



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 03:54 AM EDT

PDB ID : 9D7T / pdb\_00009d7t  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with Api137 antimicrobial peptide, mRNA, A-site release factor 1, and deacylated P-site and E-site tRNA<sup>phe</sup> at 2.70Å resolution  
Authors : Aleksandrova, E.V.; Huang, W.; Baliga, C.; Atkinson, G.C.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.  
Deposited on : 2024-08-17  
Resolution : 2.70 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                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

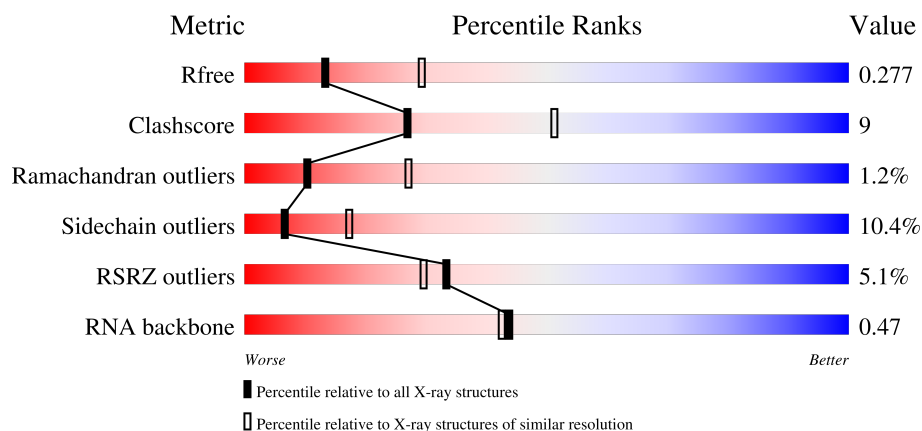
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |
| RNA backbone          | 3983                        | 1044 (2.90-2.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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   | 1A    | 2915   | <br>3% 62% 30% 7% • |
| 1   | 2A    | 2915   | <br>3% 55% 35% 6% • |
| 2   | 1B    | 121    | <br>69% 27% ••      |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | 2B    | 121    |                  |
| 3   | 1D    | 276    |                  |
| 3   | 2D    | 276    |                  |
| 4   | 1E    | 206    |                  |
| 4   | 2E    | 206    |                  |
| 5   | 1F    | 210    |                  |
| 5   | 2F    | 210    |                  |
| 6   | 1G    | 182    |                  |
| 6   | 2G    | 182    |                  |
| 7   | 1H    | 180    |                  |
| 7   | 2H    | 180    |                  |
| 8   | 1I    | 148    |                  |
| 8   | 2I    | 148    |                  |
| 9   | 1N    | 140    |                  |
| 9   | 2N    | 140    |                  |
| 10  | 1O    | 122    |                  |
| 10  | 2O    | 122    |                  |
| 11  | 1P    | 150    |                  |
| 11  | 2P    | 150    |                  |
| 12  | 1Q    | 141    |                  |
| 12  | 2Q    | 141    |                  |
| 13  | 1R    | 118    |                  |
| 13  | 2R    | 118    |                  |
| 14  | 1S    | 112    |                  |
| 14  | 2S    | 112    |                  |

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| Mol | Chain | Length | Quality of chain        |
|-----|-------|--------|-------------------------|
| 15  | 1T    | 146    | <p>2% 64% 23% 10%</p>   |
| 15  | 2T    | 146    | <p>2% 63% 25% 10%</p>   |
| 16  | 1U    | 118    | <p>% 80% 19%</p>        |
| 16  | 2U    | 118    | <p>75% 23%</p>          |
| 17  | 1V    | 101    | <p>82% 17%</p>          |
| 17  | 2V    | 101    | <p>78% 20%</p>          |
| 18  | 1W    | 113    | <p>75% 23%</p>          |
| 18  | 2W    | 113    | <p>75% 24%</p>          |
| 19  | 1X    | 96     | <p>% 70% 27%</p>        |
| 19  | 2X    | 96     | <p>4% 79% 17%</p>       |
| 20  | 1Y    | 110    | <p>75% 19%</p>          |
| 20  | 2Y    | 110    | <p>4% 54% 40%</p>       |
| 21  | 1Z    | 206    | <p>56% 30% 11%</p>      |
| 21  | 2Z    | 206    | <p>% 55% 30% 6% 10%</p> |
| 22  | 10    | 85     | <p>75% 12% 11%</p>      |
| 22  | 20    | 85     | <p>11% 64% 25% 9%</p>   |
| 23  | 11    | 98     | <p>% 86% 12%</p>        |
| 23  | 21    | 98     | <p>4% 79% 16%</p>       |
| 24  | 12    | 72     | <p>4% 68% 26%</p>       |
| 24  | 22    | 72     | <p>% 60% 32% 6%</p>     |
| 25  | 13    | 60     | <p>60% 38%</p>          |
| 25  | 23    | 60     | <p>2% 67% 32%</p>       |
| 26  | 14    | 71     | <p>13% 58% 32% 6%</p>   |
| 26  | 24    | 71     | <p>23% 46% 39% 10%</p>  |
| 27  | 15    | 60     | <p>65% 32%</p>          |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | 25    | 60     |                  |
| 28  | 16    | 54     |                  |
| 28  | 26    | 54     |                  |
| 29  | 17    | 49     |                  |
| 29  | 27    | 49     |                  |
| 30  | 18    | 65     |                  |
| 30  | 28    | 65     |                  |
| 31  | 19    | 37     |                  |
| 31  | 29    | 37     |                  |
| 32  | 1a    | 1521   |                  |
| 32  | 2a    | 1521   |                  |
| 33  | 1b    | 256    |                  |
| 33  | 2b    | 256    |                  |
| 34  | 1c    | 239    |                  |
| 34  | 2c    | 239    |                  |
| 35  | 1d    | 209    |                  |
| 35  | 2d    | 209    |                  |
| 36  | 1e    | 162    |                  |
| 36  | 2e    | 162    |                  |
| 37  | 1f    | 101    |                  |
| 37  | 2f    | 101    |                  |
| 38  | 1g    | 156    |                  |
| 38  | 2g    | 156    |                  |
| 39  | 1h    | 138    |                  |
| 39  | 2h    | 138    |                  |

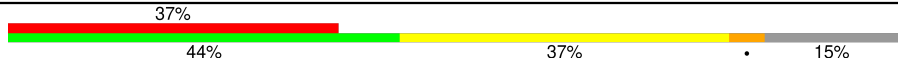
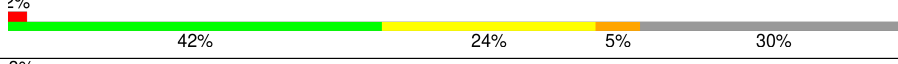
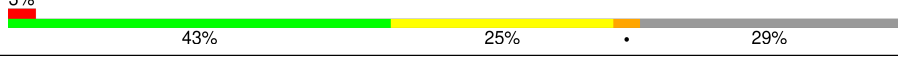
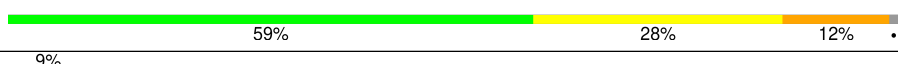
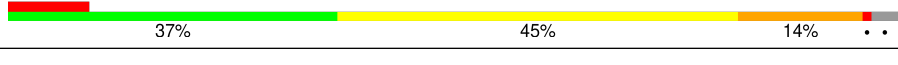
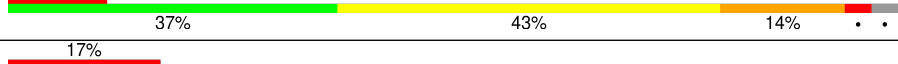
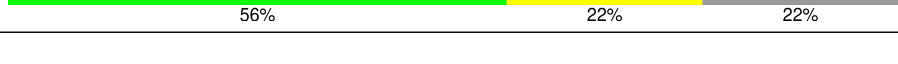
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | 1i    | 128    |                  |
| 40  | 2i    | 128    |                  |
| 41  | 1j    | 105    |                  |
| 41  | 2j    | 105    |                  |
| 42  | 1k    | 129    |                  |
| 42  | 2k    | 129    |                  |
| 43  | 1l    | 132    |                  |
| 43  | 2l    | 132    |                  |
| 44  | 1m    | 126    |                  |
| 44  | 2m    | 126    |                  |
| 45  | 1n    | 61     |                  |
| 45  | 2n    | 61     |                  |
| 46  | 1o    | 89     |                  |
| 46  | 2o    | 89     |                  |
| 47  | 1p    | 88     |                  |
| 47  | 2p    | 88     |                  |
| 48  | 1q    | 105    |                  |
| 48  | 2q    | 105    |                  |
| 49  | 1r    | 88     |                  |
| 49  | 2r    | 88     |                  |
| 50  | 1s    | 93     |                  |
| 50  | 2s    | 93     |                  |
| 51  | 1t    | 106    |                  |
| 51  | 2t    | 106    |                  |
| 52  | 1u    | 27     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 52  | 2u    | 27     |  |
| 53  | 1v    | 24     |  |
| 53  | 2v    | 24     |  |
| 54  | 1w    | 354    |  |
| 54  | 2w    | 354    |  |
| 55  | 1x    | 76     |  |
| 55  | 1y    | 76     |  |
| 55  | 2x    | 76     |  |
| 55  | 2y    | 76     |  |
| 56  | 1z    | 18     |  |
| 56  | 2z    | 18     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | 1A    | 3634 | -         | -        | -       | X                |
| 57  | MG   | 2A    | 3116 | -         | -        | -       | X                |
| 59  | SF4  | 1d    | 302  | -         | -        | X       | -                |

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 299179 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 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | 1A    | 2871     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61852 | 27531 | 11572 | 19878 | 2871 |         |         |       |
| 1   | 2A    | 2800     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60322 | 26848 | 11284 | 19390 | 2800 |         |         |       |

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | 1B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2576  | 1146 | 476 | 834 | 120 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2576  | 1146 | 476 | 834 | 120 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | 1D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |
| 3   | 2D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | 1E    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |
| 4   | 2E    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | 1F    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1584  | 1009 | 298 | 275 | 2 |         |         |       |
| 5   | 2F    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1580  | 1007 | 297 | 274 | 2 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 1G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1425  | 914 | 256 | 251 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 911 | 258 | 251 | 4 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | 1H    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 7   | 2H    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1085  | 693 | 189 | 202 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1061  | 680 | 186 | 194 | 1 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | 1N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |
| 9   | 2N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | 1O    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | 2O    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | 1P    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |
| 11  | 2P    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | 1Q    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 12  | 2Q    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | 1R    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 13  | 2R    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | 1S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |         |         |       |
| 14  | 2S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |         |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | 1T    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1091  | 680 | 225 | 185 | 1 |         |         |       |
| 15  | 2T    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 675 | 224 | 183 | 1 |         |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | 1U    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |
| 16  | 2U    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | 1V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |
| 17  | 2V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | 1W    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |
| 18  | 2W    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | 1X    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |
| 19  | 2X    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 746   | 485 | 134 | 126 | 1 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | 1Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |
| 20  | 2Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1437  | 919 | 256 | 260 | 2 |         |         |       |
| 21  | 2Z    | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1451  | 928 | 256 | 265 | 2 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 10    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 373 | 128 | 102 | 1 |         |         |       |
| 22  | 20    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | 11    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |
| 23  | 21    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | 12    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 24  | 22    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25  | 13    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 25  | 23    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 464   | 296 | 90 | 78 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 14    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 548   | 347 | 99 | 97 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 68       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 330 | 92 | 90 | 5 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | 15    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |
| 27  | 25    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | 16    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 28  | 26    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 279 | 91 | 75 | 4 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29  | 17    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 29  | 27    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30  | 18    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 511   | 328 | 99  | 82 | 2 |         |         |       |
| 30  | 28    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | 19    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 31  | 29    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 32  | 1a    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14358 | 5975 | 10413 | 1500 |         |         |       |
| 32  | 2a    | 1503     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32327 | 14396 | 5990 | 10438 | 1503 |         |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33  | 1b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1846  | 1179 | 331 | 331 | 5 |         |         |       |
| 33  | 2b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1167 | 326 | 327 | 5 |         |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | 1c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1554  | 977 | 302 | 274 | 1 |         |         |       |
| 34  | 2c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1542  | 968 | 300 | 273 | 1 |         |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35  | 1d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1659  | 1040 | 326 | 286 | 7 |         |         |       |
| 35  | 2d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1050 | 333 | 284 | 7 |         |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | 1e    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 213 | 198 | 4 |         |         |       |
| 36  | 2e    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1130  | 714 | 214 | 199 | 3 |         |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | 1f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 513 | 143 | 151 | 3 |         |         |       |
| 37  | 2f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | 1g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1231  | 766 | 243 | 216 | 6 |         |         |       |
| 38  | 2g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | 1h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |
| 39  | 2h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40  | 1i    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 983   | 623 | 193 | 167 |         |         |       |
| 40  | 2i    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 940   | 593 | 185 | 162 |         |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | 1j    | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 721   | 449 | 140 | 132 |         |         |       |
| 41  | 2j    | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 714   | 445 | 138 | 131 |         |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | 1k    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 516 | 155 | 155 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | 2k    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 833   | 519 | 156 | 155 | 3 |         |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | 1l    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 586 | 185 | 159 | 2 |         |         |       |
| 43  | 2l    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 586 | 185 | 159 | 2 |         |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | 1m    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 923   | 569 | 191 | 161 | 2 |         |         |       |
| 44  | 2m    | 115      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 889   | 546 | 183 | 158 | 2 |         |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 45  | 1n    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 45  | 2n    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 486   | 309 | 101 | 72 | 4 |         |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | 1o    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 456 | 144 | 126 | 2 |         |         |       |
| 46  | 2o    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 456 | 144 | 126 | 2 |         |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | 1p    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 433 | 134 | 113 | 1 |         |         |       |
| 47  | 2p    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 677   | 430 | 133 | 113 | 1 |         |         |       |

- Molecule 48 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | 1q    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |
| 48  | 2q    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 49  | 1r    | 68       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |  |         |         |       |
| 49  | 2r    | 68       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 551   | 353 | 108 | 90 |  |         |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | 1s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 652   | 417 | 120 | 113 | 2 |         |         |       |
| 50  | 2s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 646   | 412 | 119 | 113 | 2 |         |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | 1t    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 446 | 156 | 124 | 2 |         |         |       |
| 51  | 2t    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 446 | 155 | 124 | 2 |         |         |       |

- Molecule 52 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 52  | 1u    | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |
| 52  | 2u    | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |

- Molecule 53 is a RNA chain called PHE-Stop mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 53  | 1v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 274   | 124 | 48 | 89 | 13 |         |         |       |
| 53  | 2v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 274   | 124 | 48 | 89 | 13 |         |         |       |

- Molecule 54 is a protein called Peptide chain release factor 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 54  | 1w    | 249      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1939  | 1199 | 360 | 371 | 9 |         |         |       |
| 54  | 2w    | 253      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1954  | 1208 | 361 | 377 | 8 |         |         |       |

- Molecule 55 is a RNA chain called P-site and E-site Deacylated tRNAphe.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 55  | 1x    | 75       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1612  | 722 | 288 | 525 | 75 | 2 |         |         |       |
| 55  | 1y    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1590  | 712 | 285 | 517 | 74 | 2 |         |         |       |
| 55  | 2x    | 75       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1612  | 722 | 288 | 525 | 75 | 2 |         |         |       |
| 55  | 2y    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1592  | 713 | 285 | 518 | 74 | 2 |         |         |       |

- Molecule 56 is a protein called Api137 Antimicrobial Peptide.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 56  | 1z    | 14       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 121   | 80 | 25 | 16 |         |         |       |
| 56  | 2z    | 14       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 121   | 80 | 25 | 16 |         |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | 1A    | 807      | Total | Mg  | 0       | 0       |
|     |       |          | 807   | 807 |         |         |
| 57  | 1B    | 20       | Total | Mg  | 0       | 0       |
|     |       |          | 20    | 20  |         |         |
| 57  | 1D    | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57  | 1E    | 7        | Total<br>7 | Mg<br>7 | 0       | 0       |
| 57  | 1F    | 8        | Total<br>8 | Mg<br>8 | 0       | 0       |
| 57  | 1G    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 57  | 1N    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 57  | 1O    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | 1P    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 57  | 1Q    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 57  | 1R    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | 1T    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | 1U    | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |
| 57  | 1V    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 57  | 1W    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 57  | 1X    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 57  | 1Z    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | 10    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 57  | 11    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 57  | 12    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 57  | 13    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | 14    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 57  | 15    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 57  | 16    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | 17    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 57  | 18    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 19    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1a    | 187      | Total<br>187 | Mg<br>187 | 0       | 0       |
| 57  | 1c    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1f    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1k    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1m    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1n    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1v    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 1w    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 1x    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 57  | 1y    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2A    | 665      | Total<br>665 | Mg<br>665 | 0       | 0       |
| 57  | 2B    | 11       | Total<br>11  | Mg<br>11  | 0       | 0       |
| 57  | 2D    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 57  | 2E    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | 2F    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 57  | 2N    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2O    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | 2Q    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 2R    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2U    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2V    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2W    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2X    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 2Y    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 20    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 21    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 23    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 25    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 28    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 29    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2a    | 172      | Total<br>172 | Mg<br>172 | 0       | 0       |
| 57  | 2d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2e    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2f    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2j    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2k    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2u    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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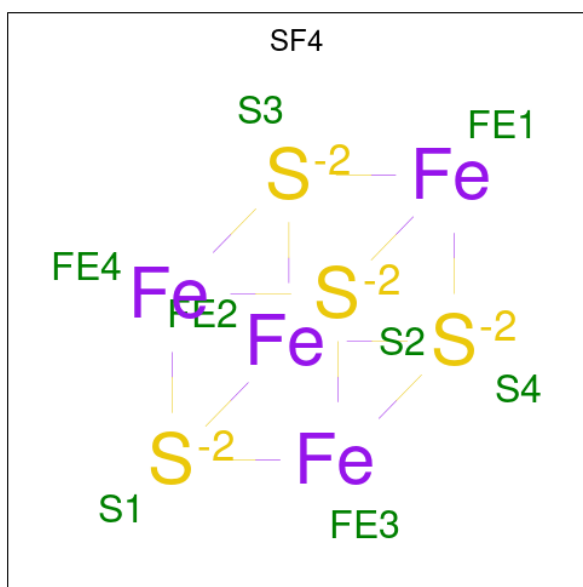
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | 2v    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 57  | 2w    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 57  | 2x    | 9        | Total | Mg | 0       | 0       |
|     |       |          | 9     | 9  |         |         |

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 29    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 2n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 59  | 1d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 59  | 2d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 60 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 60  | 1A    | 1394     | Total | O    | 0       | 0       |
|     |       |          | 1394  | 1394 |         |         |
| 60  | 1B    | 31       | Total | O    | 0       | 0       |
|     |       |          | 31    | 31   |         |         |
| 60  | 1D    | 15       | Total | O    | 0       | 0       |
|     |       |          | 15    | 15   |         |         |
| 60  | 1E    | 12       | Total | O    | 0       | 0       |
|     |       |          | 12    | 12   |         |         |
| 60  | 1F    | 6        | Total | O    | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 60  | 1G    | 1        | Total | O    | 0       | 0       |
|     |       |          | 1     | 1    |         |         |
| 60  | 1N    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 60  | 1O    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 60  | 1P    | 15       | Total | O    | 0       | 0       |
|     |       |          | 15    | 15   |         |         |
| 60  | 1Q    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 1R    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1T    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1U    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 1V    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1W    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1X    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 10    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 11    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 13    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 15    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 16    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 17    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 18    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 1a    | 194      | Total<br>194 | O<br>194 | 0       | 0       |
| 60  | 1d    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1l    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1p    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1v    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 1w    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 1x    | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 60  | 1y    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 1z    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 2A    | 997      | Total<br>997 | O<br>997 | 0       | 0       |
| 60  | 2B    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 60  | 2D    | 16       | Total<br>16  | O<br>16  | 0       | 0       |
| 60  | 2E    | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 60  | 2F    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 2N    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2O    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2P    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 60  | 2Q    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2R    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 2T    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2U    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2W    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2X    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2Y    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 20    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 60  | 21    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 23    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 25    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 27    | 3        | Total<br>3   | O<br>3   | 0       | 0       |

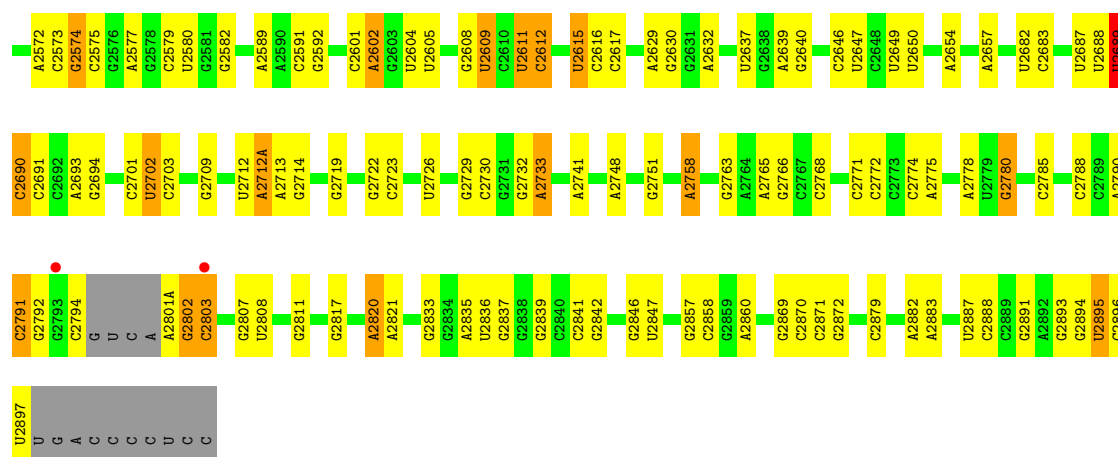
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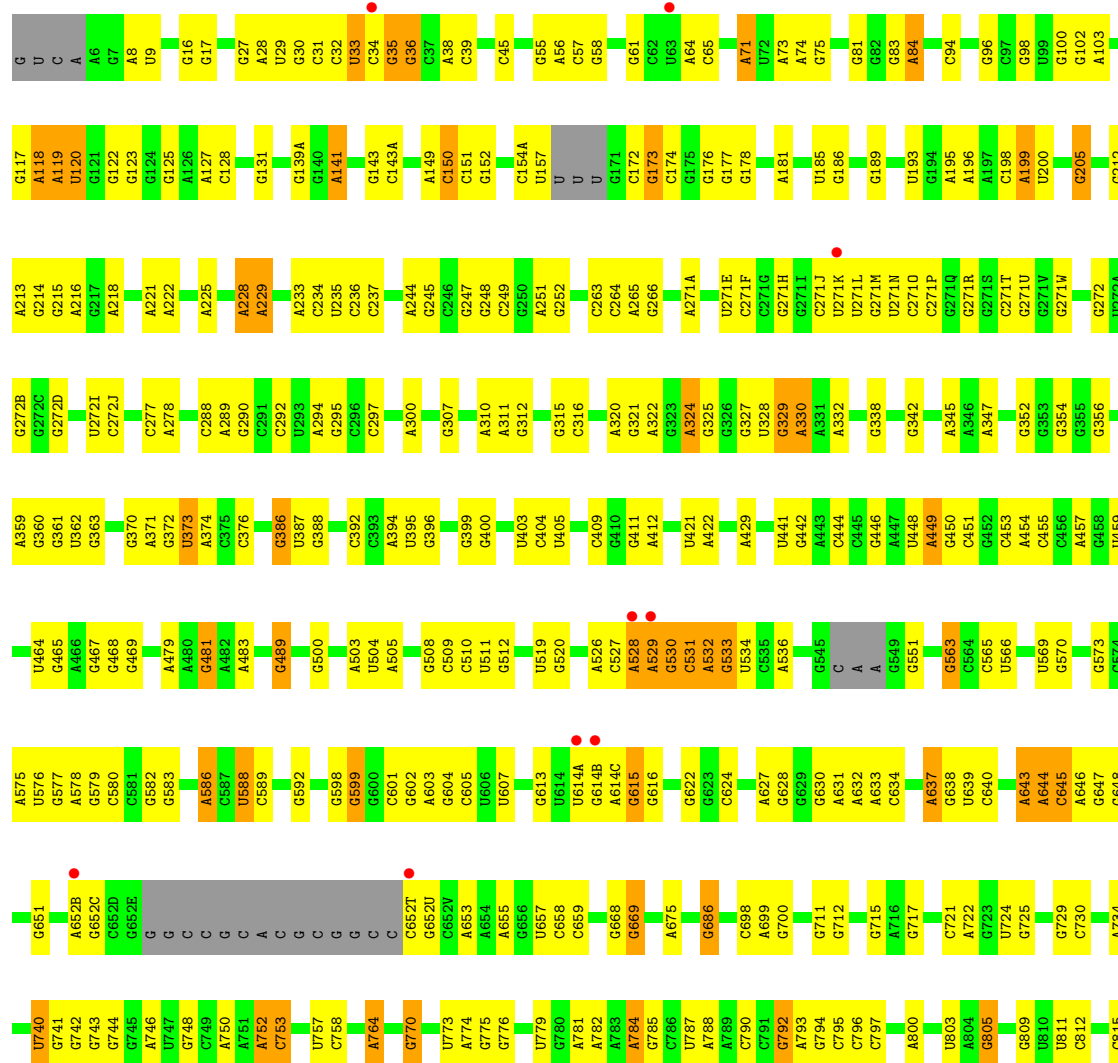
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 28    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 2a    | 154      | Total<br>154 | O<br>154 | 0       | 0       |
| 60  | 2d    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2j    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 2t    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2v    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2w    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 2x    | 13       | Total<br>13  | O<br>13  | 0       | 0       |



