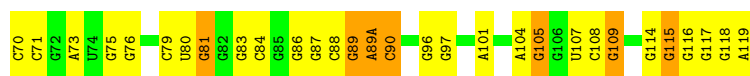
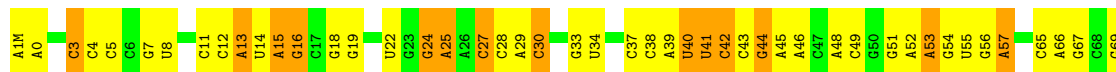
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| C2742  | G2475 | G2573 | G2475 | G2383 | G2308 | G2219 | C2147 | G2087 |       | G1886 | G1788 | G1674 | C1583  |
| G2743  | A2476 | G2574 | A2476 | G2384 | A2309 | G2224 | G2148 | C2080 | C2006 | C1887 | A1789 | C1675 | C1585  |
| G2744  | G2477 | G2575 | G2477 | G2385 | A2310 | A2225 | G2149 | A2082 | G2007 | A1889 | C1790 | C1678 | A1586  |
| U2745  | G2478 | G2576 | A2478 | G2386 | U2311 | G2226 | U2150 |       | G2008 |       |       | U1688 | U1590  |
| U2746  | G2479 |       | G2479 | G2387 | U2312 | A2227 | G2151 | U2096 | G2009 | G1899 | G1797 | G1688 | G1591  |
| G2747  |       | C2579 |       | A2388 | C2313 | G2228 | G2152 | C2097 | G2012 | A1900 | G1799 | A1689 | C1592  |
| A2748  | G2482 |       | G2482 |       | G2314 |       | A2153 |       | A2013 | G1890 | C1800 | G1696 | G1593  |
| G2749  | G2483 | G2580 | G2483 | A2392 | G2315 | C2231 | G2154 | G2093 | A2014 | G1891 | C1801 | G1697 | G1594  |
| A2750  | G2484 | G2581 | G2484 | A2393 | C2316 | U2232 | G2155 | G2094 | C2008 | A1901 | U1798 | A1698 | G1595  |
| G2751  | G2485 | G2582 | G2485 | G2394 | C2317 | U2233 | G2156 | C2095 | G2009 | C1894 | U1799 | G1699 | A1596  |
| C2752  | G2486 | G2583 |       |       | G2318 | U2234 | G2157 | U2096 |       | G1906 | G1799 | A1699 | A1597  |
| U2753  |       | U2584 | G2486 | U2401 | G2319 |       | A2158 | C2097 | G2012 | G1907 |       | A1700 | C1598  |
| G2754  | G2498 | U2585 |       | C2402 | A2320 | G2238 | G2159 | C2098 | A2013 | G1908 | C1800 | A1701 | C1599  |
| C2755  | G2502 | G2586 | G2498 | C2403 | G2321 | G2239 | U2160 | U2099 | A2014 | G1909 | C1801 | U1716 | C1600  |
| U2756  | G2503 | A2590 | G2502 | C2404 |       |       | C2161 | A2015 | A2015 | C1902 | A1802 | G1697 | G1601  |
| A2757  | G2504 | G2591 | G2502 | G2405 | G2325 | U2245 | G2162 | G2101 | U2016 | G1906 | G1799 | A1700 | U1502  |
| U2758  | G2505 | G2592 | G2505 | U2406 | C2326 | G2246 | C2163 | U2102 | U2017 | G1910 |       | A1701 |        |
| G2759  | G2506 | U2593 | U2506 | G2407 | A2327 | A2247 | C2164 | C2103 | G2018 | U1911 | A1809 | A1716 |        |
|        |       | G2594 | G2407 | G2410 | A2328 |       | G2165 | G2104 | A2019 | A1912 | A1810 | U1716 |        |
| C2760  | G2512 |       | G2410 | A2411 | G2329 | G2252 | G2166 | A2020 | A2020 | A1913 | A1811 |       |        |
| G2762  | G2513 | A2602 | A2411 |       | G2330 |       | U2167 | G2106 |       |       | A1812 |       |        |



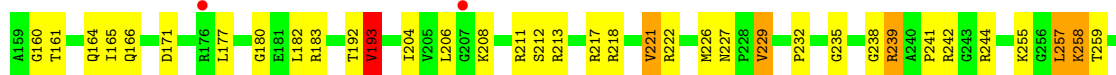
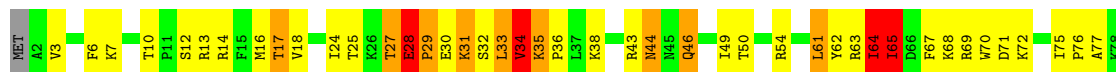
• Molecule 25: 5S RIBOSOMAL RNA



• Molecule 25: 5S RIBOSOMAL RNA

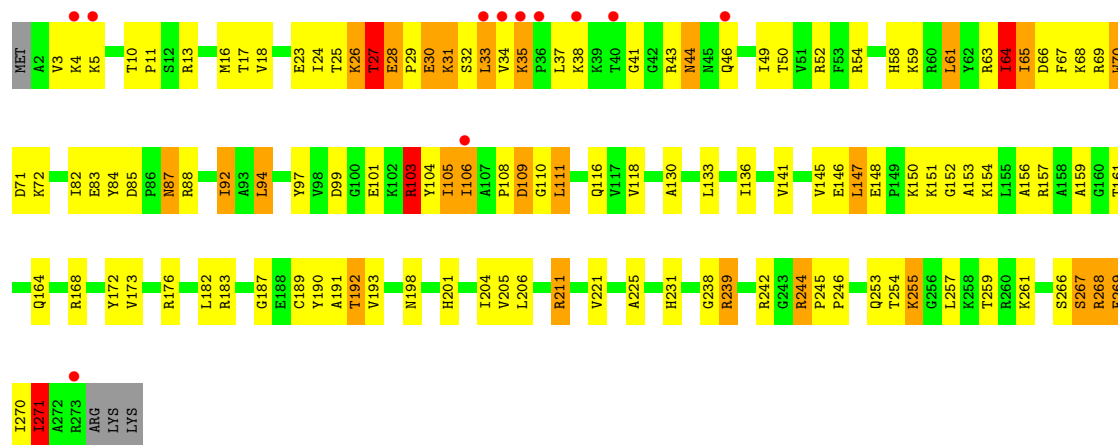


• Molecule 26: 50S ribosomal protein L2

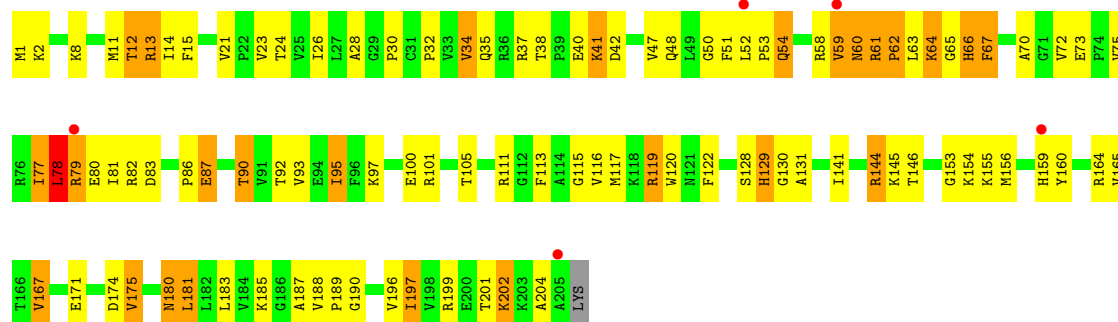


• Molecule 26: 50S ribosomal protein L2

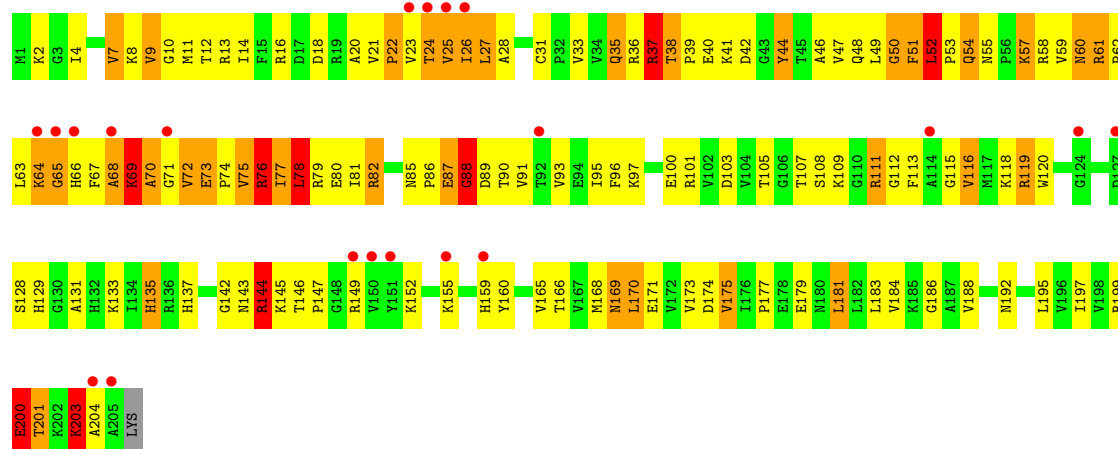




• Molecule 27: 50S ribosomal protein L3

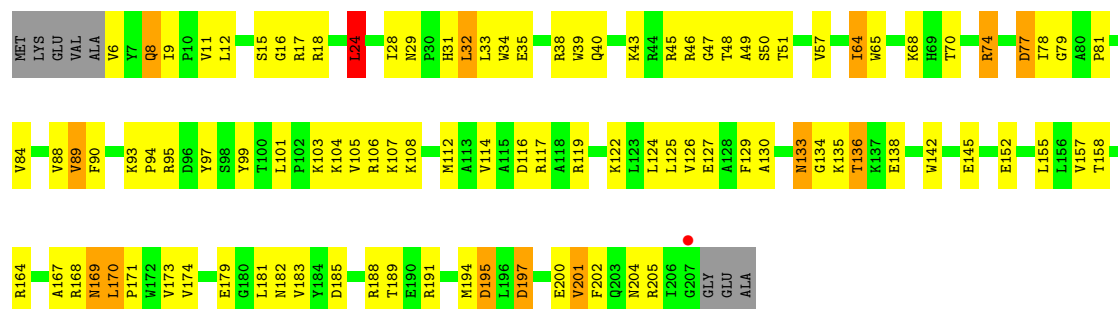


• Molecule 27: 50S ribosomal protein L3

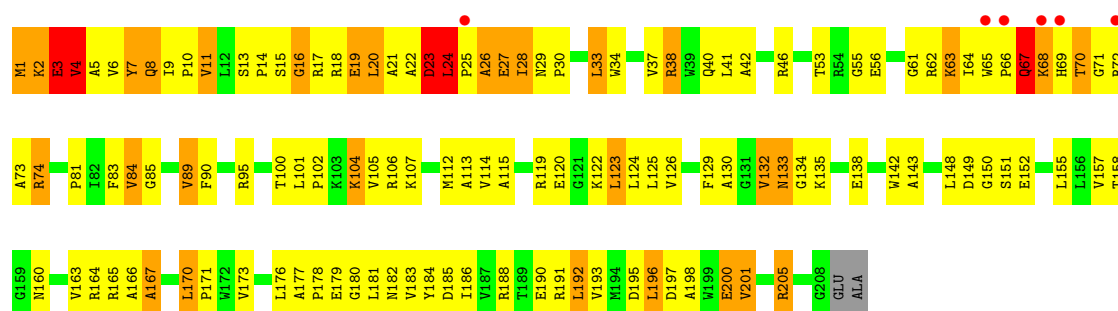


• Molecule 28: 50S ribosomal protein L4

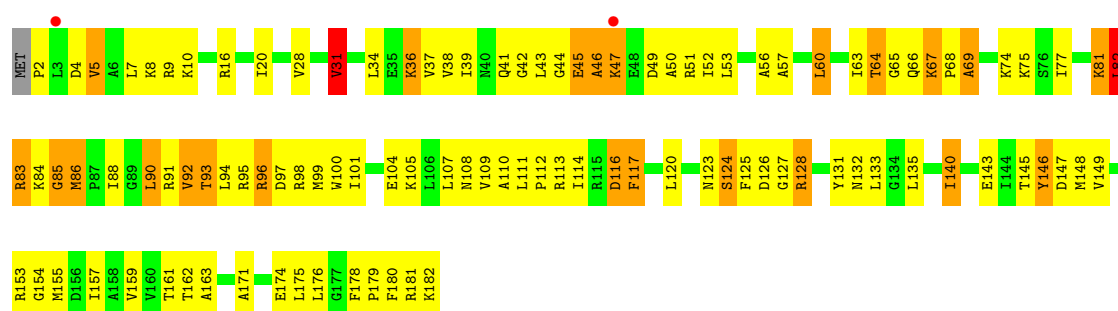
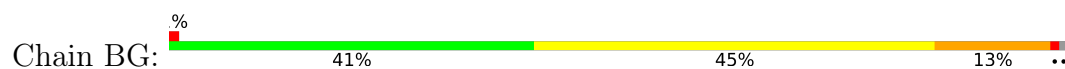




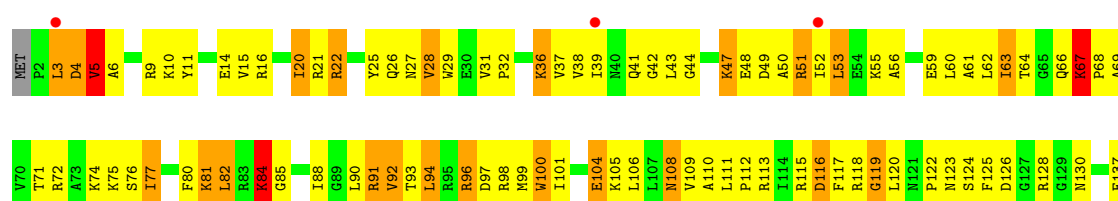
- Molecule 28: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L5

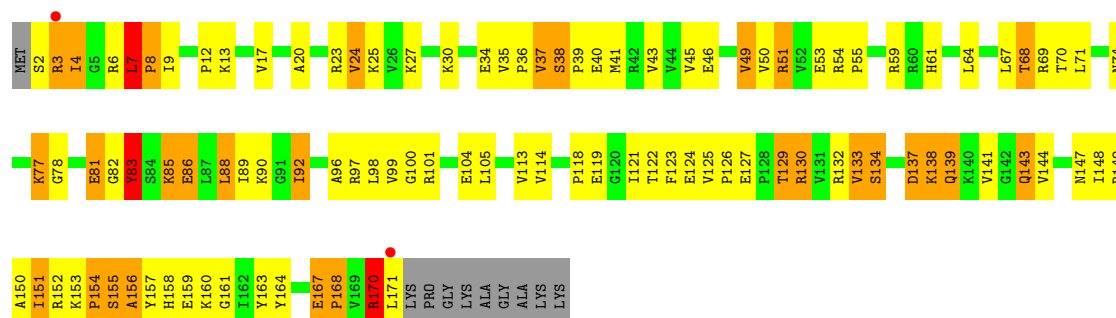


- Molecule 29: 50S ribosomal protein L5

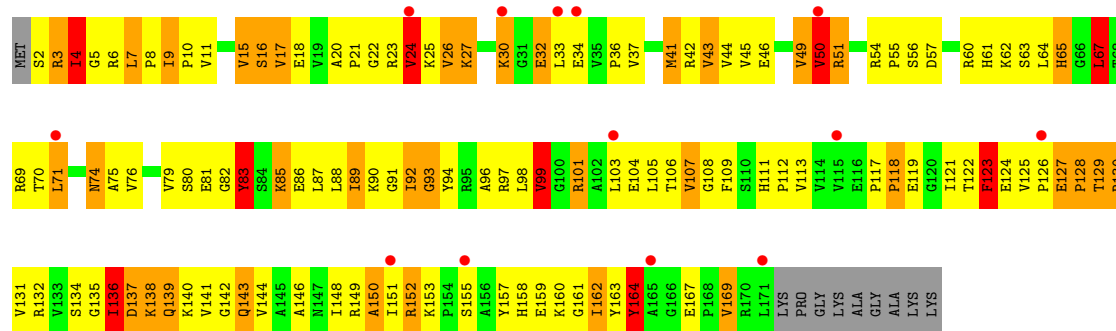




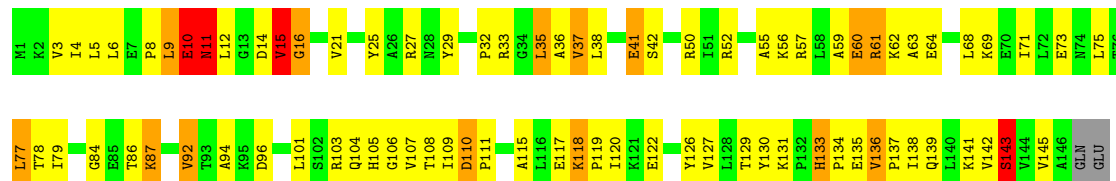
- Molecule 30: 50S ribosomal protein L6



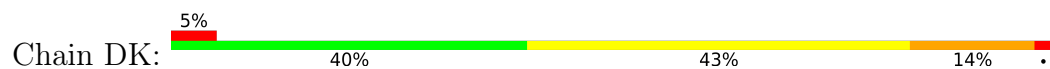
- Molecule 30: 50S ribosomal protein L6

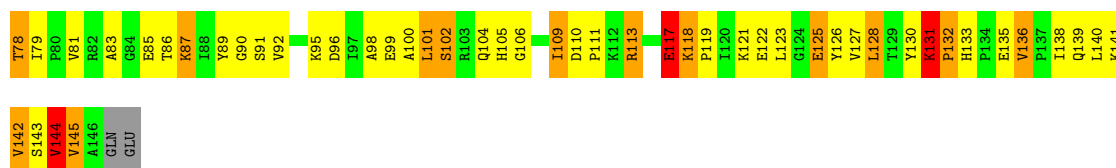


- Molecule 31: 50S ribosomal protein L9

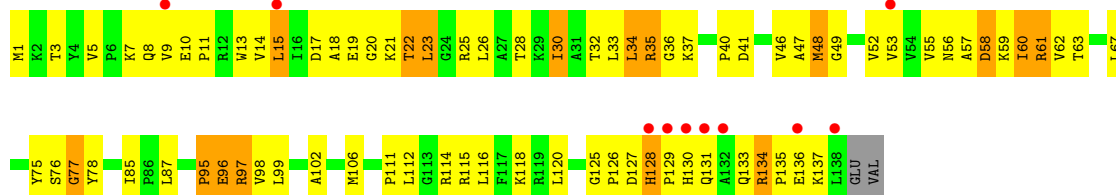
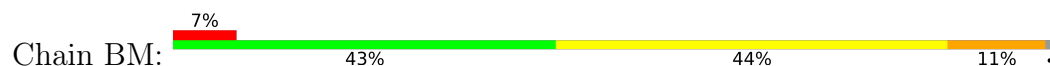


- Molecule 31: 50S ribosomal protein L9

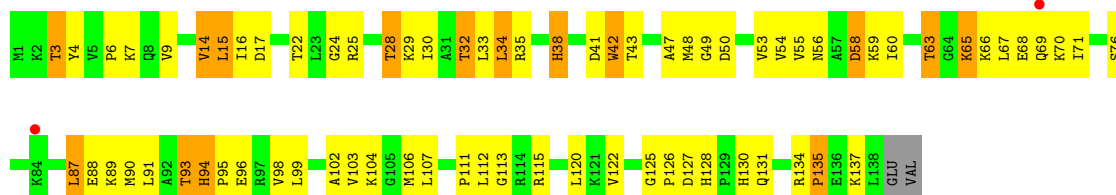




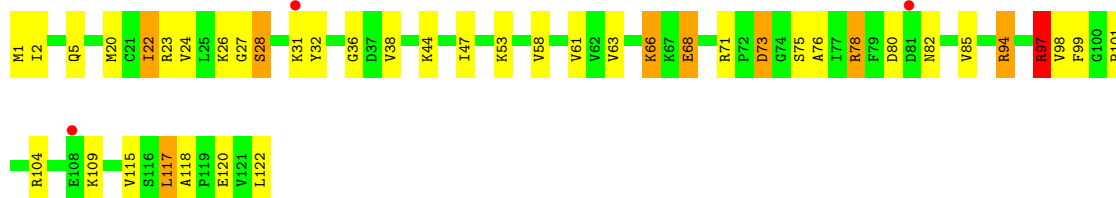
- Molecule 32: 50S ribosomal protein L13



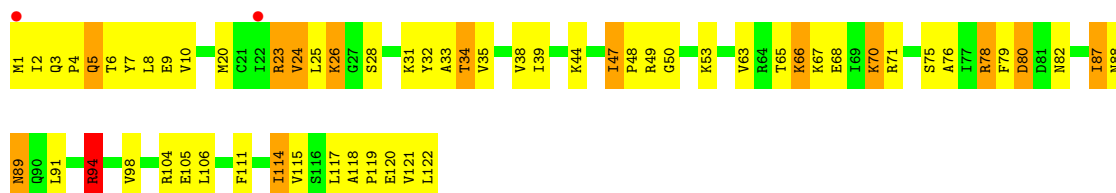
- Molecule 32: 50S ribosomal protein L13



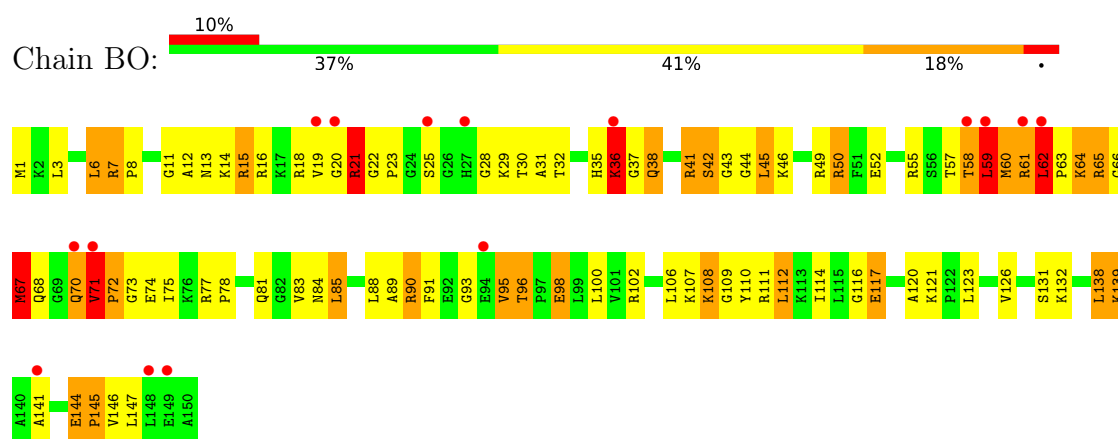
- Molecule 33: 50S ribosomal protein L14



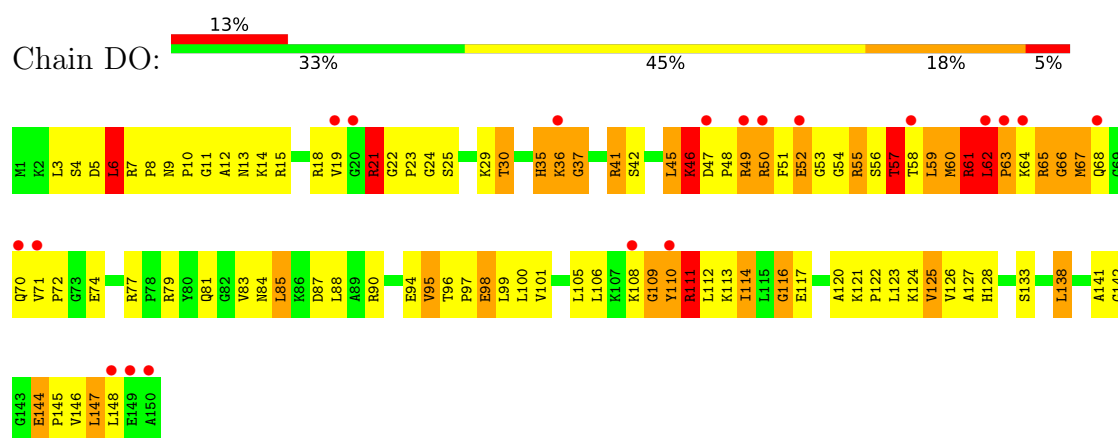
- Molecule 33: 50S ribosomal protein L14



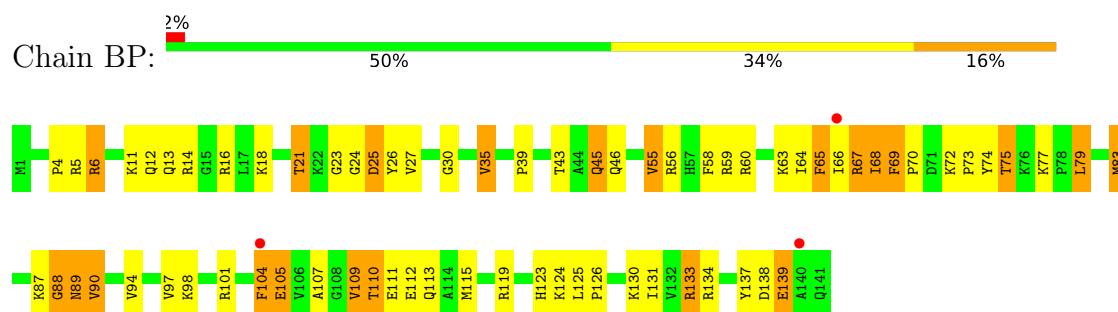
- Molecule 34: 50S ribosomal protein L15



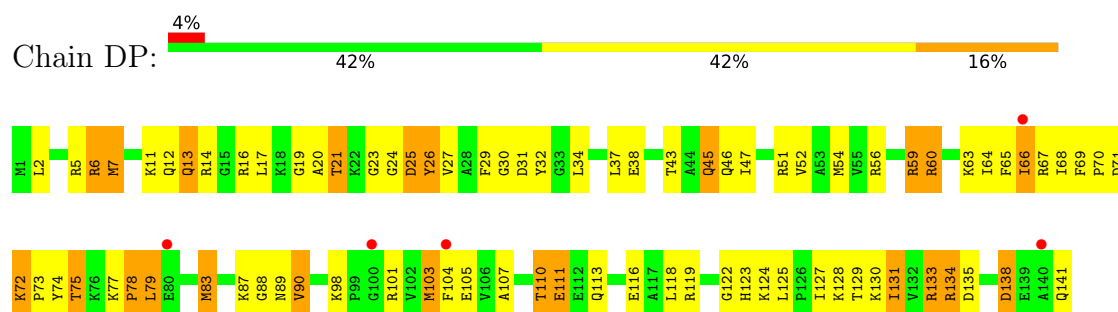
• Molecule 34: 50S ribosomal protein L15



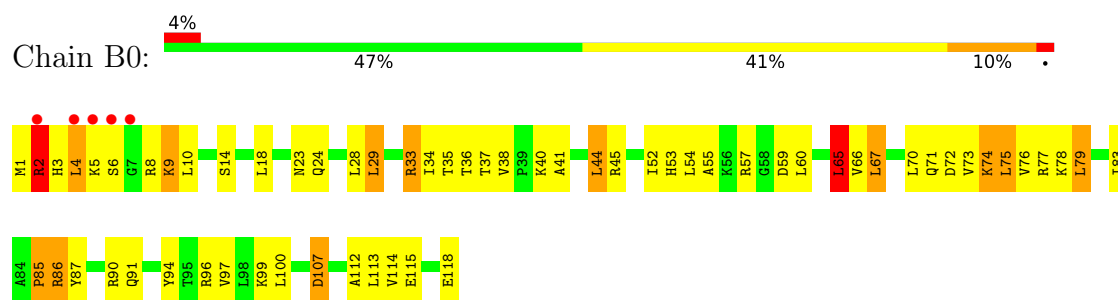
• Molecule 35: 50S ribosomal protein L16



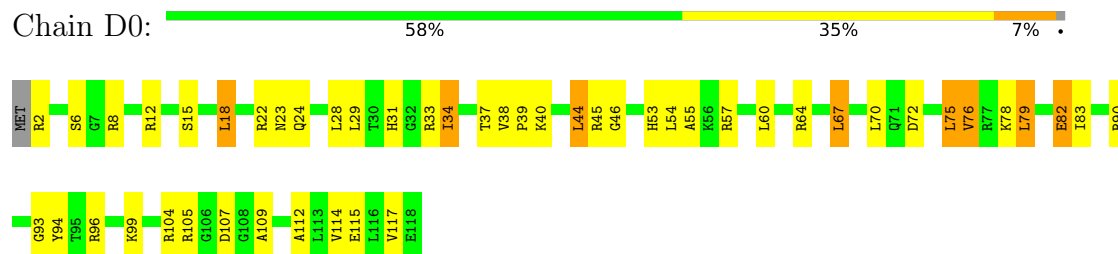
• Molecule 35: 50S ribosomal protein L16