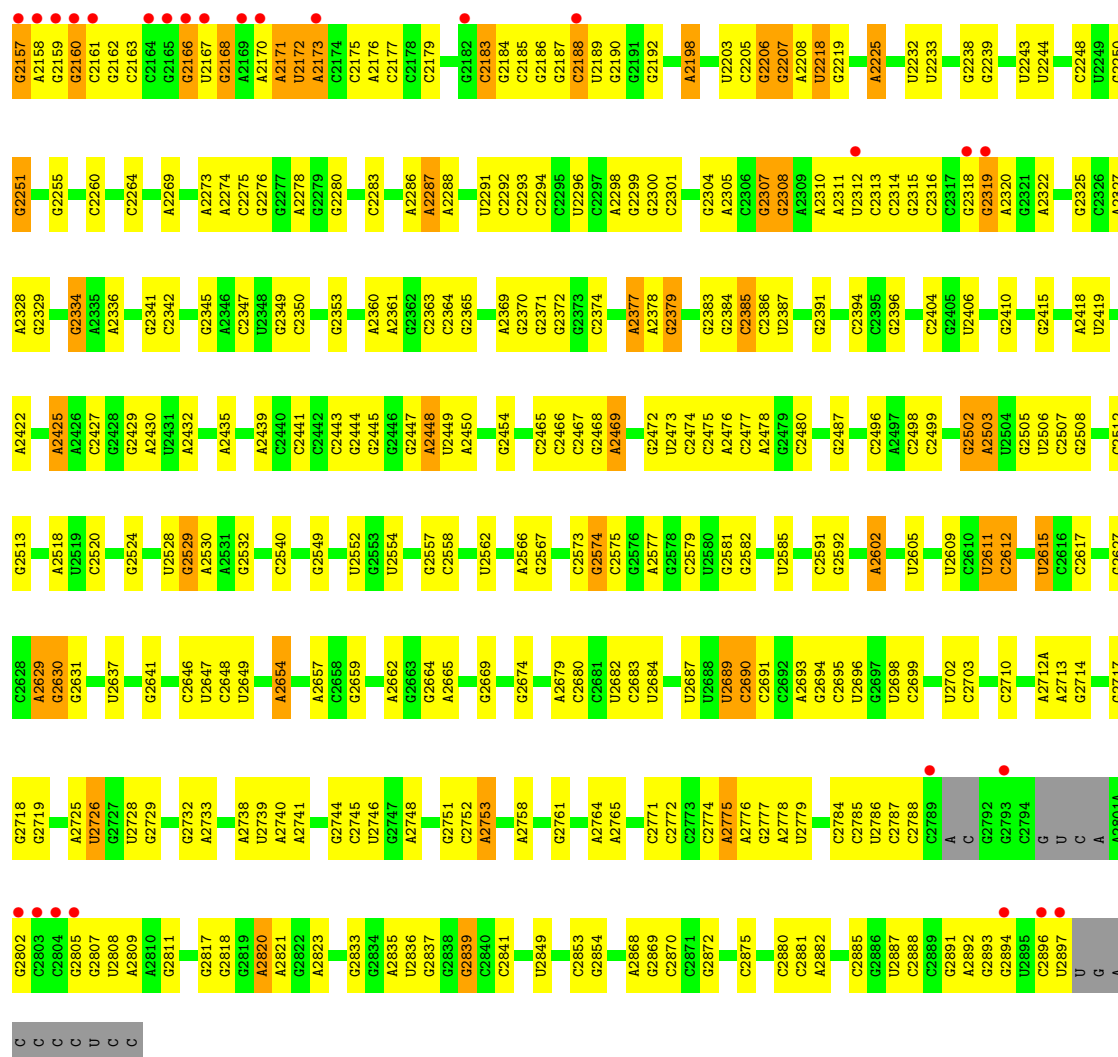
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |    |
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|----|
| C2471 | C2472 | A2476 | C2477 | A2478 | C2483 | G2484 | G2487 | U2491 | G2494 | A2497 | C2498 | C2499 | G2502 | A2503 | G2504 | G2505 | U2506 | C2507 | G2508 | A2518 | U2519 | C2520 | G2529 | G2532 | A2533 | A2534 | G2535 | G2536 | C2537 | C2538 | A2541 | G2543 | G2544 | U2552 | G2553 | U2554 | U2555 | G2556 | G2557 | U2563 | A2564 | A2565 | A2566 | G2567 | C2568 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| G2370 | G2371 | A2378 | G2379 | G2380 | G2381 | G2382 | G2383 | G2384 | G2385 | G2386 | G2387 | A2388 | G2389 | G2390 | G2391 | C2402 | C2403 | G2404 | G2405 | U2406 | G2407 | G2410 | A2422 | U2423 | G2424 | A2425 | G2428 | G2429 | A2430 | A2431 | G2432 | A2435 | U2438 | A2439 | C2440 | C2441 | G2445 | A2448 | U2452 | U2454 | G2458 | A2459 | U2460 | C2461 | U2462 | G2468 | A2469 | G2470 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| G2277 | A2278 | G2279 | G2280 | G2281 | G2282 | C2283 | C2284 | C2285 | A2286 | A2287 | A2288 | G2289 | G2290 | U2291 | C2292 | U2296 | G2297 | A2298 | G2299 | A2305 | G2308 | C2313 | G2319 | A2320 | G2325 | C2326 | A2327 | A2328 | G2329 | G2330 | G2331 | G2334 | A2335 | A2336 | G2345 | A2346 | C2347 | U2348 | G2349 | C2350 | G2354 | C2355 | C2356 | U2357 | C2364 | C2365 | A2366 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| U2172 | C2173 | C2174 | A2176 | C2177 | C2178 | C2179 | U2180 | G2181 | G2182 | C2183 | G2184 | C2185 | G2186 | G2187 | C2188 | U2189 | G2190 | G2191 | G2192 | A2198 | U2203 | C2205 | G2206 | G2207 | A2208 | G2224 | A2225 | C2226 | U2233 | G2234 | G2238 | U2243 | U2244 | A2247 | G2251 | C2254 | C2255 | C2256 | C2260 | U2261 | A2266 | A2267 | A2268 | A2269 | A2273 | A2274 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| C2111 | G2112 | U2113 | A2114 | G2115 | G2116 | A2117 | U2118 | A2119 | G2120 | G2121 | U2122 | G2123 | G2124 | A2125 | C2126 | C2127 | C2128 | C2129 | U2130 | G2131 | U2132 | G2133 | G2134 | A2135 | C2136 | C2137 | C2138 | C2139 | C2140 | G2141 | C2142 | C2143 | U2144 | C2145 | C2146 | G2147 | G2148 | U2149 | U2150 | G2151 | G2152 | G2153 | G2154 | G2155 | G2156 | G2157 | A2158 | G2159 | G2160 | C2161 | G2162 | C2163 | C2164 | G2165 | G2166 | U2167 | G2168 | A2169 | C2170 | A2171 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| A2013 | A2014 | A2015 | A2020 | G2021 | U2022 | G2023 | U2028 | G2029 | A2030 | A2031 | G2032 | A2033 | G2037 | G2038 | C2043 | G2049 | G2052 | G2053 | A2054 | G2055 | G2056 | A2060 | G2061 | G2069 | G2070 | A2071 | U2074 | U2075 | U2076 | A2077 | C2078 | U2079 | G2083 | G2094 | C2095 | U2096 | C2097 | U2098 | U2099 | G2100 | G2101 | G2104 | C2105 | G2106 | C2107 | C2108 | C2109 | C2110 | C2111 | C2112 | C2113 | C2114 | C2115 | C2116 | C2117 | C2118 | C2119 | C2120 | C2121 | C2122 | C2123 | C2124 | C2125 | C2126 | C2127 | C2128 | C2129 | C2130 | C2131 | C2132 | C2133 | C2134 | C2135 | C2136 | C2137 | C2138 | C2139 | C2140 | C2141 | C2142 | C2143 | C2144 | C2145 | C2146 | C2147 | C2148 | C2149 | C2150 | C2151 | C2152 | C2153 | C2154 | C2155 | C2156 | C2157 | C2158 | C2159 | C2160 | C2161 | C2162 | C2163 | C2164 | C2165 | C2166 | C2167 | C2168 | C2169 | C2170 | C2171 | C2172 | C2173 | C2174 | C2175 | C2176 | C2177 | C2178 | C2179 | C2180 | C2181 | C2182 | C2183 | C2184 | C2185 | C2186 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| C2312 | C2313 | C2314 | C2315 | C2316 | C2317 | C2318 | C2319 | C2320 | C2321 | C2322 | C2323 | C2324 | C2325 | C2326 | C2327 | C2328 | C2329 | C2330 | C2331 | C2332 | C2333 | C2334 | C2335 | C2336 | C2337 | C2338 | C2339 | C2340 | C2341 | C2342 | C2343 | C2344 | C2345 | C2346 | C2347 | C2348 | C2349 | C2350 | C2351 | C2352 | C2353 | C2354 | C2355 | C2356 | C2357 | C2358 | C2359 | C2360 | C2361 | C2362 | C2363 | C2364 | C2365 | C2366 | C2367 | C2368 | C2369 | C2370 | C2371 | C2372 | C2373 | C2374 | C2375 | C2376 | C2377 | C2378 | C2379 | C2380 | C2381 | C2382 | C2383 | C2384 | C2385 | C2386 | C2387 | C2388 | C2389 | C2390 | C2391 | C2392 | C2393 | C2394 | C2395 | C2396 | C2397 | C2398 | C2399 | C2400 | C2401 | C2402 | C2403 | C2404 | C2405 | C2406 | C2407 | C2408 | C2409 | C2410 | C2411 | C2412 | C2413 | C2414 | C2415 | C2416 | C2417 | C2418 | C2419 | C2420 | C2421 | C2422 | C2423 | C2424 | C2425 | C2426 | C2427 | C2428 | C2429 | C2430 | C2431 | C2432 | C2433 | C2434 | C2435 | C2436 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• Molecule 1: 23S Ribosomal RNA

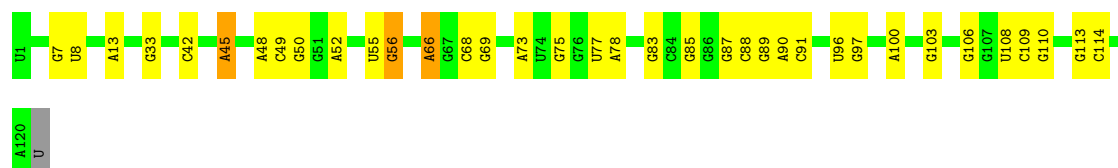


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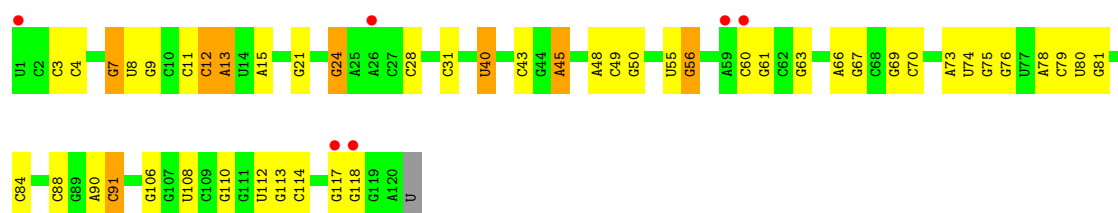
• Molecule 2: 5S Ribosomal RNA

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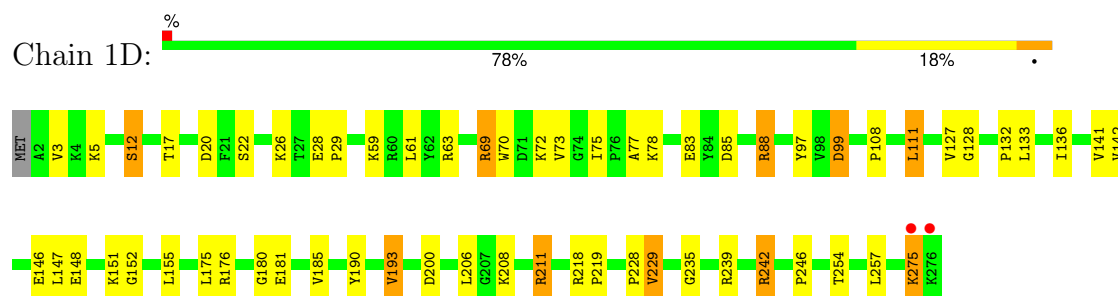


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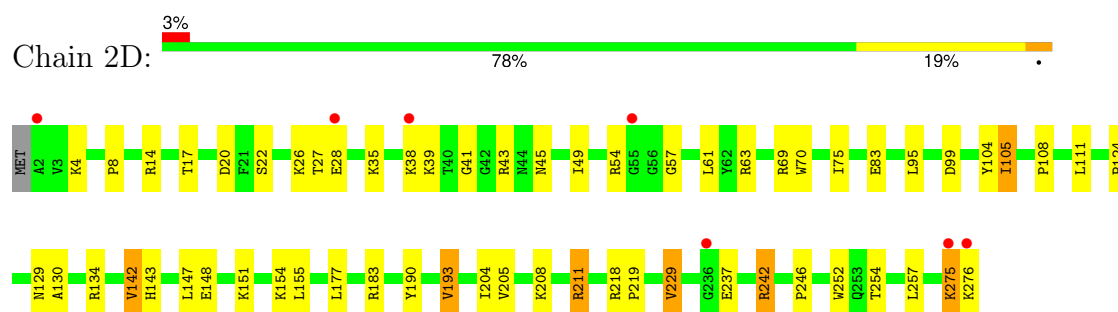
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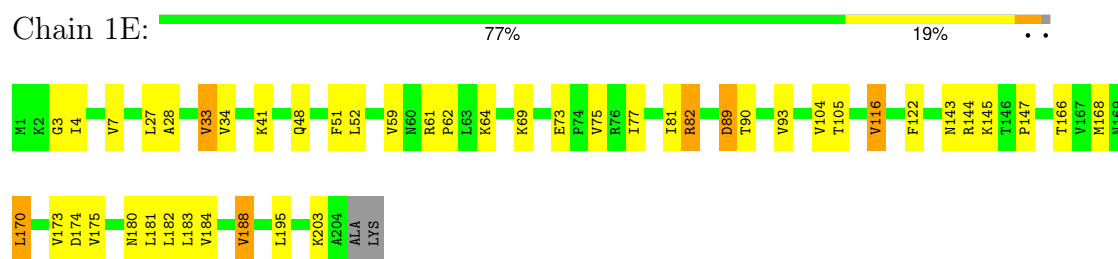
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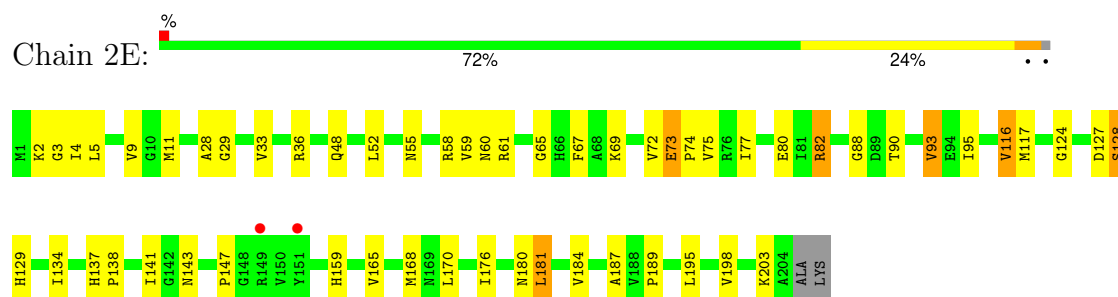
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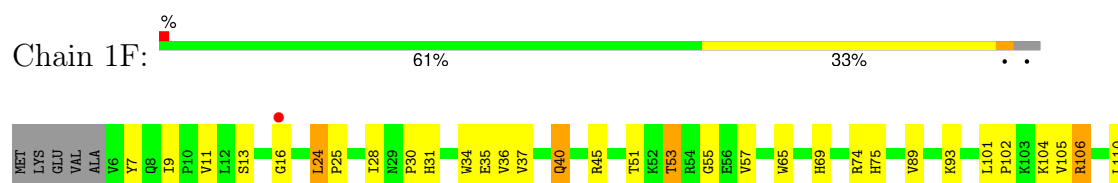
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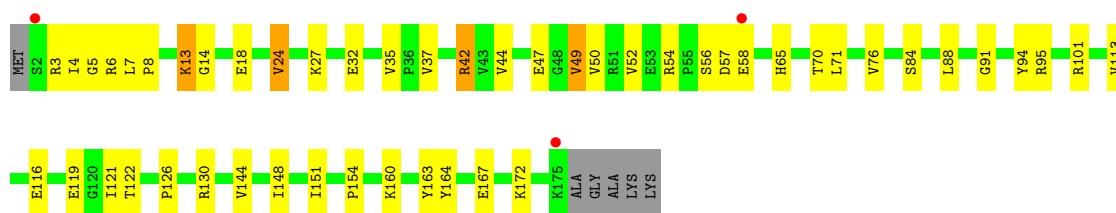
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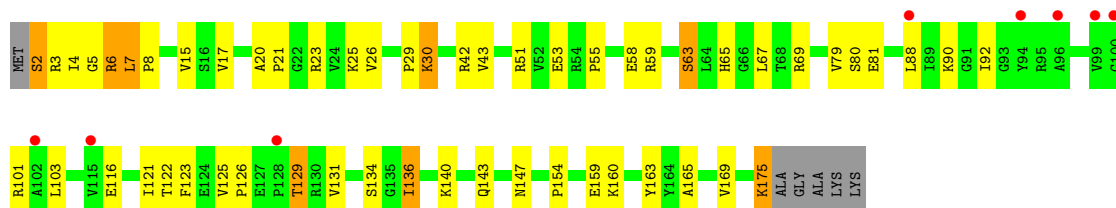
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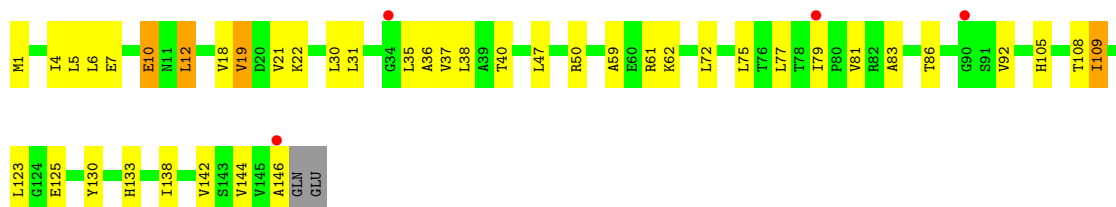




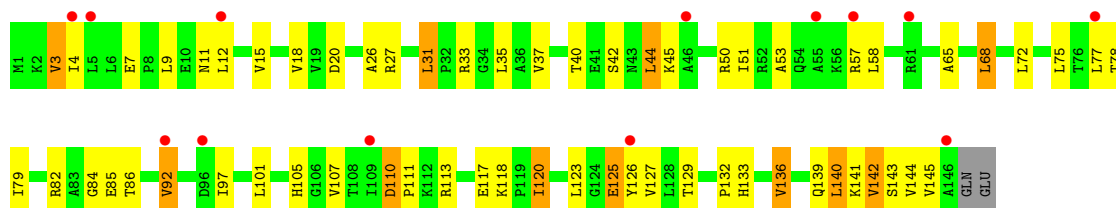
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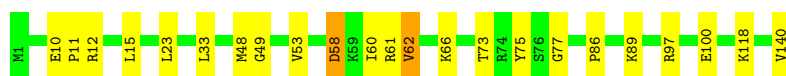
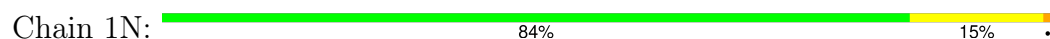
• Molecule 8: 50S ribosomal protein L9



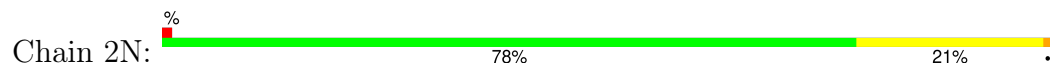
• Molecule 8: 50S ribosomal protein L9

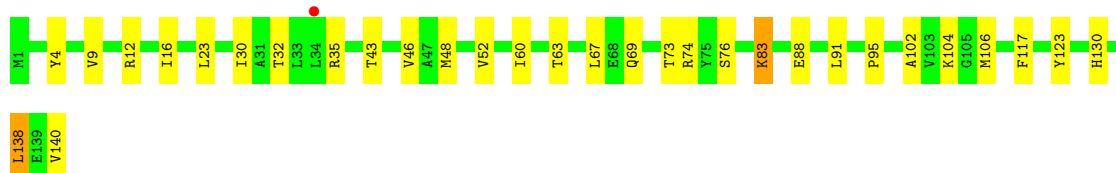


• Molecule 9: 50S ribosomal protein L13

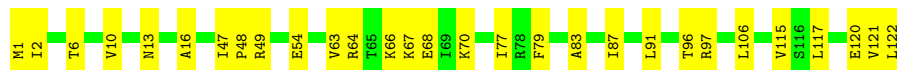


• Molecule 9: 50S ribosomal protein L13





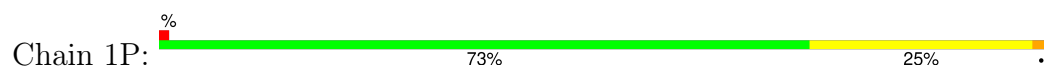
- Molecule 10: 50S ribosomal protein L14



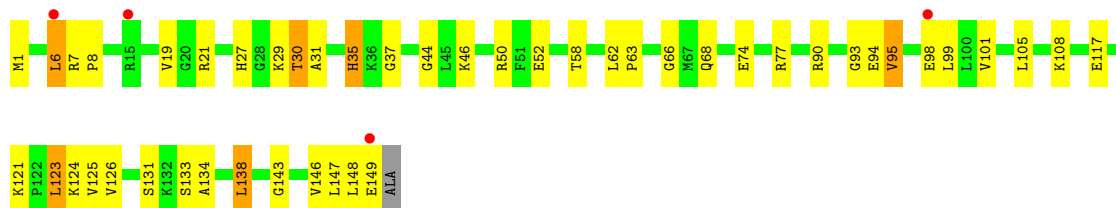
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

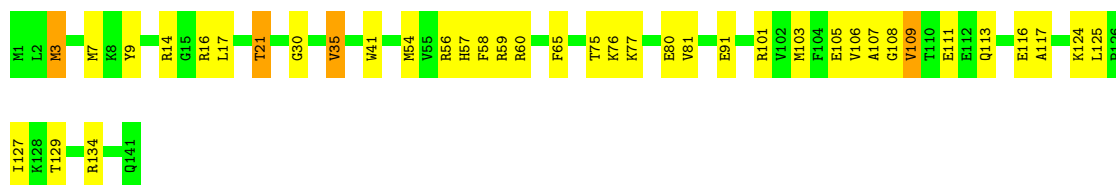


- Molecule 11: 50S ribosomal protein L15

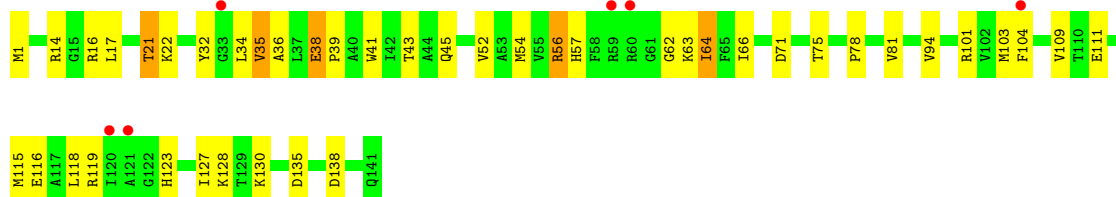


- Molecule 12: 50S ribosomal protein L16

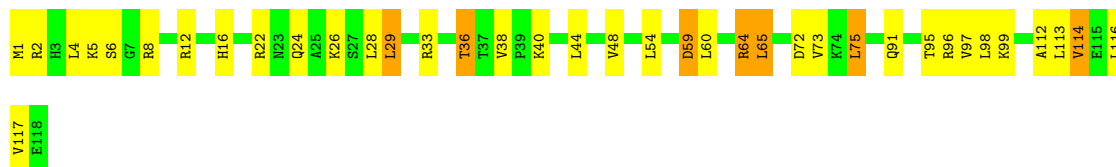




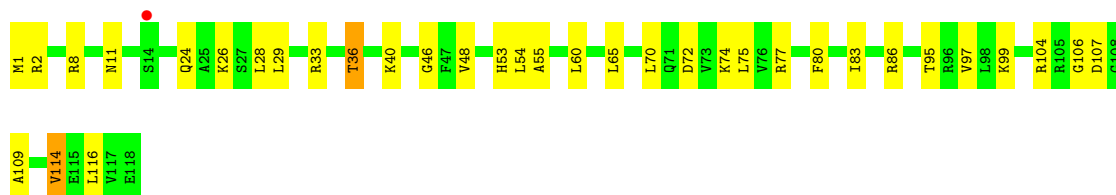
- Molecule 12: 50S ribosomal protein L16



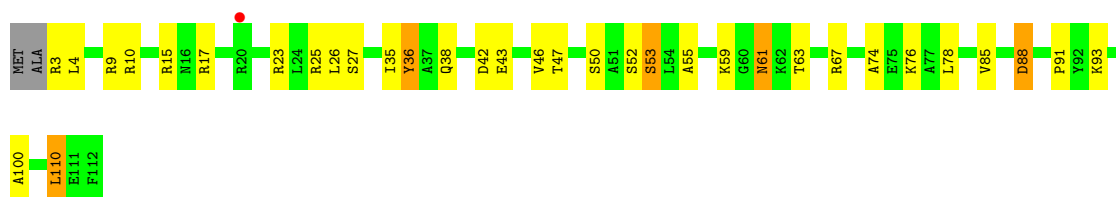
- Molecule 13: 50S ribosomal protein L17



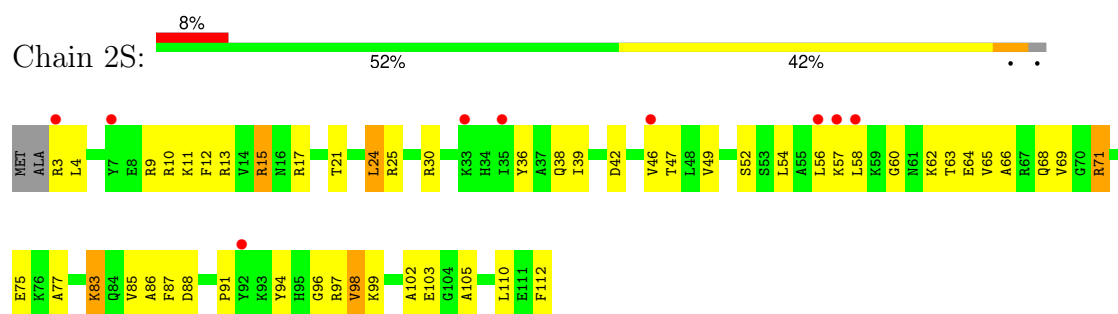
- Molecule 13: 50S ribosomal protein L17



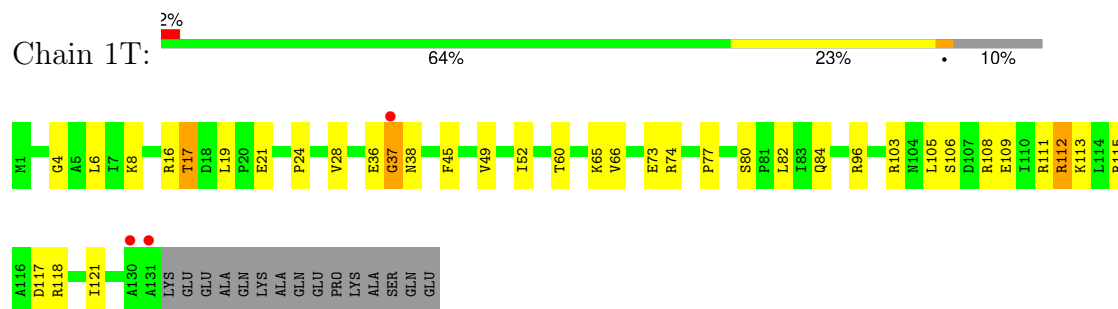
- Molecule 14: 50S ribosomal protein L18



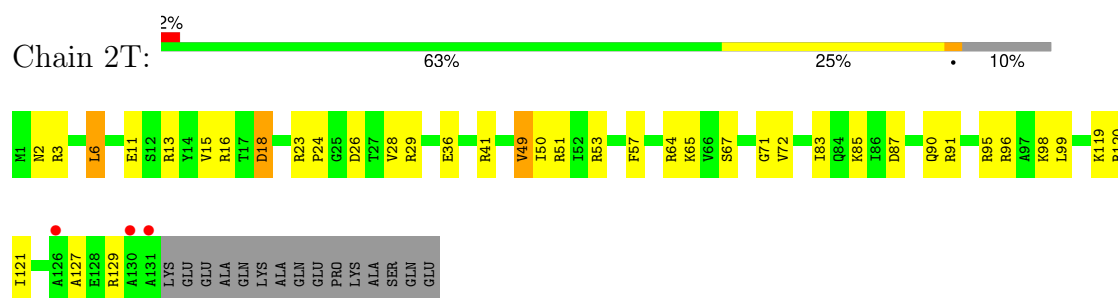
- Molecule 14: 50S ribosomal protein L18



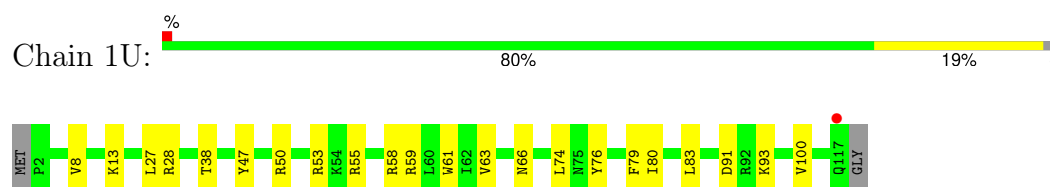
- Molecule 15: 50S ribosomal protein L19



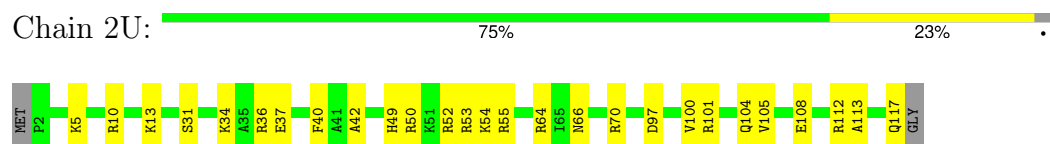
- Molecule 15: 50S ribosomal protein L19



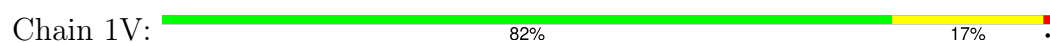
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



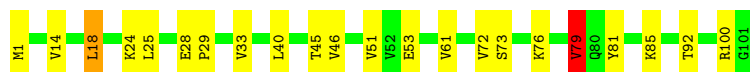
- Molecule 17: 50S ribosomal protein L21





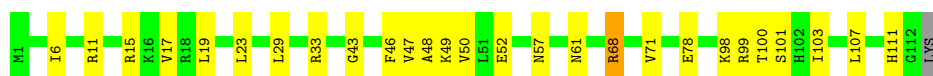
- Molecule 17: 50S ribosomal protein L21

Chain 2V: 78% 20% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 75% 23% ..