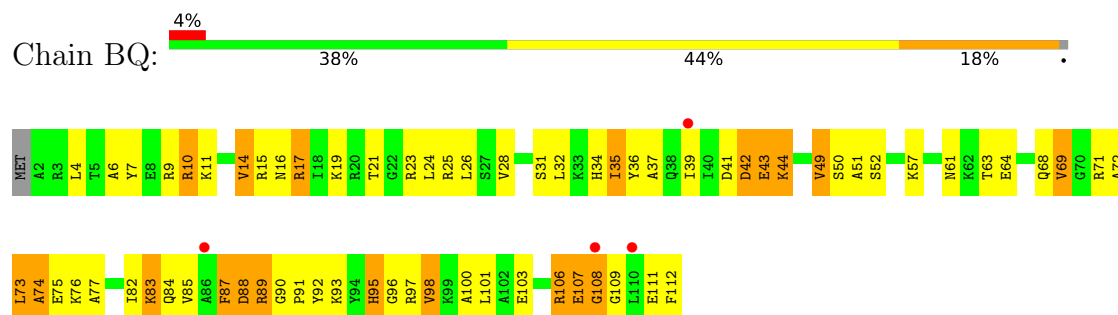
• Molecule 36: 50S ribosomal protein L17



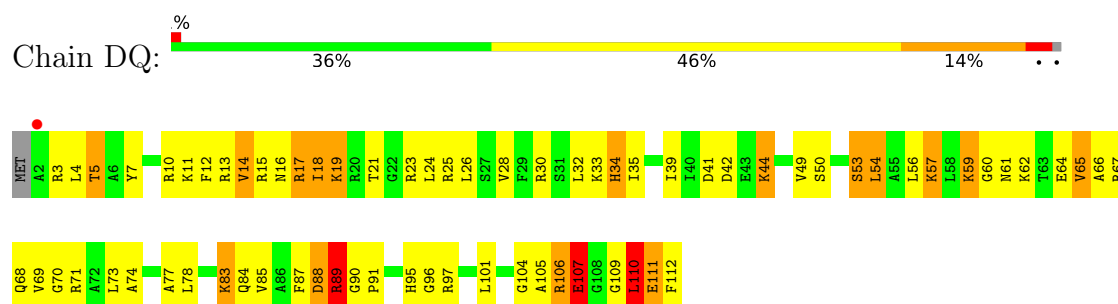
- Molecule 36: 50S ribosomal protein L17



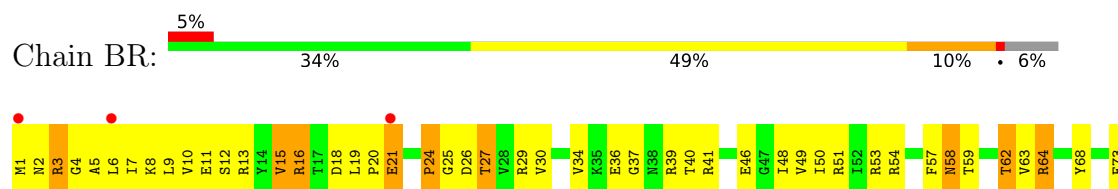
- Molecule 37: 50S ribosomal protein L18

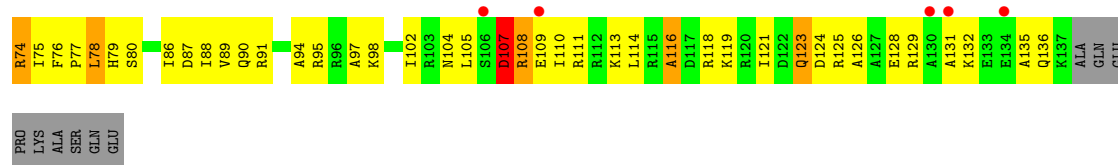


- Molecule 37: 50S ribosomal protein L18

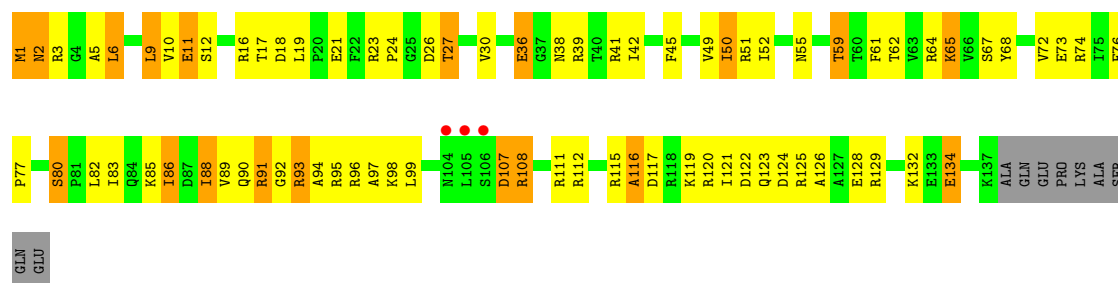


- Molecule 38: 50S ribosomal protein L19

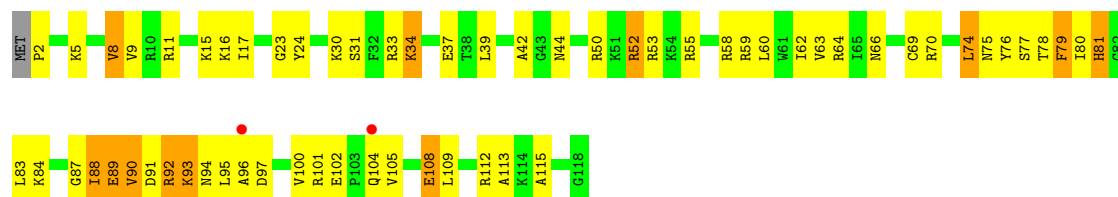




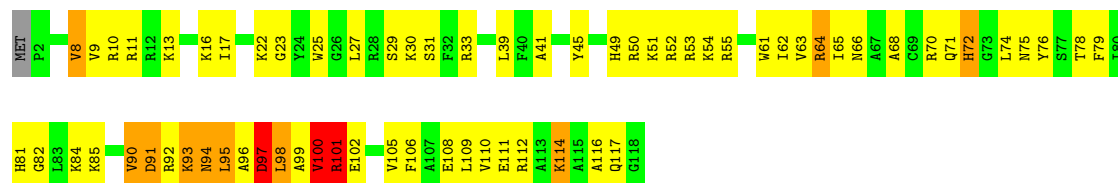
• Molecule 38: 50S ribosomal protein L19



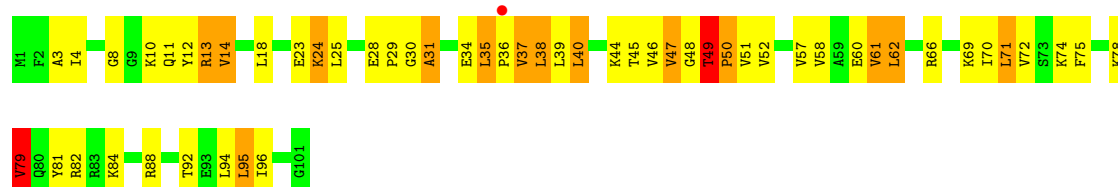
• Molecule 39: 50S ribosomal protein L20



• Molecule 39: 50S ribosomal protein L20



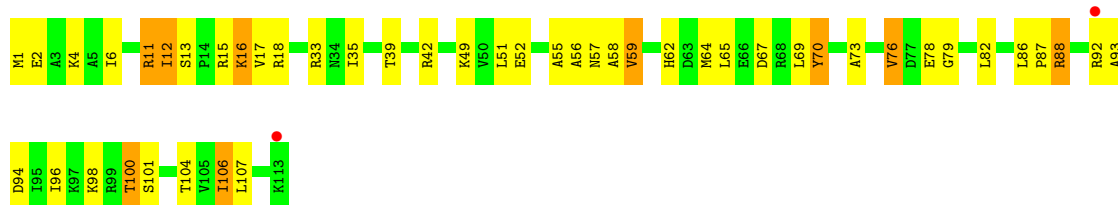
• Molecule 40: 50S ribosomal protein L21



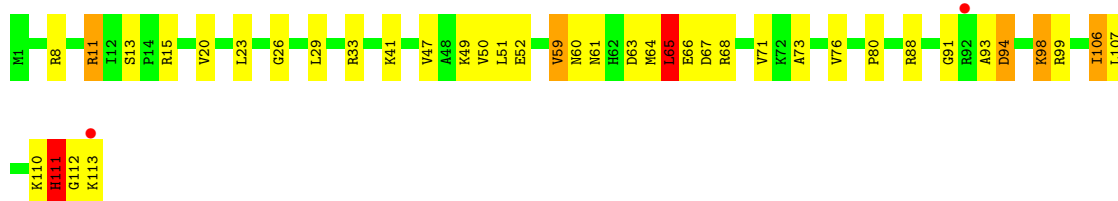
- Molecule 40: 50S ribosomal protein L21



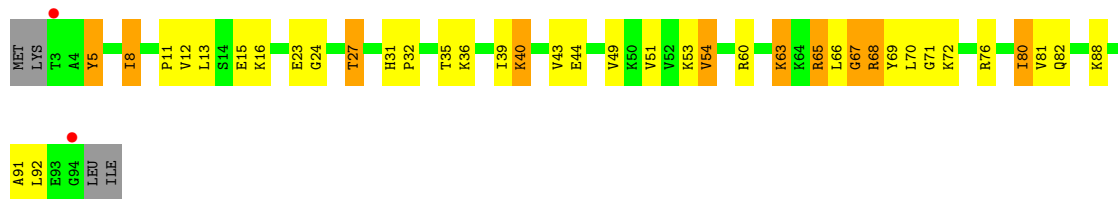
- Molecule 41: 50S ribosomal protein L22



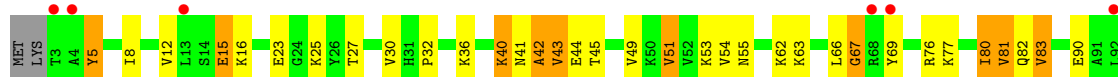
- Molecule 41: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L23

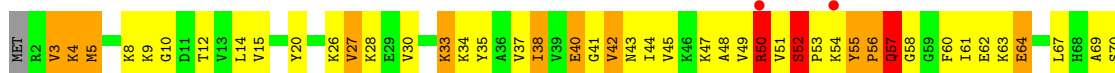


- Molecule 42: 50S ribosomal protein L23

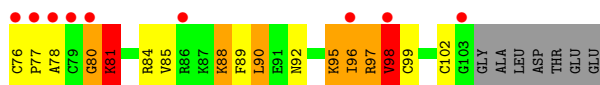
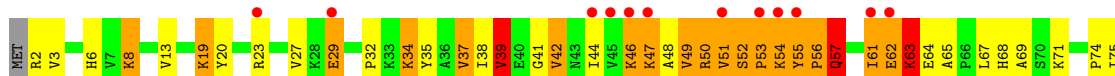




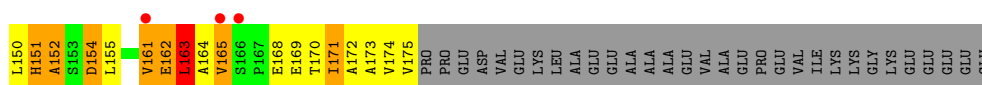
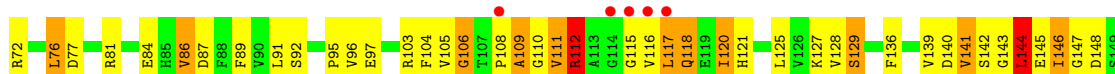
- Molecule 43: 50S ribosomal protein L24



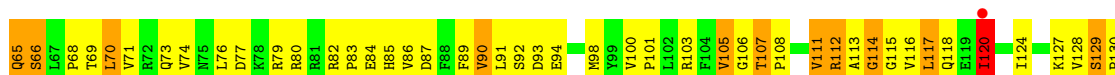
- Molecule 43: 50S ribosomal protein L24

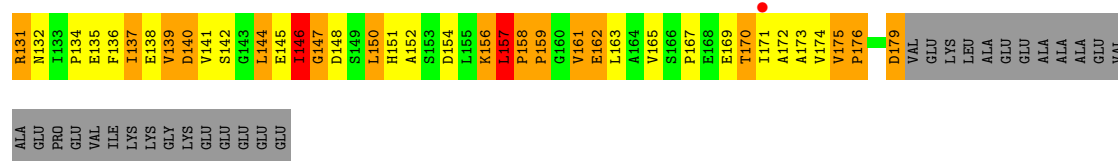


- Molecule 44: 50S ribosomal protein L25

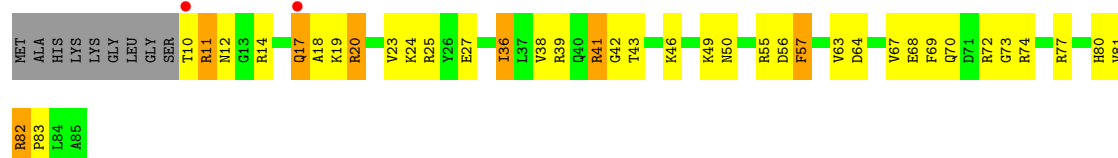


- Molecule 44: 50S ribosomal protein L25

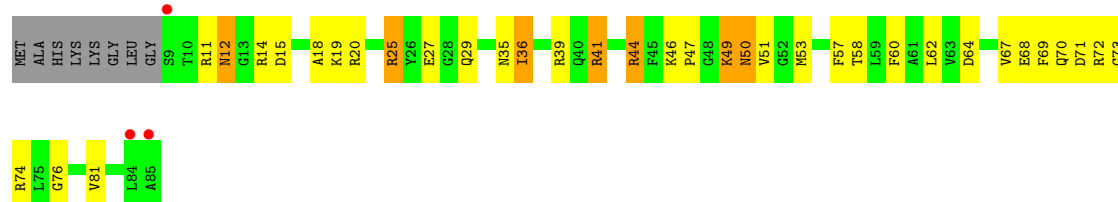




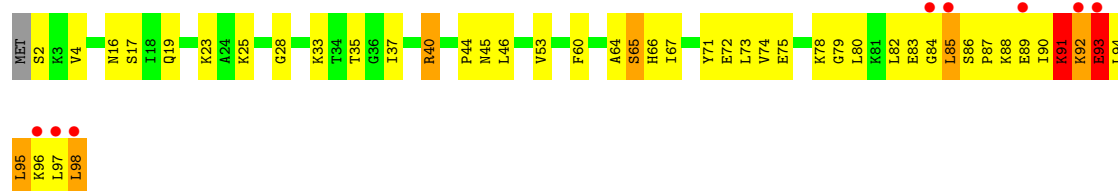
• Molecule 45: 50S ribosomal protein L27



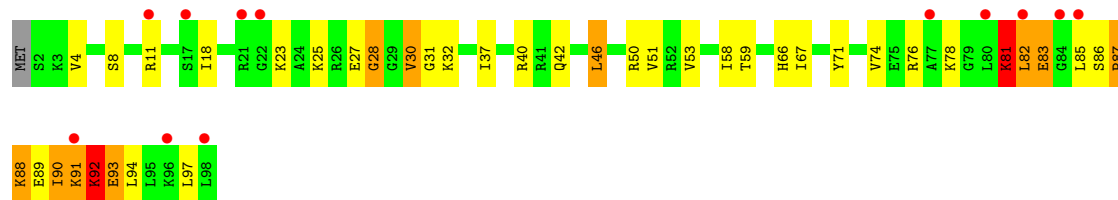
• Molecule 45: 50S ribosomal protein L27



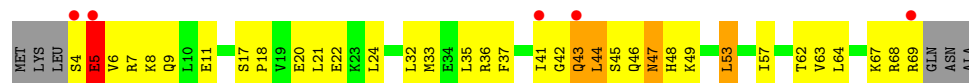
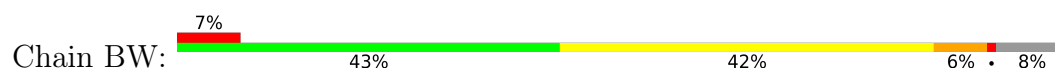
• Molecule 46: 50S ribosomal protein L28



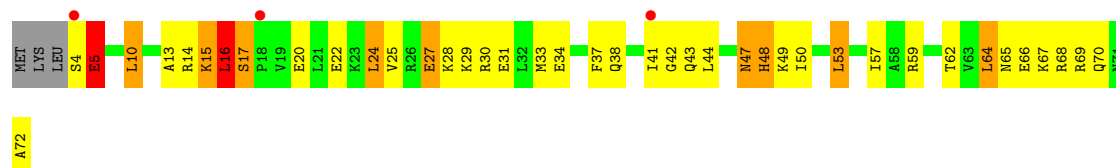
• Molecule 46: 50S ribosomal protein L28



• Molecule 47: 50S ribosomal protein L29



• Molecule 47: 50S ribosomal protein L29



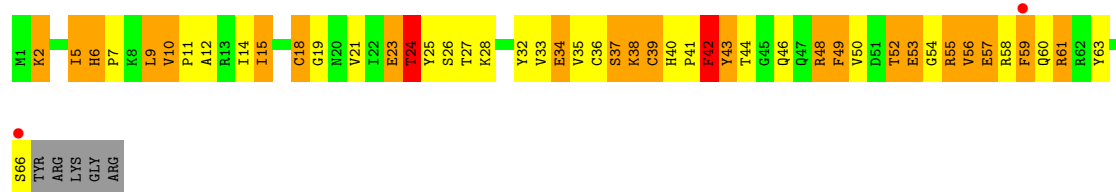
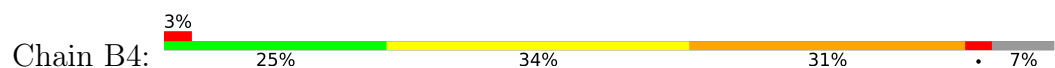
• Molecule 48: 50S ribosomal protein L30



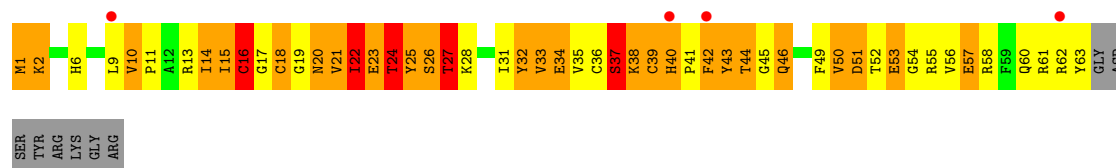
• Molecule 48: 50S ribosomal protein L30



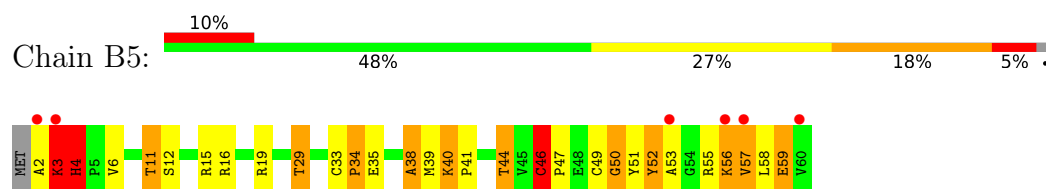
• Molecule 49: 50S ribosomal protein L31



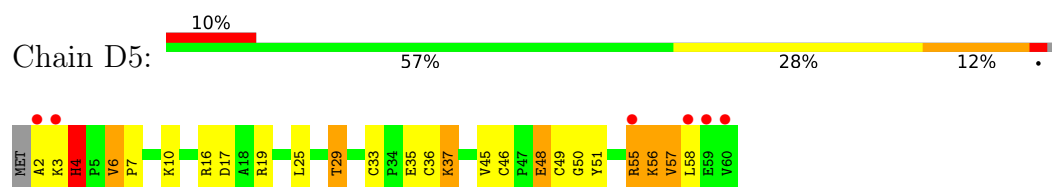
• Molecule 49: 50S ribosomal protein L31



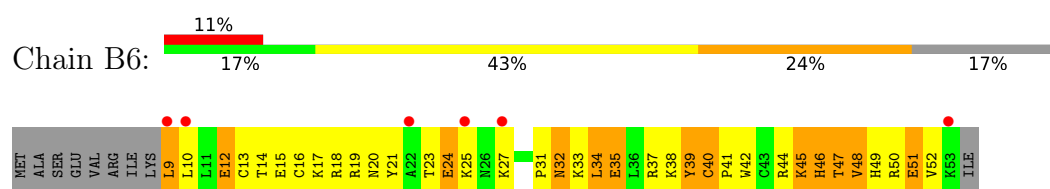
## • Molecule 50: 50S ribosomal protein L32



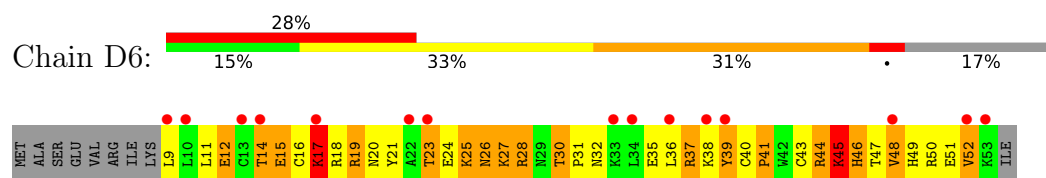
## • Molecule 50: 50S ribosomal protein L32



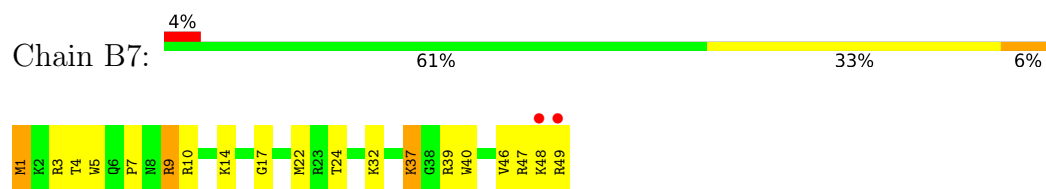
## • Molecule 51: 50S ribosomal protein L33



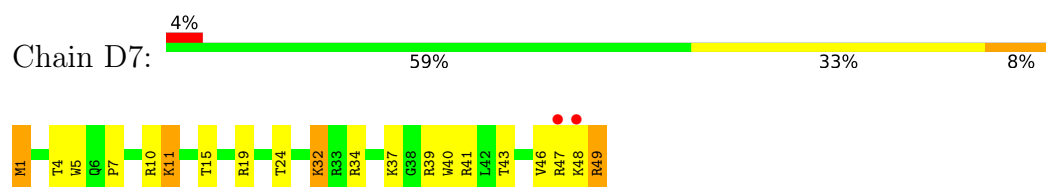
## • Molecule 51: 50S ribosomal protein L33



## • Molecule 52: 50S ribosomal protein L34

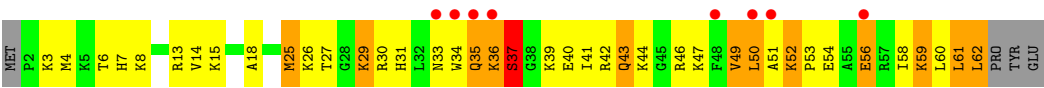


## • Molecule 52: 50S ribosomal protein L34

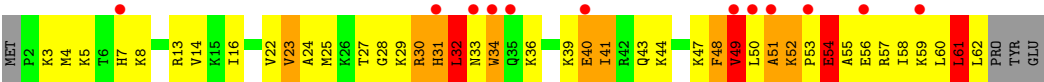


## • Molecule 53: 50S ribosomal protein L35





• Molecule 53: 50S ribosomal protein L35



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.06Å 450.27Å 616.89Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 153.59 – 3.10<br>153.59 – 3.10                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (153.59-3.10)<br>93.4 (153.59-3.10)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.47                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.89 (at 3.07Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX dev_987                                              | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.269<br>0.213 , 0.268                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (0.19%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 83.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.211                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25 , 39.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 295766                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 111.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T1C, ZN, MG