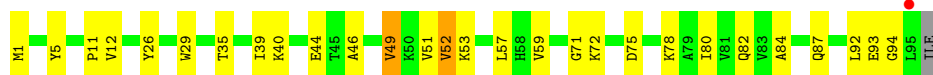
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 75% 24% .



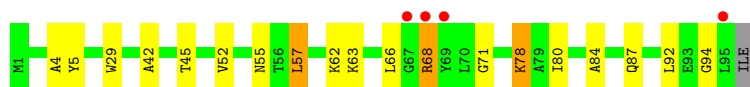
- Molecule 19: 50S ribosomal protein L23

Chain 1X: 70% 27% ..



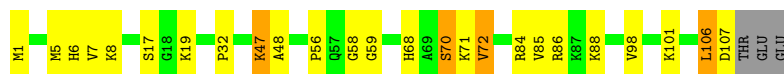
- Molecule 19: 50S ribosomal protein L23

Chain 2X: 4% 79% 17% ..



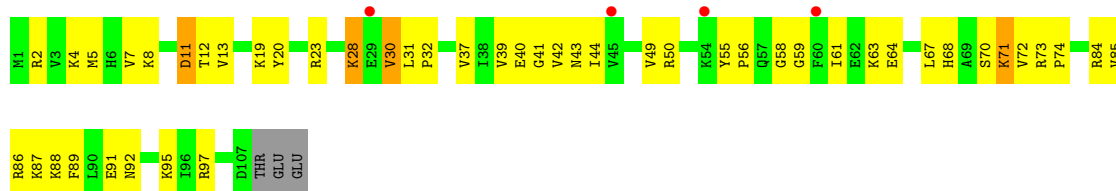
- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 75% 19% .



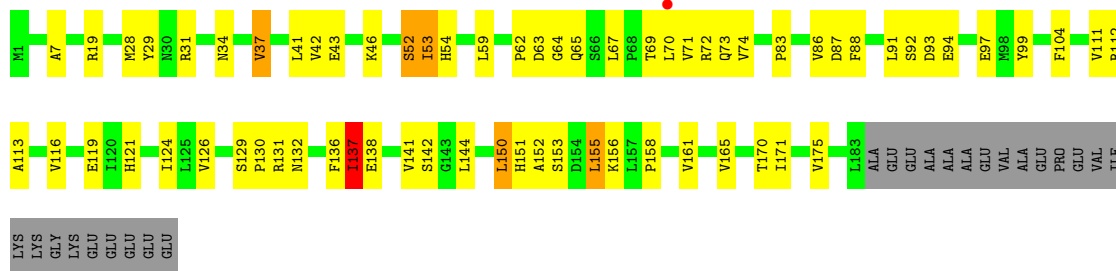
- Molecule 20: 50S ribosomal protein L24

Chain 2Y: 4% 54% 40% .



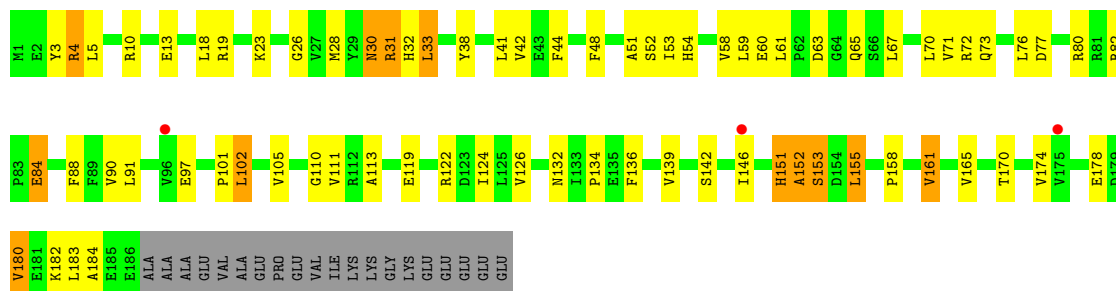
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 56% 30% 11%



- Molecule 21: 50S ribosomal protein L25

Chain 2Z: 55% 30% 6% 10%



- Molecule 22: 50S ribosomal protein L27

Chain 10: 75% 12% 11%

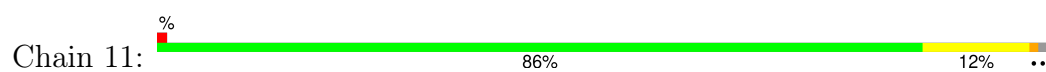


- Molecule 22: 50S ribosomal protein L27

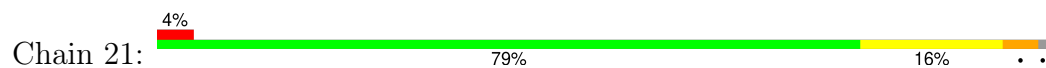
Chain 20: 11% 64% 25% 9%



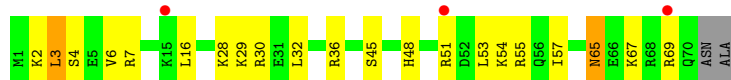
- Molecule 23: 50S ribosomal protein L28



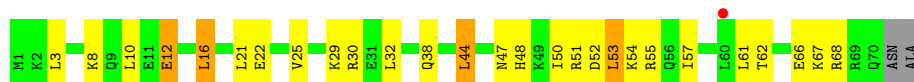
- Molecule 23: 50S ribosomal protein L28



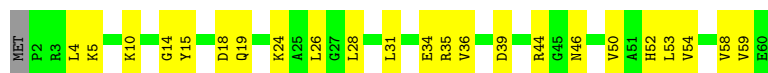
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



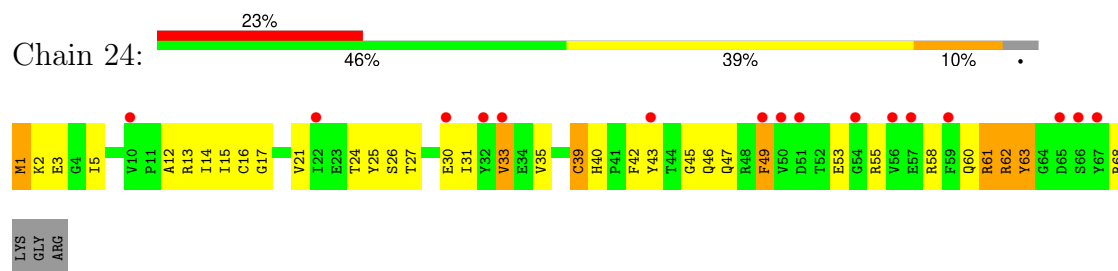
- Molecule 25: 50S ribosomal protein L30



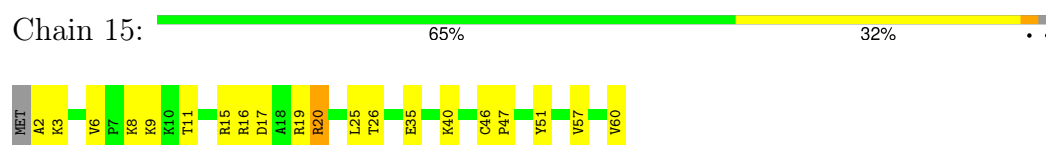
- Molecule 26: 50S ribosomal protein L31



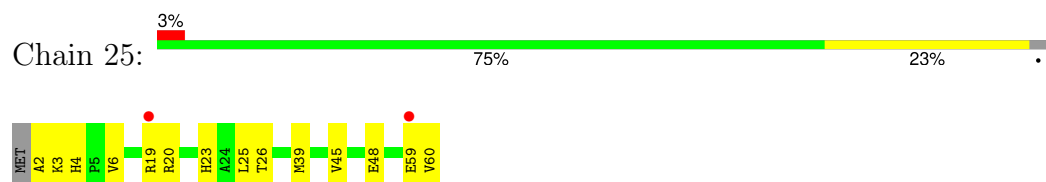
- Molecule 26: 50S ribosomal protein L31



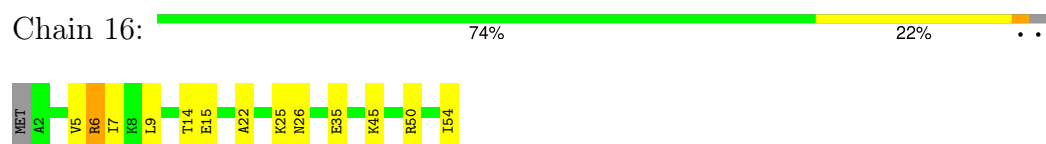
- Molecule 27: 50S ribosomal protein L32



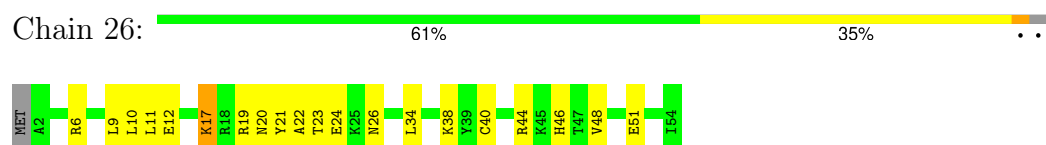
- Molecule 27: 50S ribosomal protein L32



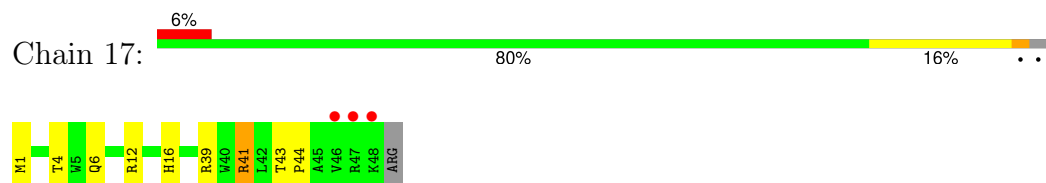
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



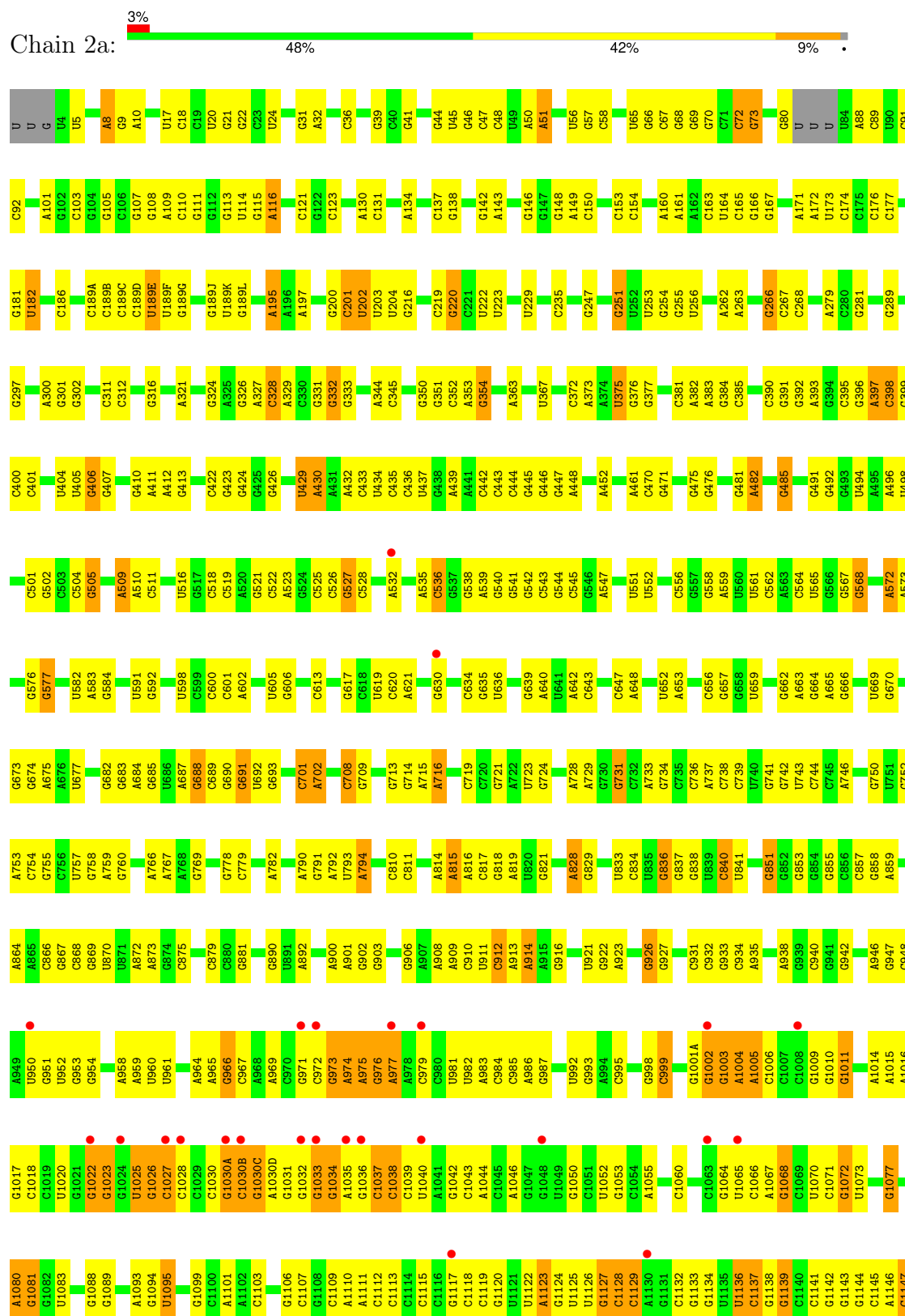
- Molecule 29: 50S ribosomal protein L34



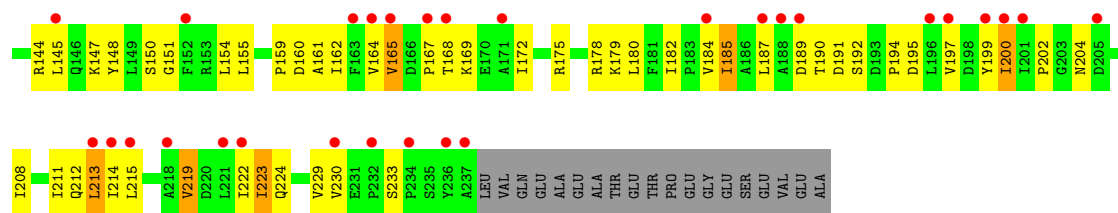




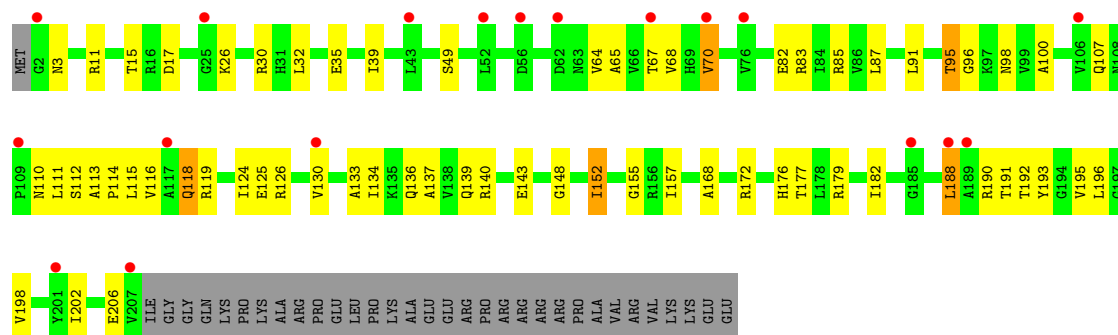
● Molecule 32: 16S Ribosomal RNA



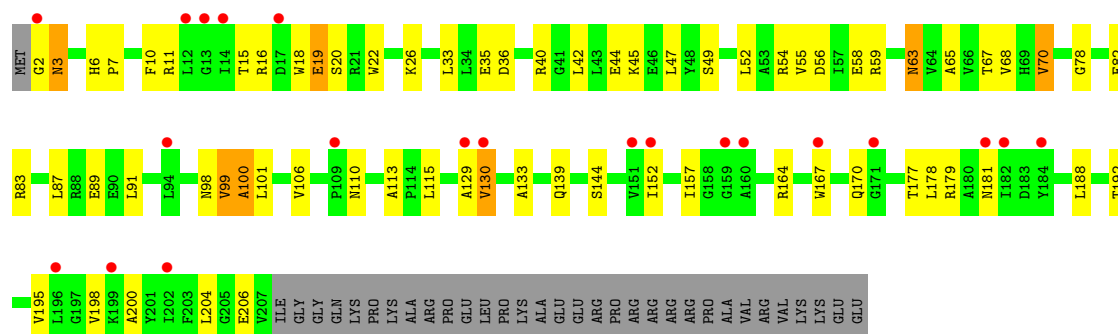




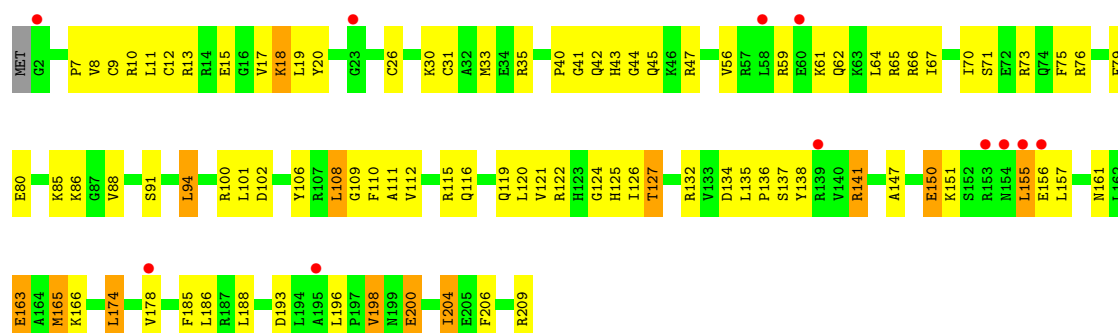
• Molecule 34: 30S ribosomal protein S3



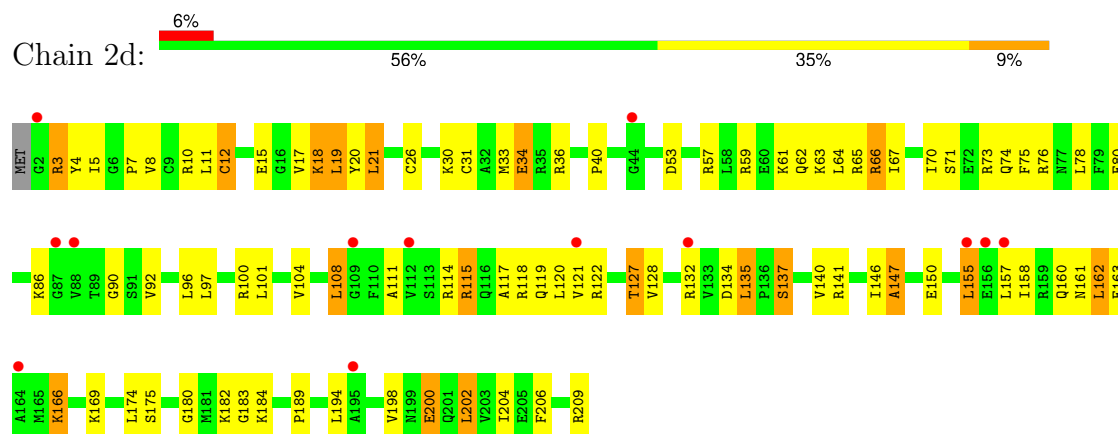
• Molecule 34: 30S ribosomal protein S3



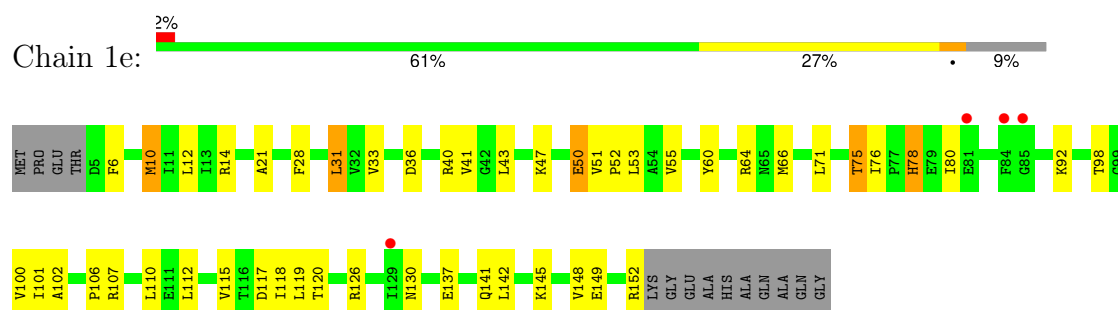
• Molecule 35: 30S ribosomal protein S4



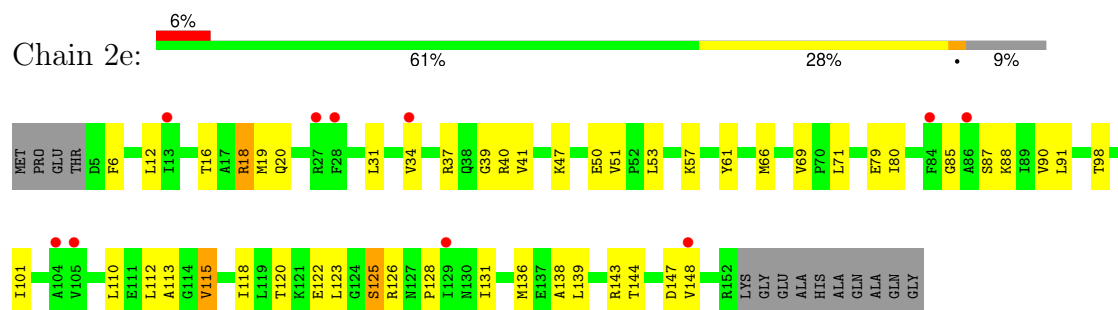
- Molecule 35: 30S ribosomal protein S4



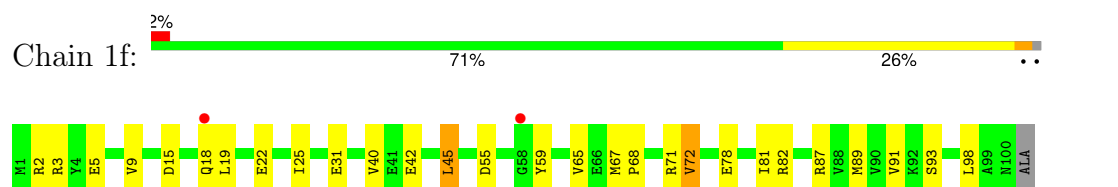
- Molecule 36: 30S ribosomal protein S5



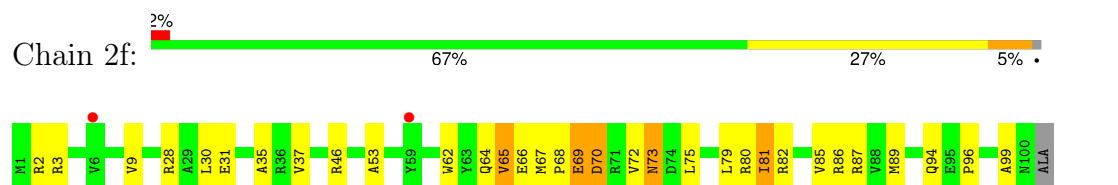
- Molecule 36: 30S ribosomal protein S5



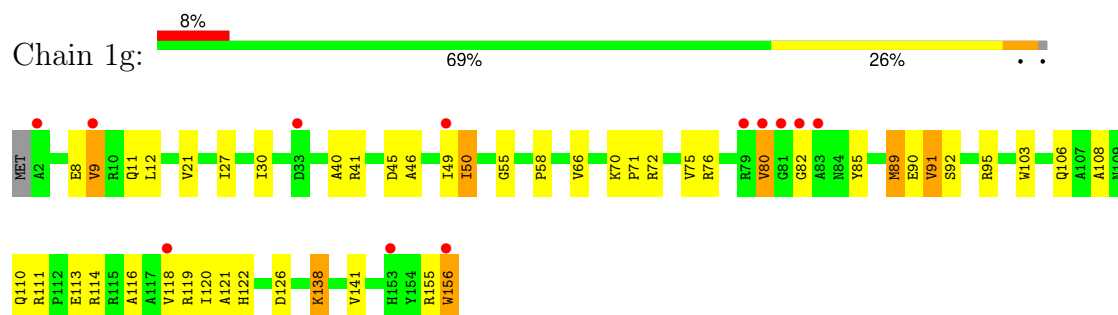
- Molecule 37: 30S ribosomal protein S6



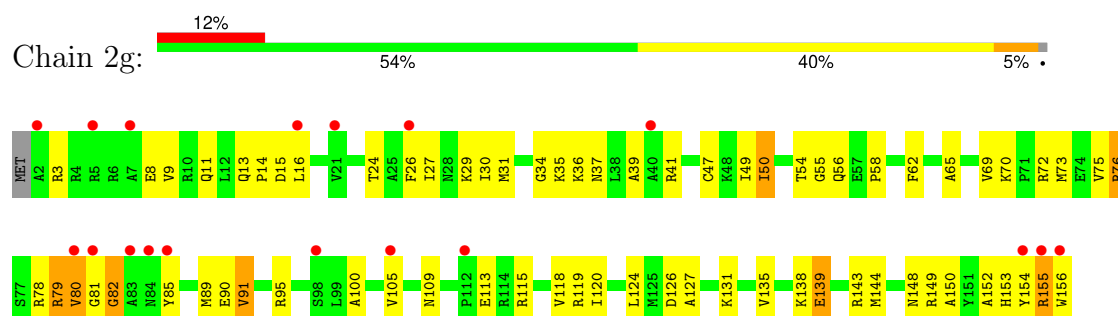
- Molecule 37: 30S ribosomal protein S6



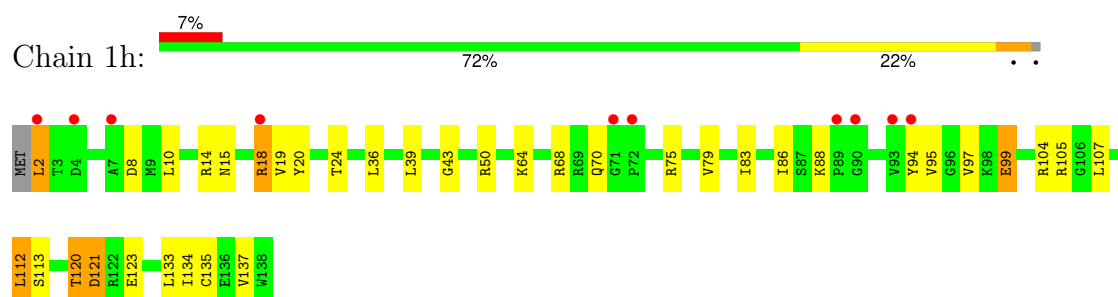
- Molecule 38: 30S ribosomal protein S7



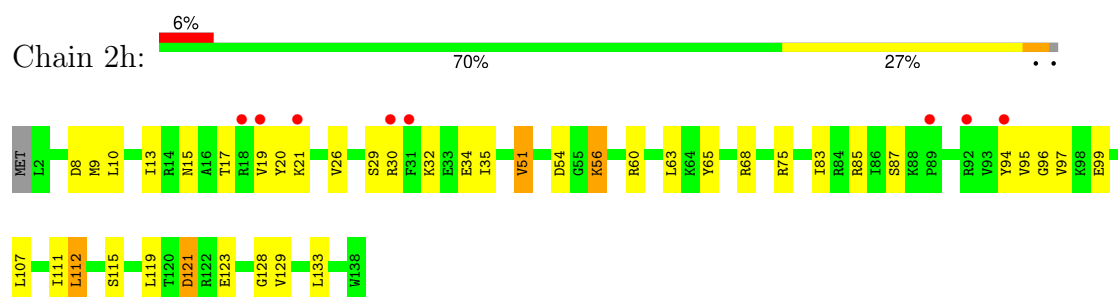
- Molecule 38: 30S ribosomal protein S7



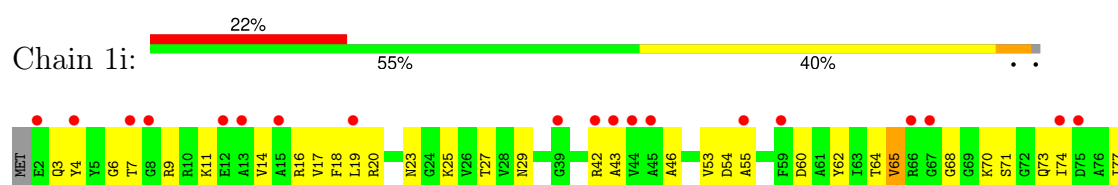
- Molecule 39: 30S ribosomal protein S8

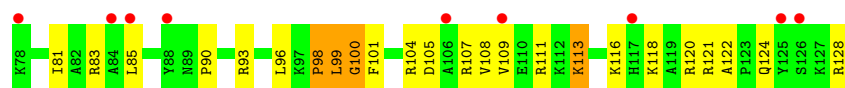


- Molecule 39: 30S ribosomal protein S8

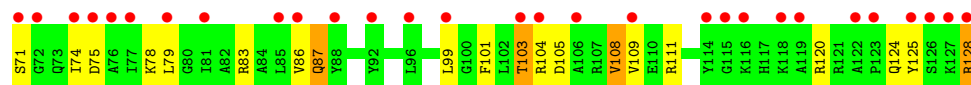
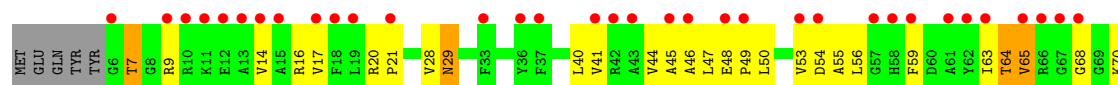


- Molecule 40: 30S ribosomal protein S9

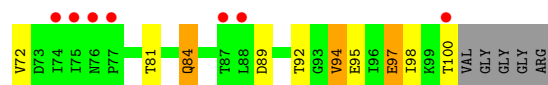
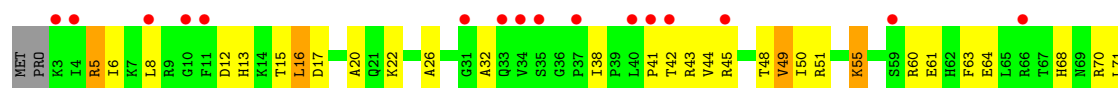




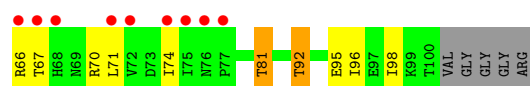
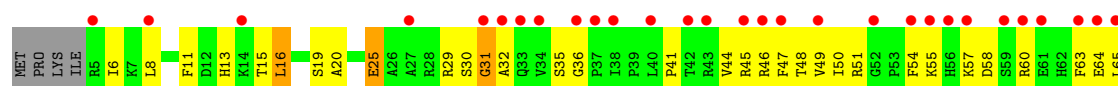
• Molecule 40: 30S ribosomal protein S9



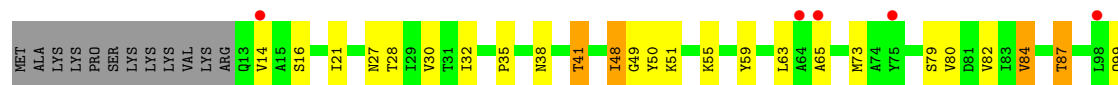
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10

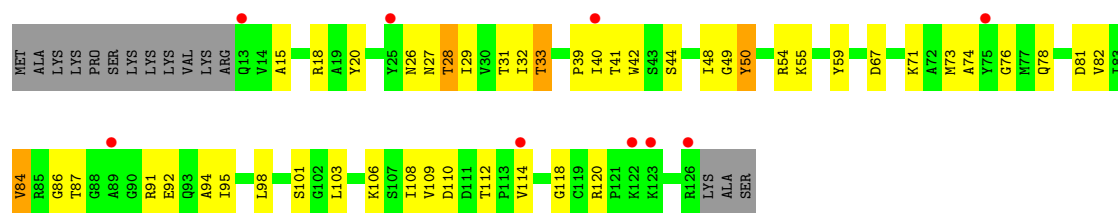


• Molecule 42: 30S ribosomal protein S11

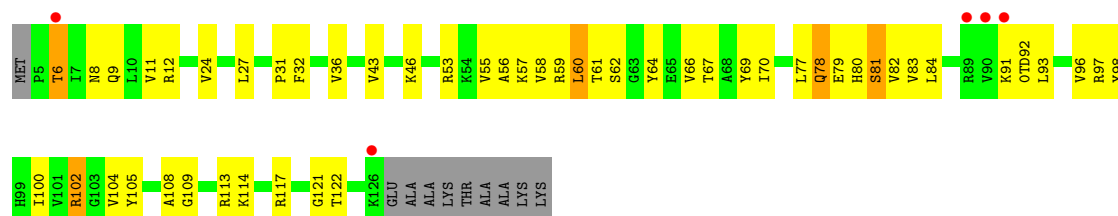


• Molecule 42: 30S ribosomal protein S11

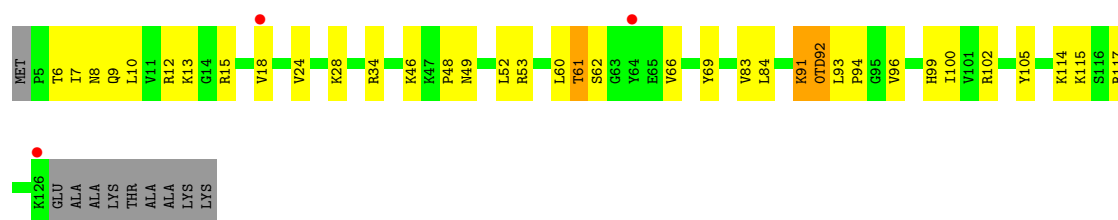




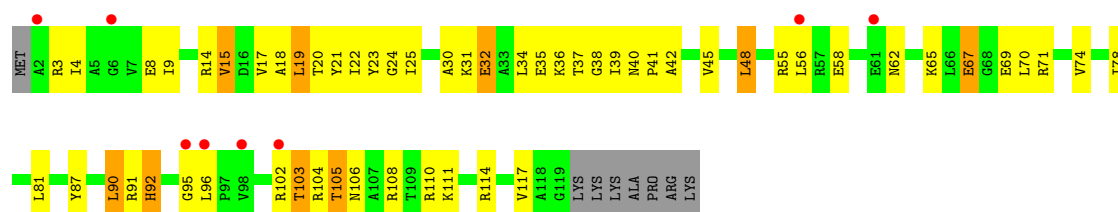
• Molecule 43: 30S ribosomal protein S12



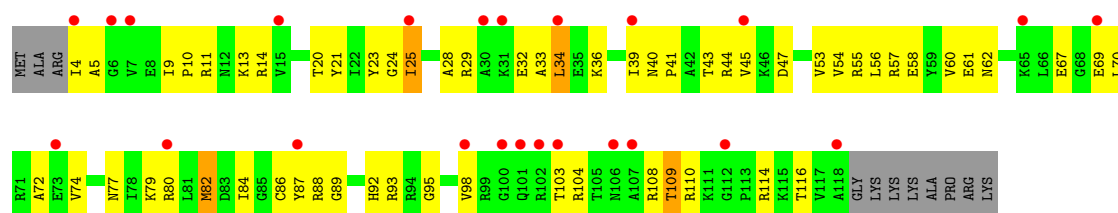
• Molecule 43: 30S ribosomal protein S12



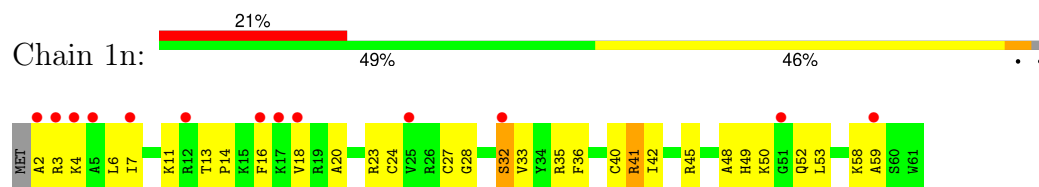
• Molecule 44: 30S ribosomal protein S13



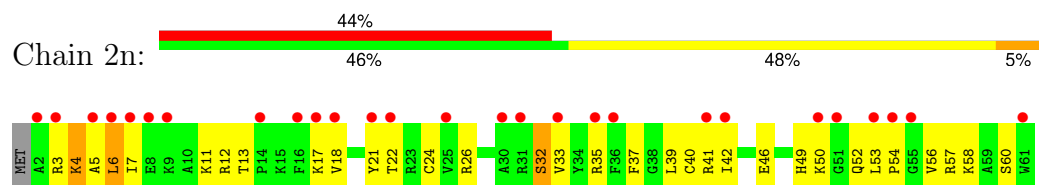
• Molecule 44: 30S ribosomal protein S13



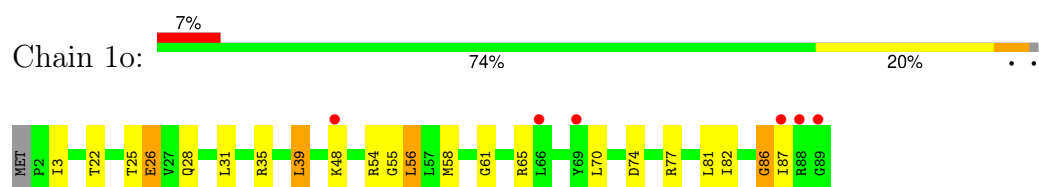
## • Molecule 45: 30S ribosomal protein S14 type Z



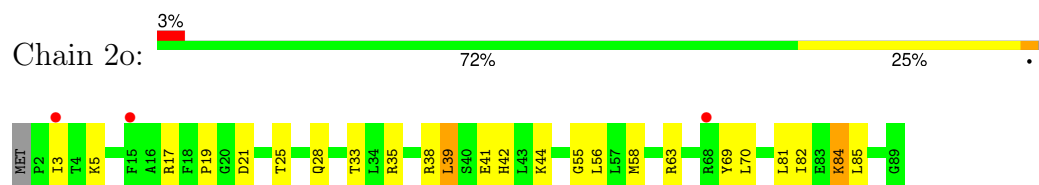
## • Molecule 45: 30S ribosomal protein S14 type Z



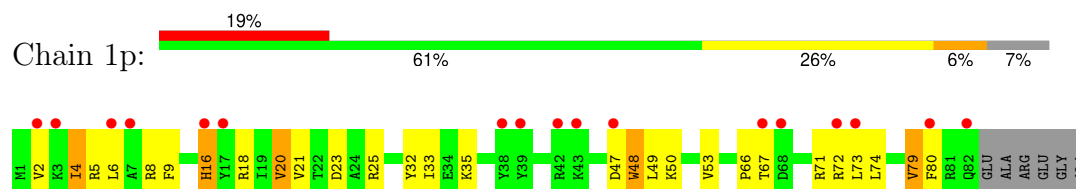
## • Molecule 46: 30S ribosomal protein S15



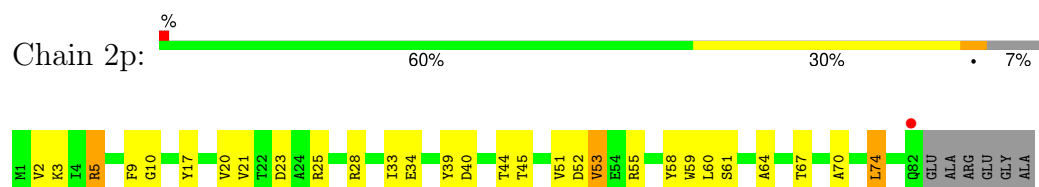
## • Molecule 46: 30S ribosomal protein S15



## • Molecule 47: 30S ribosomal protein S16

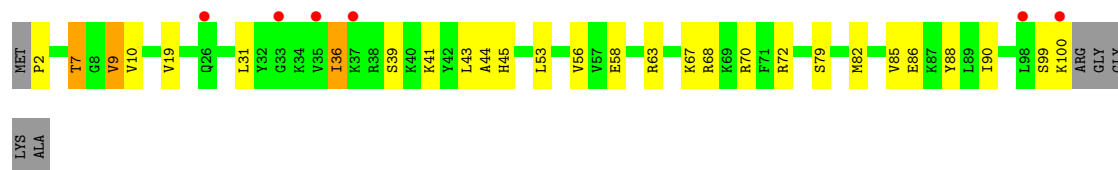


## • Molecule 47: 30S ribosomal protein S16

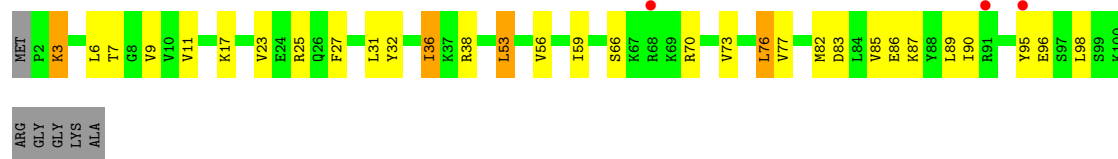


## • Molecule 48: 30S ribosomal protein S17

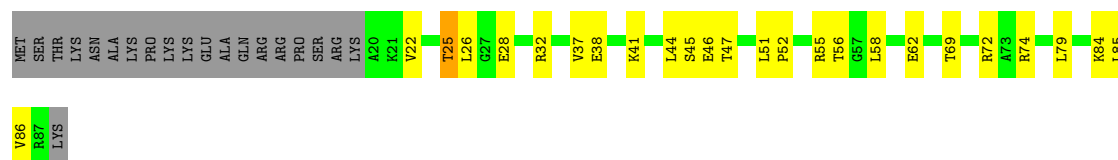




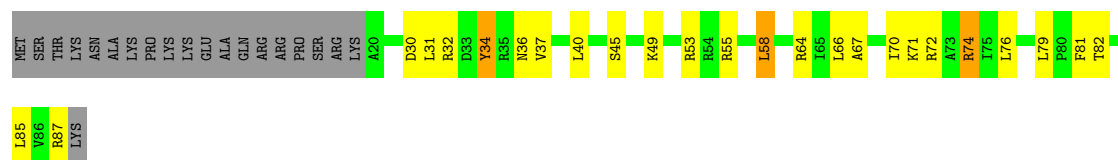
- Molecule 48: 30S ribosomal protein S17



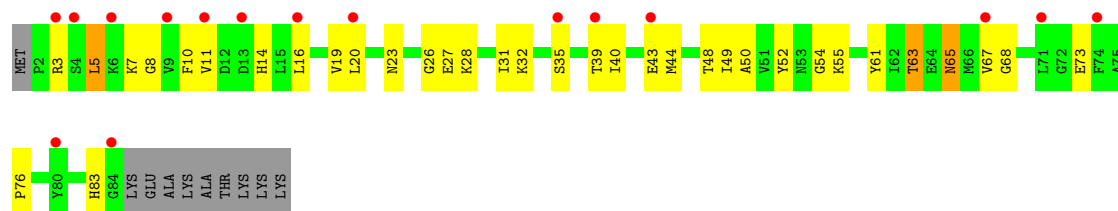
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

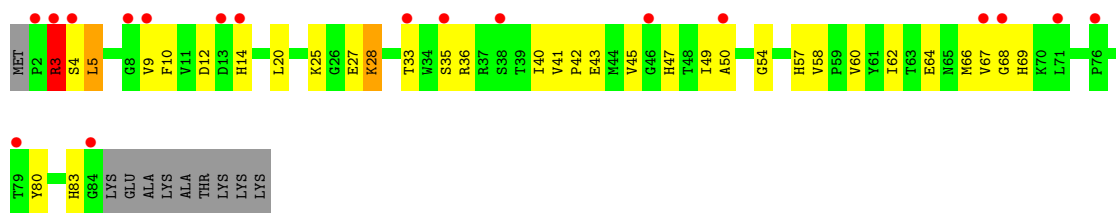


- Molecule 50: 30S ribosomal protein S19

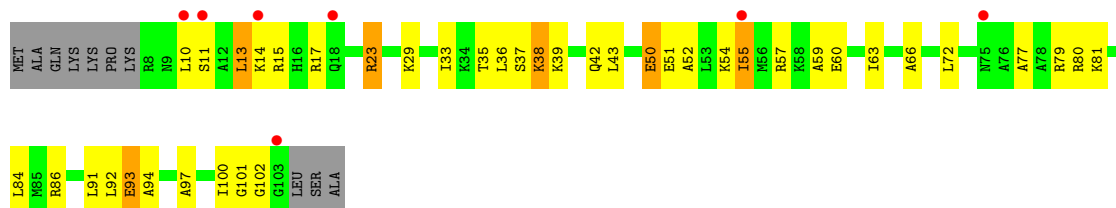


- Molecule 50: 30S ribosomal protein S19

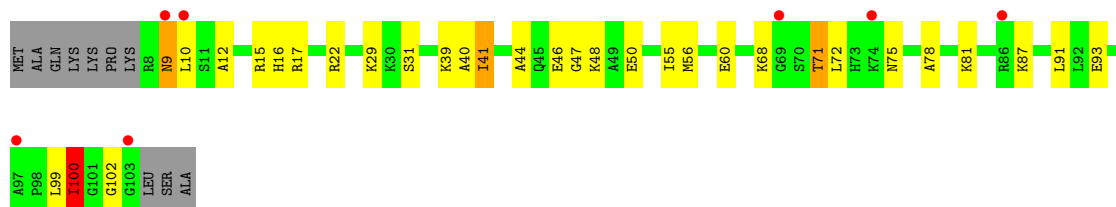




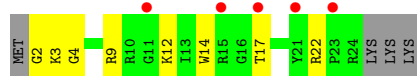
• Molecule 51: 30S ribosomal protein S20



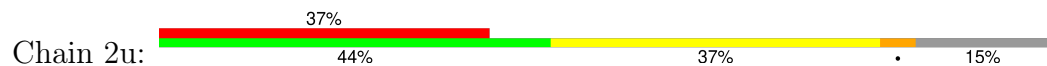
• Molecule 51: 30S ribosomal protein S20



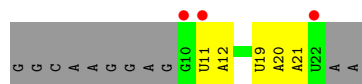
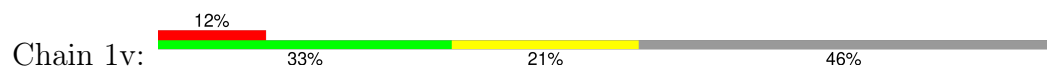
• Molecule 52: 30S ribosomal protein Thx



• Molecule 52: 30S ribosomal protein Thx

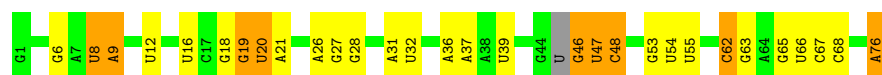


• Molecule 53: PHE-Stop mRNA



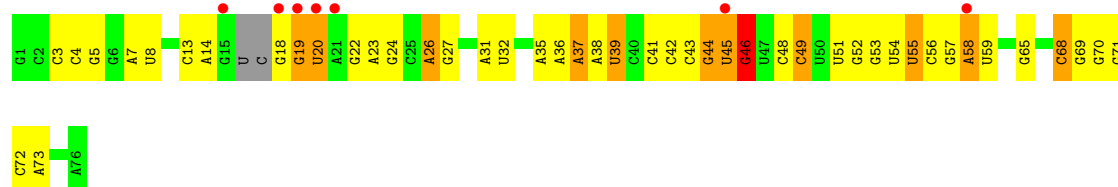


Chain 1x: 



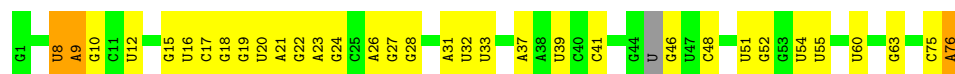
- Molecule 55: P-site and E-site Deacylated tRNAphe

Chain 1y: 



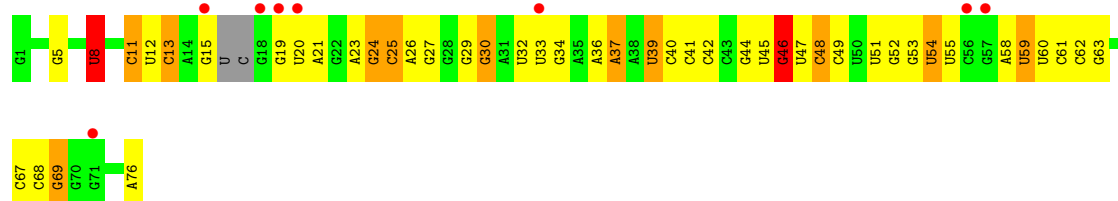
- Molecule 55: P-site and E-site Deacylated tRNAphe

Chain 2x: 



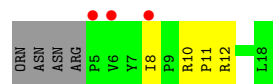
- Molecule 55: P-site and E-site Deacylated tRNAphe

Chain 2y: 



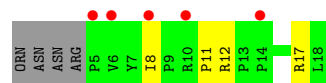
- Molecule 56: Api137 Antimicrobial Peptide

Chain 1z: 



- Molecule 56: Api137 Antimicrobial Peptide

Chain 2z: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.60Å 450.81Å 624.08Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 152.87 – 2.70<br>152.87 – 2.70                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (152.87-2.70)<br>99.1 (152.87-2.70)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.20                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.16 (at 2.69Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.2                                                | Depositor        |
| R, $R_{free}$                                                           | 0.227 , 0.278<br>0.229 , 0.277                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 79249 reflections (4.97%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.066                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 51.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 299179                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: MEQ, 2MG, G7M, MG, UR3, 4SU, OMG, OMU, 5MC, 2MA, MA6, ZN, 5MU, MIA, OMC, M2G, 0TD, SF4, 4OC, PSU