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    | 0.35         | 10/36234 (0.0%) | 0.43        | 7/56554 (0.0%) |
| 1   | CA    | 0.30         | 0/36237         | 0.40        | 0/56558        |
| 2   | AE    | 0.48         | 0/1959          | 0.96        | 4/2642 (0.2%)  |
| 2   | CE    | 0.50         | 0/1959          | 1.04        | 14/2642 (0.5%) |
| 3   | AF    | 0.49         | 0/1629          | 0.93        | 2/2195 (0.1%)  |
| 3   | CF    | 0.48         | 0/1636          | 0.88        | 5/2205 (0.2%)  |
| 4   | AG    | 0.55         | 0/1733          | 1.01        | 2/2318 (0.1%)  |
| 4   | CG    | 0.50         | 0/1733          | 0.95        | 3/2318 (0.1%)  |
| 5   | AH    | 0.53         | 0/1171          | 0.95        | 4/1576 (0.3%)  |
| 5   | CH    | 0.48         | 0/1171          | 0.95        | 4/1576 (0.3%)  |
| 6   | AI    | 0.50         | 0/856           | 0.89        | 0/1154         |
| 6   | CI    | 0.45         | 0/856           | 0.87        | 0/1154         |
| 7   | AJ    | 0.57         | 1/1276 (0.1%)   | 0.99        | 3/1709 (0.2%)  |
| 7   | CJ    | 0.47         | 0/1276          | 0.95        | 2/1709 (0.1%)  |
| 8   | AK    | 0.48         | 0/1136          | 1.05        | 4/1527 (0.3%)  |
| 8   | CK    | 0.45         | 0/1136          | 0.98        | 5/1527 (0.3%)  |
| 9   | AL    | 0.59         | 0/1029          | 0.93        | 2/1379 (0.1%)  |
| 9   | CL    | 0.52         | 0/1029          | 0.94        | 0/1379         |
| 10  | AM    | 0.47         | 0/814           | 0.89        | 1/1095 (0.1%)  |
| 10  | CM    | 0.58         | 2/814 (0.2%)    | 0.98        | 5/1095 (0.5%)  |
| 11  | AN    | 0.51         | 0/900           | 0.98        | 4/1213 (0.3%)  |
| 11  | CN    | 0.60         | 1/900 (0.1%)    | 1.01        | 1/1213 (0.1%)  |
| 12  | AO    | 0.54         | 0/991           | 0.90        | 0/1327         |
| 12  | CO    | 0.50         | 0/991           | 0.99        | 3/1327 (0.2%)  |
| 13  | AP    | 0.54         | 0/938           | 0.94        | 0/1258         |
| 13  | CP    | 0.47         | 0/943           | 0.93        | 0/1265         |
| 14  | AQ    | 0.54         | 0/501           | 1.01        | 2/664 (0.3%)   |
| 14  | CQ    | 0.49         | 0/501           | 1.01        | 2/664 (0.3%)   |
| 15  | AR    | 0.51         | 0/745           | 0.92        | 0/992          |
| 15  | CR    | 0.48         | 0/745           | 0.91        | 0/992          |
| 16  | AS    | 0.51         | 0/721           | 0.99        | 4/970 (0.4%)   |
| 16  | CS    | 0.50         | 0/721           | 0.92        | 1/970 (0.1%)   |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 17  | AT    | 0.47         | 0/847         | 0.96        | 5/1131 (0.4%)  |
| 17  | CT    | 0.46         | 0/847         | 0.90        | 2/1131 (0.2%)  |
| 18  | AU    | 0.51         | 0/596         | 0.98        | 2/790 (0.3%)   |
| 18  | CU    | 0.49         | 0/596         | 0.92        | 1/790 (0.1%)   |
| 19  | AV    | 0.62         | 0/680         | 1.11        | 2/915 (0.2%)   |
| 19  | CV    | 0.65         | 0/638         | 1.11        | 1/860 (0.1%)   |
| 20  | AW    | 0.48         | 0/765         | 1.00        | 2/1007 (0.2%)  |
| 20  | CW    | 0.48         | 0/765         | 1.01        | 2/1007 (0.2%)  |
| 21  | AX    | 0.44         | 0/221         | 0.81        | 0/288          |
| 21  | CX    | 0.50         | 0/221         | 0.92        | 0/288          |
| 22  | AC    | 0.34         | 0/1832        | 0.40        | 0/2855         |
| 22  | AD    | 0.27         | 1/1832 (0.1%) | 0.38        | 0/2855         |
| 22  | CC    | 0.30         | 1/1832 (0.1%) | 0.40        | 0/2855         |
| 22  | CD    | 0.31         | 1/1832 (0.1%) | 0.43        | 0/2855         |
| 23  | A1    | 0.39         | 0/144         | 0.38        | 0/222          |
| 23  | C1    | 0.34         | 0/144         | 0.42        | 0/222          |
| 24  | BA    | 0.38         | 0/70233       | 0.46        | 0/109643       |
| 24  | DA    | 0.35         | 0/70100       | 0.44        | 0/109435       |
| 25  | BB    | 0.36         | 0/2928        | 0.43        | 0/4568         |
| 25  | DB    | 0.30         | 0/2928        | 0.41        | 0/4568         |
| 26  | BD    | 0.70         | 1/2165 (0.0%) | 1.14        | 11/2919 (0.4%) |
| 26  | DD    | 0.69         | 1/2165 (0.0%) | 1.05        | 10/2919 (0.3%) |
| 27  | BE    | 0.59         | 0/1601        | 1.03        | 6/2160 (0.3%)  |
| 27  | DE    | 0.62         | 0/1601        | 1.00        | 9/2160 (0.4%)  |
| 28  | BF    | 0.61         | 0/1620        | 1.07        | 6/2194 (0.3%)  |
| 28  | DF    | 0.54         | 0/1662        | 1.02        | 5/2249 (0.2%)  |
| 29  | BG    | 0.53         | 0/1499        | 0.94        | 5/2016 (0.2%)  |
| 29  | DG    | 0.47         | 0/1499        | 0.98        | 7/2016 (0.3%)  |
| 30  | BH    | 0.58         | 0/1332        | 1.02        | 8/1802 (0.4%)  |
| 30  | DH    | 0.51         | 0/1332        | 1.07        | 11/1802 (0.6%) |
| 31  | BK    | 0.56         | 0/1151        | 0.97        | 1/1558 (0.1%)  |
| 31  | DK    | 0.57         | 0/1151        | 0.98        | 2/1558 (0.1%)  |
| 32  | BM    | 0.64         | 0/1131        | 0.93        | 0/1525         |
| 32  | DM    | 0.48         | 0/1131        | 0.91        | 1/1525 (0.1%)  |
| 33  | BN    | 0.60         | 0/943         | 1.01        | 3/1269 (0.2%)  |
| 33  | DN    | 0.55         | 0/943         | 0.97        | 4/1269 (0.3%)  |
| 34  | BO    | 0.67         | 0/1162        | 1.12        | 9/1544 (0.6%)  |
| 34  | DO    | 0.54         | 1/1162 (0.1%) | 1.03        | 5/1544 (0.3%)  |
| 35  | BP    | 0.59         | 0/1143        | 0.97        | 2/1527 (0.1%)  |
| 35  | DP    | 0.57         | 0/1143        | 0.97        | 4/1527 (0.3%)  |
| 36  | B0    | 0.64         | 0/982         | 0.95        | 2/1312 (0.2%)  |
| 36  | D0    | 0.56         | 0/974         | 0.93        | 0/1302         |
| 37  | BQ    | 0.62         | 0/892         | 0.99        | 0/1187         |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 37  | DQ    | 0.56         | 0/892            | 1.03        | 3/1187 (0.3%)     |
| 38  | BR    | 0.56         | 0/1155           | 1.00        | 5/1542 (0.3%)     |
| 38  | DR    | 0.51         | 0/1155           | 0.95        | 3/1542 (0.2%)     |
| 39  | B1    | 0.59         | 0/982            | 1.03        | 3/1306 (0.2%)     |
| 39  | D1    | 0.50         | 0/982            | 0.99        | 2/1306 (0.2%)     |
| 40  | B2    | 0.61         | 0/790            | 0.97        | 2/1057 (0.2%)     |
| 40  | D2    | 0.53         | 0/790            | 1.01        | 4/1057 (0.4%)     |
| 41  | BS    | 0.61         | 0/911            | 0.95        | 0/1220            |
| 41  | DS    | 0.59         | 0/911            | 0.91        | 0/1220            |
| 42  | BT    | 0.65         | 0/739            | 0.96        | 1/993 (0.1%)      |
| 42  | DT    | 0.62         | 0/739            | 0.97        | 2/993 (0.2%)      |
| 43  | BU    | 0.70         | 0/798            | 1.08        | 6/1064 (0.6%)     |
| 43  | DU    | 0.67         | 0/798            | 1.03        | 4/1064 (0.4%)     |
| 44  | BV    | 0.54         | 0/1427           | 0.97        | 2/1935 (0.1%)     |
| 44  | DV    | 0.52         | 0/1460           | 1.06        | 9/1982 (0.5%)     |
| 45  | B3    | 0.74         | 3/615 (0.5%)     | 0.95        | 0/819             |
| 45  | D3    | 0.56         | 0/621            | 0.94        | 1/827 (0.1%)      |
| 46  | BZ    | 0.62         | 0/770            | 0.95        | 0/1022            |
| 46  | DZ    | 0.62         | 0/770            | 0.95        | 0/1022            |
| 47  | BW    | 0.58         | 0/560            | 1.12        | 2/741 (0.3%)      |
| 47  | DW    | 0.51         | 0/583            | 1.14        | 6/771 (0.8%)      |
| 48  | BX    | 0.53         | 0/474            | 0.86        | 0/635             |
| 48  | DX    | 0.50         | 0/474            | 0.94        | 2/635 (0.3%)      |
| 49  | B4    | 0.68         | 0/545            | 1.15        | 5/733 (0.7%)      |
| 49  | D4    | 0.64         | 0/527            | 1.01        | 2/709 (0.3%)      |
| 50  | B5    | 0.67         | 0/473            | 1.37        | 6/639 (0.9%)      |
| 50  | D5    | 0.58         | 0/473            | 1.01        | 2/639 (0.3%)      |
| 51  | B6    | 0.63         | 0/396            | 1.06        | 3/529 (0.6%)      |
| 51  | D6    | 0.61         | 0/396            | 0.80        | 0/529             |
| 52  | B7    | 0.69         | 0/438            | 1.04        | 2/575 (0.3%)      |
| 52  | D7    | 0.65         | 0/438            | 0.97        | 0/575             |
| 53  | B8    | 0.73         | 0/494            | 1.10        | 5/649 (0.8%)      |
| 53  | D8    | 0.77         | 1/494 (0.2%)     | 1.28        | 3/649 (0.5%)      |
| All | All   | 0.42         | 24/319716 (0.0%) | 0.63        | 297/478502 (0.1%) |

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

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | AA    | 193  | C    | C5'-C4' | 11.09 | 1.67        | 1.51     |
| 1   | AA    | 1381 | U    | C1'-N1  | 10.07 | 1.63        | 1.48     |
| 1   | AA    | 193  | C    | O5'-C5' | 9.59  | 1.56        | 1.42     |
| 1   | AA    | 193  | C    | P-O5'   | 9.28  | 1.73        | 1.59     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | AA    | 192 | U    | O3'-P | 8.29 | 1.73        | 1.61     |

The worst 5 of 297 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 26  | BD    | 272 | ALA  | N-CA-C | 11.75  | 122.00      | 108.49   |
| 50  | B5    | 4   | HIS  | CA-C-N | -10.36 | 110.26      | 120.52   |
| 50  | B5    | 4   | HIS  | C-N-CA | -10.36 | 110.26      | 120.52   |
| 4   | AG    | 12  | CYS  | N-CA-C | -10.33 | 100.02      | 111.28   |
| 26  | BD    | 28  | GLU  | CA-C-N | -10.13 | 109.08      | 119.92   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32369 | 0        | 16338    | 916     | 10           |
| 1   | CA    | 32372 | 0        | 16336    | 880     | 0            |
| 2   | AE    | 1924  | 0        | 1975     | 123     | 0            |
| 2   | CE    | 1924  | 0        | 1975     | 148     | 0            |
| 3   | AF    | 1605  | 0        | 1668     | 72      | 0            |
| 3   | CF    | 1612  | 0        | 1677     | 117     | 0            |
| 4   | AG    | 1703  | 0        | 1763     | 112     | 0            |
| 4   | CG    | 1703  | 0        | 1764     | 213     | 0            |
| 5   | AH    | 1155  | 0        | 1213     | 60      | 0            |
| 5   | CH    | 1155  | 0        | 1212     | 57      | 0            |
| 6   | AI    | 843   | 0        | 857      | 44      | 0            |
| 6   | CI    | 843   | 0        | 857      | 31      | 0            |
| 7   | AJ    | 1257  | 0        | 1296     | 76      | 0            |
| 7   | CJ    | 1257  | 0        | 1296     | 68      | 0            |
| 8   | AK    | 1116  | 0        | 1177     | 60      | 0            |
| 8   | CK    | 1116  | 0        | 1177     | 46      | 0            |
| 9   | AL    | 1010  | 0        | 1037     | 90      | 0            |
| 9   | CL    | 1010  | 0        | 1037     | 96      | 0            |
| 10  | AM    | 801   | 0        | 849      | 59      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | CM    | 801   | 0        | 849      | 55      | 1            |
| 11  | AN    | 885   | 0        | 904      | 40      | 0            |
| 11  | CN    | 885   | 0        | 904      | 40      | 0            |
| 12  | AO    | 975   | 0        | 1062     | 76      | 0            |
| 12  | CO    | 975   | 0        | 1062     | 44      | 0            |
| 13  | AP    | 928   | 0        | 987      | 63      | 0            |
| 13  | CP    | 933   | 0        | 992      | 90      | 0            |
| 14  | AQ    | 492   | 0        | 529      | 41      | 0            |
| 14  | CQ    | 492   | 0        | 531      | 44      | 0            |
| 15  | AR    | 734   | 0        | 771      | 27      | 0            |
| 15  | CR    | 734   | 0        | 771      | 33      | 0            |
| 16  | AS    | 705   | 0        | 725      | 39      | 0            |
| 16  | CS    | 705   | 0        | 725      | 32      | 0            |
| 17  | AT    | 834   | 0        | 904      | 44      | 0            |
| 17  | CT    | 834   | 0        | 904      | 27      | 0            |
| 18  | AU    | 591   | 0        | 662      | 24      | 0            |
| 18  | CU    | 591   | 0        | 662      | 27      | 0            |
| 19  | AV    | 665   | 0        | 686      | 50      | 0            |
| 19  | CV    | 624   | 0        | 636      | 81      | 0            |
| 20  | AW    | 763   | 0        | 861      | 58      | 0            |
| 20  | CW    | 763   | 0        | 861      | 49      | 0            |
| 21  | AX    | 217   | 0        | 234      | 7       | 0            |
| 21  | CX    | 217   | 0        | 234      | 21      | 0            |
| 22  | AC    | 1640  | 0        | 836      | 19      | 0            |
| 22  | AD    | 1640  | 0        | 836      | 98      | 0            |
| 22  | CC    | 1640  | 0        | 836      | 23      | 0            |
| 22  | CD    | 1640  | 0        | 836      | 89      | 0            |
| 23  | A1    | 129   | 0        | 65       | 0       | 0            |
| 23  | C1    | 129   | 0        | 65       | 0       | 0            |
| 24  | BA    | 62707 | 0        | 31612    | 1389    | 0            |
| 24  | DA    | 62587 | 0        | 31554    | 1355    | 0            |
| 25  | BB    | 2617  | 0        | 1328     | 60      | 0            |
| 25  | DB    | 2617  | 0        | 1328     | 85      | 0            |
| 26  | BD    | 2115  | 0        | 2195     | 116     | 0            |
| 26  | DD    | 2115  | 0        | 2195     | 146     | 0            |
| 27  | BE    | 1568  | 0        | 1634     | 104     | 0            |
| 27  | DE    | 1568  | 0        | 1634     | 207     | 0            |
| 28  | BF    | 1585  | 0        | 1632     | 77      | 0            |
| 28  | DF    | 1627  | 0        | 1680     | 131     | 0            |
| 29  | BG    | 1474  | 0        | 1535     | 93      | 0            |
| 29  | DG    | 1474  | 0        | 1535     | 107     | 0            |
| 30  | BH    | 1307  | 0        | 1382     | 137     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 30  | DH    | 1307  | 0        | 1382     | 126     | 9            |
| 31  | BK    | 1136  | 0        | 1223     | 49      | 0            |
| 31  | DK    | 1136  | 0        | 1223     | 49      | 0            |
| 32  | BM    | 1104  | 0        | 1180     | 69      | 0            |
| 32  | DM    | 1104  | 0        | 1180     | 55      | 0            |
| 33  | BN    | 933   | 0        | 996      | 31      | 0            |
| 33  | DN    | 933   | 0        | 996      | 43      | 0            |
| 34  | BO    | 1145  | 0        | 1227     | 114     | 0            |
| 34  | DO    | 1145  | 0        | 1228     | 155     | 0            |
| 35  | BP    | 1122  | 0        | 1179     | 90      | 0            |
| 35  | DP    | 1122  | 0        | 1179     | 61      | 0            |
| 36  | B0    | 968   | 0        | 1033     | 62      | 0            |
| 36  | D0    | 960   | 0        | 1021     | 36      | 0            |
| 37  | BQ    | 882   | 0        | 943      | 54      | 0            |
| 37  | DQ    | 882   | 0        | 943      | 73      | 0            |
| 38  | BR    | 1141  | 0        | 1202     | 67      | 0            |
| 38  | DR    | 1141  | 0        | 1202     | 65      | 0            |
| 39  | B1    | 964   | 0        | 1022     | 65      | 0            |
| 39  | D1    | 964   | 0        | 1022     | 71      | 0            |
| 40  | B2    | 779   | 0        | 852      | 44      | 1            |
| 40  | D2    | 779   | 0        | 852      | 88      | 0            |
| 41  | BS    | 900   | 0        | 964      | 29      | 0            |
| 41  | DS    | 900   | 0        | 964      | 25      | 0            |
| 42  | BT    | 725   | 0        | 778      | 25      | 0            |
| 42  | DT    | 725   | 0        | 778      | 23      | 0            |
| 43  | BU    | 785   | 0        | 878      | 81      | 0            |
| 43  | DU    | 785   | 0        | 878      | 61      | 0            |
| 44  | BV    | 1397  | 0        | 1430     | 83      | 0            |
| 44  | DV    | 1428  | 0        | 1454     | 90      | 0            |
| 45  | B3    | 607   | 0        | 628      | 41      | 0            |
| 45  | D3    | 613   | 0        | 633      | 35      | 0            |
| 46  | BZ    | 763   | 0        | 848      | 31      | 0            |
| 46  | DZ    | 763   | 0        | 848      | 34      | 0            |
| 47  | BW    | 558   | 0        | 610      | 27      | 0            |
| 47  | DW    | 581   | 0        | 629      | 31      | 0            |
| 48  | BX    | 469   | 0        | 518      | 17      | 0            |
| 48  | DX    | 469   | 0        | 518      | 19      | 0            |
| 49  | B4    | 533   | 0        | 522      | 57      | 0            |
| 49  | D4    | 515   | 0        | 510      | 79      | 0            |
| 50  | B5    | 459   | 0        | 480      | 35      | 1            |
| 50  | D5    | 459   | 0        | 480      | 25      | 0            |
| 51  | B6    | 389   | 0        | 404      | 42      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 51  | D6    | 389   | 0        | 404      | 78      | 0            |
| 52  | B7    | 430   | 0        | 480      | 18      | 0            |
| 52  | D7    | 430   | 0        | 480      | 12      | 0            |
| 53  | B8    | 488   | 0        | 559      | 51      | 0            |
| 53  | D8    | 488   | 0        | 560      | 72      | 0            |
| 54  | A1    | 1     | 0        | 0        | 0       | 0            |
| 54  | AA    | 236   | 0        | 0        | 0       | 0            |
| 54  | AC    | 8     | 0        | 0        | 0       | 0            |
| 54  | AD    | 1     | 0        | 0        | 0       | 0            |
| 54  | AG    | 1     | 0        | 0        | 0       | 0            |
| 54  | AH    | 1     | 0        | 0        | 0       | 0            |
| 54  | AN    | 2     | 0        | 0        | 0       | 0            |
| 54  | AQ    | 1     | 0        | 0        | 0       | 0            |
| 54  | AT    | 1     | 0        | 0        | 0       | 0            |
| 54  | B0    | 1     | 0        | 0        | 0       | 0            |
| 54  | B1    | 1     | 0        | 0        | 0       | 0            |
| 54  | B2    | 1     | 0        | 0        | 0       | 0            |
| 54  | B3    | 2     | 0        | 0        | 0       | 0            |
| 54  | B5    | 1     | 0        | 0        | 0       | 0            |
| 54  | B7    | 3     | 0        | 0        | 0       | 0            |
| 54  | B8    | 2     | 0        | 0        | 0       | 0            |
| 54  | BA    | 632   | 0        | 0        | 0       | 0            |
| 54  | BB    | 16    | 0        | 0        | 0       | 0            |
| 54  | BD    | 1     | 0        | 0        | 0       | 0            |
| 54  | BE    | 4     | 0        | 0        | 0       | 0            |
| 54  | BF    | 2     | 0        | 0        | 0       | 0            |
| 54  | BO    | 2     | 0        | 0        | 0       | 0            |
| 54  | BU    | 2     | 0        | 0        | 0       | 0            |
| 54  | CA    | 199   | 0        | 0        | 0       | 0            |
| 54  | CC    | 9     | 0        | 0        | 0       | 0            |
| 54  | CG    | 2     | 0        | 0        | 0       | 0            |
| 54  | CL    | 1     | 0        | 0        | 0       | 0            |
| 54  | CN    | 1     | 0        | 0        | 0       | 0            |
| 54  | CS    | 1     | 0        | 0        | 0       | 0            |
| 54  | CX    | 1     | 0        | 0        | 0       | 0            |
| 54  | D1    | 1     | 0        | 0        | 0       | 0            |
| 54  | D3    | 1     | 0        | 0        | 0       | 0            |
| 54  | D5    | 1     | 0        | 0        | 0       | 0            |
| 54  | D8    | 1     | 0        | 0        | 0       | 0            |
| 54  | DA    | 523   | 0        | 0        | 0       | 0            |
| 54  | DB    | 15    | 0        | 0        | 0       | 0            |
| 54  | DE    | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 54  | DP    | 1      | 0        | 0        | 0       | 0            |
| 54  | DR    | 1      | 0        | 0        | 0       | 0            |
| 54  | DU    | 2      | 0        | 0        | 0       | 0            |
| 55  | AA    | 42     | 0        | 39       | 2       | 0            |
| 55  | CA    | 42     | 0        | 38       | 5       | 0            |
| 56  | AG    | 1      | 0        | 0        | 0       | 0            |
| 56  | AQ    | 1      | 0        | 0        | 0       | 0            |
| 56  | CG    | 1      | 0        | 0        | 0       | 0            |
| 56  | CQ    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 295766 | 0        | 199075   | 9506    | 11           |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 9506 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 24:BA:2751:G:C2  | 30:BH:3:ARG:HD3   | 1.42                     | 1.55              |
| 30:DH:127:GLU:CG | 30:DH:128:PRO:HD3 | 1.36                     | 1.54              |
| 27:DE:11:MET:SD  | 27:DE:24:THR:HG22 | 1.47                     | 1.52              |
| 40:D2:49:THR:HB  | 40:D2:50:PRO:CD   | 1.45                     | 1.47              |
| 26:DD:34:VAL:CG2 | 26:DD:35:LYS:HZ3  | 1.26                     | 1.46              |

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-------------------------|--------------------------|-------------------|
| 1:AA:85:U:O5' | 30:DH:126:PRO:CA[3_555] | 1.25                     | 0.95              |
| 1:AA:85:U:C4' | 30:DH:126:PRO:CB[3_555] | 1.47                     | 0.73              |
| 1:AA:84:U:O3' | 30:DH:127:GLU:N[3_555]  | 1.76                     | 0.44              |
| 1:AA:84:U:OP2 | 30:DH:127:GLU:CG[3_555] | 1.98                     | 0.22              |
| 1:AA:85:U:C5' | 30:DH:126:PRO:CB[3_555] | 2.00                     | 0.20              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AE    | 235/256 (92%) | 170 (72%) | 41 (17%) | 24 (10%) | 0           | 3  |
| 2   | CE    | 235/256 (92%) | 165 (70%) | 38 (16%) | 32 (14%) | 0           | 1  |
| 3   | AF    | 203/239 (85%) | 138 (68%) | 44 (22%) | 21 (10%) | 0           | 2  |
| 3   | CF    | 204/239 (85%) | 135 (66%) | 48 (24%) | 21 (10%) | 0           | 2  |
| 4   | AG    | 206/208 (99%) | 154 (75%) | 35 (17%) | 17 (8%)  | 0           | 4  |
| 4   | CG    | 206/208 (99%) | 150 (73%) | 36 (18%) | 20 (10%) | 0           | 3  |
| 5   | AH    | 149/162 (92%) | 118 (79%) | 26 (17%) | 5 (3%)   | 3           | 16 |
| 5   | CH    | 149/162 (92%) | 130 (87%) | 13 (9%)  | 6 (4%)   | 2           | 13 |
| 6   | AI    | 99/101 (98%)  | 86 (87%)  | 9 (9%)   | 4 (4%)   | 2           | 13 |
| 6   | CI    | 99/101 (98%)  | 87 (88%)  | 10 (10%) | 2 (2%)   | 6           | 25 |
| 7   | AJ    | 153/156 (98%) | 127 (83%) | 21 (14%) | 5 (3%)   | 3           | 17 |
| 7   | CJ    | 153/156 (98%) | 120 (78%) | 25 (16%) | 8 (5%)   | 1           | 10 |
| 8   | AK    | 136/138 (99%) | 103 (76%) | 23 (17%) | 10 (7%)  | 1           | 5  |
| 8   | CK    | 136/138 (99%) | 120 (88%) | 10 (7%)  | 6 (4%)   | 2           | 12 |
| 9   | AL    | 125/128 (98%) | 87 (70%)  | 26 (21%) | 12 (10%) | 0           | 3  |
| 9   | CL    | 125/128 (98%) | 90 (72%)  | 31 (25%) | 4 (3%)   | 3           | 18 |
| 10  | AM    | 97/105 (92%)  | 70 (72%)  | 18 (19%) | 9 (9%)   | 0           | 3  |
| 10  | CM    | 97/105 (92%)  | 65 (67%)  | 24 (25%) | 8 (8%)   | 0           | 4  |
| 11  | AN    | 117/129 (91%) | 90 (77%)  | 19 (16%) | 8 (7%)   | 1           | 5  |
| 11  | CN    | 117/129 (91%) | 96 (82%)  | 16 (14%) | 5 (4%)   | 2           | 12 |
| 12  | AO    | 123/128 (96%) | 87 (71%)  | 24 (20%) | 12 (10%) | 0           | 3  |
| 12  | CO    | 123/128 (96%) | 103 (84%) | 10 (8%)  | 10 (8%)  | 1           | 4  |
| 13  | AP    | 114/126 (90%) | 81 (71%)  | 20 (18%) | 13 (11%) | 0           | 1  |
| 13  | CP    | 115/126 (91%) | 75 (65%)  | 22 (19%) | 18 (16%) | 0           | 0  |
| 14  | AQ    | 58/61 (95%)   | 40 (69%)  | 7 (12%)  | 11 (19%) | 0           | 0  |
| 14  | CQ    | 58/61 (95%)   | 40 (69%)  | 12 (21%) | 6 (10%)  | 0           | 2  |
| 15  | AR    | 86/89 (97%)   | 60 (70%)  | 20 (23%) | 6 (7%)   | 1           | 5  |
| 15  | CR    | 86/89 (97%)   | 73 (85%)  | 6 (7%)   | 7 (8%)   | 1           | 4  |
| 16  | AS    | 82/88 (93%)   | 65 (79%)  | 16 (20%) | 1 (1%)   | 10          | 37 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 16  | CS    | 82/88 (93%)   | 66 (80%)  | 15 (18%) | 1 (1%)   | 10          | 37 |
| 17  | AT    | 98/105 (93%)  | 78 (80%)  | 14 (14%) | 6 (6%)   | 1           | 7  |
| 17  | CT    | 98/105 (93%)  | 85 (87%)  | 11 (11%) | 2 (2%)   | 6           | 25 |
| 18  | AU    | 70/88 (80%)   | 59 (84%)  | 7 (10%)  | 4 (6%)   | 1           | 8  |
| 18  | CU    | 70/88 (80%)   | 56 (80%)  | 7 (10%)  | 7 (10%)  | 0           | 3  |
| 19  | AV    | 81/93 (87%)   | 54 (67%)  | 19 (24%) | 8 (10%)  | 0           | 3  |
| 19  | CV    | 76/93 (82%)   | 44 (58%)  | 17 (22%) | 15 (20%) | 0           | 0  |
| 20  | AW    | 97/106 (92%)  | 72 (74%)  | 12 (12%) | 13 (13%) | 0           | 1  |
| 20  | CW    | 97/106 (92%)  | 70 (72%)  | 18 (19%) | 9 (9%)   | 0           | 3  |
| 21  | AX    | 23/27 (85%)   | 14 (61%)  | 7 (30%)  | 2 (9%)   | 0           | 4  |
| 21  | CX    | 23/27 (85%)   | 17 (74%)  | 3 (13%)  | 3 (13%)  | 0           | 1  |
| 26  | BD    | 270/276 (98%) | 231 (86%) | 26 (10%) | 13 (5%)  | 2           | 11 |
| 26  | DD    | 270/276 (98%) | 217 (80%) | 40 (15%) | 13 (5%)  | 2           | 11 |
| 27  | BE    | 203/206 (98%) | 161 (79%) | 28 (14%) | 14 (7%)  | 1           | 5  |
| 27  | DE    | 203/206 (98%) | 133 (66%) | 33 (16%) | 37 (18%) | 0           | 0  |
| 28  | BF    | 200/210 (95%) | 175 (88%) | 20 (10%) | 5 (2%)   | 4           | 21 |
| 28  | DF    | 206/210 (98%) | 151 (73%) | 29 (14%) | 26 (13%) | 0           | 1  |
| 29  | BG    | 179/182 (98%) | 120 (67%) | 42 (24%) | 17 (10%) | 0           | 3  |
| 29  | DG    | 179/182 (98%) | 121 (68%) | 38 (21%) | 20 (11%) | 0           | 2  |
| 30  | BH    | 168/180 (93%) | 124 (74%) | 24 (14%) | 20 (12%) | 0           | 1  |
| 30  | DH    | 168/180 (93%) | 92 (55%)  | 45 (27%) | 31 (18%) | 0           | 0  |
| 31  | BK    | 144/148 (97%) | 102 (71%) | 25 (17%) | 17 (12%) | 0           | 1  |
| 31  | DK    | 144/148 (97%) | 104 (72%) | 28 (19%) | 12 (8%)  | 0           | 4  |
| 32  | BM    | 136/140 (97%) | 101 (74%) | 25 (18%) | 10 (7%)  | 1           | 5  |
| 32  | DM    | 136/140 (97%) | 110 (81%) | 22 (16%) | 4 (3%)   | 3           | 19 |
| 33  | BN    | 120/122 (98%) | 113 (94%) | 5 (4%)   | 2 (2%)   | 7           | 30 |
| 33  | DN    | 120/122 (98%) | 103 (86%) | 14 (12%) | 3 (2%)   | 4           | 21 |
| 34  | BO    | 148/150 (99%) | 99 (67%)  | 21 (14%) | 28 (19%) | 0           | 0  |
| 34  | DO    | 148/150 (99%) | 83 (56%)  | 44 (30%) | 21 (14%) | 0           | 1  |
| 35  | BP    | 139/141 (99%) | 96 (69%)  | 26 (19%) | 17 (12%) | 0           | 1  |
| 35  | DP    | 139/141 (99%) | 105 (76%) | 19 (14%) | 15 (11%) | 0           | 2  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 36  | B0    | 116/118 (98%) | 88 (76%)  | 19 (16%) | 9 (8%)   | 1           | 4  |
| 36  | D0    | 115/118 (98%) | 99 (86%)  | 13 (11%) | 3 (3%)   | 4           | 21 |
| 37  | BQ    | 109/112 (97%) | 78 (72%)  | 19 (17%) | 12 (11%) | 0           | 2  |
| 37  | DQ    | 109/112 (97%) | 78 (72%)  | 20 (18%) | 11 (10%) | 0           | 3  |
| 38  | BR    | 135/146 (92%) | 101 (75%) | 25 (18%) | 9 (7%)   | 1           | 6  |
| 38  | DR    | 135/146 (92%) | 110 (82%) | 19 (14%) | 6 (4%)   | 2           | 12 |
| 39  | B1    | 115/118 (98%) | 101 (88%) | 10 (9%)  | 4 (4%)   | 3           | 16 |
| 39  | D1    | 115/118 (98%) | 88 (76%)  | 18 (16%) | 9 (8%)   | 1           | 4  |
| 40  | B2    | 99/101 (98%)  | 78 (79%)  | 11 (11%) | 10 (10%) | 0           | 3  |
| 40  | D2    | 99/101 (98%)  | 73 (74%)  | 12 (12%) | 14 (14%) | 0           | 1  |
| 41  | BS    | 111/113 (98%) | 102 (92%) | 6 (5%)   | 3 (3%)   | 4           | 20 |
| 41  | DS    | 111/113 (98%) | 98 (88%)  | 8 (7%)   | 5 (4%)   | 2           | 12 |
| 42  | BT    | 90/96 (94%)   | 78 (87%)  | 10 (11%) | 2 (2%)   | 5           | 24 |
| 42  | DT    | 90/96 (94%)   | 69 (77%)  | 13 (14%) | 8 (9%)   | 0           | 3  |
| 43  | BU    | 100/110 (91%) | 69 (69%)  | 14 (14%) | 17 (17%) | 0           | 0  |
| 43  | DU    | 100/110 (91%) | 53 (53%)  | 22 (22%) | 25 (25%) | 0           | 0  |
| 44  | BV    | 173/206 (84%) | 117 (68%) | 31 (18%) | 25 (14%) | 0           | 0  |
| 44  | DV    | 177/206 (86%) | 111 (63%) | 35 (20%) | 31 (18%) | 0           | 0  |
| 45  | B3    | 74/85 (87%)   | 65 (88%)  | 7 (10%)  | 2 (3%)   | 4           | 20 |
| 45  | D3    | 75/85 (88%)   | 66 (88%)  | 7 (9%)   | 2 (3%)   | 4           | 20 |
| 46  | BZ    | 95/98 (97%)   | 78 (82%)  | 10 (10%) | 7 (7%)   | 1           | 5  |
| 46  | DZ    | 95/98 (97%)   | 71 (75%)  | 14 (15%) | 10 (10%) | 0           | 2  |
| 47  | BW    | 64/72 (89%)   | 52 (81%)  | 9 (14%)  | 3 (5%)   | 2           | 11 |
| 47  | DW    | 67/72 (93%)   | 53 (79%)  | 6 (9%)   | 8 (12%)  | 0           | 1  |
| 48  | BX    | 57/60 (95%)   | 51 (90%)  | 4 (7%)   | 2 (4%)   | 3           | 16 |
| 48  | DX    | 57/60 (95%)   | 49 (86%)  | 5 (9%)   | 3 (5%)   | 1           | 10 |
| 49  | B4    | 64/71 (90%)   | 34 (53%)  | 15 (23%) | 15 (23%) | 0           | 0  |
| 49  | D4    | 61/71 (86%)   | 25 (41%)  | 18 (30%) | 18 (30%) | 0           | 0  |
| 50  | B5    | 57/60 (95%)   | 41 (72%)  | 9 (16%)  | 7 (12%)  | 0           | 1  |
| 50  | D5    | 57/60 (95%)   | 46 (81%)  | 7 (12%)  | 4 (7%)   | 1           | 5  |
| 51  | B6    | 43/54 (80%)   | 24 (56%)  | 14 (33%) | 5 (12%)  | 0           | 1  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers  | Percentiles |     |
|-----|-------|-------------------|------------|------------|-----------|-------------|-----|
| 51  | D6    | 43/54 (80%)       | 19 (44%)   | 13 (30%)   | 11 (26%)  | 0           | 0   |
| 52  | B7    | 47/49 (96%)       | 43 (92%)   | 4 (8%)     | 0         | 100         | 100 |
| 52  | D7    | 47/49 (96%)       | 45 (96%)   | 2 (4%)     | 0         | 100         | 100 |
| 53  | B8    | 59/65 (91%)       | 45 (76%)   | 8 (14%)    | 6 (10%)   | 0           | 3   |
| 53  | D8    | 59/65 (91%)       | 42 (71%)   | 8 (14%)    | 9 (15%)   | 0           | 0   |
| All | All   | 11341/12044 (94%) | 8521 (75%) | 1799 (16%) | 1021 (9%) | 0           | 3   |