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 1   | 1A    | 0.29         | 0/69011       | 0.47        | 2/107720 (0.0%) |
| 1   | 2A    | 0.22         | 0/67295       | 0.40        | 1/105042 (0.0%) |
| 2   | 1B    | 0.23         | 0/2881        | 0.40        | 0/4494          |
| 2   | 2B    | 0.19         | 0/2881        | 0.35        | 0/4494          |
| 3   | 1D    | 0.27         | 0/2186        | 0.50        | 0/2944          |
| 3   | 2D    | 0.22         | 0/2186        | 0.45        | 0/2944          |
| 4   | 1E    | 0.30         | 0/1592        | 0.54        | 1/2149 (0.0%)   |
| 4   | 2E    | 0.20         | 0/1592        | 0.43        | 0/2149          |
| 5   | 1F    | 0.27         | 0/1619        | 0.49        | 0/2193          |
| 5   | 2F    | 0.26         | 1/1615 (0.1%) | 0.44        | 0/2188          |
| 6   | 1G    | 0.22         | 0/1450        | 0.47        | 0/1959          |
| 6   | 2G    | 0.21         | 0/1449        | 0.45        | 0/1958          |
| 7   | 1H    | 0.23         | 0/1356        | 0.43        | 0/1834          |
| 7   | 2H    | 0.19         | 0/1356        | 0.41        | 0/1834          |
| 8   | 1I    | 0.21         | 0/1100        | 0.43        | 0/1501          |
| 8   | 2I    | 0.19         | 0/1076        | 0.43        | 0/1471          |
| 9   | 1N    | 0.27         | 0/1144        | 0.45        | 0/1543          |
| 9   | 2N    | 0.19         | 0/1144        | 0.40        | 0/1543          |
| 10  | 1O    | 0.27         | 0/943         | 0.50        | 0/1269          |
| 10  | 2O    | 0.21         | 0/943         | 0.44        | 0/1269          |
| 11  | 1P    | 0.28         | 0/1152        | 0.55        | 0/1533          |
| 11  | 2P    | 0.22         | 0/1152        | 0.47        | 0/1533          |
| 12  | 1Q    | 0.28         | 0/1143        | 0.51        | 0/1527          |
| 12  | 2Q    | 0.20         | 0/1143        | 0.41        | 0/1527          |
| 13  | 1R    | 0.29         | 0/982         | 0.52        | 0/1312          |
| 13  | 2R    | 0.21         | 0/982         | 0.44        | 0/1312          |
| 14  | 1S    | 0.22         | 0/887         | 0.52        | 0/1180          |
| 14  | 2S    | 0.21         | 0/880         | 0.47        | 0/1172          |
| 15  | 1T    | 0.26         | 0/1105        | 0.49        | 0/1477          |
| 15  | 2T    | 0.22         | 0/1097        | 0.44        | 0/1468          |
| 16  | 1U    | 0.32         | 0/977         | 0.48        | 0/1301          |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 16  | 2U    | 0.20         | 0/977          | 0.39        | 0/1301         |
| 17  | 1V    | 0.32         | 0/782          | 0.48        | 0/1049         |
| 17  | 2V    | 0.19         | 0/782          | 0.41        | 0/1049         |
| 18  | 1W    | 0.31         | 0/897          | 0.50        | 0/1205         |
| 18  | 2W    | 0.21         | 0/897          | 0.43        | 0/1205         |
| 19  | 1X    | 0.28         | 0/764          | 0.54        | 1/1025 (0.1%)  |
| 19  | 2X    | 0.20         | 0/760          | 0.35        | 0/1021         |
| 20  | 1Y    | 0.26         | 0/819          | 0.50        | 0/1095         |
| 20  | 2Y    | 0.21         | 0/823          | 0.46        | 0/1100         |
| 21  | 1Z    | 0.22         | 0/1469         | 0.48        | 0/1998         |
| 21  | 2Z    | 0.20         | 0/1483         | 0.47        | 0/2018         |
| 22  | 10    | 0.28         | 0/612          | 0.53        | 0/816          |
| 22  | 20    | 0.22         | 0/616          | 0.51        | 0/821          |
| 23  | 11    | 0.26         | 0/762          | 0.45        | 0/1014         |
| 23  | 21    | 0.22         | 0/762          | 0.44        | 0/1014         |
| 24  | 12    | 0.24         | 0/590          | 0.44        | 0/781          |
| 24  | 22    | 0.19         | 0/590          | 0.43        | 0/781          |
| 25  | 13    | 0.27         | 0/474          | 0.47        | 0/635          |
| 25  | 23    | 0.21         | 0/469          | 0.38        | 0/630          |
| 26  | 14    | 0.24         | 0/561          | 0.52        | 0/756          |
| 26  | 24    | 0.30         | 0/530          | 0.58        | 0/719          |
| 27  | 15    | 0.31         | 0/469          | 0.54        | 0/635          |
| 27  | 25    | 0.23         | 0/469          | 0.48        | 0/635          |
| 28  | 16    | 0.27         | 0/460          | 0.49        | 0/613          |
| 28  | 26    | 0.21         | 0/456          | 0.45        | 0/608          |
| 29  | 17    | 0.32         | 0/426          | 0.48        | 0/561          |
| 29  | 27    | 0.25         | 0/426          | 0.46        | 0/561          |
| 30  | 18    | 0.30         | 0/519          | 0.48        | 0/684          |
| 30  | 28    | 0.21         | 0/525          | 0.42        | 0/691          |
| 31  | 19    | 0.27         | 0/310          | 0.66        | 1/407 (0.2%)   |
| 31  | 29    | 0.22         | 0/310          | 0.49        | 0/407          |
| 32  | 1a    | 0.20         | 1/35795 (0.0%) | 0.38        | 1/55864 (0.0%) |
| 32  | 2a    | 0.20         | 2/35886 (0.0%) | 0.38        | 0/56005        |
| 33  | 1b    | 0.23         | 0/1881         | 0.50        | 0/2542         |
| 33  | 2b    | 0.30         | 0/1860         | 0.54        | 0/2518         |
| 34  | 1c    | 0.20         | 0/1578         | 0.39        | 0/2133         |
| 34  | 2c    | 0.21         | 0/1566         | 0.44        | 0/2119         |
| 35  | 1d    | 0.20         | 0/1689         | 0.49        | 0/2267         |
| 35  | 2d    | 0.21         | 0/1704         | 0.46        | 0/2284         |
| 36  | 1e    | 0.21         | 0/1145         | 0.48        | 0/1543         |
| 36  | 2e    | 0.20         | 0/1146         | 0.45        | 0/1545         |
| 37  | 1f    | 0.21         | 0/823          | 0.43        | 0/1116         |
| 37  | 2f    | 0.18         | 0/829          | 0.41        | 0/1123         |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 38  | 1g    | 0.21         | 0/1250          | 0.42        | 0/1679           |
| 38  | 2g    | 0.21         | 0/1254          | 0.43        | 0/1683           |
| 39  | 1h    | 0.20         | 0/1108          | 0.44        | 0/1494           |
| 39  | 2h    | 0.22         | 0/1108          | 0.50        | 1/1494 (0.1%)    |
| 40  | 1i    | 0.22         | 0/1002          | 0.49        | 0/1346           |
| 40  | 2i    | 0.26         | 0/957           | 0.50        | 1/1288 (0.1%)    |
| 41  | 1j    | 0.21         | 0/734           | 0.42        | 0/997            |
| 41  | 2j    | 0.24         | 0/727           | 0.46        | 0/988            |
| 42  | 1k    | 0.19         | 0/844           | 0.39        | 0/1145           |
| 42  | 2k    | 0.20         | 0/848           | 0.43        | 0/1149           |
| 43  | 1l    | 0.21         | 0/937           | 0.43        | 0/1260           |
| 43  | 2l    | 0.20         | 0/937           | 0.42        | 0/1260           |
| 44  | 1m    | 0.22         | 0/933           | 0.48        | 0/1254           |
| 44  | 2m    | 0.23         | 0/899           | 0.51        | 0/1212           |
| 45  | 1n    | 0.19         | 0/501           | 0.47        | 0/664            |
| 45  | 2n    | 0.20         | 0/495           | 0.45        | 0/657            |
| 46  | 1o    | 0.22         | 0/739           | 0.40        | 0/985            |
| 46  | 2o    | 0.18         | 0/739           | 0.39        | 0/985            |
| 47  | 1p    | 0.22         | 0/697           | 0.51        | 0/939            |
| 47  | 2p    | 0.21         | 0/693           | 0.48        | 0/935            |
| 48  | 1q    | 0.19         | 0/836           | 0.40        | 0/1117           |
| 48  | 2q    | 0.22         | 0/836           | 0.45        | 0/1117           |
| 49  | 1r    | 0.21         | 0/560           | 0.43        | 0/746            |
| 49  | 2r    | 0.20         | 0/556           | 0.44        | 0/741            |
| 50  | 1s    | 0.32         | 1/667 (0.1%)    | 0.48        | 0/900            |
| 50  | 2s    | 0.19         | 0/661           | 0.42        | 0/893            |
| 51  | 1t    | 0.21         | 0/730           | 0.46        | 0/965            |
| 51  | 2t    | 0.19         | 0/729           | 0.42        | 0/965            |
| 52  | 1u    | 0.20         | 0/203           | 0.42        | 0/266            |
| 52  | 2u    | 0.19         | 0/203           | 0.46        | 0/266            |
| 53  | 1v    | 0.23         | 0/306           | 0.42        | 0/473            |
| 53  | 2v    | 0.21         | 0/306           | 0.40        | 0/473            |
| 54  | 1w    | 0.20         | 0/1956          | 0.40        | 0/2634           |
| 54  | 2w    | 0.21         | 0/1971          | 0.44        | 1/2654 (0.0%)    |
| 55  | 1x    | 0.28         | 1/1629 (0.1%)   | 0.41        | 0/2535           |
| 55  | 1y    | 0.30         | 2/1602 (0.1%)   | 0.42        | 0/2488           |
| 55  | 2x    | 0.25         | 0/1629          | 0.36        | 0/2535           |
| 55  | 2y    | 0.31         | 1/1606 (0.1%)   | 0.36        | 0/2497           |
| 56  | 1z    | 0.27         | 0/128           | 0.49        | 0/175            |
| 56  | 2z    | 0.20         | 0/128           | 0.44        | 0/175            |
| All | All   | 0.24         | 9/317654 (0.0%) | 0.43        | 10/474763 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11  | 2P    | 0                   | 1                   |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 55  | 2y    | 46  | G7M  | O3'-P | 5.99 | 1.62        | 1.56     |
| 50  | 1s    | 65  | ASN  | CA-C  | 5.90 | 1.60        | 1.52     |
| 32  | 1a    | 527 | G7M  | O3'-P | 5.39 | 1.61        | 1.56     |
| 32  | 2a    | 527 | G7M  | O3'-P | 5.29 | 1.61        | 1.56     |
| 55  | 1y    | 46  | G7M  | O3'-P | 5.14 | 1.61        | 1.56     |

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

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | 2w    | 345  | GLU  | N-CA-C      | -9.54 | 103.75      | 114.62   |
| 39  | 2h    | 19   | VAL  | N-CA-C      | -8.59 | 104.22      | 112.29   |
| 31  | 19    | 10   | ILE  | N-CA-C      | -6.55 | 106.41      | 112.96   |
| 1   | 2A    | 1992 | G    | C2'-C3'-O3' | 5.88  | 118.33      | 109.50   |
| 1   | 1A    | 2689 | U    | C4'-C3'-O3' | 5.55  | 117.72      | 109.40   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 11  | 2P    | 35  | HIS  | Peptide |

## 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   | 1A    | 61852 | 0        | 31195    | 627     | 1            |
| 1   | 2A    | 60322 | 0        | 30426    | 720     | 0            |
| 2   | 1B    | 2576  | 0        | 1305     | 24      | 0            |
| 2   | 2B    | 2576  | 0        | 1305     | 37      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 1D    | 2136  | 0        | 2218     | 45      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 40      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 25      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 37      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 51      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 51      | 0            |
| 6   | 1G    | 1425  | 0        | 1443     | 31      | 1            |
| 6   | 2G    | 1424  | 0        | 1434     | 61      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 29      | 0            |
| 7   | 2H    | 1330  | 0        | 1407     | 30      | 0            |
| 8   | 1I    | 1085  | 0        | 1114     | 25      | 0            |
| 8   | 2I    | 1061  | 0        | 1080     | 33      | 0            |
| 9   | 1N    | 1117  | 0        | 1184     | 12      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 18      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 19      | 0            |
| 10  | 2O    | 933   | 0        | 996      | 26      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 33      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 32      | 0            |
| 12  | 1Q    | 1122  | 0        | 1178     | 23      | 0            |
| 12  | 2Q    | 1122  | 0        | 1179     | 30      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 23      | 0            |
| 13  | 2R    | 968   | 0        | 1033     | 28      | 0            |
| 14  | 1S    | 877   | 0        | 938      | 22      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 36      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 17      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 24      | 0            |
| 16  | 1U    | 959   | 0        | 1019     | 10      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 18      | 0            |
| 17  | 1V    | 771   | 0        | 829      | 10      | 0            |
| 17  | 2V    | 771   | 0        | 829      | 11      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 15      | 0            |
| 18  | 2W    | 886   | 0        | 940      | 16      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 19      | 0            |
| 19  | 2X    | 746   | 0        | 803      | 13      | 0            |
| 20  | 1Y    | 806   | 0        | 881      | 14      | 0            |
| 20  | 2Y    | 810   | 0        | 887      | 31      | 0            |
| 21  | 1Z    | 1437  | 0        | 1446     | 43      | 0            |
| 21  | 2Z    | 1451  | 0        | 1450     | 47      | 0            |
| 22  | 10    | 604   | 0        | 619      | 8       | 0            |
| 22  | 20    | 608   | 0        | 622      | 20      | 0            |
| 23  | 11    | 755   | 0        | 825      | 9       | 0            |
| 23  | 21    | 755   | 0        | 826      | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | 12    | 588   | 0        | 643      | 14      | 0            |
| 24  | 22    | 588   | 0        | 643      | 19      | 0            |
| 25  | 13    | 469   | 0        | 518      | 14      | 0            |
| 25  | 23    | 464   | 0        | 514      | 11      | 0            |
| 26  | 14    | 548   | 0        | 529      | 16      | 0            |
| 26  | 24    | 517   | 0        | 479      | 27      | 0            |
| 27  | 15    | 455   | 0        | 465      | 16      | 0            |
| 27  | 25    | 455   | 0        | 465      | 10      | 0            |
| 28  | 16    | 453   | 0        | 472      | 7       | 0            |
| 28  | 26    | 449   | 0        | 469      | 13      | 0            |
| 29  | 17    | 418   | 0        | 467      | 7       | 0            |
| 29  | 27    | 418   | 0        | 467      | 9       | 0            |
| 30  | 18    | 511   | 0        | 571      | 16      | 0            |
| 30  | 28    | 517   | 0        | 582      | 16      | 0            |
| 31  | 19    | 307   | 0        | 335      | 4       | 0            |
| 31  | 29    | 307   | 0        | 335      | 3       | 0            |
| 32  | 1a    | 32246 | 0        | 16295    | 488     | 0            |
| 32  | 2a    | 32327 | 0        | 16338    | 508     | 0            |
| 33  | 1b    | 1846  | 0        | 1867     | 77      | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 76      | 0            |
| 34  | 1c    | 1554  | 0        | 1551     | 38      | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 42      | 0            |
| 35  | 1d    | 1659  | 0        | 1676     | 63      | 0            |
| 35  | 2d    | 1674  | 0        | 1714     | 70      | 0            |
| 36  | 1e    | 1129  | 0        | 1185     | 41      | 0            |
| 36  | 2e    | 1130  | 0        | 1184     | 26      | 0            |
| 37  | 1f    | 810   | 0        | 797      | 15      | 0            |
| 37  | 2f    | 816   | 0        | 808      | 21      | 0            |
| 38  | 1g    | 1231  | 0        | 1238     | 22      | 0            |
| 38  | 2g    | 1235  | 0        | 1249     | 45      | 0            |
| 39  | 1h    | 1088  | 0        | 1126     | 28      | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 23      | 0            |
| 40  | 1i    | 983   | 0        | 986      | 42      | 0            |
| 40  | 2i    | 940   | 0        | 938      | 39      | 0            |
| 41  | 1j    | 721   | 0        | 672      | 33      | 0            |
| 41  | 2j    | 714   | 0        | 672      | 30      | 0            |
| 42  | 1k    | 829   | 0        | 825      | 23      | 0            |
| 42  | 2k    | 833   | 0        | 836      | 32      | 0            |
| 43  | 1l    | 932   | 0        | 979      | 32      | 0            |
| 43  | 2l    | 932   | 0        | 980      | 26      | 0            |
| 44  | 1m    | 923   | 0        | 962      | 41      | 0            |
| 44  | 2m    | 889   | 0        | 901      | 41      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45  | 1n    | 492   | 0        | 529      | 22      | 0            |
| 45  | 2n    | 486   | 0        | 518      | 28      | 0            |
| 46  | 1o    | 728   | 0        | 760      | 16      | 0            |
| 46  | 2o    | 728   | 0        | 760      | 16      | 0            |
| 47  | 1p    | 681   | 0        | 697      | 21      | 0            |
| 47  | 2p    | 677   | 0        | 686      | 22      | 0            |
| 48  | 1q    | 823   | 0        | 891      | 16      | 0            |
| 48  | 2q    | 823   | 0        | 891      | 14      | 0            |
| 49  | 1r    | 555   | 0        | 618      | 12      | 0            |
| 49  | 2r    | 551   | 0        | 614      | 17      | 0            |
| 50  | 1s    | 652   | 0        | 662      | 29      | 0            |
| 50  | 2s    | 646   | 0        | 644      | 23      | 0            |
| 51  | 1t    | 728   | 0        | 798      | 25      | 0            |
| 51  | 2t    | 727   | 0        | 796      | 21      | 0            |
| 52  | 1u    | 199   | 0        | 208      | 9       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 8       | 0            |
| 53  | 1v    | 274   | 0        | 139      | 2       | 0            |
| 53  | 2v    | 274   | 0        | 139      | 4       | 0            |
| 54  | 1w    | 1939  | 0        | 1925     | 60      | 0            |
| 54  | 2w    | 1954  | 0        | 1930     | 54      | 0            |
| 55  | 1x    | 1612  | 0        | 829      | 13      | 0            |
| 55  | 1y    | 1590  | 0        | 815      | 25      | 0            |
| 55  | 2x    | 1612  | 0        | 829      | 15      | 0            |
| 55  | 2y    | 1592  | 0        | 818      | 27      | 0            |
| 56  | 1z    | 121   | 0        | 128      | 2       | 0            |
| 56  | 2z    | 121   | 0        | 128      | 2       | 0            |
| 57  | 10    | 5     | 0        | 0        | 0       | 0            |
| 57  | 11    | 4     | 0        | 0        | 0       | 0            |
| 57  | 12    | 2     | 0        | 0        | 0       | 0            |
| 57  | 13    | 1     | 0        | 0        | 0       | 0            |
| 57  | 14    | 1     | 0        | 0        | 0       | 0            |
| 57  | 15    | 4     | 0        | 0        | 0       | 0            |
| 57  | 16    | 1     | 0        | 0        | 0       | 0            |
| 57  | 17    | 7     | 0        | 0        | 0       | 0            |
| 57  | 18    | 2     | 0        | 0        | 0       | 0            |
| 57  | 19    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1A    | 807   | 0        | 0        | 0       | 0            |
| 57  | 1B    | 20    | 0        | 0        | 0       | 0            |
| 57  | 1D    | 6     | 0        | 0        | 0       | 0            |
| 57  | 1E    | 7     | 0        | 0        | 0       | 0            |
| 57  | 1F    | 8     | 0        | 0        | 0       | 0            |
| 57  | 1G    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | 1N    | 4     | 0        | 0        | 0       | 0            |
| 57  | 1O    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1P    | 4     | 0        | 0        | 0       | 0            |
| 57  | 1Q    | 5     | 0        | 0        | 0       | 0            |
| 57  | 1R    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1T    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1U    | 6     | 0        | 0        | 0       | 0            |
| 57  | 1V    | 5     | 0        | 0        | 0       | 0            |
| 57  | 1W    | 4     | 0        | 0        | 0       | 0            |
| 57  | 1X    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1Z    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1a    | 187   | 0        | 0        | 0       | 0            |
| 57  | 1c    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1d    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1f    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1k    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1v    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1w    | 4     | 0        | 0        | 0       | 0            |
| 57  | 1x    | 8     | 0        | 0        | 0       | 0            |
| 57  | 1y    | 2     | 0        | 0        | 0       | 0            |
| 57  | 20    | 2     | 0        | 0        | 0       | 0            |
| 57  | 21    | 1     | 0        | 0        | 0       | 0            |
| 57  | 23    | 2     | 0        | 0        | 0       | 0            |
| 57  | 25    | 1     | 0        | 0        | 0       | 0            |
| 57  | 28    | 3     | 0        | 0        | 0       | 0            |
| 57  | 29    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2A    | 665   | 0        | 0        | 0       | 0            |
| 57  | 2B    | 11    | 0        | 0        | 0       | 0            |
| 57  | 2D    | 9     | 0        | 0        | 0       | 0            |
| 57  | 2E    | 5     | 0        | 0        | 0       | 0            |
| 57  | 2F    | 6     | 0        | 0        | 0       | 0            |
| 57  | 2N    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2O    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2Q    | 3     | 0        | 0        | 0       | 0            |
| 57  | 2R    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2U    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2V    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2W    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2X    | 4     | 0        | 0        | 0       | 0            |
| 57  | 2Y    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | 2a    | 172   | 0        | 0        | 0       | 0            |
| 57  | 2d    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2e    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2f    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2j    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2k    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2u    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2v    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2w    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2x    | 9     | 0        | 0        | 0       | 0            |
| 58  | 14    | 1     | 0        | 0        | 0       | 0            |
| 58  | 15    | 1     | 0        | 0        | 0       | 0            |
| 58  | 16    | 1     | 0        | 0        | 0       | 0            |
| 58  | 19    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 58  | 24    | 1     | 0        | 0        | 0       | 0            |
| 58  | 25    | 1     | 0        | 0        | 0       | 0            |
| 58  | 26    | 1     | 0        | 0        | 0       | 0            |
| 58  | 29    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 59  | 1d    | 8     | 0        | 0        | 2       | 0            |
| 59  | 2d    | 8     | 0        | 0        | 1       | 0            |
| 60  | 10    | 1     | 0        | 0        | 0       | 0            |
| 60  | 11    | 3     | 0        | 0        | 0       | 0            |
| 60  | 13    | 2     | 0        | 0        | 0       | 0            |
| 60  | 15    | 5     | 0        | 0        | 0       | 0            |
| 60  | 16    | 1     | 0        | 0        | 1       | 0            |
| 60  | 17    | 2     | 0        | 0        | 0       | 0            |
| 60  | 18    | 7     | 0        | 0        | 1       | 0            |
| 60  | 1A    | 1394  | 0        | 0        | 75      | 0            |
| 60  | 1B    | 31    | 0        | 0        | 1       | 0            |
| 60  | 1D    | 15    | 0        | 0        | 1       | 0            |
| 60  | 1E    | 12    | 0        | 0        | 0       | 0            |
| 60  | 1F    | 6     | 0        | 0        | 2       | 0            |
| 60  | 1G    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1N    | 3     | 0        | 0        | 1       | 0            |
| 60  | 1O    | 3     | 0        | 0        | 1       | 0            |
| 60  | 1P    | 15    | 0        | 0        | 1       | 0            |
| 60  | 1Q    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 60  | 1R    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1T    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1U    | 5     | 0        | 0        | 0       | 0            |
| 60  | 1V    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1W    | 2     | 0        | 0        | 0       | 0            |
| 60  | 1X    | 4     | 0        | 0        | 0       | 0            |
| 60  | 1a    | 194   | 0        | 0        | 23      | 0            |
| 60  | 1d    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1l    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1p    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1v    | 3     | 0        | 0        | 1       | 0            |
| 60  | 1w    | 5     | 0        | 0        | 0       | 0            |
| 60  | 1x    | 22    | 0        | 0        | 2       | 0            |
| 60  | 1y    | 1     | 0        | 0        | 1       | 0            |
| 60  | 1z    | 4     | 0        | 0        | 0       | 0            |
| 60  | 20    | 6     | 0        | 0        | 0       | 0            |
| 60  | 21    | 2     | 0        | 0        | 0       | 0            |
| 60  | 23    | 2     | 0        | 0        | 1       | 0            |
| 60  | 25    | 1     | 0        | 0        | 0       | 0            |
| 60  | 27    | 3     | 0        | 0        | 0       | 0            |
| 60  | 28    | 3     | 0        | 0        | 0       | 0            |
| 60  | 2A    | 997   | 0        | 0        | 97      | 0            |
| 60  | 2B    | 7     | 0        | 0        | 0       | 0            |
| 60  | 2D    | 16    | 0        | 0        | 0       | 0            |
| 60  | 2E    | 11    | 0        | 0        | 2       | 0            |
| 60  | 2F    | 5     | 0        | 0        | 0       | 0            |
| 60  | 2N    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2O    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2P    | 12    | 0        | 0        | 1       | 0            |
| 60  | 2Q    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2R    | 3     | 0        | 0        | 1       | 0            |
| 60  | 2T    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2U    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2W    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2X    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2Y    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2a    | 154   | 0        | 0        | 12      | 0            |
| 60  | 2d    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2j    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2t    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2v    | 2     | 0        | 0        | 0       | 0            |
| 60  | 2w    | 2     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | 2x    | 13     | 0        | 0        | 1       | 0            |
| All | All   | 299179 | 0        | 199300   | 4441    | 1            |

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 9.

The worst 5 of 4441 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 1:1A:2124:G:H1    | 1:1A:2174:C:H42 | 1.01                     | 0.97              |
| 1:2A:2129:C:N4    | 1:2A:2159:G:H1  | 1.66                     | 0.94              |
| 1:1A:1057:A:N6    | 1:1A:1081:U:H3  | 1.66                     | 0.94              |
| 1:1A:2124:G:H1    | 1:1A:2174:C:N4  | 1.68                     | 0.91              |
| 6:1G:161:THR:HG22 | 6:1G:163:ALA:H  | 1.36                     | 0.91              |