5 of 1021 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AE    | 29  | ALA  |
| 2   | AE    | 30  | ARG  |
| 2   | AE    | 95  | GLN  |
| 2   | AE    | 101 | MET  |
| 2   | AE    | 208 | ILE  |

### 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   | AE    | 205/220 (93%)  | 163 (80%) | 42 (20%) | 1           | 5  |
| 2   | CE    | 205/220 (93%)  | 160 (78%) | 45 (22%) | 1           | 4  |
| 3   | AF    | 159/188 (85%)  | 140 (88%) | 19 (12%) | 5           | 21 |
| 3   | CF    | 160/188 (85%)  | 139 (87%) | 21 (13%) | 4           | 17 |
| 4   | AG    | 180/180 (100%) | 153 (85%) | 27 (15%) | 3           | 13 |
| 4   | CG    | 180/180 (100%) | 158 (88%) | 22 (12%) | 5           | 20 |
| 5   | AH    | 116/123 (94%)  | 98 (84%)  | 18 (16%) | 2           | 12 |
| 5   | CH    | 116/123 (94%)  | 102 (88%) | 14 (12%) | 5           | 20 |
| 6   | AI    | 90/90 (100%)   | 77 (86%)  | 13 (14%) | 3           | 14 |
| 6   | CI    | 90/90 (100%)   | 75 (83%)  | 15 (17%) | 2           | 10 |
| 7   | AJ    | 126/127 (99%)  | 103 (82%) | 23 (18%) | 2           | 8  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 7   | CJ    | 126/127 (99%)  | 107 (85%) | 19 (15%) | 3           | 13  |
| 8   | AK    | 119/119 (100%) | 103 (87%) | 16 (13%) | 4           | 17  |
| 8   | CK    | 119/119 (100%) | 103 (87%) | 16 (13%) | 4           | 17  |
| 9   | AL    | 98/99 (99%)    | 74 (76%)  | 24 (24%) | 1           | 3   |
| 9   | CL    | 98/99 (99%)    | 78 (80%)  | 20 (20%) | 1           | 5   |
| 10  | AM    | 89/92 (97%)    | 78 (88%)  | 11 (12%) | 4           | 19  |
| 10  | CM    | 89/92 (97%)    | 74 (83%)  | 15 (17%) | 2           | 10  |
| 11  | AN    | 90/99 (91%)    | 77 (86%)  | 13 (14%) | 3           | 14  |
| 11  | CN    | 90/99 (91%)    | 75 (83%)  | 15 (17%) | 2           | 10  |
| 12  | AO    | 104/107 (97%)  | 88 (85%)  | 16 (15%) | 2           | 12  |
| 12  | CO    | 104/107 (97%)  | 91 (88%)  | 13 (12%) | 4           | 19  |
| 13  | AP    | 94/101 (93%)   | 86 (92%)  | 8 (8%)   | 10          | 35  |
| 13  | CP    | 94/101 (93%)   | 76 (81%)  | 18 (19%) | 1           | 7   |
| 14  | AQ    | 49/50 (98%)    | 38 (78%)  | 11 (22%) | 1           | 4   |
| 14  | CQ    | 49/50 (98%)    | 41 (84%)  | 8 (16%)  | 2           | 11  |
| 15  | AR    | 79/80 (99%)    | 68 (86%)  | 11 (14%) | 3           | 15  |
| 15  | CR    | 79/80 (99%)    | 72 (91%)  | 7 (9%)   | 9           | 33  |
| 16  | AS    | 72/74 (97%)    | 56 (78%)  | 16 (22%) | 1           | 4   |
| 16  | CS    | 72/74 (97%)    | 61 (85%)  | 11 (15%) | 3           | 12  |
| 17  | AT    | 95/97 (98%)    | 83 (87%)  | 12 (13%) | 4           | 19  |
| 17  | CT    | 95/97 (98%)    | 86 (90%)  | 9 (10%)  | 8           | 30  |
| 18  | AU    | 63/77 (82%)    | 54 (86%)  | 9 (14%)  | 3           | 14  |
| 18  | CU    | 63/77 (82%)    | 58 (92%)  | 5 (8%)   | 11          | 37  |
| 19  | AV    | 72/80 (90%)    | 55 (76%)  | 17 (24%) | 1           | 3   |
| 19  | CV    | 67/80 (84%)    | 52 (78%)  | 15 (22%) | 1           | 4   |
| 20  | AW    | 76/82 (93%)    | 64 (84%)  | 12 (16%) | 2           | 12  |
| 20  | CW    | 76/82 (93%)    | 67 (88%)  | 9 (12%)  | 5           | 21  |
| 21  | AX    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 21  | CX    | 20/22 (91%)    | 19 (95%)  | 1 (5%)   | 22          | 53  |
| 26  | BD    | 214/218 (98%)  | 175 (82%) | 39 (18%) | 2           | 8   |
| 26  | DD    | 214/218 (98%)  | 181 (85%) | 33 (15%) | 2           | 12  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 27  | BE    | 165/166 (99%)  | 139 (84%) | 26 (16%) | 2           | 12 |
| 27  | DE    | 165/166 (99%)  | 140 (85%) | 25 (15%) | 3           | 13 |
| 28  | BF    | 161/166 (97%)  | 139 (86%) | 22 (14%) | 3           | 15 |
| 28  | DF    | 165/166 (99%)  | 134 (81%) | 31 (19%) | 1           | 7  |
| 29  | BG    | 155/156 (99%)  | 136 (88%) | 19 (12%) | 4           | 20 |
| 29  | DG    | 155/156 (99%)  | 122 (79%) | 33 (21%) | 1           | 5  |
| 30  | BH    | 142/148 (96%)  | 119 (84%) | 23 (16%) | 2           | 11 |
| 30  | DH    | 142/148 (96%)  | 105 (74%) | 37 (26%) | 0           | 2  |
| 31  | BK    | 122/124 (98%)  | 100 (82%) | 22 (18%) | 2           | 8  |
| 31  | DK    | 122/124 (98%)  | 90 (74%)  | 32 (26%) | 0           | 2  |
| 32  | BM    | 117/119 (98%)  | 92 (79%)  | 25 (21%) | 1           | 5  |
| 32  | DM    | 117/119 (98%)  | 96 (82%)  | 21 (18%) | 2           | 9  |
| 33  | BN    | 100/100 (100%) | 84 (84%)  | 16 (16%) | 2           | 12 |
| 33  | DN    | 100/100 (100%) | 87 (87%)  | 13 (13%) | 4           | 18 |
| 34  | BO    | 116/116 (100%) | 88 (76%)  | 28 (24%) | 1           | 3  |
| 34  | DO    | 116/116 (100%) | 83 (72%)  | 33 (28%) | 0           | 1  |
| 35  | BP    | 111/111 (100%) | 99 (89%)  | 12 (11%) | 6           | 25 |
| 35  | DP    | 111/111 (100%) | 96 (86%)  | 15 (14%) | 4           | 16 |
| 36  | B0    | 101/101 (100%) | 81 (80%)  | 20 (20%) | 1           | 6  |
| 36  | D0    | 100/101 (99%)  | 87 (87%)  | 13 (13%) | 4           | 18 |
| 37  | BQ    | 87/88 (99%)    | 68 (78%)  | 19 (22%) | 1           | 5  |
| 37  | DQ    | 87/88 (99%)    | 69 (79%)  | 18 (21%) | 1           | 5  |
| 38  | BR    | 120/127 (94%)  | 99 (82%)  | 21 (18%) | 2           | 9  |
| 38  | DR    | 120/127 (94%)  | 99 (82%)  | 21 (18%) | 2           | 9  |
| 39  | B1    | 93/94 (99%)    | 78 (84%)  | 15 (16%) | 2           | 11 |
| 39  | D1    | 93/94 (99%)    | 81 (87%)  | 12 (13%) | 4           | 18 |
| 40  | B2    | 82/82 (100%)   | 62 (76%)  | 20 (24%) | 1           | 3  |
| 40  | D2    | 82/82 (100%)   | 60 (73%)  | 22 (27%) | 0           | 2  |
| 41  | BS    | 92/92 (100%)   | 77 (84%)  | 15 (16%) | 2           | 11 |
| 41  | DS    | 92/92 (100%)   | 78 (85%)  | 14 (15%) | 3           | 13 |
| 42  | BT    | 74/78 (95%)    | 58 (78%)  | 16 (22%) | 1           | 5  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 42  | DT    | 74/78 (95%)     | 64 (86%)   | 10 (14%)   | 4           | 16 |
| 43  | BU    | 85/91 (93%)     | 60 (71%)   | 25 (29%)   | 0           | 1  |
| 43  | DU    | 85/91 (93%)     | 61 (72%)   | 24 (28%)   | 0           | 1  |
| 44  | BV    | 154/179 (86%)   | 123 (80%)  | 31 (20%)   | 1           | 5  |
| 44  | DV    | 158/179 (88%)   | 132 (84%)  | 26 (16%)   | 2           | 11 |
| 45  | B3    | 61/67 (91%)     | 53 (87%)   | 8 (13%)    | 4           | 17 |
| 45  | D3    | 62/67 (92%)     | 56 (90%)   | 6 (10%)    | 8           | 30 |
| 46  | BZ    | 82/83 (99%)     | 68 (83%)   | 14 (17%)   | 2           | 10 |
| 46  | DZ    | 82/83 (99%)     | 71 (87%)   | 11 (13%)   | 4           | 17 |
| 47  | BW    | 62/67 (92%)     | 53 (86%)   | 9 (14%)    | 3           | 14 |
| 47  | DW    | 64/67 (96%)     | 58 (91%)   | 6 (9%)     | 8           | 31 |
| 48  | BX    | 51/52 (98%)     | 42 (82%)   | 9 (18%)    | 2           | 9  |
| 48  | DX    | 51/52 (98%)     | 43 (84%)   | 8 (16%)    | 2           | 12 |
| 49  | B4    | 59/63 (94%)     | 42 (71%)   | 17 (29%)   | 0           | 1  |
| 49  | D4    | 57/63 (90%)     | 36 (63%)   | 21 (37%)   | 0           | 0  |
| 50  | B5    | 51/52 (98%)     | 42 (82%)   | 9 (18%)    | 2           | 9  |
| 50  | D5    | 51/52 (98%)     | 43 (84%)   | 8 (16%)    | 2           | 12 |
| 51  | B6    | 44/52 (85%)     | 33 (75%)   | 11 (25%)   | 0           | 2  |
| 51  | D6    | 44/52 (85%)     | 28 (64%)   | 16 (36%)   | 0           | 0  |
| 52  | B7    | 42/42 (100%)    | 36 (86%)   | 6 (14%)    | 3           | 14 |
| 52  | D7    | 42/42 (100%)    | 32 (76%)   | 10 (24%)   | 1           | 3  |
| 53  | B8    | 51/55 (93%)     | 40 (78%)   | 11 (22%)   | 1           | 5  |
| 53  | D8    | 51/55 (93%)     | 40 (78%)   | 11 (22%)   | 1           | 5  |
| All | All   | 9584/9992 (96%) | 7930 (83%) | 1654 (17%) | 2           | 9  |

5 of 1654 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CH    | 120 | THR  |
| 26  | DD    | 157 | ARG  |
| 49  | D4    | 32  | TYR  |
| 7   | CJ    | 63  | LYS  |
| 5   | CH    | 107 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DD    | 143 | HIS  |
| 39  | D1    | 66  | ASN  |
| 27  | DE    | 55  | ASN  |
| 29  | DG    | 41  | GLN  |
| 41  | DS    | 34  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed         | Backbone Outliers | Pucker Outliers |
|-----|-------|------------------|-------------------|-----------------|
| 1   | AA    | 1506/1506 (100%) | 316 (20%)         | 26 (1%)         |
| 1   | CA    | 1505/1506 (99%)  | 312 (20%)         | 30 (1%)         |
| 22  | AC    | 76/77 (98%)      | 8 (10%)           | 1 (1%)          |
| 22  | AD    | 76/77 (98%)      | 24 (31%)          | 1 (1%)          |
| 22  | CC    | 77/77 (100%)     | 12 (15%)          | 1 (1%)          |
| 22  | CD    | 76/77 (98%)      | 45 (59%)          | 5 (6%)          |
| 23  | A1    | 5/6 (83%)        | 1 (20%)           | 0               |
| 23  | C1    | 5/6 (83%)        | 1 (20%)           | 0               |
| 24  | BA    | 2911/2912 (99%)  | 594 (20%)         | 44 (1%)         |
| 24  | DA    | 2904/2912 (99%)  | 646 (22%)         | 39 (1%)         |
| 25  | BB    | 121/122 (99%)    | 27 (22%)          | 0               |
| 25  | DB    | 121/122 (99%)    | 32 (26%)          | 0               |
| All | All   | 9383/9400 (99%)  | 2018 (21%)        | 147 (1%)        |

5 of 2018 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 6   | G    |
| 1   | AA    | 8   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 31  | G    |
| 1   | AA    | 32  | A    |

5 of 147 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | DA    | 752  | A    |
| 24  | DA    | 2747 | G    |
| 24  | DA    | 1022 | G    |
| 24  | DA    | 1912 | A    |
| 24  | BA    | 1379 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1692 ligands modelled in this entry, 1690 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 | $\# Z  > 2$ |
| 55  | T1C  | AA    | 1837 | 54   | 45,45,45     | 0.95 | 5 (11%)     | 56,72,72    | 1.88 | 11 (19%)    |
| 55  | T1C  | CA    | 1800 | 54   | 45,45,45     | 0.98 | 5 (11%)     | 56,72,72    | 1.62 | 11 (19%)    |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 55  | T1C  | AA    | 1837 | 54   | -       | 7/22/80/80 | 0/4/4/4 |
| 55  | T1C  | CA    | 1800 | 54   | -       | 9/22/80/80 | 0/4/4/4 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | CA    | 1800 | T1C  | C9-N9   | -2.61 | 1.36        | 1.41     |
| 55  | AA    | 1837 | T1C  | C1C-C12 | 2.55  | 1.54        | 1.52     |
| 55  | AA    | 1837 | T1C  | C9-N9   | -2.53 | 1.36        | 1.41     |
| 55  | AA    | 1837 | T1C  | C1C-C1  | -2.41 | 1.51        | 1.55     |
| 55  | CA    | 1800 | T1C  | C1B-C12 | -2.37 | 1.33        | 1.36     |

The worst 5 of 22 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | AA    | 1837 | T1C  | C41-C1C-C1  | -6.62 | 103.46      | 111.05   |
| 55  | AA    | 1837 | T1C  | O12-C12-C1C | 4.82  | 120.35      | 113.37   |
| 55  | AA    | 1837 | T1C  | C11-C1B-C12 | 4.29  | 122.19      | 118.80   |
| 55  | CA    | 1800 | T1C  | C1-C1C-C12  | 4.12  | 114.71      | 109.88   |
| 55  | CA    | 1800 | T1C  | O12-C12-C1C | 4.06  | 119.25      | 113.37   |

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

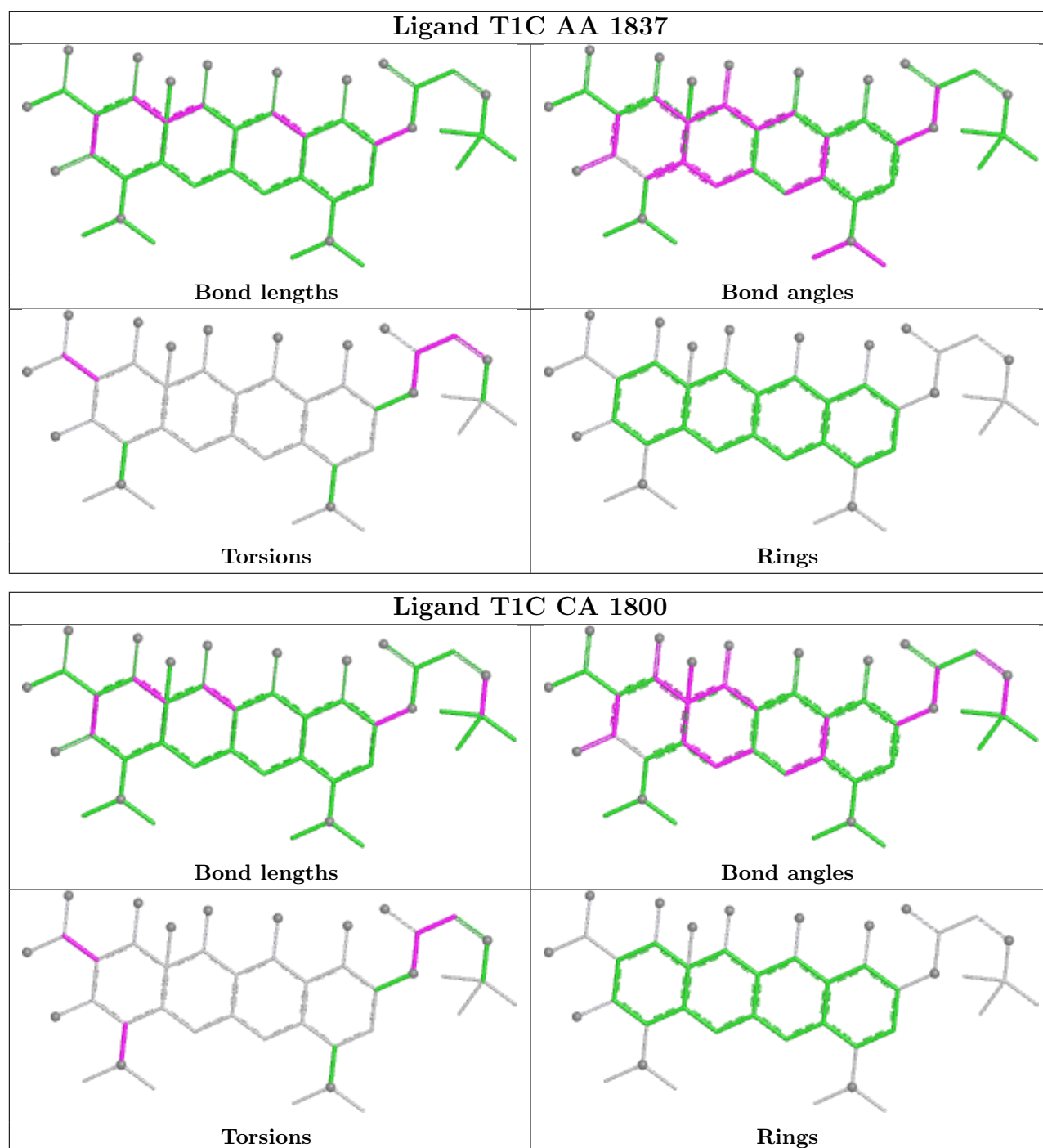
| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 55  | AA    | 1837 | T1C  | C92-C91-N9-C9 |
| 55  | AA    | 1837 | T1C  | O91-C91-N9-C9 |
| 55  | CA    | 1800 | T1C  | C92-C91-N9-C9 |
| 55  | CA    | 1800 | T1C  | O91-C91-N9-C9 |
| 55  | CA    | 1800 | T1C  | C41-C4-N4-C42 |

There are no ring outliers.