All (1) 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) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:1A:1472:A:O2' | 6:1G:21:ARG:NH1[1_455] | 2.19                     | 0.01              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 257 (94%) | 16 (6%) | 0        | 100         | 100 |
| 3   | 2D    | 273/276 (99%) | 254 (93%) | 19 (7%) | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 190 (94%) | 11 (5%) | 1 (0%)   | 24          | 48  |
| 4   | 2E    | 202/206 (98%) | 184 (91%) | 17 (8%) | 1 (0%)   | 24          | 48  |
| 5   | 1F    | 201/210 (96%) | 194 (96%) | 5 (2%)  | 2 (1%)   | 12          | 32  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 5   | 2F    | 201/210 (96%) | 187 (93%) | 11 (6%)  | 3 (2%)   | 8           | 22  |
| 6   | 1G    | 179/182 (98%) | 155 (87%) | 19 (11%) | 5 (3%)   | 4           | 9   |
| 6   | 2G    | 179/182 (98%) | 155 (87%) | 22 (12%) | 2 (1%)   | 11          | 29  |
| 7   | 1H    | 172/180 (96%) | 161 (94%) | 10 (6%)  | 1 (1%)   | 21          | 44  |
| 7   | 2H    | 172/180 (96%) | 149 (87%) | 20 (12%) | 3 (2%)   | 7           | 19  |
| 8   | 1I    | 144/148 (97%) | 123 (85%) | 19 (13%) | 2 (1%)   | 9           | 23  |
| 8   | 2I    | 144/148 (97%) | 122 (85%) | 20 (14%) | 2 (1%)   | 9           | 23  |
| 9   | 1N    | 138/140 (99%) | 134 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 133 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 10  | 1O    | 120/122 (98%) | 109 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 10  | 2O    | 120/122 (98%) | 110 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 11  | 1P    | 147/150 (98%) | 138 (94%) | 7 (5%)   | 2 (1%)   | 9           | 23  |
| 11  | 2P    | 147/150 (98%) | 127 (86%) | 19 (13%) | 1 (1%)   | 18          | 41  |
| 12  | 1Q    | 139/141 (99%) | 130 (94%) | 8 (6%)   | 1 (1%)   | 18          | 41  |
| 12  | 2Q    | 139/141 (99%) | 130 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 13  | 1R    | 116/118 (98%) | 111 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 13  | 2R    | 116/118 (98%) | 107 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 14  | 1S    | 108/112 (96%) | 98 (91%)  | 10 (9%)  | 0        | 100         | 100 |
| 14  | 2S    | 108/112 (96%) | 91 (84%)  | 11 (10%) | 6 (6%)   | 1           | 2   |
| 15  | 1T    | 129/146 (88%) | 121 (94%) | 7 (5%)   | 1 (1%)   | 16          | 37  |
| 15  | 2T    | 129/146 (88%) | 117 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 16  | 1U    | 114/118 (97%) | 113 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 112 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 91 (92%)  | 7 (7%)   | 1 (1%)   | 12          | 32  |
| 17  | 2V    | 99/101 (98%)  | 94 (95%)  | 3 (3%)   | 2 (2%)   | 6           | 16  |
| 18  | 1W    | 110/113 (97%) | 109 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 109 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 90 (97%)  | 1 (1%)   | 2 (2%)   | 5           | 14  |
| 19  | 2X    | 93/96 (97%)   | 87 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 20  | 1Y    | 105/110 (96%) | 98 (93%)  | 6 (6%)   | 1 (1%)   | 12          | 32  |
| 20  | 2Y    | 105/110 (96%) | 88 (84%)  | 17 (16%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 21  | 1Z    | 181/206 (88%) | 159 (88%) | 19 (10%) | 3 (2%)   | 7           | 19  |
| 21  | 2Z    | 184/206 (89%) | 159 (86%) | 21 (11%) | 4 (2%)   | 5           | 14  |
| 22  | 10    | 74/85 (87%)   | 70 (95%)  | 3 (4%)   | 1 (1%)   | 9           | 23  |
| 22  | 20    | 75/85 (88%)   | 67 (89%)  | 8 (11%)  | 0        | 100         | 100 |
| 23  | 11    | 95/98 (97%)   | 92 (97%)  | 2 (2%)   | 1 (1%)   | 11          | 29  |
| 23  | 21    | 95/98 (97%)   | 90 (95%)  | 4 (4%)   | 1 (1%)   | 11          | 29  |
| 24  | 12    | 68/72 (94%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 64 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 54 (95%)  | 2 (4%)   | 1 (2%)   | 6           | 18  |
| 25  | 23    | 57/60 (95%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 26  | 14    | 67/71 (94%)   | 48 (72%)  | 11 (16%) | 8 (12%)  | 0           | 0   |
| 26  | 24    | 66/71 (93%)   | 43 (65%)  | 18 (27%) | 5 (8%)   | 1           | 1   |
| 27  | 15    | 57/60 (95%)   | 56 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 54 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 49 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 46 (90%)  | 5 (10%)  | 0        | 100         | 100 |
| 29  | 17    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 61 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 57 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 33 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 193 (84%) | 29 (13%) | 7 (3%)   | 3           | 8   |
| 33  | 2b    | 229/256 (90%) | 193 (84%) | 24 (10%) | 12 (5%)  | 1           | 3   |
| 34  | 1c    | 204/239 (85%) | 175 (86%) | 27 (13%) | 2 (1%)   | 12          | 32  |
| 34  | 2c    | 204/239 (85%) | 166 (81%) | 36 (18%) | 2 (1%)   | 12          | 32  |
| 35  | 1d    | 206/209 (99%) | 180 (87%) | 24 (12%) | 2 (1%)   | 12          | 32  |
| 35  | 2d    | 206/209 (99%) | 177 (86%) | 27 (13%) | 2 (1%)   | 12          | 32  |
| 36  | 1e    | 146/162 (90%) | 129 (88%) | 17 (12%) | 0        | 100         | 100 |
| 36  | 2e    | 146/162 (90%) | 124 (85%) | 19 (13%) | 3 (2%)   | 5           | 15  |
| 37  | 1f    | 98/101 (97%)  | 92 (94%)  | 6 (6%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 37  | 2f    | 98/101 (97%)  | 85 (87%)  | 12 (12%) | 1 (1%)   | 12          | 32  |
| 38  | 1g    | 153/156 (98%) | 134 (88%) | 15 (10%) | 4 (3%)   | 4           | 11  |
| 38  | 2g    | 153/156 (98%) | 135 (88%) | 13 (8%)  | 5 (3%)   | 3           | 7   |
| 39  | 1h    | 135/138 (98%) | 125 (93%) | 9 (7%)   | 1 (1%)   | 18          | 41  |
| 39  | 2h    | 135/138 (98%) | 123 (91%) | 11 (8%)  | 1 (1%)   | 18          | 41  |
| 40  | 1i    | 125/128 (98%) | 103 (82%) | 18 (14%) | 4 (3%)   | 3           | 7   |
| 40  | 2i    | 121/128 (94%) | 99 (82%)  | 20 (16%) | 2 (2%)   | 7           | 19  |
| 41  | 1j    | 96/105 (91%)  | 88 (92%)  | 7 (7%)   | 1 (1%)   | 12          | 32  |
| 41  | 2j    | 94/105 (90%)  | 80 (85%)  | 12 (13%) | 2 (2%)   | 5           | 15  |
| 42  | 1k    | 112/129 (87%) | 103 (92%) | 7 (6%)   | 2 (2%)   | 6           | 18  |
| 42  | 2k    | 112/129 (87%) | 96 (86%)  | 15 (13%) | 1 (1%)   | 14          | 35  |
| 43  | 1l    | 119/132 (90%) | 108 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 43  | 2l    | 119/132 (90%) | 114 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 44  | 1m    | 116/126 (92%) | 102 (88%) | 13 (11%) | 1 (1%)   | 14          | 35  |
| 44  | 2m    | 113/126 (90%) | 96 (85%)  | 14 (12%) | 3 (3%)   | 4           | 10  |
| 45  | 1n    | 58/61 (95%)   | 55 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 19  |
| 45  | 2n    | 58/61 (95%)   | 53 (91%)  | 5 (9%)   | 0        | 100         | 100 |
| 46  | 1o    | 86/89 (97%)   | 81 (94%)  | 4 (5%)   | 1 (1%)   | 10          | 27  |
| 46  | 2o    | 86/89 (97%)   | 76 (88%)  | 9 (10%)  | 1 (1%)   | 10          | 27  |
| 47  | 1p    | 80/88 (91%)   | 66 (82%)  | 13 (16%) | 1 (1%)   | 9           | 25  |
| 47  | 2p    | 80/88 (91%)   | 71 (89%)  | 9 (11%)  | 0        | 100         | 100 |
| 48  | 1q    | 97/105 (92%)  | 91 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 48  | 2q    | 97/105 (92%)  | 85 (88%)  | 12 (12%) | 0        | 100         | 100 |
| 49  | 1r    | 66/88 (75%)   | 62 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 49  | 2r    | 66/88 (75%)   | 60 (91%)  | 5 (8%)   | 1 (2%)   | 8           | 22  |
| 50  | 1s    | 81/93 (87%)   | 70 (86%)  | 10 (12%) | 1 (1%)   | 10          | 27  |
| 50  | 2s    | 81/93 (87%)   | 67 (83%)  | 12 (15%) | 2 (2%)   | 4           | 11  |
| 51  | 1t    | 94/106 (89%)  | 80 (85%)  | 10 (11%) | 4 (4%)   | 2           | 4   |
| 51  | 2t    | 94/106 (89%)  | 85 (90%)  | 5 (5%)   | 4 (4%)   | 2           | 4   |
| 52  | 1u    | 21/27 (78%)   | 21 (100%) | 0        | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)   | 20 (95%)  | 1 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 54  | 1w    | 246/354 (70%)     | 228 (93%)   | 13 (5%)   | 5 (2%)   | 6           | 16  |
| 54  | 2w    | 250/354 (71%)     | 235 (94%)   | 14 (6%)   | 1 (0%)   | 30          | 54  |
| 56  | 1z    | 12/18 (67%)       | 11 (92%)    | 1 (8%)    | 0        | 100         | 100 |
| 56  | 2z    | 12/18 (67%)       | 10 (83%)    | 2 (17%)   | 0        | 100         | 100 |
| All | All   | 11922/12872 (93%) | 10772 (90%) | 1007 (8%) | 143 (1%) | 10          | 27  |

5 of 143 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1F    | 130 | ALA  |
| 6   | 1G    | 50  | ALA  |
| 8   | 1I    | 10  | GLU  |
| 17  | 1V    | 79  | VAL  |
| 23  | 1I    | 3   | LYS  |

### 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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | 1D    | 215/218 (99%) | 199 (93%) | 16 (7%)  | 13          | 32 |
| 3   | 2D    | 215/218 (99%) | 200 (93%) | 15 (7%)  | 14          | 34 |
| 4   | 1E    | 164/166 (99%) | 149 (91%) | 15 (9%)  | 9           | 22 |
| 4   | 2E    | 164/166 (99%) | 149 (91%) | 15 (9%)  | 9           | 22 |
| 5   | 1F    | 160/166 (96%) | 147 (92%) | 13 (8%)  | 11          | 27 |
| 5   | 2F    | 159/166 (96%) | 141 (89%) | 18 (11%) | 5           | 14 |
| 6   | 1G    | 143/156 (92%) | 122 (85%) | 21 (15%) | 3           | 8  |
| 6   | 2G    | 142/156 (91%) | 122 (86%) | 20 (14%) | 3           | 9  |
| 7   | 1H    | 144/148 (97%) | 128 (89%) | 16 (11%) | 6           | 15 |
| 7   | 2H    | 144/148 (97%) | 128 (89%) | 16 (11%) | 6           | 15 |
| 8   | 1I    | 110/124 (89%) | 94 (86%)  | 16 (14%) | 3           | 8  |
| 8   | 2I    | 104/124 (84%) | 76 (73%)  | 28 (27%) | 0           | 1  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 9   | 1N    | 118/119 (99%)  | 111 (94%) | 7 (6%)   | 18          | 42 |
| 9   | 2N    | 118/119 (99%)  | 112 (95%) | 6 (5%)   | 21          | 48 |
| 10  | 1O    | 100/100 (100%) | 98 (98%)  | 2 (2%)   | 48          | 76 |
| 10  | 2O    | 100/100 (100%) | 98 (98%)  | 2 (2%)   | 48          | 76 |
| 11  | 1P    | 115/116 (99%)  | 109 (95%) | 6 (5%)   | 21          | 47 |
| 11  | 2P    | 115/116 (99%)  | 106 (92%) | 9 (8%)   | 11          | 29 |
| 12  | 1Q    | 111/111 (100%) | 99 (89%)  | 12 (11%) | 6           | 16 |
| 12  | 2Q    | 111/111 (100%) | 100 (90%) | 11 (10%) | 7           | 19 |
| 13  | 1R    | 101/101 (100%) | 88 (87%)  | 13 (13%) | 4           | 10 |
| 13  | 2R    | 101/101 (100%) | 95 (94%)  | 6 (6%)   | 18          | 42 |
| 14  | 1S    | 87/88 (99%)    | 72 (83%)  | 15 (17%) | 2           | 6  |
| 14  | 2S    | 85/88 (97%)    | 74 (87%)  | 11 (13%) | 4           | 10 |
| 15  | 1T    | 115/127 (91%)  | 104 (90%) | 11 (10%) | 8           | 20 |
| 15  | 2T    | 113/127 (89%)  | 106 (94%) | 7 (6%)   | 16          | 39 |
| 16  | 1U    | 93/94 (99%)    | 87 (94%)  | 6 (6%)   | 15          | 37 |
| 16  | 2U    | 93/94 (99%)    | 90 (97%)  | 3 (3%)   | 34          | 64 |
| 17  | 1V    | 80/82 (98%)    | 76 (95%)  | 4 (5%)   | 22          | 48 |
| 17  | 2V    | 80/82 (98%)    | 71 (89%)  | 9 (11%)  | 5           | 14 |
| 18  | 1W    | 90/92 (98%)    | 85 (94%)  | 5 (6%)   | 19          | 44 |
| 18  | 2W    | 90/92 (98%)    | 85 (94%)  | 5 (6%)   | 19          | 44 |
| 19  | 1X    | 77/78 (99%)    | 74 (96%)  | 3 (4%)   | 28          | 57 |
| 19  | 2X    | 76/78 (97%)    | 71 (93%)  | 5 (7%)   | 15          | 36 |
| 20  | 1Y    | 85/91 (93%)    | 76 (89%)  | 9 (11%)  | 6           | 17 |
| 20  | 2Y    | 86/91 (94%)    | 75 (87%)  | 11 (13%) | 4           | 11 |
| 21  | 1Z    | 155/179 (87%)  | 141 (91%) | 14 (9%)  | 9           | 23 |
| 21  | 2Z    | 155/179 (87%)  | 137 (88%) | 18 (12%) | 5           | 13 |
| 22  | 10    | 61/67 (91%)    | 56 (92%)  | 5 (8%)   | 10          | 27 |
| 22  | 20    | 61/67 (91%)    | 54 (88%)  | 7 (12%)  | 5           | 14 |
| 23  | 11    | 80/83 (96%)    | 76 (95%)  | 4 (5%)   | 22          | 48 |
| 23  | 21    | 80/83 (96%)    | 74 (92%)  | 6 (8%)   | 12          | 31 |
| 24  | 12    | 65/67 (97%)    | 61 (94%)  | 4 (6%)   | 16          | 39 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 24  | 22    | 65/67 (97%)   | 58 (89%)  | 7 (11%)  | 6           | 16 |
| 25  | 13    | 51/52 (98%)   | 49 (96%)  | 2 (4%)   | 28          | 57 |
| 25  | 23    | 50/52 (96%)   | 47 (94%)  | 3 (6%)   | 17          | 41 |
| 26  | 14    | 58/63 (92%)   | 52 (90%)  | 6 (10%)  | 7           | 18 |
| 26  | 24    | 51/63 (81%)   | 41 (80%)  | 10 (20%) | 1           | 4  |
| 27  | 15    | 50/52 (96%)   | 47 (94%)  | 3 (6%)   | 17          | 41 |
| 27  | 25    | 50/52 (96%)   | 47 (94%)  | 3 (6%)   | 17          | 41 |
| 28  | 16    | 51/52 (98%)   | 47 (92%)  | 4 (8%)   | 11          | 29 |
| 28  | 26    | 50/52 (96%)   | 45 (90%)  | 5 (10%)  | 7           | 19 |
| 29  | 17    | 41/42 (98%)   | 39 (95%)  | 2 (5%)   | 22          | 49 |
| 29  | 27    | 41/42 (98%)   | 39 (95%)  | 2 (5%)   | 22          | 49 |
| 30  | 18    | 53/55 (96%)   | 45 (85%)  | 8 (15%)  | 3           | 7  |
| 30  | 28    | 54/55 (98%)   | 51 (94%)  | 3 (6%)   | 19          | 44 |
| 31  | 19    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 37          | 67 |
| 31  | 29    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 37          | 67 |
| 33  | 1b    | 192/220 (87%) | 156 (81%) | 36 (19%) | 1           | 4  |
| 33  | 2b    | 187/220 (85%) | 154 (82%) | 33 (18%) | 2           | 5  |
| 34  | 1c    | 144/188 (77%) | 127 (88%) | 17 (12%) | 5           | 13 |
| 34  | 2c    | 140/188 (74%) | 120 (86%) | 20 (14%) | 3           | 8  |
| 35  | 1d    | 170/181 (94%) | 142 (84%) | 28 (16%) | 2           | 6  |
| 35  | 2d    | 173/181 (96%) | 148 (86%) | 25 (14%) | 3           | 8  |
| 36  | 1e    | 113/123 (92%) | 106 (94%) | 7 (6%)   | 16          | 39 |
| 36  | 2e    | 113/123 (92%) | 103 (91%) | 10 (9%)  | 9           | 23 |
| 37  | 1f    | 84/90 (93%)   | 76 (90%)  | 8 (10%)  | 8           | 20 |
| 37  | 2f    | 85/90 (94%)   | 78 (92%)  | 7 (8%)   | 10          | 27 |
| 38  | 1g    | 119/127 (94%) | 104 (87%) | 15 (13%) | 4           | 11 |
| 38  | 2g    | 120/127 (94%) | 109 (91%) | 11 (9%)  | 8           | 22 |
| 39  | 1h    | 114/119 (96%) | 102 (90%) | 12 (10%) | 6           | 17 |
| 39  | 2h    | 114/119 (96%) | 105 (92%) | 9 (8%)   | 11          | 28 |
| 40  | 1i    | 90/99 (91%)   | 83 (92%)  | 7 (8%)   | 11          | 29 |
| 40  | 2i    | 86/99 (87%)   | 72 (84%)  | 14 (16%) | 2           | 6  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|------------------|------------|------------|-------------|-----|
| 41  | 1j    | 68/92 (74%)      | 56 (82%)   | 12 (18%)   | 2           | 5   |
| 41  | 2j    | 69/92 (75%)      | 59 (86%)   | 10 (14%)   | 3           | 8   |
| 42  | 1k    | 82/99 (83%)      | 73 (89%)   | 9 (11%)    | 6           | 15  |
| 42  | 2k    | 83/99 (84%)      | 75 (90%)   | 8 (10%)    | 8           | 20  |
| 43  | 1l    | 96/108 (89%)     | 86 (90%)   | 10 (10%)   | 7           | 17  |
| 43  | 2l    | 96/108 (89%)     | 88 (92%)   | 8 (8%)     | 10          | 26  |
| 44  | 1m    | 90/101 (89%)     | 78 (87%)   | 12 (13%)   | 4           | 10  |
| 44  | 2m    | 85/101 (84%)     | 79 (93%)   | 6 (7%)     | 13          | 33  |
| 45  | 1n    | 49/50 (98%)      | 43 (88%)   | 6 (12%)    | 5           | 12  |
| 45  | 2n    | 48/50 (96%)      | 38 (79%)   | 10 (21%)   | 1           | 3   |
| 46  | 1o    | 78/80 (98%)      | 73 (94%)   | 5 (6%)     | 16          | 38  |
| 46  | 2o    | 78/80 (98%)      | 73 (94%)   | 5 (6%)     | 16          | 38  |
| 47  | 1p    | 69/74 (93%)      | 60 (87%)   | 9 (13%)    | 4           | 10  |
| 47  | 2p    | 68/74 (92%)      | 61 (90%)   | 7 (10%)    | 7           | 18  |
| 48  | 1q    | 94/97 (97%)      | 85 (90%)   | 9 (10%)    | 8           | 20  |
| 48  | 2q    | 94/97 (97%)      | 80 (85%)   | 14 (15%)   | 3           | 8   |
| 49  | 1r    | 59/77 (77%)      | 51 (86%)   | 8 (14%)    | 3           | 9   |
| 49  | 2r    | 58/77 (75%)      | 48 (83%)   | 10 (17%)   | 2           | 6   |
| 50  | 1s    | 69/80 (86%)      | 64 (93%)   | 5 (7%)     | 13          | 32  |
| 50  | 2s    | 67/80 (84%)      | 57 (85%)   | 10 (15%)   | 3           | 8   |
| 51  | 1t    | 70/82 (85%)      | 61 (87%)   | 9 (13%)    | 4           | 10  |
| 51  | 2t    | 70/82 (85%)      | 64 (91%)   | 6 (9%)     | 10          | 25  |
| 52  | 1u    | 18/22 (82%)      | 18 (100%)  | 0          | 100         | 100 |
| 52  | 2u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)     | 19          | 44  |
| 54  | 1w    | 203/298 (68%)    | 177 (87%)  | 26 (13%)   | 4           | 11  |
| 54  | 2w    | 202/298 (68%)    | 167 (83%)  | 35 (17%)   | 2           | 5   |
| 56  | 1z    | 14/17 (82%)      | 12 (86%)   | 2 (14%)    | 3           | 8   |
| 56  | 2z    | 14/17 (82%)      | 12 (86%)   | 2 (14%)    | 3           | 8   |
| All | All   | 9747/10694 (91%) | 8729 (90%) | 1018 (10%) | 7           | 17  |

5 of 1018 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | 1t    | 55  | ILE  |
| 41  | 2j    | 13  | HIS  |
| 7   | 2H    | 122 | THR  |
| 40  | 2i    | 64  | THR  |
| 48  | 2q    | 76  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2d    | 42  | GLN  |
| 35  | 2d    | 119 | GLN  |
| 40  | 2i    | 87  | GLN  |
| 40  | 1i    | 31  | GLN  |
| 39  | 1h    | 82  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2864/2915 (98%) | 468 (16%)         | 28 (0%)         |
| 1   | 2A    | 2791/2915 (95%) | 490 (17%)         | 25 (0%)         |
| 2   | 1B    | 119/121 (98%)   | 11 (9%)           | 0               |
| 2   | 2B    | 119/121 (98%)   | 18 (15%)          | 0               |
| 32  | 1a    | 1497/1521 (98%) | 318 (21%)         | 0               |
| 32  | 2a    | 1501/1521 (98%) | 323 (21%)         | 0               |
| 53  | 1v    | 10/24 (41%)     | 3 (30%)           | 0               |
| 53  | 2v    | 10/24 (41%)     | 2 (20%)           | 0               |
| 55  | 1x    | 73/76 (96%)     | 13 (17%)          | 0               |
| 55  | 1y    | 71/76 (93%)     | 22 (30%)          | 0               |
| 55  | 2x    | 73/76 (96%)     | 12 (16%)          | 0               |
| 55  | 2y    | 72/76 (94%)     | 26 (36%)          | 0               |
| All | All   | 9200/9466 (97%) | 1706 (18%)        | 53 (0%)         |

5 of 1706 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 13  | A    |
| 1   | 1A    | 15  | G    |
| 1   | 1A    | 34  | C    |
| 1   | 1A    | 45  | C    |

5 of 53 RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 34     | C    |
| 1   | 2A    | 746    | A    |
| 1   | 2A    | 2119   | A    |
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 271(M) | G    |

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

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

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

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | PSU  | 1y    | 55   | 55      | 18,21,22     | 1.41 | 2 (11%)  | 21,30,33    | 1.91 | 3 (14%)  |
| 1   | OMG  | 1A    | 2251 | 1,57,55 | 23,26,27     | 1.25 | 3 (13%)  | 32,38,41    | 2.09 | 7 (21%)  |
| 32  | 4OC  | 2a    | 1402 | 57,32   | 20,23,24     | 0.79 | 0        | 25,32,35    | 0.92 | 0        |
| 32  | 2MG  | 2a    | 1207 | 32      | 23,26,27     | 1.22 | 2 (8%)   | 33,38,41    | 2.21 | 8 (24%)  |
| 1   | 2MA  | 2A    | 2503 | 1,57    | 22,25,26     | 1.48 | 4 (18%)  | 32,37,40    | 2.24 | 9 (28%)  |
| 55  | PSU  | 1x    | 55   | 55      | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 55  | PSU  | 1y    | 39   | 55      | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 1.94 | 3 (14%)  |
| 32  | UR3  | 2a    | 1498 | 57,32   | 19,22,23     | 0.96 | 0        | 26,32,35    | 1.70 | 2 (7%)   |
| 32  | PSU  | 2a    | 516  | 57,32   | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.02 | 5 (23%)  |
| 1   | 5MU  | 1A    | 1915 | 1,57,54 | 19,22,23     | 1.48 | 5 (26%)  | 27,32,35    | 2.11 | 6 (22%)  |
| 55  | PSU  | 1x    | 39   | 55      | 18,21,22     | 1.42 | 2 (11%)  | 21,30,33    | 1.86 | 3 (14%)  |
| 55  | MIA  | 2y    | 37   | 55      | 28,31,32     | 2.45 | 6 (21%)  | 38,44,47    | 2.81 | 13 (34%) |
| 55  | G7M  | 1y    | 46   | 55      | 23,26,27     | 1.55 | 4 (17%)  | 34,39,42    | 1.81 | 5 (14%)  |
| 55  | PSU  | 2y    | 55   | 55      | 18,21,22     | 1.37 | 3 (16%)  | 21,30,33    | 1.98 | 3 (14%)  |
| 55  | 4SU  | 1y    | 8    | 55      | 18,21,22     | 1.74 | 4 (22%)  | 25,30,33    | 2.46 | 6 (24%)  |
| 1   | 5MU  | 1A    | 1939 | 1,57    | 19,22,23     | 1.46 | 6 (31%)  | 27,32,35    | 2.30 | 6 (22%)  |
| 55  | PSU  | 2x    | 55   | 55      | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 2.02 | 3 (14%)  |
| 32  | MA6  | 2a    | 1519 | 32      | 23,26,27     | 0.41 | 0        | 33,38,41    | 2.11 | 8 (24%)  |

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | PSU  | 1y    | 32   | 55      | 18,21,22     | 1.40 | 3 (16%)  | 21,30,33    | 1.94 | 3 (14%)  |
| 1   | OMC  | 2A    | 1920 | 1,57    | 19,22,23     | 0.82 | 0        | 25,31,34    | 0.89 | 0        |
| 1   | 5MC  | 2A    | 1962 | 1,57    | 19,22,23     | 1.57 | 3 (15%)  | 26,32,35    | 1.14 | 2 (7%)   |
| 55  | MIA  | 1y    | 37   | 55      | 28,31,32     | 2.36 | 5 (17%)  | 38,44,47    | 2.53 | 12 (31%) |
| 1   | PSU  | 2A    | 1917 | 1       | 18,21,22     | 1.36 | 3 (16%)  | 21,30,33    | 2.09 | 4 (19%)  |
| 55  | MIA  | 1x    | 37   | 55      | 28,31,32     | 2.36 | 7 (25%)  | 38,44,47    | 2.62 | 13 (34%) |
| 32  | PSU  | 1a    | 516  | 57,32   | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.00 | 5 (23%)  |
| 32  | MA6  | 1a    | 1518 | 32      | 23,26,27     | 0.41 | 0        | 33,38,41    | 1.96 | 9 (27%)  |
| 55  | G7M  | 2x    | 46   | 55      | 23,26,27     | 1.51 | 3 (13%)  | 34,39,42    | 1.75 | 5 (14%)  |
| 1   | PSU  | 1A    | 2605 | 1,57    | 18,21,22     | 1.49 | 4 (22%)  | 21,30,33    | 1.99 | 4 (19%)  |
| 32  | G7M  | 1a    | 527  | 57,32   | 23,26,27     | 1.56 | 3 (13%)  | 34,39,42    | 1.73 | 5 (14%)  |
| 1   | OMU  | 2A    | 2552 | 1,57    | 19,22,23     | 1.25 | 3 (15%)  | 25,31,34    | 1.90 | 5 (20%)  |
| 32  | M2G  | 2a    | 966  | 32      | 24,27,28     | 1.30 | 4 (16%)  | 33,40,43    | 1.88 | 6 (18%)  |
| 55  | 5MU  | 2y    | 54   | 55      | 19,22,23     | 1.44 | 5 (26%)  | 27,32,35    | 2.15 | 8 (29%)  |
| 1   | PSU  | 1A    | 1911 | 1       | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 2.12 | 5 (23%)  |
| 32  | MA6  | 2a    | 1518 | 32      | 23,26,27     | 0.41 | 0        | 33,38,41    | 2.06 | 9 (27%)  |
| 1   | OMC  | 1A    | 1920 | 1       | 19,22,23     | 0.80 | 0        | 25,31,34    | 1.03 | 2 (8%)   |
| 1   | OMG  | 2A    | 2251 | 1,57,55 | 23,26,27     | 1.29 | 3 (13%)  | 32,38,41    | 1.93 | 6 (18%)  |
| 32  | 5MC  | 1a    | 1407 | 32      | 19,22,23     | 1.43 | 2 (10%)  | 26,32,35    | 1.06 | 2 (7%)   |
| 32  | MA6  | 1a    | 1519 | 32      | 23,26,27     | 0.45 | 0        | 33,38,41    | 2.14 | 10 (30%) |
| 1   | 5MC  | 2A    | 1942 | 1       | 19,22,23     | 1.74 | 3 (15%)  | 26,32,35    | 1.21 | 2 (7%)   |
| 55  | 5MU  | 1y    | 54   | 55      | 19,22,23     | 1.43 | 4 (21%)  | 27,32,35    | 1.68 | 6 (22%)  |
| 55  | G7M  | 1x    | 46   | 55      | 23,26,27     | 1.55 | 4 (17%)  | 34,39,42    | 1.78 | 4 (11%)  |
| 32  | G7M  | 2a    | 527  | 32      | 23,26,27     | 1.49 | 3 (13%)  | 34,39,42    | 1.71 | 5 (14%)  |
| 32  | 5MC  | 2a    | 967  | 32      | 19,22,23     | 1.61 | 3 (15%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 55  | G7M  | 2y    | 46   | 55      | 23,26,27     | 1.55 | 4 (17%)  | 34,39,42    | 1.78 | 5 (14%)  |
| 32  | M2G  | 1a    | 966  | 32      | 24,27,28     | 1.31 | 3 (12%)  | 33,40,43    | 1.92 | 7 (21%)  |
| 43  | 0TD  | 1l    | 92   | 43      | 8,9,10       | 4.34 | 1 (12%)  | 6,11,13     | 7.76 | 1 (16%)  |
| 32  | 5MC  | 1a    | 967  | 32      | 19,22,23     | 1.65 | 3 (15%)  | 26,32,35    | 1.14 | 2 (7%)   |
| 1   | 5MU  | 2A    | 1915 | 1,57    | 19,22,23     | 1.44 | 5 (26%)  | 27,32,35    | 2.14 | 6 (22%)  |
| 1   | PSU  | 2A    | 2605 | 1       | 18,21,22     | 1.30 | 2 (11%)  | 21,30,33    | 2.08 | 3 (14%)  |
| 1   | 5MU  | 2A    | 1939 | 1,57    | 19,22,23     | 1.48 | 6 (31%)  | 27,32,35    | 2.15 | 6 (22%)  |
| 1   | OMU  | 1A    | 2552 | 1,57    | 19,22,23     | 1.27 | 3 (15%)  | 25,31,34    | 1.93 | 5 (20%)  |
| 32  | 5MC  | 2a    | 1400 | 32      | 19,22,23     | 1.65 | 3 (15%)  | 26,32,35    | 1.24 | 4 (15%)  |
| 1   | 2MA  | 1A    | 2503 | 1,57    | 22,25,26     | 1.51 | 4 (18%)  | 32,37,40    | 2.32 | 7 (21%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5MC  | 1A    | 1942 | 1     | 19,22,23     | 1.50 | 3 (15%)  | 26,32,35    | 1.14 | 3 (11%)  |
| 55  | 5MU  | 1x    | 54   | 55    | 19,22,23     | 1.40 | 4 (21%)  | 27,32,35    | 1.78 | 7 (25%)  |
| 32  | 4OC  | 1a    | 1402 | 57,32 | 20,23,24     | 0.80 | 1 (5%)   | 25,32,35    | 0.96 | 1 (4%)   |
| 55  | PSU  | 2x    | 39   | 55    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.86 | 3 (14%)  |
| 55  | PSU  | 1x    | 32   | 55    | 18,21,22     | 1.38 | 3 (16%)  | 21,30,33    | 2.09 | 5 (23%)  |
| 1   | 5MC  | 1A    | 1962 | 1,57  | 19,22,23     | 1.55 | 3 (15%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 55  | 4SU  | 1x    | 8    | 55    | 18,21,22     | 1.78 | 5 (27%)  | 25,30,33    | 2.16 | 5 (20%)  |
| 55  | 4SU  | 2y    | 8    | 55    | 18,21,22     | 1.83 | 6 (33%)  | 25,30,33    | 1.67 | 5 (20%)  |
| 55  | PSU  | 2y    | 32   | 55    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.90 | 3 (14%)  |
| 1   | PSU  | 1A    | 1917 | 1     | 18,21,22     | 1.42 | 2 (11%)  | 21,30,33    | 2.12 | 5 (23%)  |
| 54  | MEQ  | 1w    | 230  | 54    | 8,9,10       | 1.00 | 0        | 5,10,12     | 0.78 | 0        |
| 32  | 5MC  | 2a    | 1404 | 32    | 19,22,23     | 1.60 | 2 (10%)  | 26,32,35    | 1.16 | 3 (11%)  |
| 32  | 5MC  | 2a    | 1407 | 32    | 19,22,23     | 1.59 | 3 (15%)  | 26,32,35    | 1.14 | 3 (11%)  |
| 43  | 0TD  | 2l    | 92   | 43    | 8,9,10       | 4.44 | 2 (25%)  | 6,11,13     | 5.67 | 1 (16%)  |
| 55  | 5MU  | 2x    | 54   | 55    | 19,22,23     | 1.40 | 5 (26%)  | 27,32,35    | 1.80 | 6 (22%)  |
| 32  | 2MG  | 1a    | 1207 | 32    | 23,26,27     | 1.24 | 4 (17%)  | 33,38,41    | 2.20 | 8 (24%)  |
| 55  | PSU  | 2x    | 32   | 55    | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.03 | 3 (14%)  |
| 32  | UR3  | 1a    | 1498 | 32    | 19,22,23     | 1.08 | 2 (10%)  | 26,32,35    | 1.66 | 4 (15%)  |
| 55  | 4SU  | 2x    | 8    | 55    | 18,21,22     | 1.87 | 5 (27%)  | 25,30,33    | 2.04 | 5 (20%)  |
| 54  | MEQ  | 2w    | 230  | 54    | 8,9,10       | 0.91 | 0        | 5,10,12     | 0.50 | 0        |
| 55  | MIA  | 2x    | 37   | 55    | 28,31,32     | 2.41 | 5 (17%)  | 38,44,47    | 2.70 | 14 (36%) |
| 32  | 5MC  | 1a    | 1400 | 32    | 19,22,23     | 1.75 | 3 (15%)  | 26,32,35    | 1.15 | 2 (7%)   |
| 1   | PSU  | 2A    | 1911 | 1     | 18,21,22     | 1.40 | 3 (16%)  | 21,30,33    | 2.10 | 5 (23%)  |
| 55  | PSU  | 2y    | 39   | 55    | 18,21,22     | 1.42 | 2 (11%)  | 21,30,33    | 1.66 | 3 (14%)  |
| 32  | 5MC  | 1a    | 1404 | 32    | 19,22,23     | 1.62 | 3 (15%)  | 26,32,35    | 1.10 | 2 (7%)   |