2 monomers are involved in 7 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55  | AA    | 1837 | T1C  | 2       | 0            |
| 55  | CA    | 1800 | T1C  | 5       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1506/1506 (100%) | -0.42  | 8 (0%) 87 73  | 66, 112, 190, 248     | 0     |
| 1   | CA    | 1506/1506 (100%) | -0.43  | 4 (0%) 90 80  | 76, 117, 189, 249     | 0     |
| 2   | AE    | 237/256 (92%)    | -0.00  | 0 100 100     | 116, 147, 183, 192    | 0     |
| 2   | CE    | 237/256 (92%)    | -0.00  | 4 (1%) 69 48  | 126, 162, 192, 208    | 0     |
| 3   | AF    | 205/239 (85%)    | 0.34   | 5 (2%) 59 38  | 99, 124, 157, 164     | 0     |
| 3   | CF    | 206/239 (86%)    | 0.36   | 8 (3%) 43 24  | 121, 145, 174, 184    | 0     |
| 4   | AG    | 208/208 (100%)   | 0.44   | 10 (4%) 35 19 | 95, 118, 140, 145     | 0     |
| 4   | CG    | 208/208 (100%)   | 0.45   | 9 (4%) 40 22  | 93, 113, 133, 142     | 0     |
| 5   | AH    | 151/162 (93%)    | 0.14   | 2 (1%) 75 56  | 90, 110, 132, 163     | 0     |
| 5   | CH    | 151/162 (93%)    | 0.13   | 0 100 100     | 97, 117, 139, 165     | 0     |
| 6   | AI    | 101/101 (100%)   | 0.03   | 1 (0%) 79 61  | 91, 112, 125, 144     | 0     |
| 6   | CI    | 101/101 (100%)   | -0.22  | 0 100 100     | 90, 107, 128, 148     | 0     |
| 7   | AJ    | 155/156 (99%)    | 0.24   | 9 (5%) 29 16  | 111, 129, 157, 167    | 0     |
| 7   | CJ    | 155/156 (99%)    | 0.26   | 4 (2%) 57 36  | 116, 133, 162, 173    | 0     |
| 8   | AK    | 138/138 (100%)   | 0.20   | 4 (2%) 53 32  | 97, 117, 127, 137     | 0     |
| 8   | CK    | 138/138 (100%)   | -0.09  | 0 100 100     | 105, 122, 135, 143    | 0     |
| 9   | AL    | 127/128 (99%)    | 0.13   | 9 (7%) 22 12  | 100, 144, 163, 167    | 0     |
| 9   | CL    | 127/128 (99%)    | 0.28   | 7 (5%) 30 16  | 114, 155, 170, 176    | 0     |
| 10  | AM    | 99/105 (94%)     | 0.38   | 6 (6%) 27 15  | 100, 146, 171, 175    | 0     |
| 10  | CM    | 99/105 (94%)     | 0.15   | 1 (1%) 79 61  | 117, 159, 174, 180    | 0     |
| 11  | AN    | 119/129 (92%)    | 0.45   | 5 (4%) 40 22  | 83, 108, 138, 168     | 0     |
| 11  | CN    | 119/129 (92%)    | 0.33   | 6 (5%) 34 18  | 91, 112, 138, 163     | 0     |
| 12  | AO    | 125/128 (97%)    | 0.41   | 7 (5%) 30 16  | 78, 92, 116, 168      | 0     |
| 12  | CO    | 125/128 (97%)    | 0.43   | 13 (10%) 11 6 | 84, 104, 129, 170     | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 13  | AP    | 116/126 (92%)    | 0.22   | 3 (2%) 57 36  | 100, 133, 147, 157    | 0     |
| 13  | CP    | 117/126 (92%)    | 0.26   | 3 (2%) 57 36  | 121, 155, 170, 177    | 0     |
| 14  | AQ    | 60/61 (98%)      | 0.47   | 3 (5%) 34 18  | 103, 114, 127, 135    | 0     |
| 14  | CQ    | 60/61 (98%)      | 0.57   | 1 (1%) 69 48  | 130, 139, 155, 162    | 0     |
| 15  | AR    | 88/89 (98%)      | 0.01   | 0 100 100     | 89, 108, 124, 127     | 0     |
| 15  | CR    | 88/89 (98%)      | -0.01  | 0 100 100     | 89, 113, 131, 136     | 0     |
| 16  | AS    | 84/88 (95%)      | 0.31   | 0 100 100     | 107, 122, 145, 171    | 0     |
| 16  | CS    | 84/88 (95%)      | -0.01  | 1 (1%) 76 58  | 91, 107, 126, 167     | 0     |
| 17  | AT    | 100/105 (95%)    | 0.25   | 3 (3%) 52 31  | 96, 114, 126, 133     | 0     |
| 17  | CT    | 100/105 (95%)    | 0.54   | 7 (7%) 22 12  | 91, 111, 128, 149     | 0     |
| 18  | AU    | 72/88 (81%)      | -0.01  | 2 (2%) 55 34  | 95, 112, 141, 169     | 0     |
| 18  | CU    | 72/88 (81%)      | -0.13  | 1 (1%) 73 53  | 96, 117, 152, 173     | 0     |
| 19  | AV    | 83/93 (89%)      | 0.03   | 4 (4%) 35 19  | 115, 136, 151, 157    | 0     |
| 19  | CV    | 78/93 (83%)      | 0.34   | 4 (5%) 33 18  | 135, 166, 181, 188    | 0     |
| 20  | AW    | 99/106 (93%)     | 0.10   | 0 100 100     | 111, 127, 157, 162    | 0     |
| 20  | CW    | 99/106 (93%)     | -0.12  | 1 (1%) 79 61  | 91, 116, 148, 165     | 0     |
| 21  | AX    | 25/27 (92%)      | 0.18   | 0 100 100     | 111, 120, 140, 160    | 0     |
| 21  | CX    | 25/27 (92%)      | 0.61   | 2 (8%) 18 10  | 117, 138, 154, 170    | 0     |
| 22  | AC    | 77/77 (100%)     | -0.21  | 1 (1%) 75 56  | 77, 100, 135, 151     | 0     |
| 22  | AD    | 77/77 (100%)     | 0.18   | 2 (2%) 57 36  | 93, 214, 228, 234     | 0     |
| 22  | CC    | 77/77 (100%)     | -0.32  | 1 (1%) 75 56  | 80, 118, 151, 171     | 0     |
| 22  | CD    | 77/77 (100%)     | 0.48   | 4 (5%) 33 17  | 93, 220, 238, 248     | 0     |
| 23  | A1    | 6/6 (100%)       | 0.63   | 2 (33%) 1 0   | 85, 89, 129, 143      | 0     |
| 23  | C1    | 6/6 (100%)       | 0.88   | 1 (16%) 4 2   | 103, 111, 138, 153    | 0     |
| 24  | BA    | 2912/2912 (100%) | -0.62  | 17 (0%) 85 70 | 53, 82, 212, 247      | 0     |
| 24  | DA    | 2906/2912 (99%)  | -0.54  | 12 (0%) 88 76 | 60, 90, 232, 251      | 0     |
| 25  | BB    | 122/122 (100%)   | -0.56  | 0 100 100     | 78, 106, 126, 184     | 0     |
| 25  | DB    | 122/122 (100%)   | -0.40  | 0 100 100     | 91, 127, 154, 200     | 0     |
| 26  | BD    | 272/276 (98%)    | 0.04   | 2 (0%) 84 68  | 55, 75, 94, 102       | 0     |
| 26  | DD    | 272/276 (98%)    | 0.12   | 11 (4%) 42 23 | 58, 81, 99, 122       | 0     |
| 27  | BE    | 205/206 (99%)    | 0.28   | 5 (2%) 59 38  | 60, 92, 135, 153      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27  | DE    | 205/206 (99%)  | 0.54   | 20 (9%) 13 7  | 60, 97, 142, 165      | 0     |
| 28  | BF    | 202/210 (96%)  | -0.20  | 1 (0%) 87 73  | 54, 84, 118, 133      | 0     |
| 28  | DF    | 208/210 (99%)  | 0.14   | 6 (2%) 53 32  | 66, 102, 156, 182     | 0     |
| 29  | BG    | 181/182 (99%)  | 0.09   | 2 (1%) 78 59  | 95, 116, 145, 154     | 0     |
| 29  | DG    | 181/182 (99%)  | 0.31   | 7 (3%) 43 24  | 117, 141, 165, 177    | 0     |
| 30  | BH    | 170/180 (94%)  | 0.06   | 2 (1%) 76 58  | 88, 113, 132, 151     | 0     |
| 30  | DH    | 170/180 (94%)  | 0.73   | 13 (7%) 20 11 | 146, 200, 223, 235    | 0     |
| 31  | BK    | 146/148 (98%)  | -0.13  | 0 100 100     | 87, 129, 146, 151     | 0     |
| 31  | DK    | 146/148 (98%)  | 0.14   | 7 (4%) 35 19  | 88, 132, 151, 159     | 0     |
| 32  | BM    | 138/140 (98%)  | 0.56   | 10 (7%) 21 11 | 78, 93, 128, 145      | 0     |
| 32  | DM    | 138/140 (98%)  | 0.04   | 2 (1%) 73 53  | 80, 107, 137, 157     | 0     |
| 33  | BN    | 122/122 (100%) | 0.26   | 3 (2%) 58 37  | 69, 87, 102, 112      | 0     |
| 33  | DN    | 122/122 (100%) | 0.22   | 2 (1%) 70 49  | 70, 91, 109, 116      | 0     |
| 34  | BO    | 150/150 (100%) | 0.59   | 15 (10%) 12 6 | 60, 91, 114, 167      | 0     |
| 34  | DO    | 150/150 (100%) | 0.55   | 19 (12%) 8 4  | 66, 105, 140, 179     | 0     |
| 35  | BP    | 141/141 (100%) | 0.16   | 3 (2%) 63 42  | 68, 91, 113, 135      | 0     |
| 35  | DP    | 141/141 (100%) | 0.44   | 5 (3%) 47 27  | 80, 106, 130, 152     | 0     |
| 36  | B0    | 118/118 (100%) | 0.13   | 5 (4%) 40 22  | 72, 89, 104, 118      | 0     |
| 36  | D0    | 117/118 (99%)  | 0.11   | 0 100 100     | 71, 89, 108, 119      | 0     |
| 37  | BQ    | 111/112 (99%)  | 0.17   | 4 (3%) 46 26  | 85, 104, 127, 137     | 0     |
| 37  | DQ    | 111/112 (99%)  | 0.08   | 1 (0%) 81 63  | 98, 121, 142, 151     | 0     |
| 38  | BR    | 137/146 (93%)  | 0.67   | 8 (5%) 29 16  | 80, 102, 150, 169     | 0     |
| 38  | DR    | 137/146 (93%)  | 0.23   | 3 (2%) 62 41  | 80, 99, 159, 185      | 0     |
| 39  | B1    | 117/118 (99%)  | 0.13   | 2 (1%) 69 48  | 63, 83, 112, 138      | 0     |
| 39  | D1    | 117/118 (99%)  | -0.26  | 0 100 100     | 72, 101, 136, 154     | 0     |
| 40  | B2    | 101/101 (100%) | 0.21   | 1 (0%) 79 61  | 64, 102, 126, 145     | 0     |
| 40  | D2    | 101/101 (100%) | 0.18   | 3 (2%) 52 31  | 71, 123, 139, 148     | 0     |
| 41  | BS    | 113/113 (100%) | -0.04  | 2 (1%) 67 47  | 63, 80, 110, 161      | 0     |
| 41  | DS    | 113/113 (100%) | 0.12   | 2 (1%) 67 47  | 68, 83, 113, 161      | 0     |
| 42  | BT    | 92/96 (95%)    | 0.14   | 2 (2%) 62 41  | 64, 78, 100, 111      | 0     |
| 42  | DT    | 92/96 (95%)    | 0.21   | 7 (7%) 20 11  | 77, 94, 118, 128      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 43  | BU    | 102/110 (92%)     | 0.50   | 10 (9%) 13 7   | 75, 99, 149, 163      | 0     |
| 43  | DU    | 102/110 (92%)     | 1.27   | 21 (20%) 2 1   | 93, 118, 160, 182     | 0     |
| 44  | BV    | 175/206 (84%)     | 0.43   | 10 (5%) 29 16  | 97, 131, 195, 201     | 0     |
| 44  | DV    | 179/206 (86%)     | 0.53   | 2 (1%) 78 59   | 118, 157, 213, 219    | 0     |
| 45  | B3    | 76/85 (89%)       | 0.21   | 2 (2%) 57 36   | 69, 85, 101, 140      | 0     |
| 45  | D3    | 77/85 (90%)       | 0.20   | 3 (3%) 43 24   | 74, 95, 111, 151      | 0     |
| 46  | BZ    | 97/98 (98%)       | 0.32   | 8 (8%) 17 10   | 65, 85, 132, 164      | 0     |
| 46  | DZ    | 97/98 (98%)       | 0.82   | 12 (12%) 8 5   | 67, 91, 135, 157      | 0     |
| 47  | BW    | 66/72 (91%)       | 0.48   | 5 (7%) 20 11   | 70, 87, 108, 132      | 0     |
| 47  | DW    | 69/72 (95%)       | 0.00   | 3 (4%) 40 22   | 90, 112, 133, 164     | 0     |
| 48  | BX    | 59/60 (98%)       | 0.14   | 1 (1%) 69 48   | 73, 86, 121, 137      | 0     |
| 48  | DX    | 59/60 (98%)       | 0.16   | 1 (1%) 69 48   | 79, 102, 144, 162     | 0     |
| 49  | B4    | 66/71 (92%)       | 0.20   | 2 (3%) 52 31   | 122, 158, 180, 186    | 0     |
| 49  | D4    | 63/71 (88%)       | 0.46   | 4 (6%) 26 14   | 154, 187, 197, 205    | 0     |
| 50  | B5    | 59/60 (98%)       | 0.62   | 6 (10%) 12 6   | 57, 90, 166, 172      | 0     |
| 50  | D5    | 59/60 (98%)       | 0.48   | 6 (10%) 12 6   | 68, 91, 178, 192      | 0     |
| 51  | B6    | 45/54 (83%)       | 1.30   | 6 (13%) 7 4    | 128, 153, 163, 164    | 0     |
| 51  | D6    | 45/54 (83%)       | 1.78   | 15 (33%) 1 0   | 138, 164, 181, 183    | 0     |
| 52  | B7    | 49/49 (100%)      | 0.07   | 2 (4%) 41 23   | 55, 61, 92, 120       | 0     |
| 52  | D7    | 49/49 (100%)      | 0.37   | 2 (4%) 41 23   | 63, 70, 107, 130      | 0     |
| 53  | B8    | 61/65 (93%)       | 0.77   | 8 (13%) 7 4    | 66, 81, 98, 124       | 0     |
| 53  | D8    | 61/65 (93%)       | 0.99   | 12 (19%) 3 1   | 73, 87, 106, 121      | 0     |
| All | All   | 20927/21444 (97%) | -0.09  | 513 (2%) 58 37 | 53, 106, 186, 251     | 0     |

The worst 5 of 513 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | DO    | 62   | LEU  | 8.8  |
| 11  | AN    | 127  | LYS  | 8.6  |
| 17  | CT    | 101  | ARG  | 8.2  |
| 24  | BA    | 2899 | G    | 6.9  |
| 11  | AN    | 128  | ALA  | 6.2  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3301 | 1/1   | -0.12 | 0.15 | 140,140,140,140             | 0     |
| 54  | MG   | AA    | 1785 | 1/1   | 0.06  | 0.20 | 146,146,146,146             | 0     |
| 54  | MG   | AA    | 1673 | 1/1   | 0.27  | 0.18 | 131,131,131,131             | 0     |
| 54  | MG   | CA    | 1765 | 1/1   | 0.27  | 0.16 | 122,122,122,122             | 0     |
| 54  | MG   | AA    | 1782 | 1/1   | 0.27  | 0.28 | 124,124,124,124             | 0     |
| 54  | MG   | AA    | 1739 | 1/1   | 0.29  | 0.12 | 191,191,191,191             | 0     |
| 54  | MG   | CA    | 1622 | 1/1   | 0.30  | 0.46 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3427 | 1/1   | 0.31  | 0.12 | 160,160,160,160             | 0     |
| 54  | MG   | CA    | 1705 | 1/1   | 0.31  | 0.13 | 135,135,135,135             | 0     |
| 54  | MG   | AA    | 1773 | 1/1   | 0.32  | 0.21 | 125,125,125,125             | 0     |
| 54  | MG   | CA    | 1787 | 1/1   | 0.32  | 0.30 | 136,136,136,136             | 0     |
| 54  | MG   | BA    | 3597 | 1/1   | 0.32  | 0.20 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3444 | 1/1   | 0.32  | 0.12 | 133,133,133,133             | 0     |
| 54  | MG   | AA    | 1629 | 1/1   | 0.33  | 0.15 | 134,134,134,134             | 0     |
| 54  | MG   | AA    | 1827 | 1/1   | 0.33  | 0.17 | 112,112,112,112             | 0     |
| 54  | MG   | BB    | 209  | 1/1   | 0.33  | 0.13 | 112,112,112,112             | 0     |
| 54  | MG   | DB    | 207  | 1/1   | 0.33  | 0.25 | 133,133,133,133             | 0     |
| 54  | MG   | CA    | 1739 | 1/1   | 0.35  | 0.28 | 120,120,120,120             | 0     |
| 54  | MG   | AA    | 1749 | 1/1   | 0.35  | 0.16 | 130,130,130,130             | 0     |
| 54  | MG   | AA    | 1769 | 1/1   | 0.36  | 0.18 | 122,122,122,122             | 0     |
| 54  | MG   | AA    | 1786 | 1/1   | 0.37  | 0.14 | 145,145,145,145             | 0     |
| 54  | MG   | AA    | 1675 | 1/1   | 0.37  | 0.36 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3296 | 1/1   | 0.37  | 0.24 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3399 | 1/1   | 0.38  | 0.15 | 103,103,103,103             | 0     |
| 54  | MG   | DB    | 206  | 1/1   | 0.39  | 0.33 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1664 | 1/1   | 0.39  | 0.17 | 169,169,169,169             | 0     |
| 54  | MG   | CA    | 1781 | 1/1   | 0.40  | 0.21 | 148,148,148,148             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3308 | 1/1   | 0.41 | 0.24 | 108,108,108,108             | 0     |
| 54  | MG   | CC    | 108  | 1/1   | 0.42 | 0.15 | 120,120,120,120             | 0     |
| 54  | MG   | AA    | 1614 | 1/1   | 0.43 | 0.16 | 132,132,132,132             | 0     |
| 54  | MG   | CA    | 1658 | 1/1   | 0.44 | 0.26 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3348 | 1/1   | 0.44 | 0.12 | 140,140,140,140             | 0     |
| 54  | MG   | CA    | 1722 | 1/1   | 0.45 | 0.36 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1653 | 1/1   | 0.46 | 0.17 | 124,124,124,124             | 0     |
| 54  | MG   | DA    | 3038 | 1/1   | 0.46 | 0.26 | 119,119,119,119             | 0     |
| 54  | MG   | BA    | 3352 | 1/1   | 0.47 | 0.24 | 112,112,112,112             | 0     |
| 54  | MG   | AC    | 105  | 1/1   | 0.47 | 0.21 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3088 | 1/1   | 0.49 | 0.28 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1625 | 1/1   | 0.50 | 0.21 | 115,115,115,115             | 0     |
| 54  | MG   | DA    | 3406 | 1/1   | 0.50 | 0.27 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3293 | 1/1   | 0.50 | 0.23 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1818 | 1/1   | 0.50 | 0.37 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3338 | 1/1   | 0.50 | 0.33 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1748 | 1/1   | 0.51 | 0.20 | 110,110,110,110             | 0     |
| 54  | MG   | AA    | 1637 | 1/1   | 0.51 | 0.20 | 122,122,122,122             | 0     |
| 54  | MG   | CA    | 1642 | 1/1   | 0.51 | 0.26 | 116,116,116,116             | 0     |
| 54  | MG   | DA    | 3289 | 1/1   | 0.52 | 0.26 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3288 | 1/1   | 0.52 | 0.24 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 3056 | 1/1   | 0.52 | 0.35 | 109,109,109,109             | 0     |
| 54  | MG   | CA    | 1700 | 1/1   | 0.53 | 0.15 | 133,133,133,133             | 0     |
| 54  | MG   | BA    | 3231 | 1/1   | 0.54 | 0.20 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3072 | 1/1   | 0.54 | 0.17 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1752 | 1/1   | 0.54 | 0.09 | 134,134,134,134             | 0     |
| 54  | MG   | AA    | 1682 | 1/1   | 0.54 | 0.25 | 103,103,103,103             | 0     |
| 54  | MG   | CL    | 201  | 1/1   | 0.55 | 0.46 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3435 | 1/1   | 0.55 | 0.31 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3405 | 1/1   | 0.56 | 0.12 | 153,153,153,153             | 0     |
| 54  | MG   | DA    | 3071 | 1/1   | 0.56 | 0.14 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1716 | 1/1   | 0.56 | 0.24 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3500 | 1/1   | 0.56 | 0.27 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3503 | 1/1   | 0.56 | 0.24 | 117,117,117,117             | 0     |
| 54  | MG   | AA    | 1756 | 1/1   | 0.56 | 0.17 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3117 | 1/1   | 0.57 | 0.19 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1713 | 1/1   | 0.57 | 0.21 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3149 | 1/1   | 0.57 | 0.14 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3040 | 1/1   | 0.57 | 0.24 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3274 | 1/1   | 0.58 | 0.32 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1617 | 1/1   | 0.58 | 0.29 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1764 | 1/1   | 0.58 | 0.24 | 111,111,111,111             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1741 | 1/1   | 0.58 | 0.19 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 3130 | 1/1   | 0.59 | 0.27 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3324 | 1/1   | 0.59 | 0.47 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1620 | 1/1   | 0.59 | 0.09 | 140,140,140,140             | 0     |
| 54  | MG   | AC    | 104  | 1/1   | 0.59 | 0.28 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3414 | 1/1   | 0.59 | 0.13 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1812 | 1/1   | 0.59 | 0.31 | 99,99,99,99                 | 0     |
| 54  | MG   | CA    | 1626 | 1/1   | 0.59 | 0.24 | 115,115,115,115             | 0     |
| 54  | MG   | DA    | 3460 | 1/1   | 0.59 | 0.09 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3495 | 1/1   | 0.59 | 0.17 | 125,125,125,125             | 0     |
| 54  | MG   | CA    | 1794 | 1/1   | 0.59 | 0.28 | 112,112,112,112             | 0     |
| 54  | MG   | CA    | 1714 | 1/1   | 0.59 | 0.12 | 161,161,161,161             | 0     |
| 54  | MG   | AA    | 1710 | 1/1   | 0.59 | 0.11 | 118,118,118,118             | 0     |
| 54  | MG   | AA    | 1789 | 1/1   | 0.60 | 0.34 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1646 | 1/1   | 0.60 | 0.30 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3370 | 1/1   | 0.60 | 0.31 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1724 | 1/1   | 0.60 | 0.24 | 126,126,126,126             | 0     |
| 54  | MG   | DA    | 3151 | 1/1   | 0.60 | 0.24 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3322 | 1/1   | 0.60 | 0.20 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3435 | 1/1   | 0.61 | 0.10 | 134,134,134,134             | 0     |
| 54  | MG   | DA    | 3442 | 1/1   | 0.61 | 0.28 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1724 | 1/1   | 0.61 | 0.30 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3278 | 1/1   | 0.61 | 0.24 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1682 | 1/1   | 0.61 | 0.30 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1753 | 1/1   | 0.61 | 0.41 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1761 | 1/1   | 0.61 | 0.24 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3067 | 1/1   | 0.61 | 0.49 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3430 | 1/1   | 0.62 | 0.25 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3315 | 1/1   | 0.62 | 0.28 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3036 | 1/1   | 0.62 | 0.30 | 114,114,114,114             | 0     |
| 54  | MG   | CA    | 1719 | 1/1   | 0.62 | 0.23 | 104,104,104,104             | 0     |
| 54  | MG   | AA    | 1808 | 1/1   | 0.62 | 0.23 | 125,125,125,125             | 0     |
| 54  | MG   | CA    | 1696 | 1/1   | 0.62 | 0.15 | 121,121,121,121             | 0     |
| 54  | MG   | CA    | 1732 | 1/1   | 0.62 | 0.26 | 108,108,108,108             | 0     |
| 54  | MG   | CX    | 101  | 1/1   | 0.62 | 0.27 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1624 | 1/1   | 0.62 | 0.16 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1772 | 1/1   | 0.63 | 0.12 | 128,128,128,128             | 0     |
| 54  | MG   | DA    | 3192 | 1/1   | 0.63 | 0.31 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3091 | 1/1   | 0.63 | 0.26 | 128,128,128,128             | 0     |
| 54  | MG   | BA    | 3280 | 1/1   | 0.63 | 0.07 | 106,106,106,106             | 0     |
| 54  | MG   | AD    | 101  | 1/1   | 0.63 | 0.24 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1823 | 1/1   | 0.63 | 0.11 | 151,151,151,151             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DB    | 215  | 1/1   | 0.63 | 0.13 | 120,120,120,120             | 0     |
| 54  | MG   | DA    | 3348 | 1/1   | 0.64 | 0.34 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3566 | 1/1   | 0.64 | 0.45 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3373 | 1/1   | 0.64 | 0.34 | 107,107,107,107             | 0     |
| 54  | MG   | BA    | 3180 | 1/1   | 0.64 | 0.39 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3118 | 1/1   | 0.64 | 0.34 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1654 | 1/1   | 0.64 | 0.30 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3077 | 1/1   | 0.64 | 0.25 | 110,110,110,110             | 0     |
| 54  | MG   | AA    | 1612 | 1/1   | 0.64 | 0.12 | 131,131,131,131             | 0     |
| 54  | MG   | DA    | 3138 | 1/1   | 0.65 | 0.15 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3358 | 1/1   | 0.65 | 0.23 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3468 | 1/1   | 0.65 | 0.25 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3418 | 1/1   | 0.65 | 0.30 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3466 | 1/1   | 0.65 | 0.17 | 123,123,123,123             | 0     |
| 54  | MG   | DA    | 3381 | 1/1   | 0.65 | 0.22 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3319 | 1/1   | 0.65 | 0.15 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3506 | 1/1   | 0.65 | 0.38 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3423 | 1/1   | 0.65 | 0.20 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3464 | 1/1   | 0.65 | 0.12 | 101,101,101,101             | 0     |
| 54  | MG   | CA    | 1746 | 1/1   | 0.65 | 0.43 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1773 | 1/1   | 0.66 | 0.25 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3362 | 1/1   | 0.66 | 0.32 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1785 | 1/1   | 0.66 | 0.21 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3443 | 1/1   | 0.66 | 0.14 | 116,116,116,116             | 0     |
| 54  | MG   | BB    | 213  | 1/1   | 0.66 | 0.16 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1603 | 1/1   | 0.66 | 0.40 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 3453 | 1/1   | 0.66 | 0.18 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3307 | 1/1   | 0.66 | 0.25 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1709 | 1/1   | 0.66 | 0.10 | 106,106,106,106             | 0     |
| 54  | MG   | CA    | 1629 | 1/1   | 0.66 | 0.18 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3287 | 1/1   | 0.66 | 0.18 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1776 | 1/1   | 0.66 | 0.26 | 102,102,102,102             | 0     |
| 54  | MG   | DB    | 209  | 1/1   | 0.66 | 0.14 | 97,97,97,97                 | 0     |
| 54  | MG   | DB    | 212  | 1/1   | 0.66 | 0.27 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1690 | 1/1   | 0.66 | 0.12 | 131,131,131,131             | 0     |
| 54  | MG   | DA    | 3345 | 1/1   | 0.67 | 0.30 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3493 | 1/1   | 0.67 | 0.38 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1709 | 1/1   | 0.67 | 0.10 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3360 | 1/1   | 0.67 | 0.34 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1732 | 1/1   | 0.67 | 0.24 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3341 | 1/1   | 0.67 | 0.29 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3145 | 1/1   | 0.67 | 0.19 | 86,86,86,86                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BB    | 214  | 1/1   | 0.67 | 0.17 | 99,99,99,99                 | 0     |
| 54  | MG   | CA    | 1725 | 1/1   | 0.68 | 0.22 | 115,115,115,115             | 0     |
| 54  | MG   | AA    | 1726 | 1/1   | 0.68 | 0.17 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1677 | 1/1   | 0.68 | 0.28 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3086 | 1/1   | 0.68 | 0.12 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3500 | 1/1   | 0.68 | 0.12 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1734 | 1/1   | 0.68 | 0.13 | 135,135,135,135             | 0     |
| 54  | MG   | DA    | 3459 | 1/1   | 0.68 | 0.30 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3121 | 1/1   | 0.68 | 0.27 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3522 | 1/1   | 0.68 | 0.19 | 100,100,100,100             | 0     |
| 54  | MG   | CC    | 107  | 1/1   | 0.68 | 0.24 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3149 | 1/1   | 0.68 | 0.21 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1736 | 1/1   | 0.68 | 0.26 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3520 | 1/1   | 0.68 | 0.27 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3167 | 1/1   | 0.68 | 0.45 | 105,105,105,105             | 0     |
| 54  | MG   | BA    | 3446 | 1/1   | 0.68 | 0.35 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3625 | 1/1   | 0.68 | 0.13 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1711 | 1/1   | 0.68 | 0.09 | 132,132,132,132             | 0     |
| 54  | MG   | BA    | 3227 | 1/1   | 0.68 | 0.27 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3432 | 1/1   | 0.69 | 0.19 | 102,102,102,102             | 0     |
| 54  | MG   | CC    | 109  | 1/1   | 0.69 | 0.22 | 111,111,111,111             | 0     |
| 54  | MG   | DA    | 3029 | 1/1   | 0.69 | 0.14 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1662 | 1/1   | 0.69 | 0.12 | 110,110,110,110             | 0     |
| 54  | MG   | AA    | 1828 | 1/1   | 0.69 | 0.20 | 107,107,107,107             | 0     |
| 54  | MG   | BA    | 3621 | 1/1   | 0.69 | 0.29 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3157 | 1/1   | 0.69 | 0.17 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3394 | 1/1   | 0.69 | 0.16 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3271 | 1/1   | 0.69 | 0.20 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3074 | 1/1   | 0.69 | 0.29 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1708 | 1/1   | 0.69 | 0.29 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3391 | 1/1   | 0.69 | 0.25 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1757 | 1/1   | 0.69 | 0.21 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1656 | 1/1   | 0.69 | 0.16 | 127,127,127,127             | 0     |
| 54  | MG   | BA    | 3196 | 1/1   | 0.69 | 0.16 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1715 | 1/1   | 0.69 | 0.38 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1608 | 1/1   | 0.70 | 0.32 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3446 | 1/1   | 0.70 | 0.25 | 99,99,99,99                 | 0     |
| 54  | MG   | CA    | 1628 | 1/1   | 0.70 | 0.09 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3608 | 1/1   | 0.70 | 0.16 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1676 | 1/1   | 0.70 | 0.20 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1706 | 1/1   | 0.70 | 0.21 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1731 | 1/1   | 0.70 | 0.19 | 97,97,97,97                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1697 | 1/1   | 0.70 | 0.29 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3507 | 1/1   | 0.70 | 0.09 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3250 | 1/1   | 0.70 | 0.19 | 105,105,105,105             | 0     |
| 54  | MG   | DB    | 205  | 1/1   | 0.70 | 0.31 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1655 | 1/1   | 0.70 | 0.38 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1703 | 1/1   | 0.70 | 0.37 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3434 | 1/1   | 0.70 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3357 | 1/1   | 0.70 | 0.16 | 123,123,123,123             | 0     |
| 54  | MG   | AA    | 1765 | 1/1   | 0.70 | 0.24 | 122,122,122,122             | 0     |
| 54  | MG   | DA    | 3024 | 1/1   | 0.71 | 0.20 | 110,110,110,110             | 0     |
| 54  | MG   | AC    | 106  | 1/1   | 0.71 | 0.18 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3134 | 1/1   | 0.71 | 0.19 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3509 | 1/1   | 0.71 | 0.11 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3331 | 1/1   | 0.71 | 0.21 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3382 | 1/1   | 0.71 | 0.39 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3403 | 1/1   | 0.71 | 0.14 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3452 | 1/1   | 0.71 | 0.28 | 95,95,95,95                 | 0     |
| 54  | MG   | CA    | 1649 | 1/1   | 0.71 | 0.31 | 88,88,88,88                 | 0     |
| 54  | MG   | CG    | 301  | 1/1   | 0.71 | 0.24 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3096 | 1/1   | 0.71 | 0.38 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1729 | 1/1   | 0.72 | 0.16 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3615 | 1/1   | 0.72 | 0.24 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3075 | 1/1   | 0.72 | 0.23 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1721 | 1/1   | 0.72 | 0.22 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3085 | 1/1   | 0.72 | 0.46 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3281 | 1/1   | 0.72 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3004 | 1/1   | 0.72 | 0.33 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1722 | 1/1   | 0.72 | 0.23 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3493 | 1/1   | 0.72 | 0.15 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1742 | 1/1   | 0.72 | 0.38 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3387 | 1/1   | 0.72 | 0.24 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1616 | 1/1   | 0.72 | 0.17 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1618 | 1/1   | 0.72 | 0.18 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3517 | 1/1   | 0.72 | 0.31 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1621 | 1/1   | 0.72 | 0.30 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3049 | 1/1   | 0.72 | 0.21 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3407 | 1/1   | 0.72 | 0.12 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3426 | 1/1   | 0.72 | 0.35 | 95,95,95,95                 | 0     |
| 54  | MG   | DB    | 208  | 1/1   | 0.72 | 0.27 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3065 | 1/1   | 0.72 | 0.29 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1754 | 1/1   | 0.72 | 0.27 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3245 | 1/1   | 0.72 | 0.23 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1705 | 1/1   | 0.73 | 0.14 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3284 | 1/1   | 0.73 | 0.27 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3456 | 1/1   | 0.73 | 0.14 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1639 | 1/1   | 0.73 | 0.30 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3629 | 1/1   | 0.73 | 0.21 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3123 | 1/1   | 0.73 | 0.38 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1610 | 1/1   | 0.73 | 0.18 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1801 | 1/1   | 0.73 | 0.10 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3141 | 1/1   | 0.73 | 0.28 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1725 | 1/1   | 0.73 | 0.24 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1760 | 1/1   | 0.73 | 0.30 | 109,109,109,109             | 0     |
| 54  | MG   | BB    | 215  | 1/1   | 0.73 | 0.14 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3410 | 1/1   | 0.73 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3335 | 1/1   | 0.73 | 0.31 | 91,91,91,91                 | 0     |
| 54  | MG   | B8    | 101  | 1/1   | 0.73 | 0.14 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3604 | 1/1   | 0.73 | 0.34 | 92,92,92,92                 | 0     |
| 54  | MG   | AG    | 301  | 1/1   | 0.73 | 0.10 | 122,122,122,122             | 0     |
| 54  | MG   | DA    | 3355 | 1/1   | 0.73 | 0.36 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1779 | 1/1   | 0.73 | 0.46 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3290 | 1/1   | 0.73 | 0.25 | 82,82,82,82                 | 0     |
| 54  | MG   | DE    | 302  | 1/1   | 0.73 | 0.15 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3330 | 1/1   | 0.74 | 0.29 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3426 | 1/1   | 0.74 | 0.34 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1797 | 1/1   | 0.74 | 0.30 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1751 | 1/1   | 0.74 | 0.23 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1693 | 1/1   | 0.74 | 0.17 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3346 | 1/1   | 0.74 | 0.21 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3442 | 1/1   | 0.74 | 0.20 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1755 | 1/1   | 0.74 | 0.25 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3605 | 1/1   | 0.74 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | AC    | 108  | 1/1   | 0.74 | 0.27 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3164 | 1/1   | 0.74 | 0.26 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1636 | 1/1   | 0.74 | 0.25 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3269 | 1/1   | 0.74 | 0.25 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3447 | 1/1   | 0.74 | 0.30 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3450 | 1/1   | 0.74 | 0.09 | 166,166,166,166             | 0     |
| 54  | MG   | BA    | 3451 | 1/1   | 0.74 | 0.27 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3368 | 1/1   | 0.74 | 0.13 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3375 | 1/1   | 0.74 | 0.37 | 99,99,99,99                 | 0     |
| 54  | MG   | AA    | 1719 | 1/1   | 0.74 | 0.20 | 98,98,98,98                 | 0     |
| 54  | MG   | CA    | 1660 | 1/1   | 0.74 | 0.18 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1829 | 1/1   | 0.74 | 0.27 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3092 | 1/1   | 0.74 | 0.36 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1788 | 1/1   | 0.74 | 0.29 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1758 | 1/1   | 0.74 | 0.21 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3330 | 1/1   | 0.74 | 0.25 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1673 | 1/1   | 0.75 | 0.38 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1720 | 1/1   | 0.75 | 0.14 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3369 | 1/1   | 0.75 | 0.27 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3453 | 1/1   | 0.75 | 0.50 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3054 | 1/1   | 0.75 | 0.22 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1695 | 1/1   | 0.75 | 0.15 | 119,119,119,119             | 0     |
| 54  | MG   | BA    | 3264 | 1/1   | 0.75 | 0.23 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1712 | 1/1   | 0.75 | 0.29 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1683 | 1/1   | 0.75 | 0.15 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1652 | 1/1   | 0.75 | 0.27 | 106,106,106,106             | 0     |
| 54  | MG   | CA    | 1615 | 1/1   | 0.75 | 0.23 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3171 | 1/1   | 0.75 | 0.47 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3483 | 1/1   | 0.75 | 0.21 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3154 | 1/1   | 0.75 | 0.13 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1752 | 1/1   | 0.75 | 0.26 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3415 | 1/1   | 0.75 | 0.33 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3424 | 1/1   | 0.75 | 0.26 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 3111 | 1/1   | 0.75 | 0.41 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1638 | 1/1   | 0.75 | 0.19 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3258 | 1/1   | 0.75 | 0.43 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3383 | 1/1   | 0.75 | 0.22 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3122 | 1/1   | 0.75 | 0.28 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3090 | 1/1   | 0.75 | 0.14 | 119,119,119,119             | 0     |
| 54  | MG   | AA    | 1772 | 1/1   | 0.76 | 0.35 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1684 | 1/1   | 0.76 | 0.21 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3418 | 1/1   | 0.76 | 0.45 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1686 | 1/1   | 0.76 | 0.19 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1756 | 1/1   | 0.76 | 0.34 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3319 | 1/1   | 0.76 | 0.23 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3321 | 1/1   | 0.76 | 0.25 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3318 | 1/1   | 0.76 | 0.29 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1821 | 1/1   | 0.76 | 0.16 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3551 | 1/1   | 0.76 | 0.14 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3554 | 1/1   | 0.76 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1776 | 1/1   | 0.76 | 0.29 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3555 | 1/1   | 0.76 | 0.17 | 105,105,105,105             | 0     |
| 54  | MG   | BA    | 3235 | 1/1   | 0.76 | 0.24 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3576 | 1/1   | 0.76 | 0.19 | 93,93,93,93                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3594 | 1/1   | 0.76 | 0.09 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3062 | 1/1   | 0.76 | 0.17 | 106,106,106,106             | 0     |
| 54  | MG   | BA    | 3075 | 1/1   | 0.76 | 0.16 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3082 | 1/1   | 0.76 | 0.43 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1643 | 1/1   | 0.76 | 0.24 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1707 | 1/1   | 0.76 | 0.07 | 127,127,127,127             | 0     |
| 54  | MG   | AA    | 1621 | 1/1   | 0.76 | 0.34 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3183 | 1/1   | 0.76 | 0.25 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3392 | 1/1   | 0.76 | 0.10 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3049 | 1/1   | 0.76 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3521 | 1/1   | 0.76 | 0.41 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3631 | 1/1   | 0.76 | 0.32 | 96,96,96,96                 | 0     |
| 54  | MG   | BB    | 202  | 1/1   | 0.76 | 0.21 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3037 | 1/1   | 0.76 | 0.24 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3261 | 1/1   | 0.76 | 0.31 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3304 | 1/1   | 0.76 | 0.32 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3477 | 1/1   | 0.76 | 0.15 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3406 | 1/1   | 0.76 | 0.31 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3207 | 1/1   | 0.76 | 0.29 | 78,78,78,78                 | 0     |
| 55  | T1C  | AA    | 1837 | 42/42 | 0.76 | 0.20 | 81,103,111,117              | 0     |
| 54  | MG   | BA    | 3540 | 1/1   | 0.77 | 0.35 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1689 | 1/1   | 0.77 | 0.32 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3412 | 1/1   | 0.77 | 0.18 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1628 | 1/1   | 0.77 | 0.28 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1758 | 1/1   | 0.77 | 0.24 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3429 | 1/1   | 0.77 | 0.30 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3360 | 1/1   | 0.77 | 0.24 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3089 | 1/1   | 0.77 | 0.30 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3570 | 1/1   | 0.77 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3363 | 1/1   | 0.77 | 0.21 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3089 | 1/1   | 0.77 | 0.24 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3323 | 1/1   | 0.77 | 0.23 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1741 | 1/1   | 0.77 | 0.17 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3109 | 1/1   | 0.77 | 0.20 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1631 | 1/1   | 0.77 | 0.12 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3377 | 1/1   | 0.77 | 0.17 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1804 | 1/1   | 0.77 | 0.34 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3114 | 1/1   | 0.77 | 0.11 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1634 | 1/1   | 0.77 | 0.26 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3397 | 1/1   | 0.77 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3473 | 1/1   | 0.77 | 0.27 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3469 | 1/1   | 0.77 | 0.06 | 94,94,94,94                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1684 | 1/1   | 0.77 | 0.33 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3481 | 1/1   | 0.77 | 0.14 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1737 | 1/1   | 0.77 | 0.18 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3363 | 1/1   | 0.77 | 0.30 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3153 | 1/1   | 0.77 | 0.28 | 88,88,88,88                 | 0     |
| 54  | MG   | AC    | 102  | 1/1   | 0.77 | 0.29 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1740 | 1/1   | 0.77 | 0.27 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3408 | 1/1   | 0.77 | 0.22 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1715 | 1/1   | 0.77 | 0.20 | 112,112,112,112             | 0     |
| 54  | MG   | AA    | 1738 | 1/1   | 0.77 | 0.20 | 120,120,120,120             | 0     |
| 54  | MG   | BA    | 3347 | 1/1   | 0.77 | 0.30 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3392 | 1/1   | 0.77 | 0.16 | 82,82,82,82                 | 0     |
| 54  | MG   | BF    | 302  | 1/1   | 0.77 | 0.28 | 71,71,71,71                 | 0     |
| 54  | MG   | DB    | 213  | 1/1   | 0.77 | 0.10 | 111,111,111,111             | 0     |
| 54  | MG   | DB    | 214  | 1/1   | 0.77 | 0.12 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3400 | 1/1   | 0.77 | 0.26 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3510 | 1/1   | 0.77 | 0.43 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3163 | 1/1   | 0.77 | 0.19 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3327 | 1/1   | 0.78 | 0.34 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3033 | 1/1   | 0.78 | 0.19 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1720 | 1/1   | 0.78 | 0.25 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1679 | 1/1   | 0.78 | 0.21 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3436 | 1/1   | 0.78 | 0.32 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3248 | 1/1   | 0.78 | 0.22 | 76,76,76,76                 | 0     |
| 54  | MG   | BB    | 211  | 1/1   | 0.78 | 0.16 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3150 | 1/1   | 0.78 | 0.40 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1727 | 1/1   | 0.78 | 0.14 | 128,128,128,128             | 0     |
| 54  | MG   | DA    | 3060 | 1/1   | 0.78 | 0.35 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3064 | 1/1   | 0.78 | 0.41 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3457 | 1/1   | 0.78 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3458 | 1/1   | 0.78 | 0.11 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3380 | 1/1   | 0.78 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1730 | 1/1   | 0.78 | 0.13 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3248 | 1/1   | 0.78 | 0.26 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1601 | 1/1   | 0.78 | 0.28 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3197 | 1/1   | 0.78 | 0.23 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3273 | 1/1   | 0.78 | 0.20 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1816 | 1/1   | 0.78 | 0.32 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3270 | 1/1   | 0.78 | 0.32 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3221 | 1/1   | 0.78 | 0.30 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3083 | 1/1   | 0.78 | 0.34 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1798 | 1/1   | 0.78 | 0.21 | 115,115,115,115             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1691 | 1/1   | 0.78 | 0.17 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3087 | 1/1   | 0.78 | 0.34 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1751 | 1/1   | 0.78 | 0.17 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3534 | 1/1   | 0.78 | 0.08 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3622 | 1/1   | 0.78 | 0.23 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1710 | 1/1   | 0.78 | 0.20 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3094 | 1/1   | 0.78 | 0.16 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3414 | 1/1   | 0.78 | 0.18 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3232 | 1/1   | 0.78 | 0.28 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1735 | 1/1   | 0.78 | 0.23 | 104,104,104,104             | 0     |
| 54  | MG   | AA    | 1775 | 1/1   | 0.78 | 0.12 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3316 | 1/1   | 0.78 | 0.23 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1748 | 1/1   | 0.79 | 0.08 | 152,152,152,152             | 0     |
| 54  | MG   | DA    | 3305 | 1/1   | 0.79 | 0.31 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1652 | 1/1   | 0.79 | 0.37 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3017 | 1/1   | 0.79 | 0.28 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3100 | 1/1   | 0.79 | 0.40 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3367 | 1/1   | 0.79 | 0.23 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3306 | 1/1   | 0.79 | 0.26 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3518 | 1/1   | 0.79 | 0.36 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3325 | 1/1   | 0.79 | 0.21 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3034 | 1/1   | 0.79 | 0.17 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3328 | 1/1   | 0.79 | 0.18 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3520 | 1/1   | 0.79 | 0.17 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1645 | 1/1   | 0.79 | 0.33 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3099 | 1/1   | 0.79 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3336 | 1/1   | 0.79 | 0.35 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1759 | 1/1   | 0.79 | 0.10 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3043 | 1/1   | 0.79 | 0.25 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1687 | 1/1   | 0.79 | 0.08 | 137,137,137,137             | 0     |
| 54  | MG   | AA    | 1688 | 1/1   | 0.79 | 0.20 | 118,118,118,118             | 0     |
| 54  | MG   | BA    | 3192 | 1/1   | 0.79 | 0.30 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3158 | 1/1   | 0.79 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1657 | 1/1   | 0.79 | 0.18 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 3327 | 1/1   | 0.79 | 0.32 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3217 | 1/1   | 0.79 | 0.30 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3238 | 1/1   | 0.79 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | B7    | 103  | 1/1   | 0.79 | 0.24 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3268 | 1/1   | 0.79 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3253 | 1/1   | 0.79 | 0.26 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3340 | 1/1   | 0.79 | 0.19 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1670 | 1/1   | 0.79 | 0.29 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1754 | 1/1   | 0.79 | 0.18 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3079 | 1/1   | 0.79 | 0.20 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3064 | 1/1   | 0.79 | 0.24 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3204 | 1/1   | 0.79 | 0.37 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1755 | 1/1   | 0.79 | 0.24 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1683 | 1/1   | 0.79 | 0.40 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3419 | 1/1   | 0.79 | 0.24 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3489 | 1/1   | 0.79 | 0.19 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3291 | 1/1   | 0.79 | 0.33 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1702 | 1/1   | 0.79 | 0.27 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3301 | 1/1   | 0.80 | 0.28 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3039 | 1/1   | 0.80 | 0.27 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3513 | 1/1   | 0.80 | 0.20 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3042 | 1/1   | 0.80 | 0.19 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3517 | 1/1   | 0.80 | 0.30 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3218 | 1/1   | 0.80 | 0.24 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3056 | 1/1   | 0.80 | 0.27 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1641 | 1/1   | 0.80 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3438 | 1/1   | 0.80 | 0.26 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3225 | 1/1   | 0.80 | 0.25 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1613 | 1/1   | 0.80 | 0.28 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3084 | 1/1   | 0.80 | 0.07 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1625 | 1/1   | 0.80 | 0.19 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3165 | 1/1   | 0.80 | 0.29 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3166 | 1/1   | 0.80 | 0.43 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1822 | 1/1   | 0.80 | 0.24 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1798 | 1/1   | 0.80 | 0.15 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1609 | 1/1   | 0.80 | 0.11 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3362 | 1/1   | 0.80 | 0.34 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1797 | 1/1   | 0.80 | 0.31 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1824 | 1/1   | 0.80 | 0.33 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3582 | 1/1   | 0.80 | 0.32 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1626 | 1/1   | 0.80 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1735 | 1/1   | 0.80 | 0.29 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3282 | 1/1   | 0.80 | 0.22 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1681 | 1/1   | 0.80 | 0.45 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3515 | 1/1   | 0.80 | 0.29 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3389 | 1/1   | 0.80 | 0.19 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1662 | 1/1   | 0.80 | 0.17 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3485 | 1/1   | 0.80 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1666 | 1/1   | 0.80 | 0.21 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3355 | 1/1   | 0.80 | 0.30 | 86,86,86,86                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3299 | 1/1   | 0.80 | 0.17 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3200 | 1/1   | 0.80 | 0.31 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1694 | 1/1   | 0.80 | 0.26 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3409 | 1/1   | 0.80 | 0.31 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3617 | 1/1   | 0.80 | 0.19 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3411 | 1/1   | 0.80 | 0.33 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1836 | 1/1   | 0.80 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1668 | 1/1   | 0.80 | 0.31 | 81,81,81,81                 | 0     |
| 54  | MG   | DU    | 201  | 1/1   | 0.80 | 0.18 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1638 | 1/1   | 0.80 | 0.25 | 100,100,100,100             | 0     |
| 55  | T1C  | CA    | 1800 | 42/42 | 0.80 | 0.18 | 101,116,124,127             | 0     |
| 54  | MG   | CA    | 1767 | 1/1   | 0.81 | 0.25 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1768 | 1/1   | 0.81 | 0.26 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3050 | 1/1   | 0.81 | 0.20 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3387 | 1/1   | 0.81 | 0.25 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3474 | 1/1   | 0.81 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3092 | 1/1   | 0.81 | 0.25 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1711 | 1/1   | 0.81 | 0.14 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1805 | 1/1   | 0.81 | 0.42 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3419 | 1/1   | 0.81 | 0.29 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3421 | 1/1   | 0.81 | 0.34 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3102 | 1/1   | 0.81 | 0.27 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3400 | 1/1   | 0.81 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3429 | 1/1   | 0.81 | 0.17 | 103,103,103,103             | 0     |
| 54  | MG   | AA    | 1704 | 1/1   | 0.81 | 0.25 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3306 | 1/1   | 0.81 | 0.14 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1809 | 1/1   | 0.81 | 0.19 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1743 | 1/1   | 0.81 | 0.23 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3071 | 1/1   | 0.81 | 0.28 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3095 | 1/1   | 0.81 | 0.17 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3508 | 1/1   | 0.81 | 0.29 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3074 | 1/1   | 0.81 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3274 | 1/1   | 0.81 | 0.17 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3511 | 1/1   | 0.81 | 0.20 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3002 | 1/1   | 0.81 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3128 | 1/1   | 0.81 | 0.10 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3283 | 1/1   | 0.81 | 0.25 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1672 | 1/1   | 0.81 | 0.25 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3142 | 1/1   | 0.81 | 0.23 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3337 | 1/1   | 0.81 | 0.31 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3143 | 1/1   | 0.81 | 0.13 | 84,84,84,84                 | 0     |
| 54  | MG   | BB    | 216  | 1/1   | 0.81 | 0.07 | 111,111,111,111             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3490 | 1/1   | 0.81 | 0.18 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3287 | 1/1   | 0.81 | 0.45 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1799 | 1/1   | 0.81 | 0.22 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3361 | 1/1   | 0.81 | 0.31 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3152 | 1/1   | 0.81 | 0.22 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3523 | 1/1   | 0.81 | 0.23 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3440 | 1/1   | 0.81 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1750 | 1/1   | 0.81 | 0.29 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3135 | 1/1   | 0.81 | 0.33 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3187 | 1/1   | 0.81 | 0.31 | 83,83,83,83                 | 0     |
| 54  | MG   | DB    | 202  | 1/1   | 0.81 | 0.16 | 116,116,116,116             | 0     |
| 54  | MG   | BA    | 3291 | 1/1   | 0.81 | 0.23 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3371 | 1/1   | 0.81 | 0.23 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1696 | 1/1   | 0.81 | 0.15 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3045 | 1/1   | 0.81 | 0.21 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3299 | 1/1   | 0.81 | 0.28 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3151 | 1/1   | 0.81 | 0.25 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1833 | 1/1   | 0.81 | 0.26 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1679 | 1/1   | 0.81 | 0.16 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3382 | 1/1   | 0.81 | 0.34 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3265 | 1/1   | 0.81 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1701 | 1/1   | 0.81 | 0.23 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3068 | 1/1   | 0.81 | 0.26 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3466 | 1/1   | 0.81 | 0.18 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3100 | 1/1   | 0.82 | 0.16 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1606 | 1/1   | 0.82 | 0.20 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3590 | 1/1   | 0.82 | 0.23 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3344 | 1/1   | 0.82 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3222 | 1/1   | 0.82 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3072 | 1/1   | 0.82 | 0.20 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3081 | 1/1   | 0.82 | 0.27 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1664 | 1/1   | 0.82 | 0.44 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3416 | 1/1   | 0.82 | 0.17 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3614 | 1/1   | 0.82 | 0.09 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1653 | 1/1   | 0.82 | 0.25 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1792 | 1/1   | 0.82 | 0.15 | 105,105,105,105             | 0     |
| 54  | MG   | BA    | 3359 | 1/1   | 0.82 | 0.21 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3080 | 1/1   | 0.82 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3300 | 1/1   | 0.82 | 0.17 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3182 | 1/1   | 0.82 | 0.30 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1654 | 1/1   | 0.82 | 0.19 | 107,107,107,107             | 0     |
| 54  | MG   | CS    | 101  | 1/1   | 0.82 | 0.28 | 95,95,95,95                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1615 | 1/1   | 0.82 | 0.12 | 114,114,114,114             | 0     |
| 54  | MG   | CC    | 101  | 1/1   | 0.82 | 0.10 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3450 | 1/1   | 0.82 | 0.21 | 94,94,94,94                 | 0     |
| 54  | MG   | CC    | 106  | 1/1   | 0.82 | 0.14 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3630 | 1/1   | 0.82 | 0.18 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3305 | 1/1   | 0.82 | 0.31 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3191 | 1/1   | 0.82 | 0.19 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3370 | 1/1   | 0.82 | 0.09 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3519 | 1/1   | 0.82 | 0.19 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 3372 | 1/1   | 0.82 | 0.37 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3344 | 1/1   | 0.82 | 0.28 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3018 | 1/1   | 0.82 | 0.21 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3250 | 1/1   | 0.82 | 0.32 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1811 | 1/1   | 0.82 | 0.19 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3525 | 1/1   | 0.82 | 0.25 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3313 | 1/1   | 0.82 | 0.43 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1745 | 1/1   | 0.82 | 0.16 | 102,102,102,102             | 0     |
| 54  | MG   | BU    | 202  | 1/1   | 0.82 | 0.09 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3511 | 1/1   | 0.82 | 0.25 | 77,77,77,77                 | 0     |
| 54  | MG   | B3    | 102  | 1/1   | 0.82 | 0.09 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3516 | 1/1   | 0.82 | 0.30 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1749 | 1/1   | 0.82 | 0.30 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3177 | 1/1   | 0.82 | 0.41 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3088 | 1/1   | 0.82 | 0.09 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3544 | 1/1   | 0.82 | 0.22 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1601 | 1/1   | 0.82 | 0.24 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3044 | 1/1   | 0.82 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3243 | 1/1   | 0.82 | 0.22 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3246 | 1/1   | 0.82 | 0.25 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3549 | 1/1   | 0.82 | 0.13 | 74,74,74,74                 | 0     |
| 54  | MG   | DB    | 211  | 1/1   | 0.82 | 0.44 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1655 | 1/1   | 0.82 | 0.28 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1692 | 1/1   | 0.82 | 0.34 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1814 | 1/1   | 0.82 | 0.24 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3063 | 1/1   | 0.82 | 0.26 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3063 | 1/1   | 0.82 | 0.29 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3393 | 1/1   | 0.82 | 0.27 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1815 | 1/1   | 0.82 | 0.36 | 98,98,98,98                 | 0     |
| 54  | MG   | CA    | 1762 | 1/1   | 0.82 | 0.23 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1647 | 1/1   | 0.83 | 0.31 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3206 | 1/1   | 0.83 | 0.34 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3289 | 1/1   | 0.83 | 0.22 | 94,94,94,94                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3082 | 1/1   | 0.83 | 0.24 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3148 | 1/1   | 0.83 | 0.29 | 85,85,85,85                 | 0     |
| 54  | MG   | BB    | 208  | 1/1   | 0.83 | 0.10 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1728 | 1/1   | 0.83 | 0.30 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3215 | 1/1   | 0.83 | 0.33 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1649 | 1/1   | 0.83 | 0.27 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1708 | 1/1   | 0.83 | 0.17 | 96,96,96,96                 | 0     |
| 54  | MG   | CC    | 105  | 1/1   | 0.83 | 0.34 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3444 | 1/1   | 0.83 | 0.30 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3153 | 1/1   | 0.83 | 0.20 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3223 | 1/1   | 0.83 | 0.30 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3543 | 1/1   | 0.83 | 0.17 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3154 | 1/1   | 0.83 | 0.30 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3101 | 1/1   | 0.83 | 0.26 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3114 | 1/1   | 0.83 | 0.26 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3548 | 1/1   | 0.83 | 0.34 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1790 | 1/1   | 0.83 | 0.20 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3057 | 1/1   | 0.83 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3060 | 1/1   | 0.83 | 0.18 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3326 | 1/1   | 0.83 | 0.28 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1717 | 1/1   | 0.83 | 0.26 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3386 | 1/1   | 0.83 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3236 | 1/1   | 0.83 | 0.44 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3455 | 1/1   | 0.83 | 0.27 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3472 | 1/1   | 0.83 | 0.16 | 114,114,114,114             | 0     |
| 54  | MG   | DA    | 3333 | 1/1   | 0.83 | 0.29 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1681 | 1/1   | 0.83 | 0.16 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1631 | 1/1   | 0.83 | 0.26 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1733 | 1/1   | 0.83 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3596 | 1/1   | 0.83 | 0.39 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3343 | 1/1   | 0.83 | 0.38 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1777 | 1/1   | 0.83 | 0.14 | 117,117,117,117             | 0     |
| 54  | MG   | CA    | 1698 | 1/1   | 0.83 | 0.36 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1676 | 1/1   | 0.83 | 0.19 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3337 | 1/1   | 0.83 | 0.34 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3353 | 1/1   | 0.83 | 0.33 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3047 | 1/1   | 0.83 | 0.38 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3168 | 1/1   | 0.83 | 0.09 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3169 | 1/1   | 0.83 | 0.27 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3119 | 1/1   | 0.83 | 0.20 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3178 | 1/1   | 0.83 | 0.48 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1763 | 1/1   | 0.83 | 0.25 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3057 | 1/1   | 0.83 | 0.32 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1825 | 1/1   | 0.83 | 0.16 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3231 | 1/1   | 0.83 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1639 | 1/1   | 0.83 | 0.36 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3276 | 1/1   | 0.83 | 0.35 | 91,91,91,91                 | 0     |
| 54  | MG   | A1    | 101  | 1/1   | 0.83 | 0.17 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3386 | 1/1   | 0.83 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1778 | 1/1   | 0.83 | 0.23 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3388 | 1/1   | 0.83 | 0.20 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3281 | 1/1   | 0.83 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1648 | 1/1   | 0.83 | 0.22 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3254 | 1/1   | 0.83 | 0.49 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3398 | 1/1   | 0.83 | 0.22 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3131 | 1/1   | 0.83 | 0.26 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1651 | 1/1   | 0.83 | 0.10 | 114,114,114,114             | 0     |
| 54  | MG   | CA    | 1791 | 1/1   | 0.83 | 0.09 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3099 | 1/1   | 0.84 | 0.26 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3601 | 1/1   | 0.84 | 0.27 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3257 | 1/1   | 0.84 | 0.23 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3108 | 1/1   | 0.84 | 0.32 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3113 | 1/1   | 0.84 | 0.37 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1690 | 1/1   | 0.84 | 0.25 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1624 | 1/1   | 0.84 | 0.18 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3416 | 1/1   | 0.84 | 0.25 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3303 | 1/1   | 0.84 | 0.10 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1768 | 1/1   | 0.84 | 0.13 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1699 | 1/1   | 0.84 | 0.11 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3391 | 1/1   | 0.84 | 0.28 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3270 | 1/1   | 0.84 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3120 | 1/1   | 0.84 | 0.19 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3320 | 1/1   | 0.84 | 0.11 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1759 | 1/1   | 0.84 | 0.28 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1633 | 1/1   | 0.84 | 0.26 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3039 | 1/1   | 0.84 | 0.27 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3147 | 1/1   | 0.84 | 0.28 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3437 | 1/1   | 0.84 | 0.24 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3454 | 1/1   | 0.84 | 0.25 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1764 | 1/1   | 0.84 | 0.20 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3623 | 1/1   | 0.84 | 0.11 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1780 | 1/1   | 0.84 | 0.23 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3448 | 1/1   | 0.84 | 0.29 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3533 | 1/1   | 0.84 | 0.13 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1771 | 1/1   | 0.84 | 0.32 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3356 | 1/1   | 0.84 | 0.36 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3166 | 1/1   | 0.84 | 0.21 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3536 | 1/1   | 0.84 | 0.27 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1712 | 1/1   | 0.84 | 0.16 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3342 | 1/1   | 0.84 | 0.27 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1671 | 1/1   | 0.84 | 0.25 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3175 | 1/1   | 0.84 | 0.25 | 71,71,71,71                 | 0     |
| 54  | MG   | BB    | 205  | 1/1   | 0.84 | 0.26 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1826 | 1/1   | 0.84 | 0.13 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3184 | 1/1   | 0.84 | 0.08 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3312 | 1/1   | 0.84 | 0.34 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3188 | 1/1   | 0.84 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3055 | 1/1   | 0.84 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3207 | 1/1   | 0.84 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3240 | 1/1   | 0.84 | 0.20 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1694 | 1/1   | 0.84 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1819 | 1/1   | 0.84 | 0.28 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3364 | 1/1   | 0.84 | 0.14 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1692 | 1/1   | 0.84 | 0.19 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3559 | 1/1   | 0.84 | 0.47 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3252 | 1/1   | 0.84 | 0.49 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3334 | 1/1   | 0.84 | 0.14 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3573 | 1/1   | 0.84 | 0.27 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3494 | 1/1   | 0.84 | 0.15 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3336 | 1/1   | 0.84 | 0.21 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3260 | 1/1   | 0.84 | 0.31 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1674 | 1/1   | 0.84 | 0.31 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3430 | 1/1   | 0.84 | 0.18 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1607 | 1/1   | 0.84 | 0.42 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3253 | 1/1   | 0.84 | 0.31 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3393 | 1/1   | 0.84 | 0.30 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3381 | 1/1   | 0.84 | 0.27 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3276 | 1/1   | 0.84 | 0.18 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3339 | 1/1   | 0.84 | 0.28 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3599 | 1/1   | 0.84 | 0.19 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3016 | 1/1   | 0.84 | 0.30 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1648 | 1/1   | 0.85 | 0.07 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 3259 | 1/1   | 0.85 | 0.30 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3078 | 1/1   | 0.85 | 0.23 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3422 | 1/1   | 0.85 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3136 | 1/1   | 0.85 | 0.17 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3470 | 1/1   | 0.85 | 0.21 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3428 | 1/1   | 0.85 | 0.08 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1688 | 1/1   | 0.85 | 0.32 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1729 | 1/1   | 0.85 | 0.11 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3473 | 1/1   | 0.85 | 0.28 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3205 | 1/1   | 0.85 | 0.23 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1672 | 1/1   | 0.85 | 0.30 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3214 | 1/1   | 0.85 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3628 | 1/1   | 0.85 | 0.31 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3425 | 1/1   | 0.85 | 0.13 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3439 | 1/1   | 0.85 | 0.15 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1792 | 1/1   | 0.85 | 0.16 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3482 | 1/1   | 0.85 | 0.31 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3632 | 1/1   | 0.85 | 0.12 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1820 | 1/1   | 0.85 | 0.07 | 112,112,112,112             | 0     |
| 54  | MG   | AA    | 1714 | 1/1   | 0.85 | 0.10 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3451 | 1/1   | 0.85 | 0.22 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3251 | 1/1   | 0.85 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3354 | 1/1   | 0.85 | 0.06 | 126,126,126,126             | 0     |
| 54  | MG   | DA    | 3021 | 1/1   | 0.85 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3552 | 1/1   | 0.85 | 0.12 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3155 | 1/1   | 0.85 | 0.40 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3490 | 1/1   | 0.85 | 0.31 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1746 | 1/1   | 0.85 | 0.14 | 110,110,110,110             | 0     |
| 54  | MG   | AA    | 1747 | 1/1   | 0.85 | 0.22 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3498 | 1/1   | 0.85 | 0.23 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3367 | 1/1   | 0.85 | 0.42 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3499 | 1/1   | 0.85 | 0.22 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3094 | 1/1   | 0.85 | 0.24 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3285 | 1/1   | 0.85 | 0.30 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3129 | 1/1   | 0.85 | 0.24 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3279 | 1/1   | 0.85 | 0.29 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3132 | 1/1   | 0.85 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1769 | 1/1   | 0.85 | 0.27 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3514 | 1/1   | 0.85 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3395 | 1/1   | 0.85 | 0.30 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1716 | 1/1   | 0.85 | 0.21 | 103,103,103,103             | 0     |
| 54  | MG   | AN    | 202  | 1/1   | 0.85 | 0.10 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1774 | 1/1   | 0.85 | 0.16 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3295 | 1/1   | 0.85 | 0.14 | 128,128,128,128             | 0     |
| 54  | MG   | BA    | 3595 | 1/1   | 0.85 | 0.13 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3249 | 1/1   | 0.85 | 0.26 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1800 | 1/1   | 0.85 | 0.20 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1780 | 1/1   | 0.85 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3402 | 1/1   | 0.85 | 0.13 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3304 | 1/1   | 0.85 | 0.18 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3217 | 1/1   | 0.85 | 0.24 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3170 | 1/1   | 0.85 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1614 | 1/1   | 0.85 | 0.30 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3316 | 1/1   | 0.85 | 0.28 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3410 | 1/1   | 0.85 | 0.26 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3462 | 1/1   | 0.85 | 0.18 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1678 | 1/1   | 0.85 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1617 | 1/1   | 0.85 | 0.23 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3411 | 1/1   | 0.85 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3441 | 1/1   | 0.86 | 0.26 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3505 | 1/1   | 0.86 | 0.21 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3137 | 1/1   | 0.86 | 0.26 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1835 | 1/1   | 0.86 | 0.33 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1693 | 1/1   | 0.86 | 0.35 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1757 | 1/1   | 0.86 | 0.34 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1643 | 1/1   | 0.86 | 0.16 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1802 | 1/1   | 0.86 | 0.08 | 100,100,100,100             | 0     |
| 54  | MG   | AH    | 201  | 1/1   | 0.86 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3095 | 1/1   | 0.86 | 0.40 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3420 | 1/1   | 0.86 | 0.16 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1744 | 1/1   | 0.86 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1632 | 1/1   | 0.86 | 0.19 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3349 | 1/1   | 0.86 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3619 | 1/1   | 0.86 | 0.27 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1704 | 1/1   | 0.86 | 0.27 | 99,99,99,99                 | 0     |
| 54  | MG   | CA    | 1634 | 1/1   | 0.86 | 0.21 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3164 | 1/1   | 0.86 | 0.23 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3258 | 1/1   | 0.86 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3433 | 1/1   | 0.86 | 0.21 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3459 | 1/1   | 0.86 | 0.32 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3302 | 1/1   | 0.86 | 0.39 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3624 | 1/1   | 0.86 | 0.15 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3404 | 1/1   | 0.86 | 0.40 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3531 | 1/1   | 0.86 | 0.08 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3332 | 1/1   | 0.86 | 0.21 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3303 | 1/1   | 0.86 | 0.23 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3443 | 1/1   | 0.86 | 0.12 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1667 | 1/1   | 0.86 | 0.35 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3185 | 1/1   | 0.86 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1774 | 1/1   | 0.86 | 0.32 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3539 | 1/1   | 0.86 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3191 | 1/1   | 0.86 | 0.32 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3267 | 1/1   | 0.86 | 0.34 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3542 | 1/1   | 0.86 | 0.19 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3471 | 1/1   | 0.86 | 0.42 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3209 | 1/1   | 0.86 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3347 | 1/1   | 0.86 | 0.09 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1791 | 1/1   | 0.86 | 0.16 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1795 | 1/1   | 0.86 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3219 | 1/1   | 0.86 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3461 | 1/1   | 0.86 | 0.16 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3221 | 1/1   | 0.86 | 0.30 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3472 | 1/1   | 0.86 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1727 | 1/1   | 0.86 | 0.18 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3475 | 1/1   | 0.86 | 0.28 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3488 | 1/1   | 0.86 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1650 | 1/1   | 0.86 | 0.39 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1656 | 1/1   | 0.86 | 0.32 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3314 | 1/1   | 0.86 | 0.36 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3497 | 1/1   | 0.86 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3424 | 1/1   | 0.86 | 0.22 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3503 | 1/1   | 0.86 | 0.34 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3008 | 1/1   | 0.86 | 0.33 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3079 | 1/1   | 0.86 | 0.34 | 103,103,103,103             | 0     |
| 54  | MG   | CC    | 102  | 1/1   | 0.86 | 0.28 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3488 | 1/1   | 0.86 | 0.31 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3093 | 1/1   | 0.86 | 0.31 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3022 | 1/1   | 0.86 | 0.26 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3375 | 1/1   | 0.86 | 0.28 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3519 | 1/1   | 0.86 | 0.15 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3376 | 1/1   | 0.86 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3380 | 1/1   | 0.86 | 0.15 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3036 | 1/1   | 0.86 | 0.28 | 73,73,73,73                 | 0     |
| 54  | MG   | B8    | 102  | 1/1   | 0.86 | 0.15 | 107,107,107,107             | 0     |
| 54  | MG   | CA    | 1743 | 1/1   | 0.86 | 0.13 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1611 | 1/1   | 0.86 | 0.12 | 118,118,118,118             | 0     |
| 54  | MG   | BA    | 3237 | 1/1   | 0.86 | 0.34 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3275 | 1/1   | 0.86 | 0.24 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3011 | 1/1   | 0.86 | 0.11 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3583 | 1/1   | 0.86 | 0.26 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3588 | 1/1   | 0.86 | 0.33 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3436 | 1/1   | 0.86 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3438 | 1/1   | 0.86 | 0.15 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1753 | 1/1   | 0.86 | 0.17 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3286 | 1/1   | 0.86 | 0.30 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3127 | 1/1   | 0.86 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3025 | 1/1   | 0.86 | 0.21 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1779 | 1/1   | 0.87 | 0.34 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1605 | 1/1   | 0.87 | 0.29 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3035 | 1/1   | 0.87 | 0.18 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3309 | 1/1   | 0.87 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1685 | 1/1   | 0.87 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3495 | 1/1   | 0.87 | 0.16 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3431 | 1/1   | 0.87 | 0.22 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1669 | 1/1   | 0.87 | 0.27 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3378 | 1/1   | 0.87 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3229 | 1/1   | 0.87 | 0.32 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3326 | 1/1   | 0.87 | 0.31 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1660 | 1/1   | 0.87 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3115 | 1/1   | 0.87 | 0.35 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3046 | 1/1   | 0.87 | 0.47 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1770 | 1/1   | 0.87 | 0.07 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1623 | 1/1   | 0.87 | 0.07 | 142,142,142,142             | 0     |
| 54  | MG   | DA    | 3329 | 1/1   | 0.87 | 0.32 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3030 | 1/1   | 0.87 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3390 | 1/1   | 0.87 | 0.23 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3058 | 1/1   | 0.87 | 0.22 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3607 | 1/1   | 0.87 | 0.37 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3181 | 1/1   | 0.87 | 0.21 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1702 | 1/1   | 0.87 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3516 | 1/1   | 0.87 | 0.31 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3186 | 1/1   | 0.87 | 0.27 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3032 | 1/1   | 0.87 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3034 | 1/1   | 0.87 | 0.34 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1632 | 1/1   | 0.87 | 0.22 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3069 | 1/1   | 0.87 | 0.25 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1817 | 1/1   | 0.87 | 0.07 | 137,137,137,137             | 0     |
| 54  | MG   | BA    | 3247 | 1/1   | 0.87 | 0.28 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3342 | 1/1   | 0.87 | 0.20 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3343 | 1/1   | 0.87 | 0.35 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3215 | 1/1   | 0.87 | 0.27 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1636 | 1/1   | 0.87 | 0.14 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1641 | 1/1   | 0.87 | 0.23 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3462 | 1/1   | 0.87 | 0.10 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3463 | 1/1   | 0.87 | 0.29 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3464 | 1/1   | 0.87 | 0.22 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1788 | 1/1   | 0.87 | 0.30 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3225 | 1/1   | 0.87 | 0.32 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1790 | 1/1   | 0.87 | 0.15 | 105,105,105,105             | 0     |
| 54  | MG   | BA    | 3527 | 1/1   | 0.87 | 0.18 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3530 | 1/1   | 0.87 | 0.16 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3365 | 1/1   | 0.87 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1717 | 1/1   | 0.87 | 0.32 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3463 | 1/1   | 0.87 | 0.26 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3496 | 1/1   | 0.87 | 0.27 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3402 | 1/1   | 0.87 | 0.40 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3297 | 1/1   | 0.87 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3298 | 1/1   | 0.87 | 0.32 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1750 | 1/1   | 0.87 | 0.14 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3407 | 1/1   | 0.87 | 0.26 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1803 | 1/1   | 0.87 | 0.34 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3354 | 1/1   | 0.87 | 0.21 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1678 | 1/1   | 0.87 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | CC    | 104  | 1/1   | 0.87 | 0.20 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3098 | 1/1   | 0.87 | 0.07 | 112,112,112,112             | 0     |
| 54  | MG   | CA    | 1731 | 1/1   | 0.87 | 0.18 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3143 | 1/1   | 0.87 | 0.34 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3390 | 1/1   | 0.87 | 0.22 | 76,76,76,76                 | 0     |
| 54  | MG   | DB    | 201  | 1/1   | 0.87 | 0.24 | 90,90,90,90                 | 0     |
| 54  | MG   | BB    | 212  | 1/1   | 0.87 | 0.26 | 82,82,82,82                 | 0     |
| 54  | MG   | AC    | 101  | 1/1   | 0.87 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3479 | 1/1   | 0.87 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1603 | 1/1   | 0.87 | 0.15 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1807 | 1/1   | 0.87 | 0.33 | 79,79,79,79                 | 0     |
| 54  | MG   | BE    | 304  | 1/1   | 0.87 | 0.11 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3152 | 1/1   | 0.87 | 0.07 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3558 | 1/1   | 0.87 | 0.32 | 58,58,58,58                 | 0     |
| 54  | MG   | AA    | 1674 | 1/1   | 0.87 | 0.21 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3130 | 1/1   | 0.87 | 0.36 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3020 | 1/1   | 0.87 | 0.36 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1700 | 1/1   | 0.87 | 0.07 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1794 | 1/1   | 0.87 | 0.34 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3107 | 1/1   | 0.87 | 0.29 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3160 | 1/1   | 0.87 | 0.26 | 92,92,92,92                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3371 | 1/1   | 0.88 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1635 | 1/1   | 0.88 | 0.13 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3491 | 1/1   | 0.88 | 0.14 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1604 | 1/1   | 0.88 | 0.28 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1742 | 1/1   | 0.88 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3577 | 1/1   | 0.88 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1608 | 1/1   | 0.88 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3376 | 1/1   | 0.88 | 0.18 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3298 | 1/1   | 0.88 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1611 | 1/1   | 0.88 | 0.37 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3300 | 1/1   | 0.88 | 0.25 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3148 | 1/1   | 0.88 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3177 | 1/1   | 0.88 | 0.21 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1737 | 1/1   | 0.88 | 0.22 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3433 | 1/1   | 0.88 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3379 | 1/1   | 0.88 | 0.17 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3308 | 1/1   | 0.88 | 0.26 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3427 | 1/1   | 0.88 | 0.27 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3502 | 1/1   | 0.88 | 0.10 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3048 | 1/1   | 0.88 | 0.29 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3101 | 1/1   | 0.88 | 0.29 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3160 | 1/1   | 0.88 | 0.32 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3437 | 1/1   | 0.88 | 0.26 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3598 | 1/1   | 0.88 | 0.29 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3332 | 1/1   | 0.88 | 0.31 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3145 | 1/1   | 0.88 | 0.33 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3602 | 1/1   | 0.88 | 0.30 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3146 | 1/1   | 0.88 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1767 | 1/1   | 0.88 | 0.25 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3066 | 1/1   | 0.88 | 0.24 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3606 | 1/1   | 0.88 | 0.12 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3182 | 1/1   | 0.88 | 0.32 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3445 | 1/1   | 0.88 | 0.28 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3243 | 1/1   | 0.88 | 0.30 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3388 | 1/1   | 0.88 | 0.14 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3389 | 1/1   | 0.88 | 0.22 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3193 | 1/1   | 0.88 | 0.30 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1834 | 1/1   | 0.88 | 0.25 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3296 | 1/1   | 0.88 | 0.22 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1640 | 1/1   | 0.88 | 0.21 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3195 | 1/1   | 0.88 | 0.38 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3341 | 1/1   | 0.88 | 0.36 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3197 | 1/1   | 0.88 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3204 | 1/1   | 0.88 | 0.27 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1723 | 1/1   | 0.88 | 0.28 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3199 | 1/1   | 0.88 | 0.24 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1728 | 1/1   | 0.88 | 0.35 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3210 | 1/1   | 0.88 | 0.26 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3213 | 1/1   | 0.88 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3350 | 1/1   | 0.88 | 0.29 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1740 | 1/1   | 0.88 | 0.36 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3399 | 1/1   | 0.88 | 0.18 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3084 | 1/1   | 0.88 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3476 | 1/1   | 0.88 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3218 | 1/1   | 0.88 | 0.41 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3489 | 1/1   | 0.88 | 0.18 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1761 | 1/1   | 0.88 | 0.13 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3359 | 1/1   | 0.88 | 0.36 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3350 | 1/1   | 0.88 | 0.31 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3012 | 1/1   | 0.88 | 0.24 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3226 | 1/1   | 0.88 | 0.37 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3227 | 1/1   | 0.88 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3501 | 1/1   | 0.88 | 0.13 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3353 | 1/1   | 0.88 | 0.26 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3366 | 1/1   | 0.88 | 0.25 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3537 | 1/1   | 0.88 | 0.18 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3240 | 1/1   | 0.88 | 0.22 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3405 | 1/1   | 0.88 | 0.13 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3209 | 1/1   | 0.88 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3156 | 1/1   | 0.88 | 0.28 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3374 | 1/1   | 0.88 | 0.34 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3263 | 1/1   | 0.88 | 0.22 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3059 | 1/1   | 0.88 | 0.11 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3379 | 1/1   | 0.88 | 0.31 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3523 | 1/1   | 0.88 | 0.22 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3001 | 1/1   | 0.88 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3090 | 1/1   | 0.88 | 0.12 | 85,85,85,85                 | 0     |
| 54  | MG   | DB    | 203  | 1/1   | 0.88 | 0.23 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3257 | 1/1   | 0.88 | 0.33 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3219 | 1/1   | 0.88 | 0.10 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3008 | 1/1   | 0.88 | 0.21 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3309 | 1/1   | 0.88 | 0.31 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3018 | 1/1   | 0.88 | 0.36 | 55,55,55,55                 | 0     |
| 54  | MG   | DB    | 210  | 1/1   | 0.88 | 0.25 | 95,95,95,95                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1795 | 1/1   | 0.88 | 0.31 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3129 | 1/1   | 0.88 | 0.30 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3557 | 1/1   | 0.88 | 0.25 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3487 | 1/1   | 0.88 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3023 | 1/1   | 0.88 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | AT    | 201  | 1/1   | 0.88 | 0.28 | 87,87,87,87                 | 0     |
| 54  | MG   | D1    | 201  | 1/1   | 0.88 | 0.33 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3562 | 1/1   | 0.88 | 0.30 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3401 | 1/1   | 0.88 | 0.32 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3563 | 1/1   | 0.88 | 0.29 | 59,59,59,59                 | 0     |
| 56  | ZN   | AQ    | 102  | 1/1   | 0.88 | 0.17 | 138,138,138,138             | 0     |
| 54  | MG   | BA    | 3603 | 1/1   | 0.89 | 0.35 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3122 | 1/1   | 0.89 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3331 | 1/1   | 0.89 | 0.15 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3125 | 1/1   | 0.89 | 0.27 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3126 | 1/1   | 0.89 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3385 | 1/1   | 0.89 | 0.27 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3514 | 1/1   | 0.89 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3294 | 1/1   | 0.89 | 0.26 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3417 | 1/1   | 0.89 | 0.28 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1635 | 1/1   | 0.89 | 0.21 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3006 | 1/1   | 0.89 | 0.44 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3133 | 1/1   | 0.89 | 0.14 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1713 | 1/1   | 0.89 | 0.34 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3168 | 1/1   | 0.89 | 0.23 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3015 | 1/1   | 0.89 | 0.36 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3140 | 1/1   | 0.89 | 0.38 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3612 | 1/1   | 0.89 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3284 | 1/1   | 0.89 | 0.23 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3013 | 1/1   | 0.89 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | AQ    | 101  | 1/1   | 0.89 | 0.07 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1736 | 1/1   | 0.89 | 0.16 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3312 | 1/1   | 0.89 | 0.29 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3521 | 1/1   | 0.89 | 0.42 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1644 | 1/1   | 0.89 | 0.36 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3134 | 1/1   | 0.89 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3025 | 1/1   | 0.89 | 0.26 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3031 | 1/1   | 0.89 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3032 | 1/1   | 0.89 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3526 | 1/1   | 0.89 | 0.09 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1651 | 1/1   | 0.89 | 0.32 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3529 | 1/1   | 0.89 | 0.29 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3456 | 1/1   | 0.89 | 0.07 | 225,225,225,225             | 0     |
| 54  | MG   | CA    | 1747 | 1/1   | 0.89 | 0.38 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3241 | 1/1   | 0.89 | 0.15 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3449 | 1/1   | 0.89 | 0.33 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3532 | 1/1   | 0.89 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3396 | 1/1   | 0.89 | 0.09 | 117,117,117,117             | 0     |
| 54  | MG   | BB    | 201  | 1/1   | 0.89 | 0.21 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1659 | 1/1   | 0.89 | 0.20 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3345 | 1/1   | 0.89 | 0.53 | 91,91,91,91                 | 0     |
| 54  | MG   | BB    | 203  | 1/1   | 0.89 | 0.25 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3184 | 1/1   | 0.89 | 0.16 | 66,66,66,66                 | 0     |
| 54  | MG   | BB    | 206  | 1/1   | 0.89 | 0.20 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3186 | 1/1   | 0.89 | 0.32 | 69,69,69,69                 | 0     |
| 54  | MG   | AA    | 1627 | 1/1   | 0.89 | 0.40 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3144 | 1/1   | 0.89 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3541 | 1/1   | 0.89 | 0.28 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3190 | 1/1   | 0.89 | 0.27 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3068 | 1/1   | 0.89 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3465 | 1/1   | 0.89 | 0.28 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3069 | 1/1   | 0.89 | 0.29 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1630 | 1/1   | 0.89 | 0.15 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3103 | 1/1   | 0.89 | 0.21 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3349 | 1/1   | 0.89 | 0.22 | 78,78,78,78                 | 0     |
| 54  | MG   | BE    | 301  | 1/1   | 0.89 | 0.36 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3483 | 1/1   | 0.89 | 0.41 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1718 | 1/1   | 0.89 | 0.28 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3409 | 1/1   | 0.89 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3478 | 1/1   | 0.89 | 0.33 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3357 | 1/1   | 0.89 | 0.33 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1665 | 1/1   | 0.89 | 0.34 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3413 | 1/1   | 0.89 | 0.07 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1775 | 1/1   | 0.89 | 0.11 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3499 | 1/1   | 0.89 | 0.31 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3047 | 1/1   | 0.89 | 0.28 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3484 | 1/1   | 0.89 | 0.21 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1602 | 1/1   | 0.89 | 0.18 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3262 | 1/1   | 0.89 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1796 | 1/1   | 0.89 | 0.30 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3510 | 1/1   | 0.89 | 0.12 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1782 | 1/1   | 0.89 | 0.25 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1642 | 1/1   | 0.89 | 0.36 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1786 | 1/1   | 0.89 | 0.26 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1606 | 1/1   | 0.89 | 0.19 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3311 | 1/1   | 0.89 | 0.23 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3053 | 1/1   | 0.89 | 0.28 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1771 | 1/1   | 0.89 | 0.13 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3086 | 1/1   | 0.89 | 0.35 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3377 | 1/1   | 0.89 | 0.17 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3161 | 1/1   | 0.89 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3428 | 1/1   | 0.89 | 0.13 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1706 | 1/1   | 0.89 | 0.32 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3586 | 1/1   | 0.89 | 0.37 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3317 | 1/1   | 0.89 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3318 | 1/1   | 0.89 | 0.28 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3259 | 1/1   | 0.89 | 0.30 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3272 | 1/1   | 0.89 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3432 | 1/1   | 0.89 | 0.23 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3262 | 1/1   | 0.89 | 0.13 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3263 | 1/1   | 0.89 | 0.33 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3162 | 1/1   | 0.89 | 0.18 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3394 | 1/1   | 0.89 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3504 | 1/1   | 0.89 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3102 | 1/1   | 0.89 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3325 | 1/1   | 0.89 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1616 | 1/1   | 0.89 | 0.29 | 81,81,81,81                 | 0     |
| 54  | MG   | D3    | 101  | 1/1   | 0.89 | 0.31 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3123 | 1/1   | 0.89 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3115 | 1/1   | 0.89 | 0.28 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3127 | 1/1   | 0.89 | 0.14 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1669 | 1/1   | 0.90 | 0.27 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3528 | 1/1   | 0.90 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3346 | 1/1   | 0.90 | 0.17 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3202 | 1/1   | 0.90 | 0.26 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3138 | 1/1   | 0.90 | 0.27 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3014 | 1/1   | 0.90 | 0.33 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3206 | 1/1   | 0.90 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1675 | 1/1   | 0.90 | 0.20 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3334 | 1/1   | 0.90 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3238 | 1/1   | 0.90 | 0.33 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3005 | 1/1   | 0.90 | 0.44 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3440 | 1/1   | 0.90 | 0.16 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3434 | 1/1   | 0.90 | 0.10 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3017 | 1/1   | 0.90 | 0.22 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3045 | 1/1   | 0.90 | 0.15 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3277 | 1/1   | 0.90 | 0.14 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1612 | 1/1   | 0.90 | 0.09 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1613 | 1/1   | 0.90 | 0.20 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3242 | 1/1   | 0.90 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3121 | 1/1   | 0.90 | 0.21 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3110 | 1/1   | 0.90 | 0.27 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3492 | 1/1   | 0.90 | 0.19 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1697 | 1/1   | 0.90 | 0.15 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3454 | 1/1   | 0.90 | 0.29 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3234 | 1/1   | 0.90 | 0.16 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3019 | 1/1   | 0.90 | 0.22 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1620 | 1/1   | 0.90 | 0.27 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3028 | 1/1   | 0.90 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3150 | 1/1   | 0.90 | 0.34 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3546 | 1/1   | 0.90 | 0.21 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3124 | 1/1   | 0.90 | 0.24 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3496 | 1/1   | 0.90 | 0.25 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3124 | 1/1   | 0.90 | 0.38 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3550 | 1/1   | 0.90 | 0.24 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3256 | 1/1   | 0.90 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3322 | 1/1   | 0.90 | 0.23 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1766 | 1/1   | 0.90 | 0.30 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3323 | 1/1   | 0.90 | 0.24 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1605 | 1/1   | 0.90 | 0.07 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3364 | 1/1   | 0.90 | 0.21 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3135 | 1/1   | 0.90 | 0.18 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3484 | 1/1   | 0.90 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3485 | 1/1   | 0.90 | 0.30 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3487 | 1/1   | 0.90 | 0.25 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3220 | 1/1   | 0.90 | 0.10 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3006 | 1/1   | 0.90 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3268 | 1/1   | 0.90 | 0.35 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3507 | 1/1   | 0.90 | 0.20 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3455 | 1/1   | 0.90 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1707 | 1/1   | 0.90 | 0.26 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3328 | 1/1   | 0.90 | 0.25 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1777 | 1/1   | 0.90 | 0.18 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3565 | 1/1   | 0.90 | 0.32 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3383 | 1/1   | 0.90 | 0.21 | 87,87,87,87                 | 0     |
| 54  | MG   | BB    | 207  | 1/1   | 0.90 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3504 | 1/1   | 0.90 | 0.38 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3254 | 1/1   | 0.90 | 0.21 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3567 | 1/1   | 0.90 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3256 | 1/1   | 0.90 | 0.36 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3028 | 1/1   | 0.90 | 0.29 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3062 | 1/1   | 0.90 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 1762 | 1/1   | 0.90 | 0.28 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1646 | 1/1   | 0.90 | 0.08 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3293 | 1/1   | 0.90 | 0.29 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3518 | 1/1   | 0.90 | 0.30 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3415 | 1/1   | 0.90 | 0.31 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3162 | 1/1   | 0.90 | 0.13 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3163 | 1/1   | 0.90 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3522 | 1/1   | 0.90 | 0.24 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1789 | 1/1   | 0.90 | 0.15 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3165 | 1/1   | 0.90 | 0.31 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3404 | 1/1   | 0.90 | 0.17 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3335 | 1/1   | 0.90 | 0.17 | 75,75,75,75                 | 0     |
| 54  | MG   | DB    | 204  | 1/1   | 0.90 | 0.16 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3224 | 1/1   | 0.90 | 0.46 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3260 | 1/1   | 0.90 | 0.33 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3070 | 1/1   | 0.90 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3172 | 1/1   | 0.90 | 0.34 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3113 | 1/1   | 0.90 | 0.27 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3589 | 1/1   | 0.90 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | BO    | 201  | 1/1   | 0.90 | 0.20 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3310 | 1/1   | 0.90 | 0.43 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3180 | 1/1   | 0.90 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3132 | 1/1   | 0.90 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | AA    | 1686 | 1/1   | 0.90 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | B7    | 101  | 1/1   | 0.90 | 0.35 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3265 | 1/1   | 0.90 | 0.18 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1831 | 1/1   | 0.90 | 0.27 | 91,91,91,91                 | 0     |
| 54  | MG   | DU    | 202  | 1/1   | 0.90 | 0.09 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3116 | 1/1   | 0.90 | 0.20 | 84,84,84,84                 | 0     |
| 54  | MG   | D8    | 101  | 1/1   | 0.90 | 0.29 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1663 | 1/1   | 0.90 | 0.14 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3198 | 1/1   | 0.90 | 0.33 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1738 | 1/1   | 0.90 | 0.36 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3285 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3417 | 1/1   | 0.91 | 0.31 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3368 | 1/1   | 0.91 | 0.23 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3524 | 1/1   | 0.91 | 0.24 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3031 | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3290 | 1/1   | 0.91 | 0.24 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3087 | 1/1   | 0.91 | 0.24 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3234 | 1/1   | 0.91 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3201 | 1/1   | 0.91 | 0.26 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3315 | 1/1   | 0.91 | 0.25 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3581 | 1/1   | 0.91 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3297 | 1/1   | 0.91 | 0.40 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3369 | 1/1   | 0.91 | 0.33 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3201 | 1/1   | 0.91 | 0.34 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3460 | 1/1   | 0.91 | 0.07 | 189,189,189,189             | 0     |
| 54  | MG   | BA    | 3066 | 1/1   | 0.91 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3470 | 1/1   | 0.91 | 0.22 | 54,54,54,54                 | 0     |
| 54  | MG   | BB    | 204  | 1/1   | 0.91 | 0.31 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1813 | 1/1   | 0.91 | 0.23 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3474 | 1/1   | 0.91 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3003 | 1/1   | 0.91 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3175 | 1/1   | 0.91 | 0.23 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3477 | 1/1   | 0.91 | 0.13 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3480 | 1/1   | 0.91 | 0.57 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3373 | 1/1   | 0.91 | 0.21 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3211 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3591 | 1/1   | 0.91 | 0.25 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3311 | 1/1   | 0.91 | 0.32 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3467 | 1/1   | 0.91 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3176 | 1/1   | 0.91 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3073 | 1/1   | 0.91 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3492 | 1/1   | 0.91 | 0.19 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3012 | 1/1   | 0.91 | 0.29 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3013 | 1/1   | 0.91 | 0.24 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1830 | 1/1   | 0.91 | 0.12 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3403 | 1/1   | 0.91 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3498 | 1/1   | 0.91 | 0.13 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3144 | 1/1   | 0.91 | 0.19 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3020 | 1/1   | 0.91 | 0.25 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3146 | 1/1   | 0.91 | 0.23 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3502 | 1/1   | 0.91 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3133 | 1/1   | 0.91 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1730 | 1/1   | 0.91 | 0.20 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3236 | 1/1   | 0.91 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3237 | 1/1   | 0.91 | 0.30 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3246 | 1/1   | 0.91 | 0.28 | 62,62,62,62                 | 0     |
| 54  | MG   | AA    | 1760 | 1/1   | 0.91 | 0.19 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3241 | 1/1   | 0.91 | 0.32 | 74,74,74,74                 | 0     |
| 54  | MG   | BE    | 303  | 1/1   | 0.91 | 0.17 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3547 | 1/1   | 0.91 | 0.13 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3058 | 1/1   | 0.91 | 0.29 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3512 | 1/1   | 0.91 | 0.16 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3157 | 1/1   | 0.91 | 0.27 | 58,58,58,58                 | 0     |
| 54  | MG   | CA    | 1783 | 1/1   | 0.91 | 0.33 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1784 | 1/1   | 0.91 | 0.27 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3339 | 1/1   | 0.91 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3161 | 1/1   | 0.91 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | B2    | 201  | 1/1   | 0.91 | 0.19 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3077 | 1/1   | 0.91 | 0.15 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3140 | 1/1   | 0.91 | 0.37 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3515 | 1/1   | 0.91 | 0.26 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3431 | 1/1   | 0.91 | 0.12 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3480 | 1/1   | 0.91 | 0.35 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3412 | 1/1   | 0.91 | 0.25 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3097 | 1/1   | 0.91 | 0.14 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3046 | 1/1   | 0.91 | 0.28 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3170 | 1/1   | 0.91 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | CA    | 1699 | 1/1   | 0.91 | 0.30 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3174 | 1/1   | 0.91 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | AA    | 1695 | 1/1   | 0.91 | 0.09 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3356 | 1/1   | 0.91 | 0.13 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3441 | 1/1   | 0.91 | 0.06 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3618 | 1/1   | 0.91 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | DR    | 201  | 1/1   | 0.91 | 0.07 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3048 | 1/1   | 0.91 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3277 | 1/1   | 0.91 | 0.27 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3179 | 1/1   | 0.91 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3104 | 1/1   | 0.91 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3447 | 1/1   | 0.91 | 0.11 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3005 | 1/1   | 0.91 | 0.28 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3448 | 1/1   | 0.91 | 0.24 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3112 | 1/1   | 0.91 | 0.24 | 58,58,58,58                 | 0     |
| 56  | ZN   | CG    | 303  | 1/1   | 0.91 | 0.13 | 139,139,139,139             | 0     |
| 54  | MG   | DA    | 3050 | 1/1   | 0.92 | 0.24 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3051 | 1/1   | 0.92 | 0.39 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3054 | 1/1   | 0.92 | 0.35 | 65,65,65,65                 | 0     |
| 54  | MG   | AA    | 1698 | 1/1   | 0.92 | 0.14 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3275 | 1/1   | 0.92 | 0.33 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1647 | 1/1   | 0.92 | 0.13 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BE    | 302  | 1/1   | 0.92 | 0.09 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3203 | 1/1   | 0.92 | 0.10 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1718 | 1/1   | 0.92 | 0.09 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3156 | 1/1   | 0.92 | 0.28 | 49,49,49,49                 | 0     |
| 54  | MG   | CA    | 1650 | 1/1   | 0.92 | 0.16 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3592 | 1/1   | 0.92 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3038 | 1/1   | 0.92 | 0.27 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3141 | 1/1   | 0.92 | 0.25 | 76,76,76,76                 | 0     |
| 54  | MG   | BO    | 202  | 1/1   | 0.92 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1726 | 1/1   | 0.92 | 0.37 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3372 | 1/1   | 0.92 | 0.21 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1796 | 1/1   | 0.92 | 0.20 | 81,81,81,81                 | 0     |
| 54  | MG   | B1    | 201  | 1/1   | 0.92 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | AC    | 107  | 1/1   | 0.92 | 0.09 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3040 | 1/1   | 0.92 | 0.29 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3211 | 1/1   | 0.92 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3042 | 1/1   | 0.92 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3600 | 1/1   | 0.92 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | CA    | 1734 | 1/1   | 0.92 | 0.28 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3479 | 1/1   | 0.92 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1661 | 1/1   | 0.92 | 0.25 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3482 | 1/1   | 0.92 | 0.31 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3173 | 1/1   | 0.92 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3384 | 1/1   | 0.92 | 0.36 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3016 | 1/1   | 0.92 | 0.28 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3401 | 1/1   | 0.92 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1667 | 1/1   | 0.92 | 0.27 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3445 | 1/1   | 0.92 | 0.36 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3147 | 1/1   | 0.92 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3067 | 1/1   | 0.92 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 1806 | 1/1   | 0.92 | 0.40 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3365 | 1/1   | 0.92 | 0.24 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3366 | 1/1   | 0.92 | 0.31 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3452 | 1/1   | 0.92 | 0.20 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3181 | 1/1   | 0.92 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3616 | 1/1   | 0.92 | 0.30 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3009 | 1/1   | 0.92 | 0.22 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3295 | 1/1   | 0.92 | 0.32 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1787 | 1/1   | 0.92 | 0.12 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3096 | 1/1   | 0.92 | 0.31 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3198 | 1/1   | 0.92 | 0.26 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3505 | 1/1   | 0.92 | 0.32 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3014 | 1/1   | 0.92 | 0.35 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3333 | 1/1   | 0.92 | 0.16 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3509 | 1/1   | 0.92 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1685 | 1/1   | 0.92 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3556 | 1/1   | 0.92 | 0.32 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3513 | 1/1   | 0.92 | 0.39 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3001 | 1/1   | 0.92 | 0.34 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3019 | 1/1   | 0.92 | 0.19 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1619 | 1/1   | 0.92 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3374 | 1/1   | 0.92 | 0.22 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1691 | 1/1   | 0.92 | 0.27 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3212 | 1/1   | 0.92 | 0.26 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3228 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3560 | 1/1   | 0.92 | 0.20 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3026 | 1/1   | 0.92 | 0.26 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3027 | 1/1   | 0.92 | 0.13 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3465 | 1/1   | 0.92 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3423 | 1/1   | 0.92 | 0.15 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3003 | 1/1   | 0.92 | 0.20 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3338 | 1/1   | 0.92 | 0.13 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3230 | 1/1   | 0.92 | 0.14 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1659 | 1/1   | 0.92 | 0.21 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3568 | 1/1   | 0.92 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3228 | 1/1   | 0.92 | 0.26 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3569 | 1/1   | 0.92 | 0.29 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3232 | 1/1   | 0.92 | 0.23 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1770 | 1/1   | 0.92 | 0.12 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3266 | 1/1   | 0.92 | 0.28 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3340 | 1/1   | 0.92 | 0.34 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1810 | 1/1   | 0.92 | 0.43 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3574 | 1/1   | 0.92 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3007 | 1/1   | 0.92 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1784 | 1/1   | 0.92 | 0.13 | 82,82,82,82                 | 0     |
| 54  | MG   | BB    | 210  | 1/1   | 0.92 | 0.37 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3384 | 1/1   | 0.92 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3011 | 1/1   | 0.92 | 0.24 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3249 | 1/1   | 0.92 | 0.20 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3112 | 1/1   | 0.92 | 0.42 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3310 | 1/1   | 0.92 | 0.24 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3351 | 1/1   | 0.92 | 0.18 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1680 | 1/1   | 0.92 | 0.09 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1644 | 1/1   | 0.92 | 0.22 | 85,85,85,85                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1701 | 1/1   | 0.93 | 0.07 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3076 | 1/1   | 0.93 | 0.22 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3061 | 1/1   | 0.93 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1633 | 1/1   | 0.93 | 0.25 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3408 | 1/1   | 0.93 | 0.24 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3358 | 1/1   | 0.93 | 0.30 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3178 | 1/1   | 0.93 | 0.23 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3189 | 1/1   | 0.93 | 0.33 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3278 | 1/1   | 0.93 | 0.36 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3413 | 1/1   | 0.93 | 0.13 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3267 | 1/1   | 0.93 | 0.23 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1793 | 1/1   | 0.93 | 0.36 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3255 | 1/1   | 0.93 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3587 | 1/1   | 0.93 | 0.10 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3196 | 1/1   | 0.93 | 0.28 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1677 | 1/1   | 0.93 | 0.31 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3080 | 1/1   | 0.93 | 0.22 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3626 | 1/1   | 0.93 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3033 | 1/1   | 0.93 | 0.29 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3021 | 1/1   | 0.93 | 0.24 | 63,63,63,63                 | 0     |
| 54  | MG   | CG    | 302  | 1/1   | 0.93 | 0.08 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1645 | 1/1   | 0.93 | 0.22 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3421 | 1/1   | 0.93 | 0.30 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3486 | 1/1   | 0.93 | 0.29 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1763 | 1/1   | 0.93 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1723 | 1/1   | 0.93 | 0.31 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3288 | 1/1   | 0.93 | 0.27 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3508 | 1/1   | 0.93 | 0.34 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3023 | 1/1   | 0.93 | 0.26 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3091 | 1/1   | 0.93 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3286 | 1/1   | 0.93 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1687 | 1/1   | 0.93 | 0.18 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3216 | 1/1   | 0.93 | 0.07 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3216 | 1/1   | 0.93 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3142 | 1/1   | 0.93 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3239 | 1/1   | 0.93 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3220 | 1/1   | 0.93 | 0.21 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3024 | 1/1   | 0.93 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3222 | 1/1   | 0.93 | 0.39 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3105 | 1/1   | 0.93 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3302 | 1/1   | 0.93 | 0.16 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3159 | 1/1   | 0.93 | 0.19 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3106 | 1/1   | 0.93 | 0.36 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3294 | 1/1   | 0.93 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3230 | 1/1   | 0.93 | 0.35 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1766 | 1/1   | 0.93 | 0.07 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3378 | 1/1   | 0.93 | 0.26 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3052 | 1/1   | 0.93 | 0.27 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3320 | 1/1   | 0.93 | 0.33 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3235 | 1/1   | 0.93 | 0.36 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3105 | 1/1   | 0.93 | 0.23 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3106 | 1/1   | 0.93 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3007 | 1/1   | 0.93 | 0.30 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3317 | 1/1   | 0.93 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3239 | 1/1   | 0.93 | 0.28 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3564 | 1/1   | 0.93 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3111 | 1/1   | 0.93 | 0.40 | 105,105,105,105             | 0     |
| 54  | MG   | BA    | 3027 | 1/1   | 0.93 | 0.23 | 53,53,53,53                 | 0     |
| 54  | MG   | DE    | 303  | 1/1   | 0.93 | 0.25 | 85,85,85,85                 | 0     |
| 54  | MG   | DE    | 304  | 1/1   | 0.93 | 0.29 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3244 | 1/1   | 0.93 | 0.05 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3245 | 1/1   | 0.93 | 0.24 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3110 | 1/1   | 0.93 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | AA    | 1618 | 1/1   | 0.93 | 0.17 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3609 | 1/1   | 0.93 | 0.32 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3611 | 1/1   | 0.93 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3120 | 1/1   | 0.93 | 0.27 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3324 | 1/1   | 0.93 | 0.32 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1661 | 1/1   | 0.93 | 0.36 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3535 | 1/1   | 0.93 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | B0    | 201  | 1/1   | 0.94 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3009 | 1/1   | 0.94 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3194 | 1/1   | 0.94 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3076 | 1/1   | 0.94 | 0.15 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3469 | 1/1   | 0.94 | 0.34 | 50,50,50,50                 | 0     |
| 54  | MG   | BU    | 201  | 1/1   | 0.94 | 0.09 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3506 | 1/1   | 0.94 | 0.33 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1689 | 1/1   | 0.94 | 0.33 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3026 | 1/1   | 0.94 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3223 | 1/1   | 0.94 | 0.31 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3139 | 1/1   | 0.94 | 0.36 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1640 | 1/1   | 0.94 | 0.26 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1670 | 1/1   | 0.94 | 0.21 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1778 | 1/1   | 0.94 | 0.33 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3229 | 1/1   | 0.94 | 0.37 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3202 | 1/1   | 0.94 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3313 | 1/1   | 0.94 | 0.28 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3314 | 1/1   | 0.94 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3155 | 1/1   | 0.94 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3022 | 1/1   | 0.94 | 0.21 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3233 | 1/1   | 0.94 | 0.18 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3561 | 1/1   | 0.94 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3167 | 1/1   | 0.94 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3070 | 1/1   | 0.94 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3494 | 1/1   | 0.94 | 0.35 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1721 | 1/1   | 0.94 | 0.34 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3620 | 1/1   | 0.94 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3169 | 1/1   | 0.94 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3052 | 1/1   | 0.94 | 0.28 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3279 | 1/1   | 0.94 | 0.29 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1610 | 1/1   | 0.94 | 0.11 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3208 | 1/1   | 0.94 | 0.49 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3475 | 1/1   | 0.94 | 0.09 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3476 | 1/1   | 0.94 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3247 | 1/1   | 0.94 | 0.32 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3015 | 1/1   | 0.94 | 0.07 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3210 | 1/1   | 0.94 | 0.18 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1602 | 1/1   | 0.94 | 0.14 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3212 | 1/1   | 0.94 | 0.31 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3252 | 1/1   | 0.94 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3214 | 1/1   | 0.94 | 0.18 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3580 | 1/1   | 0.94 | 0.34 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3512 | 1/1   | 0.94 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1658 | 1/1   | 0.94 | 0.21 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3439 | 1/1   | 0.94 | 0.25 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3251 | 1/1   | 0.94 | 0.31 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1781 | 1/1   | 0.94 | 0.04 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3125 | 1/1   | 0.94 | 0.26 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3004 | 1/1   | 0.94 | 0.21 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3292 | 1/1   | 0.94 | 0.10 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1627 | 1/1   | 0.94 | 0.08 | 111,111,111,111             | 0     |
| 54  | MG   | DA    | 3264 | 1/1   | 0.94 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3329 | 1/1   | 0.94 | 0.34 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3266 | 1/1   | 0.94 | 0.13 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1619 | 1/1   | 0.94 | 0.11 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1630 | 1/1   | 0.94 | 0.08 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1832 | 1/1   | 0.94 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3593 | 1/1   | 0.94 | 0.21 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3271 | 1/1   | 0.94 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3272 | 1/1   | 0.94 | 0.11 | 65,65,65,65                 | 0     |
| 54  | MG   | AA    | 1783 | 1/1   | 0.94 | 0.32 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3194 | 1/1   | 0.94 | 0.41 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3059 | 1/1   | 0.94 | 0.33 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3449 | 1/1   | 0.94 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3361 | 1/1   | 0.94 | 0.36 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3083 | 1/1   | 0.94 | 0.29 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3128 | 1/1   | 0.94 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3199 | 1/1   | 0.94 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3041 | 1/1   | 0.94 | 0.43 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1637 | 1/1   | 0.94 | 0.09 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3203 | 1/1   | 0.94 | 0.35 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3131 | 1/1   | 0.94 | 0.28 | 77,77,77,77                 | 0     |
| 54  | MG   | BD    | 301  | 1/1   | 0.94 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3085 | 1/1   | 0.94 | 0.27 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3497 | 1/1   | 0.94 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3261 | 1/1   | 0.94 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3190 | 1/1   | 0.94 | 0.29 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3292 | 1/1   | 0.94 | 0.21 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1793 | 1/1   | 0.94 | 0.15 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3139 | 1/1   | 0.94 | 0.14 | 63,63,63,63                 | 0     |
| 56  | ZN   | AG    | 302  | 1/1   | 0.94 | 0.19 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 3159 | 1/1   | 0.94 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3458 | 1/1   | 0.94 | 0.33 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3093 | 1/1   | 0.95 | 0.06 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3585 | 1/1   | 0.95 | 0.38 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3116 | 1/1   | 0.95 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | AN    | 201  | 1/1   | 0.95 | 0.06 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3118 | 1/1   | 0.95 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3119 | 1/1   | 0.95 | 0.31 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3613 | 1/1   | 0.95 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3398 | 1/1   | 0.95 | 0.29 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3010 | 1/1   | 0.95 | 0.31 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3185 | 1/1   | 0.95 | 0.37 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3467 | 1/1   | 0.95 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3104 | 1/1   | 0.95 | 0.20 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3425 | 1/1   | 0.95 | 0.22 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3471 | 1/1   | 0.95 | 0.26 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3538 | 1/1   | 0.95 | 0.19 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3233 | 1/1   | 0.95 | 0.09 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3420 | 1/1   | 0.95 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3187 | 1/1   | 0.95 | 0.30 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3501 | 1/1   | 0.95 | 0.26 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1665 | 1/1   | 0.95 | 0.14 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1666 | 1/1   | 0.95 | 0.10 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3282 | 1/1   | 0.95 | 0.27 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3171 | 1/1   | 0.95 | 0.42 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3126 | 1/1   | 0.95 | 0.30 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3173 | 1/1   | 0.95 | 0.28 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3545 | 1/1   | 0.95 | 0.26 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1671 | 1/1   | 0.95 | 0.12 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3176 | 1/1   | 0.95 | 0.45 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3396 | 1/1   | 0.95 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3035 | 1/1   | 0.95 | 0.24 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3491 | 1/1   | 0.95 | 0.11 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1663 | 1/1   | 0.95 | 0.11 | 72,72,72,72                 | 0     |
| 54  | MG   | DE    | 301  | 1/1   | 0.95 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | BF    | 301  | 1/1   | 0.95 | 0.06 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3269 | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3098 | 1/1   | 0.95 | 0.23 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3575 | 1/1   | 0.95 | 0.22 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3030 | 1/1   | 0.95 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3108 | 1/1   | 0.95 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3002 | 1/1   | 0.95 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | CA    | 1680 | 1/1   | 0.95 | 0.06 | 104,104,104,104             | 0     |
| 54  | MG   | D5    | 101  | 1/1   | 0.95 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3578 | 1/1   | 0.95 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3051 | 1/1   | 0.95 | 0.26 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1609 | 1/1   | 0.95 | 0.30 | 61,61,61,61                 | 0     |
| 54  | MG   | B3    | 101  | 1/1   | 0.95 | 0.41 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3213 | 1/1   | 0.95 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3193 | 1/1   | 0.95 | 0.21 | 76,76,76,76                 | 0     |
| 54  | MG   | CC    | 103  | 1/1   | 0.96 | 0.24 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3137 | 1/1   | 0.96 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3481 | 1/1   | 0.96 | 0.26 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3351 | 1/1   | 0.96 | 0.21 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3188 | 1/1   | 0.96 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3065 | 1/1   | 0.96 | 0.44 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1744 | 1/1   | 0.96 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3486 | 1/1   | 0.96 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1604 | 1/1   | 0.96 | 0.09 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3208 | 1/1   | 0.96 | 0.24 | 57,57,57,57                 | 0     |
| 54  | MG   | B5    | 1701 | 1/1   | 0.96 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3205 | 1/1   | 0.96 | 0.23 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3179 | 1/1   | 0.96 | 0.41 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3627 | 1/1   | 0.96 | 0.35 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3273 | 1/1   | 0.96 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3242 | 1/1   | 0.96 | 0.37 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3081 | 1/1   | 0.96 | 0.15 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3103 | 1/1   | 0.96 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3553 | 1/1   | 0.96 | 0.22 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3055 | 1/1   | 0.96 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3385 | 1/1   | 0.96 | 0.33 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3610 | 1/1   | 0.96 | 0.21 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3280 | 1/1   | 0.96 | 0.23 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3107 | 1/1   | 0.96 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3571 | 1/1   | 0.96 | 0.24 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3283 | 1/1   | 0.96 | 0.09 | 69,69,69,69                 | 0     |
| 54  | MG   | DP    | 201  | 1/1   | 0.96 | 0.15 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3136 | 1/1   | 0.96 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | AC    | 103  | 1/1   | 0.96 | 0.36 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3321 | 1/1   | 0.96 | 0.37 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3195 | 1/1   | 0.96 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1703 | 1/1   | 0.96 | 0.27 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3224 | 1/1   | 0.96 | 0.41 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3255 | 1/1   | 0.96 | 0.34 | 62,62,62,62                 | 0     |
| 54  | MG   | AA    | 1657 | 1/1   | 0.96 | 0.30 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3172 | 1/1   | 0.96 | 0.42 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3044 | 1/1   | 0.96 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3078 | 1/1   | 0.96 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3244 | 1/1   | 0.96 | 0.21 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3043 | 1/1   | 0.97 | 0.27 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3174 | 1/1   | 0.97 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3037 | 1/1   | 0.97 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3041 | 1/1   | 0.97 | 0.09 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1745 | 1/1   | 0.97 | 0.39 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1733 | 1/1   | 0.97 | 0.32 | 79,79,79,79                 | 0     |
| 54  | MG   | CN    | 201  | 1/1   | 0.97 | 0.05 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1622 | 1/1   | 0.97 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3584 | 1/1   | 0.97 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3468 | 1/1   | 0.97 | 0.31 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3097 | 1/1   | 0.97 | 0.40 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3109 | 1/1   | 0.97 | 0.32 | 61,61,61,61                 | 0     |