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  | PSU  | 1y    | 55   | 55      | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | 1A    | 2251 | 1,57,55 | -       | 0/9/27/28 | 0/3/3/3 |
| 32  | 4OC  | 2a    | 1402 | 57,32   | -       | 2/9/29/30 | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32      | -       | 1/9/27/28 | 0/3/3/3 |
| 1   | 2MA  | 2A    | 2503 | 1,57    | -       | 2/7/25/26 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link    | Chirals | Torsions   | Rings   |
|-----|------|-------|------|---------|---------|------------|---------|
| 55  | PSU  | 1x    | 55   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 1y    | 39   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | UR3  | 2a    | 1498 | 57,32   | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 57,32   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1,57,54 | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 1x    | 39   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | MIA  | 2y    | 37   | 55      | -       | 3/15/33/34 | 0/3/3/3 |
| 55  | G7M  | 1y    | 46   | 55      | -       | 3/7/25/26  | 0/3/3/3 |
| 55  | PSU  | 2y    | 55   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 1y    | 8    | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 1,57    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 2x    | 55   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1519 | 32      | -       | 3/11/29/30 | 0/3/3/3 |
| 55  | PSU  | 1y    | 32   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 2A    | 1920 | 1,57    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 1,57    | -       | 2/7/25/26  | 0/2/2/2 |
| 55  | MIA  | 1y    | 37   | 55      | -       | 4/15/33/34 | 0/3/3/3 |
| 1   | PSU  | 2A    | 1917 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | MIA  | 1x    | 37   | 55      | -       | 5/15/33/34 | 0/3/3/3 |
| 32  | PSU  | 1a    | 516  | 57,32   | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1518 | 32      | -       | 0/11/29/30 | 0/3/3/3 |
| 55  | G7M  | 2x    | 46   | 55      | -       | 3/7/25/26  | 0/3/3/3 |
| 1   | PSU  | 1A    | 2605 | 1,57    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | G7M  | 1a    | 527  | 57,32   | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | OMU  | 2A    | 2552 | 1,57    | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | M2G  | 2a    | 966  | 32      | -       | 0/11/29/30 | 0/3/3/3 |
| 55  | 5MU  | 2y    | 54   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1911 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1518 | 32      | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | OMC  | 1A    | 1920 | 1       | -       | 3/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 1,57,55 | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1407 | 32      | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1519 | 32      | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | 5MC  | 2A    | 1942 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU  | 1y    | 54   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | G7M  | 1x    | 46   | 55      | -       | 3/7/25/26  | 0/3/3/3 |
| 32  | G7M  | 2a    | 527  | 32      | -       | 0/7/25/26  | 0/3/3/3 |
| 32  | 5MC  | 2a    | 967  | 32      | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | G7M  | 2y    | 46   | 55      | -       | 2/7/25/26  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 32  | M2G  | 1a    | 966  | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 43  | 0TD  | 1l    | 92   | 43    | -       | 3/7/12/14  | -       |
| 32  | 5MC  | 1a    | 967  | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1915 | 1,57  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 2605 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 1,57  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 1A    | 2552 | 1,57  | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1400 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2503 | 1,57  | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1942 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU  | 1x    | 54   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 4OC  | 1a    | 1402 | 57,32 | -       | 2/9/29/30  | 0/2/2/2 |
| 55  | PSU  | 2x    | 39   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 1x    | 32   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1962 | 1,57  | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 1x    | 8    | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 2y    | 8    | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 2y    | 32   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MEQ  | 1w    | 230  | 54    | -       | 3/8/9/11   | -       |
| 32  | 5MC  | 2a    | 1404 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43    | -       | 5/7/12/14  | -       |
| 55  | 5MU  | 2x    | 54   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32    | -       | 0/9/27/28  | 0/3/3/3 |
| 55  | PSU  | 2x    | 32   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | UR3  | 1a    | 1498 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 2x    | 8    | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MEQ  | 2w    | 230  | 54    | -       | 2/8/9/11   | -       |
| 55  | MIA  | 2x    | 37   | 55    | -       | 3/15/33/34 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1400 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 2y    | 39   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1404 | 32    | -       | 0/7/25/26  | 0/2/2/2 |

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

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 43  | 2l    | 92  | 0TD  | CB-SB  | -12.01 | 1.70        | 1.82     |
| 43  | 1l    | 92  | 0TD  | CB-SB  | -11.84 | 1.70        | 1.82     |
| 55  | 2y    | 37  | MIA  | C2-S10 | -7.45  | 1.69        | 1.75     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 55  | 1x    | 37  | MIA  | C2-S10  | -7.12 | 1.69        | 1.75     |
| 55  | 2x    | 37  | MIA  | C13-C14 | 7.06  | 1.53        | 1.32     |

The worst 5 of 372 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB   | 18.90 | 136.33      | 102.36   |
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB   | 13.78 | 127.14      | 102.36   |
| 55  | 2y    | 37   | MIA  | C12-C13-C14 | -8.81 | 111.21      | 127.01   |
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3    | -8.24 | 118.50      | 127.18   |
| 55  | 1x    | 37   | MIA  | C12-C13-C14 | -8.09 | 112.49      | 127.01   |

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 32  | 1a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 54  | 1w    | 230  | MEQ  | C-CA-CB-CG      |
| 55  | 1x    | 37   | MIA  | C12-C13-C14-C15 |
| 55  | 1x    | 37   | MIA  | C12-C13-C14-C16 |
| 55  | 1x    | 46   | G7M  | C4'-C5'-O5'-P   |

There are no ring outliers.

35 monomers are involved in 45 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55  | 1y    | 55   | PSU  | 1       | 0            |
| 1   | 1A    | 2251 | OMG  | 1       | 0            |
| 32  | 2a    | 1402 | 4OC  | 2       | 0            |
| 32  | 2a    | 1207 | 2MG  | 1       | 0            |
| 1   | 2A    | 2503 | 2MA  | 1       | 0            |
| 55  | 1y    | 39   | PSU  | 1       | 0            |
| 55  | 2y    | 37   | MIA  | 1       | 0            |
| 55  | 1y    | 46   | G7M  | 2       | 0            |
| 1   | 1A    | 1939 | 5MU  | 1       | 0            |
| 32  | 2a    | 1519 | MA6  | 2       | 0            |
| 55  | 1y    | 37   | MIA  | 3       | 0            |
| 1   | 2A    | 1917 | PSU  | 1       | 0            |
| 32  | 1a    | 1518 | MA6  | 2       | 0            |
| 55  | 2y    | 54   | 5MU  | 1       | 0            |
| 32  | 2a    | 1518 | MA6  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1A    | 1920 | OMC  | 1       | 0            |
| 1   | 2A    | 2251 | OMG  | 1       | 0            |
| 32  | 1a    | 1519 | MA6  | 3       | 0            |
| 55  | 1x    | 46   | G7M  | 1       | 0            |
| 32  | 2a    | 527  | G7M  | 1       | 0            |
| 55  | 2y    | 46   | G7M  | 1       | 0            |
| 32  | 1a    | 966  | M2G  | 1       | 0            |
| 32  | 1a    | 967  | 5MC  | 1       | 0            |
| 1   | 1A    | 2552 | OMU  | 1       | 0            |
| 1   | 1A    | 2503 | 2MA  | 2       | 0            |
| 32  | 1a    | 1402 | 4OC  | 2       | 0            |
| 55  | 1x    | 8    | 4SU  | 1       | 0            |
| 55  | 2y    | 8    | 4SU  | 4       | 0            |
| 1   | 1A    | 1917 | PSU  | 1       | 0            |
| 32  | 2a    | 1404 | 5MC  | 1       | 0            |
| 43  | 2l    | 92   | 0TD  | 2       | 0            |
| 32  | 1a    | 1207 | 2MG  | 2       | 0            |
| 55  | 2x    | 8    | 4SU  | 1       | 0            |
| 54  | 2w    | 230  | MEQ  | 1       | 0            |
| 55  | 2y    | 39   | PSU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2056 ligands modelled in this entry, 2054 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 | $\# Z  > 2$ |
| 59  | SF4  | 2d    | 302 | 35   | 0,12,12      | -    | -           | -           |      |             |
| 59  | SF4  | 1d    | 302 | 35   | 0,12,12      | -    | -           | -           |      |             |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 59  | SF4  | 2d    | 302 | 35   | -       | -        | 0/6/5/5 |
| 59  | SF4  | 1d    | 302 | 35   | -       | -        | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 59  | 2d    | 302 | SF4  | 1       | 0            |
| 59  | 1d    | 302 | SF4  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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   | 1A    | 2860/2915 (98%) | -0.51  | 91 (3%)  | 50  | 46  | 16, 33, 90, 104       | 0     |
| 1   | 2A    | 2789/2915 (95%) | -0.02  | 78 (2%)  | 55  | 51  | 29, 56, 89, 104       | 0     |
| 2   | 1B    | 120/121 (99%)   | -0.44  | 0        | 100 | 100 | 25, 48, 61, 77        | 0     |
| 2   | 2B    | 120/121 (99%)   | 0.66   | 6 (5%)   | 34  | 30  | 59, 79, 88, 98        | 0     |
| 3   | 1D    | 275/276 (99%)   | -0.18  | 2 (0%)   | 84  | 83  | 17, 35, 51, 75        | 0     |
| 3   | 2D    | 275/276 (99%)   | 0.41   | 7 (2%)   | 58  | 55  | 31, 50, 64, 77        | 0     |
| 4   | 1E    | 204/206 (99%)   | -0.15  | 0        | 100 | 100 | 17, 36, 55, 67        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.38   | 2 (0%)   | 79  | 78  | 35, 56, 69, 77        | 0     |
| 5   | 1F    | 203/210 (96%)   | -0.15  | 2 (0%)   | 79  | 78  | 18, 38, 65, 82        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.48   | 1 (0%)   | 87  | 86  | 36, 63, 76, 89        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.59   | 12 (6%)  | 24  | 21  | 43, 56, 71, 84        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.35   | 37 (20%) | 3   | 2   | 63, 79, 85, 89        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.17   | 3 (1%)   | 69  | 67  | 34, 51, 65, 69        | 0     |
| 7   | 2H    | 174/180 (96%)   | 0.91   | 8 (4%)   | 37  | 34  | 64, 77, 84, 91        | 0     |
| 8   | 1I    | 146/148 (98%)   | 0.51   | 4 (2%)   | 56  | 53  | 42, 67, 76, 80        | 0     |
| 8   | 2I    | 146/148 (98%)   | 1.01   | 13 (8%)  | 15  | 13  | 55, 72, 79, 83        | 0     |
| 9   | 1N    | 140/140 (100%)  | -0.31  | 0        | 100 | 100 | 21, 32, 54, 61        | 0     |
| 9   | 2N    | 140/140 (100%)  | 0.44   | 1 (0%)   | 84  | 83  | 45, 61, 72, 80        | 0     |
| 10  | 1O    | 122/122 (100%)  | -0.13  | 0        | 100 | 100 | 27, 38, 54, 60        | 0     |
| 10  | 2O    | 122/122 (100%)  | 0.09   | 0        | 100 | 100 | 38, 53, 63, 73        | 0     |
| 11  | 1P    | 149/150 (99%)   | 0.03   | 2 (1%)   | 75  | 73  | 15, 39, 59, 67        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.61   | 4 (2%)   | 56  | 53  | 37, 65, 77, 88        | 0     |
| 12  | 1Q    | 141/141 (100%)  | -0.11  | 0        | 100 | 100 | 23, 37, 52, 71        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 0.60   | 6 (4%)   | 40  | 36  | 48, 60, 70, 84        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | -0.22  | 0 100 100    | 21, 31, 44, 57        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.33   | 1 (0%) 82 81 | 38, 53, 64, 71        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.11   | 1 (0%) 81 80 | 37, 47, 60, 64        | 0     |
| 14  | 2S    | 110/112 (98%)  | 1.05   | 9 (8%) 17 15 | 62, 71, 76, 81        | 0     |
| 15  | 1T    | 131/146 (89%)  | -0.00  | 3 (2%) 61 58 | 29, 41, 66, 81        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.47   | 3 (2%) 61 58 | 46, 56, 72, 83        | 0     |
| 16  | 1U    | 116/118 (98%)  | -0.27  | 1 (0%) 81 80 | 18, 26, 39, 58        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.32   | 0 100 100    | 41, 57, 70, 76        | 0     |
| 17  | 1V    | 101/101 (100%) | -0.26  | 0 100 100    | 18, 35, 52, 58        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.46   | 0 100 100    | 40, 65, 75, 81        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.37  | 0 100 100    | 21, 27, 42, 81        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.15   | 0 100 100    | 40, 50, 66, 84        | 0     |
| 19  | 1X    | 95/96 (98%)    | -0.08  | 1 (1%) 78 76 | 24, 35, 54, 68        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.74   | 4 (4%) 40 37 | 49, 61, 69, 80        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.15   | 0 100 100    | 27, 44, 63, 74        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 0.78   | 4 (3%) 45 41 | 56, 69, 77, 82        | 0     |
| 21  | 1Z    | 183/206 (88%)  | 0.30   | 1 (0%) 87 86 | 35, 54, 69, 74        | 0     |
| 21  | 2Z    | 186/206 (90%)  | 0.69   | 3 (1%) 70 68 | 59, 73, 80, 89        | 0     |
| 22  | 10    | 76/85 (89%)    | -0.08  | 0 100 100    | 25, 35, 48, 61        | 0     |
| 22  | 20    | 77/85 (90%)    | 1.02   | 9 (11%) 9 7  | 50, 62, 70, 77        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.09   | 1 (1%) 79 78 | 26, 40, 66, 70        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.63   | 4 (4%) 41 37 | 41, 58, 74, 79        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.12   | 3 (4%) 40 36 | 34, 46, 58, 74        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.41   | 1 (1%) 73 72 | 57, 67, 73, 78        | 0     |
| 25  | 13    | 59/60 (98%)    | -0.27  | 0 100 100    | 20, 31, 55, 72        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.40   | 1 (1%) 69 67 | 50, 58, 71, 78        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.93   | 9 (13%) 7 6  | 53, 73, 86, 88        | 0     |
| 26  | 24    | 68/71 (95%)    | 1.29   | 16 (23%) 2 1 | 76, 84, 89, 94        | 0     |
| 27  | 15    | 59/60 (98%)    | -0.46  | 0 100 100    | 16, 28, 45, 55        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.37   | 2 (3%) 48 44 | 34, 50, 66, 82        | 0     |
| 28  | 16    | 53/54 (98%)    | -0.14  | 0 100 100    | 30, 40, 54, 58        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.56   | 0 100 100      | 54, 61, 68, 73        | 0     |
| 29  | 17    | 48/49 (97%)     | -0.10  | 3 (6%) 26 23   | 21, 26, 64, 66        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.31   | 4 (8%) 17 14   | 36, 44, 65, 79        | 0     |
| 30  | 18    | 64/65 (98%)     | 0.04   | 0 100 100      | 24, 30, 37, 46        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.52   | 1 (1%) 70 68   | 43, 51, 60, 62        | 0     |
| 31  | 19    | 37/37 (100%)    | 0.00   | 0 100 100      | 27, 39, 52, 57        | 0     |
| 31  | 29    | 37/37 (100%)    | 0.71   | 0 100 100      | 56, 64, 73, 76        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.45   | 56 (3%) 44 40  | 35, 71, 92, 103       | 0     |
| 32  | 2a    | 1491/1521 (98%) | 0.50   | 46 (3%) 51 48  | 44, 74, 92, 104       | 0     |
| 33  | 1b    | 231/256 (90%)   | 1.02   | 25 (10%) 11 9  | 63, 75, 85, 90        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.43   | 63 (27%) 1 1   | 63, 79, 87, 96        | 0     |
| 34  | 1c    | 206/239 (86%)   | 1.07   | 18 (8%) 16 13  | 63, 77, 84, 91        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.07   | 21 (10%) 12 10 | 67, 78, 84, 87        | 0     |
| 35  | 1d    | 208/209 (99%)   | 0.99   | 11 (5%) 32 28  | 53, 72, 79, 89        | 0     |
| 35  | 2d    | 208/209 (99%)   | 0.86   | 13 (6%) 26 23  | 53, 68, 76, 86        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.64   | 4 (2%) 56 53   | 53, 64, 73, 81        | 0     |
| 36  | 2e    | 148/162 (91%)   | 0.89   | 10 (6%) 23 20  | 58, 70, 76, 88        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.62   | 2 (2%) 65 62   | 55, 68, 75, 80        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.75   | 2 (2%) 65 62   | 57, 70, 76, 79        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.85   | 12 (7%) 19 17  | 60, 73, 82, 90        | 0     |
| 38  | 2g    | 155/156 (99%)   | 1.03   | 18 (11%) 9 8   | 66, 79, 85, 91        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.59   | 10 (7%) 21 18  | 56, 65, 73, 76        | 0     |
| 39  | 2h    | 137/138 (99%)   | 0.87   | 8 (5%) 29 25   | 59, 70, 77, 83        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.40   | 28 (22%) 2 2   | 60, 77, 83, 89        | 0     |
| 40  | 2i    | 123/128 (96%)   | 2.11   | 63 (51%) 0 0   | 70, 82, 87, 91        | 0     |
| 41  | 1j    | 98/105 (93%)    | 1.46   | 23 (23%) 2 1   | 63, 79, 85, 89        | 0     |
| 41  | 2j    | 96/105 (91%)    | 1.94   | 38 (39%) 1 0   | 72, 82, 88, 91        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.57   | 5 (4%) 39 35   | 45, 65, 75, 78        | 0     |
| 42  | 2k    | 114/129 (88%)   | 0.92   | 9 (7%) 18 16   | 62, 73, 80, 85        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.52   | 5 (4%) 41 37   | 47, 59, 70, 73        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.57   | 3 (2%) 58 55   | 49, 61, 69, 76        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 118/126 (93%)     | 1.16   | 8 (6%) 23 20    | 60, 73, 78, 84        | 0     |
| 44  | 2m    | 115/126 (91%)     | 1.49   | 24 (20%) 2 2    | 69, 81, 87, 88        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.43   | 13 (21%) 2 2    | 67, 74, 80, 81        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.25   | 27 (45%) 0 0    | 72, 80, 86, 92        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.72   | 6 (6%) 23 20    | 49, 63, 73, 79        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.85   | 3 (3%) 48 44    | 60, 69, 77, 81        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.35   | 17 (20%) 2 2    | 58, 71, 80, 82        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.85   | 1 (1%) 76 75    | 56, 67, 74, 78        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.70   | 6 (6%) 27 24    | 50, 63, 71, 75        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.67   | 3 (3%) 52 49    | 57, 67, 74, 78        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.44   | 0 100 100       | 53, 64, 74, 80        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.80   | 0 100 100       | 61, 71, 76, 80        | 0     |
| 50  | 1s    | 83/93 (89%)       | 1.43   | 16 (19%) 3 3    | 66, 76, 81, 83        | 0     |
| 50  | 2s    | 83/93 (89%)       | 1.46   | 18 (21%) 2 2    | 74, 82, 88, 90        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.88   | 7 (7%) 21 18    | 54, 67, 78, 83        | 0     |
| 51  | 2t    | 96/106 (90%)      | 0.81   | 7 (7%) 21 18    | 56, 68, 78, 83        | 0     |
| 52  | 1u    | 23/27 (85%)       | 1.53   | 5 (21%) 2 2     | 65, 71, 74, 79        | 0     |
| 52  | 2u    | 23/27 (85%)       | 1.81   | 10 (43%) 0 0    | 72, 82, 85, 86        | 0     |
| 53  | 1v    | 13/24 (54%)       | 0.72   | 3 (23%) 2 2     | 52, 64, 92, 92        | 0     |
| 53  | 2v    | 13/24 (54%)       | 1.44   | 5 (38%) 1 0     | 68, 75, 98, 100       | 0     |
| 54  | 1w    | 248/354 (70%)     | 0.29   | 8 (3%) 50 46    | 29, 65, 79, 87        | 0     |
| 54  | 2w    | 252/354 (71%)     | 0.69   | 12 (4%) 35 32   | 48, 73, 83, 88        | 0     |
| 55  | 1x    | 68/76 (89%)       | -0.20  | 0 100 100       | 27, 59, 73, 82        | 0     |
| 55  | 1y    | 67/76 (88%)       | 0.81   | 7 (10%) 11 10   | 41, 91, 97, 99        | 0     |
| 55  | 2x    | 68/76 (89%)       | 0.22   | 0 100 100       | 48, 74, 82, 94        | 0     |
| 55  | 2y    | 67/76 (88%)       | 1.26   | 8 (11%) 9 7     | 61, 97, 101, 103      | 0     |
| 56  | 1z    | 14/18 (77%)       | 1.19   | 3 (21%) 2 2     | 31, 49, 71, 80        | 0     |
| 56  | 2z    | 14/18 (77%)       | 1.77   | 5 (35%) 1 0     | 52, 65, 77, 82        | 0     |
| All | All   | 21290/22338 (95%) | 0.34   | 1079 (5%) 33 29 | 15, 62, 86, 104       | 0     |