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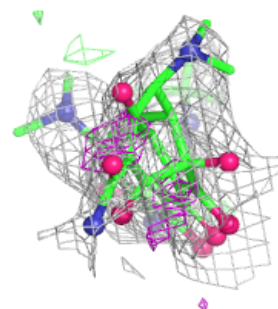
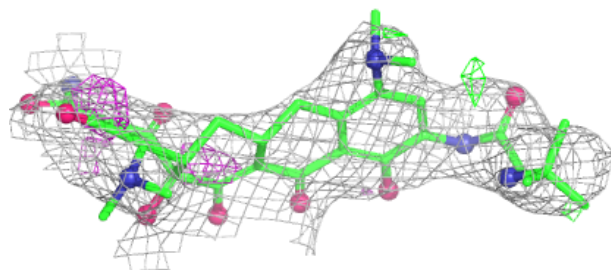
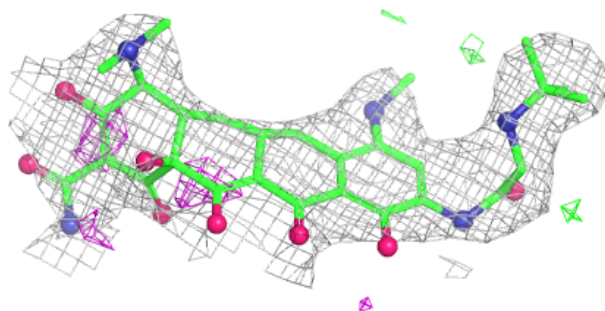
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3457 | 1/1   | 0.97 | 0.35 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3307 | 1/1   | 0.97 | 0.23 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3189 | 1/1   | 0.97 | 0.36 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3422 | 1/1   | 0.97 | 0.23 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3029 | 1/1   | 0.97 | 0.25 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3461 | 1/1   | 0.97 | 0.23 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3053 | 1/1   | 0.97 | 0.37 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1607 | 1/1   | 0.97 | 0.08 | 89,89,89,89                 | 0     |
| 54  | MG   | B7    | 102  | 1/1   | 0.97 | 0.33 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3010 | 1/1   | 0.97 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3117 | 1/1   | 0.97 | 0.25 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3183 | 1/1   | 0.97 | 0.30 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3395 | 1/1   | 0.98 | 0.06 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3572 | 1/1   | 0.98 | 0.29 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3397 | 1/1   | 0.98 | 0.33 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3158 | 1/1   | 0.98 | 0.08 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3352 | 1/1   | 0.98 | 0.25 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3200 | 1/1   | 0.98 | 0.31 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3478 | 1/1   | 0.98 | 0.43 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1623 | 1/1   | 0.98 | 0.08 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3061 | 1/1   | 0.98 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3226 | 1/1   | 0.98 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3073 | 1/1   | 0.98 | 0.07 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1799 | 1/1   | 0.98 | 0.04 | 115,115,115,115             | 0     |
| 56  | ZN   | CQ    | 101  | 1/1   | 0.98 | 0.04 | 123,123,123,123             | 0     |
| 54  | MG   | BA    | 3579 | 1/1   | 0.99 | 0.38 | 51,51,51,51                 | 0     |
| 54  | MG   | CA    | 1668 | 1/1   | 0.99 | 0.35 | 61,61,61,61                 | 0     |

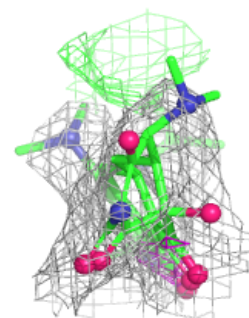
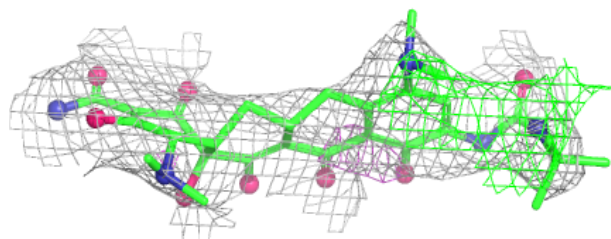
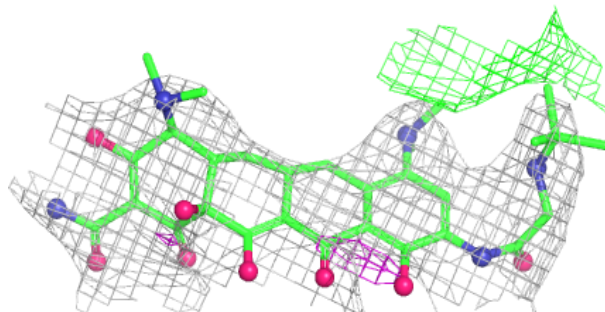
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around T1C AA 1837:**

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

**Electron density around T1C CA 1800:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.