The worst 5 of 1079 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | 2n    | 2    | ALA  | 7.6  |
| 23  | 11    | 2    | SER  | 6.3  |
| 44  | 1m    | 2    | ALA  | 5.9  |
| 40  | 2i    | 14   | VAL  | 5.9  |
| 1   | 1A    | 1088 | A    | 5.5  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MIA  | 2y    | 37   | 29/30 | 0.56 | 0.18 | 82,91,98,107               | 0     |
| 55  | PSU  | 2y    | 32   | 20/21 | 0.61 | 0.15 | 86,94,101,104              | 0     |
| 55  | G7M  | 2y    | 46   | 24/25 | 0.61 | 0.13 | 85,97,109,126              | 0     |
| 55  | 4SU  | 2y    | 8    | 20/21 | 0.62 | 0.13 | 94,98,108,118              | 0     |
| 55  | 5MU  | 1y    | 54   | 21/22 | 0.63 | 0.12 | 82,90,99,103               | 0     |
| 55  | PSU  | 2y    | 55   | 20/21 | 0.63 | 0.16 | 88,99,107,107              | 0     |
| 55  | 5MU  | 2y    | 54   | 21/22 | 0.65 | 0.14 | 89,97,103,117              | 0     |
| 55  | PSU  | 1y    | 55   | 20/21 | 0.66 | 0.13 | 82,96,103,107              | 0     |
| 55  | PSU  | 2y    | 39   | 20/21 | 0.68 | 0.13 | 87,96,107,118              | 0     |
| 55  | G7M  | 1y    | 46   | 24/25 | 0.69 | 0.14 | 79,92,98,111               | 0     |
| 55  | MIA  | 1y    | 37   | 29/30 | 0.71 | 0.16 | 73,88,99,113               | 0     |
| 55  | 4SU  | 1y    | 8    | 20/21 | 0.75 | 0.12 | 80,92,98,103               | 0     |
| 55  | PSU  | 1y    | 32   | 20/21 | 0.81 | 0.12 | 72,83,91,96                | 0     |
| 55  | PSU  | 1y    | 39   | 20/21 | 0.81 | 0.09 | 76,87,94,98                | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.83 | 0.13 | 72,83,87,87                | 0     |
| 55  | G7M  | 2x    | 46   | 24/25 | 0.85 | 0.12 | 65,73,81,100               | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.86 | 0.15 | 60,63,67,79                | 0     |
| 55  | PSU  | 2x    | 32   | 20/21 | 0.86 | 0.13 | 72,79,86,86                | 0     |
| 55  | MIA  | 2x    | 37   | 29/30 | 0.88 | 0.15 | 65,76,83,102               | 0     |
| 55  | G7M  | 1x    | 46   | 24/25 | 0.88 | 0.10 | 50,60,73,97                | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.88 | 0.11 | 73,78,83,84                | 0     |
| 55  | PSU  | 2x    | 55   | 20/21 | 0.89 | 0.09 | 70,76,82,90                | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.90 | 0.10 | 69,77,84,86                | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.90 | 0.15 | 63,69,76,76                | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.91 | 0.14 | 57,73,74,79                | 0     |
| 55  | 5MU  | 1x    | 54   | 21/22 | 0.92 | 0.09 | 58,64,70,73                | 0     |
| 55  | 4SU  | 2x    | 8    | 20/21 | 0.92 | 0.09 | 60,70,77,78                | 0     |
| 32  | G7M  | 2a    | 527  | 24/25 | 0.92 | 0.11 | 60,68,71,73                | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.92 | 0.13 | 61,67,78,83                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MIA  | 1x    | 37   | 29/30 | 0.92 | 0.11 | 43,58,65,90                 | 0     |
| 55  | 5MU  | 2x    | 54   | 21/22 | 0.92 | 0.09 | 62,70,78,80                 | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.92 | 0.09 | 62,68,75,79                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.93 | 0.12 | 49,61,69,75                 | 0     |
| 55  | PSU  | 1x    | 32   | 20/21 | 0.93 | 0.10 | 52,61,71,71                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.93 | 0.10 | 51,67,75,75                 | 0     |
| 55  | PSU  | 2x    | 39   | 20/21 | 0.93 | 0.09 | 56,72,78,78                 | 0     |
| 55  | PSU  | 1x    | 39   | 20/21 | 0.93 | 0.09 | 54,59,63,69                 | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.93 | 0.13 | 51,57,62,63                 | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.93 | 0.11 | 52,64,68,81                 | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.94 | 0.10 | 46,51,58,62                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.94 | 0.09 | 59,63,67,68                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.94 | 0.11 | 47,60,68,73                 | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.94 | 0.12 | 54,61,65,66                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.94 | 0.10 | 55,62,67,69                 | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.94 | 0.09 | 52,61,66,68                 | 0     |
| 54  | MEQ  | 2w    | 230  | 10/11 | 0.94 | 0.12 | 52,54,56,57                 | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.95 | 0.10 | 51,62,71,74                 | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.95 | 0.10 | 49,58,65,67                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.95 | 0.10 | 47,56,61,64                 | 0     |
| 55  | PSU  | 1x    | 55   | 20/21 | 0.95 | 0.08 | 55,60,64,71                 | 0     |
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.96 | 0.07 | 42,48,53,54                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.96 | 0.09 | 22,29,36,37                 | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.96 | 0.09 | 41,47,53,54                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.96 | 0.09 | 40,46,52,59                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.96 | 0.09 | 36,42,48,50                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.96 | 0.10 | 36,43,48,60                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.96 | 0.09 | 36,47,55,55                 | 0     |
| 55  | 4SU  | 1x    | 8    | 20/21 | 0.96 | 0.07 | 39,48,55,59                 | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.96 | 0.09 | 53,57,62,63                 | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.96 | 0.10 | 48,53,62,68                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.96 | 0.09 | 37,43,47,57                 | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.96 | 0.11 | 51,57,62,63                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.96 | 0.09 | 24,39,45,50                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.96 | 0.07 | 31,35,41,42                 | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.97 | 0.08 | 30,36,41,48                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.07 | 33,39,46,49                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.97 | 0.09 | 38,42,48,50                 | 0     |
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.97 | 0.08 | 19,26,30,35                 | 0     |
| 54  | MEQ  | 1w    | 230  | 10/11 | 0.97 | 0.07 | 25,30,33,33                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.08 | 36,41,46,48                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.97 | 0.07 | 44,52,56,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.97 | 0.07 | 20,25,35,36                 | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.07 | 30,33,39,45                 | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.97 | 0.08 | 34,43,46,50                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.06 | 19,23,26,29                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.07 | 18,26,30,31                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.98 | 0.07 | 38,45,50,53                 | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.99 | 0.05 | 14,19,22,22                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3634 | 1/1   | 0.56 | 0.58 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3490 | 1/1   | 0.58 | 0.20 | 75,75,75,75                 | 0     |
| 57  | MG   | 1A    | 3658 | 1/1   | 0.59 | 0.22 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3726 | 1/1   | 0.64 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3148 | 1/1   | 0.66 | 0.26 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3116 | 1/1   | 0.67 | 0.42 | 81,81,81,81                 | 0     |
| 57  | MG   | 2a    | 1694 | 1/1   | 0.67 | 0.26 | 78,78,78,78                 | 0     |
| 57  | MG   | 1A    | 3650 | 1/1   | 0.68 | 0.20 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3638 | 1/1   | 0.70 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3641 | 1/1   | 0.70 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 1638 | 1/1   | 0.71 | 0.32 | 79,79,79,79                 | 0     |
| 57  | MG   | 2A    | 3511 | 1/1   | 0.71 | 0.17 | 77,77,77,77                 | 0     |
| 57  | MG   | 2A    | 3110 | 1/1   | 0.72 | 0.13 | 75,75,75,75                 | 0     |
| 57  | MG   | 2A    | 3598 | 1/1   | 0.72 | 0.19 | 82,82,82,82                 | 0     |
| 57  | MG   | 2A    | 3379 | 1/1   | 0.72 | 0.14 | 67,67,67,67                 | 0     |
| 57  | MG   | 2a    | 1602 | 1/1   | 0.72 | 0.14 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3410 | 1/1   | 0.72 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3431 | 1/1   | 0.73 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | 1w    | 404  | 1/1   | 0.73 | 0.18 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3182 | 1/1   | 0.73 | 0.23 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3336 | 1/1   | 0.74 | 0.13 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3624 | 1/1   | 0.74 | 0.30 | 72,72,72,72                 | 0     |
| 57  | MG   | 1a    | 1738 | 1/1   | 0.74 | 0.22 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3535 | 1/1   | 0.74 | 0.23 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3262 | 1/1   | 0.75 | 0.28 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3486 | 1/1   | 0.75 | 0.14 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3648 | 1/1   | 0.75 | 0.15 | 77,77,77,77                 | 0     |
| 57  | MG   | 1A    | 3644 | 1/1   | 0.75 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3144 | 1/1   | 0.75 | 0.16 | 71,71,71,71                 | 0     |
| 57  | MG   | 2a    | 1759 | 1/1   | 0.75 | 0.14 | 78,78,78,78                 | 0     |
| 57  | MG   | 2A    | 3578 | 1/1   | 0.76 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1752 | 1/1   | 0.76 | 0.25 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3639 | 1/1   | 0.76 | 0.15 | 78,78,78,78                 | 0     |
| 57  | MG   | 2A    | 3348 | 1/1   | 0.77 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1707 | 1/1   | 0.77 | 0.23 | 71,71,71,71                 | 0     |
| 57  | MG   | 2a    | 1720 | 1/1   | 0.77 | 0.20 | 76,76,76,76                 | 0     |
| 57  | MG   | 2A    | 3055 | 1/1   | 0.77 | 0.20 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3662 | 1/1   | 0.77 | 0.29 | 73,73,73,73                 | 0     |
| 57  | MG   | 2e    | 201  | 1/1   | 0.77 | 0.11 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 3771 | 1/1   | 0.78 | 0.16 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3481 | 1/1   | 0.78 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 1O    | 202  | 1/1   | 0.78 | 0.16 | 67,67,67,67                 | 0     |
| 57  | MG   | 2X    | 104  | 1/1   | 0.78 | 0.15 | 83,83,83,83                 | 0     |
| 57  | MG   | 2A    | 3137 | 1/1   | 0.78 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3532 | 1/1   | 0.78 | 0.19 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3354 | 1/1   | 0.78 | 0.18 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3664 | 1/1   | 0.78 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 1758 | 1/1   | 0.78 | 0.24 | 69,69,69,69                 | 0     |
| 57  | MG   | 1a    | 1669 | 1/1   | 0.78 | 0.29 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3422 | 1/1   | 0.78 | 0.22 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3665 | 1/1   | 0.79 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3371 | 1/1   | 0.79 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3219 | 1/1   | 0.79 | 0.18 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 1665 | 1/1   | 0.79 | 0.39 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3256 | 1/1   | 0.79 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1E    | 307  | 1/1   | 0.79 | 0.19 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3434 | 1/1   | 0.79 | 0.15 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3284 | 1/1   | 0.79 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3021 | 1/1   | 0.79 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1612 | 1/1   | 0.79 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3516 | 1/1   | 0.80 | 0.23 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3603 | 1/1   | 0.80 | 0.13 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 1643 | 1/1   | 0.80 | 0.24 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3618 | 1/1   | 0.80 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3105 | 1/1   | 0.80 | 0.32 | 67,67,67,67                 | 0     |
| 57  | MG   | 1c    | 301  | 1/1   | 0.80 | 0.28 | 71,71,71,71                 | 0     |
| 57  | MG   | 2a    | 1735 | 1/1   | 0.80 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3647 | 1/1   | 0.80 | 0.16 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3572 | 1/1   | 0.80 | 0.19 | 75,75,75,75                 | 0     |
| 57  | MG   | 1A    | 3690 | 1/1   | 0.80 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3580 | 1/1   | 0.80 | 0.19 | 61,61,61,61                 | 0     |
| 57  | MG   | 2x    | 108  | 1/1   | 0.80 | 0.29 | 77,77,77,77                 | 0     |
| 57  | MG   | 1a    | 1771 | 1/1   | 0.81 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 1783 | 1/1   | 0.81 | 0.25 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3505 | 1/1   | 0.81 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 3455 | 1/1   | 0.81 | 0.14 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3314 | 1/1   | 0.81 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3305 | 1/1   | 0.81 | 0.23 | 67,67,67,67                 | 0     |
| 57  | MG   | 2a    | 1657 | 1/1   | 0.81 | 0.16 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3328 | 1/1   | 0.81 | 0.21 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 1683 | 1/1   | 0.81 | 0.18 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3359 | 1/1   | 0.81 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 1688 | 1/1   | 0.81 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3596 | 1/1   | 0.81 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3416 | 1/1   | 0.81 | 0.32 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1718 | 1/1   | 0.81 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 1769 | 1/1   | 0.81 | 0.33 | 77,77,77,77                 | 0     |
| 57  | MG   | 1a    | 1733 | 1/1   | 0.81 | 0.25 | 62,62,62,62                 | 0     |
| 57  | MG   | 2x    | 101  | 1/1   | 0.81 | 0.20 | 72,72,72,72                 | 0     |
| 57  | MG   | 1l    | 103  | 1/1   | 0.81 | 0.26 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1756 | 1/1   | 0.82 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3374 | 1/1   | 0.82 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3195 | 1/1   | 0.82 | 0.23 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3201 | 1/1   | 0.82 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3211 | 1/1   | 0.82 | 0.10 | 81,81,81,81                 | 0     |
| 57  | MG   | 2a    | 1668 | 1/1   | 0.82 | 0.34 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3589 | 1/1   | 0.82 | 0.26 | 70,70,70,70                 | 0     |
| 57  | MG   | 2a    | 1708 | 1/1   | 0.82 | 0.22 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3674 | 1/1   | 0.82 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3746 | 1/1   | 0.82 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3102 | 1/1   | 0.82 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3472 | 1/1   | 0.82 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3473 | 1/1   | 0.82 | 0.21 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3288 | 1/1   | 0.82 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 1771 | 1/1   | 0.82 | 0.14 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3807 | 1/1   | 0.82 | 0.19 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3037 | 1/1   | 0.82 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3048 | 1/1   | 0.82 | 0.30 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3652 | 1/1   | 0.83 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3655 | 1/1   | 0.83 | 0.19 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3369 | 1/1   | 0.83 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3513 | 1/1   | 0.83 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | 2B    | 206  | 1/1   | 0.83 | 0.37 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3523 | 1/1   | 0.83 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3362 | 1/1   | 0.83 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3753 | 1/1   | 0.83 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1652 | 1/1   | 0.83 | 0.17 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3555 | 1/1   | 0.83 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3556 | 1/1   | 0.83 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3244 | 1/1   | 0.83 | 0.30 | 79,79,79,79                 | 0     |
| 57  | MG   | 2a    | 1674 | 1/1   | 0.83 | 0.23 | 65,65,65,65                 | 0     |
| 57  | MG   | 2a    | 1684 | 1/1   | 0.83 | 0.19 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3129 | 1/1   | 0.83 | 0.30 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1701 | 1/1   | 0.83 | 0.18 | 82,82,82,82                 | 0     |
| 57  | MG   | 1A    | 3049 | 1/1   | 0.83 | 0.28 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3584 | 1/1   | 0.83 | 0.14 | 81,81,81,81                 | 0     |
| 57  | MG   | 2A    | 3138 | 1/1   | 0.83 | 0.14 | 71,71,71,71                 | 0     |
| 57  | MG   | 1A    | 3524 | 1/1   | 0.83 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 1750 | 1/1   | 0.83 | 0.24 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3610 | 1/1   | 0.83 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3314 | 1/1   | 0.83 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3173 | 1/1   | 0.83 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3153 | 1/1   | 0.83 | 0.09 | 76,76,76,76                 | 0     |
| 57  | MG   | 2A    | 3503 | 1/1   | 0.83 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3604 | 1/1   | 0.83 | 0.09 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3274 | 1/1   | 0.84 | 0.23 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3461 | 1/1   | 0.84 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3589 | 1/1   | 0.84 | 0.09 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3025 | 1/1   | 0.84 | 0.25 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3020 | 1/1   | 0.84 | 0.24 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 1725 | 1/1   | 0.84 | 0.26 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3501 | 1/1   | 0.84 | 0.28 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 3404 | 1/1   | 0.84 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3617 | 1/1   | 0.84 | 0.25 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3775 | 1/1   | 0.84 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3622 | 1/1   | 0.84 | 0.15 | 81,81,81,81                 | 0     |
| 57  | MG   | 2A    | 3626 | 1/1   | 0.84 | 0.18 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 1652 | 1/1   | 0.84 | 0.22 | 76,76,76,76                 | 0     |
| 57  | MG   | 2A    | 3405 | 1/1   | 0.84 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 1661 | 1/1   | 0.84 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1767 | 1/1   | 0.84 | 0.25 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3798 | 1/1   | 0.84 | 0.19 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3537 | 1/1   | 0.84 | 0.17 | 75,75,75,75                 | 0     |
| 57  | MG   | 2A    | 3656 | 1/1   | 0.84 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3543 | 1/1   | 0.84 | 0.13 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3423 | 1/1   | 0.84 | 0.23 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3646 | 1/1   | 0.84 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 1B    | 212  | 1/1   | 0.85 | 0.29 | 67,67,67,67                 | 0     |
| 57  | MG   | 1a    | 1702 | 1/1   | 0.85 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3274 | 1/1   | 0.85 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3046 | 1/1   | 0.85 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3286 | 1/1   | 0.85 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3661 | 1/1   | 0.85 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3491 | 1/1   | 0.85 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3071 | 1/1   | 0.85 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 2B    | 205  | 1/1   | 0.85 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3496 | 1/1   | 0.85 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 1731 | 1/1   | 0.85 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3536 | 1/1   | 0.85 | 0.19 | 72,72,72,72                 | 0     |
| 57  | MG   | 2a    | 1605 | 1/1   | 0.85 | 0.17 | 66,66,66,66                 | 0     |
| 57  | MG   | 1a    | 1611 | 1/1   | 0.85 | 0.23 | 68,68,68,68                 | 0     |
| 57  | MG   | 2a    | 1648 | 1/1   | 0.85 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3761 | 1/1   | 0.85 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 1623 | 1/1   | 0.85 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 1658 | 1/1   | 0.85 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1633 | 1/1   | 0.85 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3564 | 1/1   | 0.85 | 0.19 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3401 | 1/1   | 0.85 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3610 | 1/1   | 0.85 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 1769 | 1/1   | 0.85 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3583 | 1/1   | 0.85 | 0.26 | 73,73,73,73                 | 0     |
| 57  | MG   | 1A    | 3423 | 1/1   | 0.85 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 2a    | 1713 | 1/1   | 0.85 | 0.11 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 1782 | 1/1   | 0.85 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3105 | 1/1   | 0.85 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3197 | 1/1   | 0.85 | 0.19 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3571 | 1/1   | 0.85 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3443 | 1/1   | 0.85 | 0.14 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3448 | 1/1   | 0.85 | 0.10 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1w    | 402  | 1/1   | 0.85 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3227 | 1/1   | 0.85 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3240 | 1/1   | 0.85 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1B    | 211  | 1/1   | 0.85 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3482 | 1/1   | 0.86 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 1626 | 1/1   | 0.86 | 0.33 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3500 | 1/1   | 0.86 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3370 | 1/1   | 0.86 | 0.20 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3492 | 1/1   | 0.86 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3319 | 1/1   | 0.86 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3339 | 1/1   | 0.86 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3341 | 1/1   | 0.86 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 1648 | 1/1   | 0.86 | 0.21 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3661 | 1/1   | 0.86 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1656 | 1/1   | 0.86 | 0.24 | 53,53,53,53                 | 0     |
| 57  | MG   | 20    | 101  | 1/1   | 0.86 | 0.10 | 77,77,77,77                 | 0     |
| 57  | MG   | 21    | 101  | 1/1   | 0.86 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 1659 | 1/1   | 0.86 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3161 | 1/1   | 0.86 | 0.29 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 1626 | 1/1   | 0.86 | 0.26 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1632 | 1/1   | 0.86 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3171 | 1/1   | 0.86 | 0.25 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3397 | 1/1   | 0.86 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3399 | 1/1   | 0.86 | 0.29 | 68,68,68,68                 | 0     |
| 57  | MG   | 1a    | 1778 | 1/1   | 0.86 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3175 | 1/1   | 0.86 | 0.28 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3615 | 1/1   | 0.86 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3466 | 1/1   | 0.86 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3418 | 1/1   | 0.86 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3716 | 1/1   | 0.86 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 1693 | 1/1   | 0.86 | 0.20 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3591 | 1/1   | 0.86 | 0.26 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 1701 | 1/1   | 0.86 | 0.09 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3601 | 1/1   | 0.86 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3470 | 1/1   | 0.86 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3544 | 1/1   | 0.86 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1744 | 1/1   | 0.86 | 0.24 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3611 | 1/1   | 0.86 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 2a    | 1756 | 1/1   | 0.86 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3613 | 1/1   | 0.86 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3749 | 1/1   | 0.86 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 1721 | 1/1   | 0.86 | 0.16 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3468 | 1/1   | 0.86 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3488 | 1/1   | 0.86 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3281 | 1/1   | 0.86 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3045 | 1/1   | 0.86 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 1B    | 201  | 1/1   | 0.87 | 0.08 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3072 | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3081 | 1/1   | 0.87 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3594 | 1/1   | 0.87 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3383 | 1/1   | 0.87 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3612 | 1/1   | 0.87 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3393 | 1/1   | 0.87 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3281 | 1/1   | 0.87 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3112 | 1/1   | 0.87 | 0.24 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3346 | 1/1   | 0.87 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3126 | 1/1   | 0.87 | 0.24 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3634 | 1/1   | 0.87 | 0.07 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3406 | 1/1   | 0.87 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3503 | 1/1   | 0.87 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3613 | 1/1   | 0.87 | 0.47 | 30,30,30,30                 | 0     |
| 57  | MG   | 18    | 101  | 1/1   | 0.87 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3350 | 1/1   | 0.87 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3654 | 1/1   | 0.87 | 0.25 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3147 | 1/1   | 0.87 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3059 | 1/1   | 0.87 | 0.17 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3151 | 1/1   | 0.87 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3159 | 1/1   | 0.87 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 1617 | 1/1   | 0.87 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3455 | 1/1   | 0.87 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3168 | 1/1   | 0.87 | 0.31 | 64,64,64,64                 | 0     |
| 57  | MG   | 2X    | 102  | 1/1   | 0.87 | 0.12 | 74,74,74,74                 | 0     |
| 57  | MG   | 2A    | 3467 | 1/1   | 0.87 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 1740 | 1/1   | 0.87 | 0.20 | 73,73,73,73                 | 0     |
| 57  | MG   | 1A    | 3736 | 1/1   | 0.87 | 0.23 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3629 | 1/1   | 0.87 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 1758 | 1/1   | 0.87 | 0.23 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 1759 | 1/1   | 0.87 | 0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3543 | 1/1   | 0.87 | 0.12 | 17,17,17,17                 | 0     |
| 57  | MG   | 2a    | 1636 | 1/1   | 0.87 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3210 | 1/1   | 0.87 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3636 | 1/1   | 0.87 | 0.29 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3758 | 1/1   | 0.87 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 1773 | 1/1   | 0.87 | 0.14 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3302 | 1/1   | 0.87 | 0.34 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3765 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 1657 | 1/1   | 0.87 | 0.20 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3526 | 1/1   | 0.87 | 0.27 | 67,67,67,67                 | 0     |
| 57  | MG   | 2a    | 1677 | 1/1   | 0.87 | 0.25 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3531 | 1/1   | 0.87 | 0.18 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3770 | 1/1   | 0.87 | 0.38 | 43,43,43,43                 | 0     |
| 57  | MG   | 1v    | 101  | 1/1   | 0.87 | 0.12 | 71,71,71,71                 | 0     |
| 57  | MG   | 1A    | 3552 | 1/1   | 0.87 | 0.09 | 16,16,16,16                 | 0     |
| 57  | MG   | 1a    | 1667 | 1/1   | 0.87 | 0.39 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1717 | 1/1   | 0.87 | 0.20 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3542 | 1/1   | 0.87 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 1728 | 1/1   | 0.87 | 0.24 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3295 | 1/1   | 0.87 | 0.11 | 74,74,74,74                 | 0     |
| 57  | MG   | 2A    | 3298 | 1/1   | 0.87 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 1y    | 101  | 1/1   | 0.87 | 0.22 | 77,77,77,77                 | 0     |
| 57  | MG   | 1A    | 3122 | 1/1   | 0.87 | 0.21 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1673 | 1/1   | 0.87 | 0.29 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3335 | 1/1   | 0.87 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 1761 | 1/1   | 0.87 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3647 | 1/1   | 0.87 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 1686 | 1/1   | 0.87 | 0.10 | 75,75,75,75                 | 0     |
| 57  | MG   | 2A    | 3347 | 1/1   | 0.87 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2j    | 201  | 1/1   | 0.87 | 0.15 | 74,74,74,74                 | 0     |
| 57  | MG   | 1A    | 3016 | 1/1   | 0.87 | 0.19 | 40,40,40,40                 | 0     |
| 57  | MG   | 2x    | 102  | 1/1   | 0.87 | 0.24 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3059 | 1/1   | 0.87 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3186 | 1/1   | 0.88 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3194 | 1/1   | 0.88 | 0.35 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3390 | 1/1   | 0.88 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | 2B    | 209  | 1/1   | 0.88 | 0.31 | 63,63,63,63                 | 0     |
| 57  | MG   | 2D    | 306  | 1/1   | 0.88 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3108 | 1/1   | 0.88 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 1668 | 1/1   | 0.88 | 0.29 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3198 | 1/1   | 0.88 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3645 | 1/1   | 0.88 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3538 | 1/1   | 0.88 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 1679 | 1/1   | 0.88 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1612 | 1/1   | 0.88 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1624 | 1/1   | 0.88 | 0.22 | 61,61,61,61                 | 0     |
| 57  | MG   | 1B    | 210  | 1/1   | 0.88 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1624 | 1/1   | 0.88 | 0.10 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3579 | 1/1   | 0.88 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3111 | 1/1   | 0.88 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3248 | 1/1   | 0.88 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1650 | 1/1   | 0.88 | 0.33 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3250 | 1/1   | 0.88 | 0.26 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3588 | 1/1   | 0.88 | 0.20 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3428 | 1/1   | 0.88 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1659 | 1/1   | 0.88 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3115 | 1/1   | 0.88 | 0.32 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3477 | 1/1   | 0.88 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 1671 | 1/1   | 0.88 | 0.29 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 1634 | 1/1   | 0.88 | 0.34 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3602 | 1/1   | 0.88 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1680 | 1/1   | 0.88 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 1779 | 1/1   | 0.88 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3134 | 1/1   | 0.88 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3375 | 1/1   | 0.88 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3292 | 1/1   | 0.88 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | 1a    | 1703 | 1/1   | 0.88 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3140 | 1/1   | 0.88 | 0.11 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3141 | 1/1   | 0.88 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3620 | 1/1   | 0.88 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3476 | 1/1   | 0.88 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3741 | 1/1   | 0.88 | 0.25 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3629 | 1/1   | 0.88 | 0.20 | 70,70,70,70                 | 0     |
| 57  | MG   | 1a    | 1649 | 1/1   | 0.88 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1Z    | 301  | 1/1   | 0.88 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3459 | 1/1   | 0.88 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3340 | 1/1   | 0.88 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 1763 | 1/1   | 0.88 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1764 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 1729 | 1/1   | 0.88 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 14    | 502  | 1/1   | 0.88 | 0.28 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3164 | 1/1   | 0.88 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 2f    | 201  | 1/1   | 0.88 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3796 | 1/1   | 0.88 | 0.25 | 69,69,69,69                 | 0     |
| 57  | MG   | 2t    | 201  | 1/1   | 0.88 | 0.21 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3039 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 1734 | 1/1   | 0.88 | 0.26 | 71,71,71,71                 | 0     |
| 57  | MG   | 1a    | 1605 | 1/1   | 0.88 | 0.35 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3346 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3029 | 1/1   | 0.89 | 0.20 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3033 | 1/1   | 0.89 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3352 | 1/1   | 0.89 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2F    | 303  | 1/1   | 0.89 | 0.11 | 64,64,64,64                 | 0     |
| 57  | MG   | 2Q    | 203  | 1/1   | 0.89 | 0.28 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3744 | 1/1   | 0.89 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3356 | 1/1   | 0.89 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 1732 | 1/1   | 0.89 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3362 | 1/1   | 0.89 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 28    | 101  | 1/1   | 0.89 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3195 | 1/1   | 0.89 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3518 | 1/1   | 0.89 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1610 | 1/1   | 0.89 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3544 | 1/1   | 0.89 | 0.13 | 67,67,67,67                 | 0     |
| 57  | MG   | 2a    | 1620 | 1/1   | 0.89 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3546 | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3751 | 1/1   | 0.89 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 1630 | 1/1   | 0.89 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3648 | 1/1   | 0.89 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 1744 | 1/1   | 0.89 | 0.27 | 74,74,74,74                 | 0     |
| 57  | MG   | 2A    | 3570 | 1/1   | 0.89 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1645 | 1/1   | 0.89 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1665 | 1/1   | 0.89 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3074 | 1/1   | 0.89 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3207 | 1/1   | 0.89 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1653 | 1/1   | 0.89 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3075 | 1/1   | 0.89 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3064 | 1/1   | 0.89 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3212 | 1/1   | 0.89 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3587 | 1/1   | 0.89 | 0.12 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3407 | 1/1   | 0.89 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3083 | 1/1   | 0.89 | 0.23 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3413 | 1/1   | 0.89 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3233 | 1/1   | 0.89 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3239 | 1/1   | 0.89 | 0.20 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3419 | 1/1   | 0.89 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 2a    | 1685 | 1/1   | 0.89 | 0.28 | 65,65,65,65                 | 0     |
| 57  | MG   | 2a    | 1688 | 1/1   | 0.89 | 0.28 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3267 | 1/1   | 0.89 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3085 | 1/1   | 0.89 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3767 | 1/1   | 0.89 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3626 | 1/1   | 0.89 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3670 | 1/1   | 0.89 | 0.24 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3261 | 1/1   | 0.89 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 1727 | 1/1   | 0.89 | 0.20 | 76,76,76,76                 | 0     |
| 57  | MG   | 1a    | 1620 | 1/1   | 0.89 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1730 | 1/1   | 0.89 | 0.19 | 71,71,71,71                 | 0     |
| 57  | MG   | 1A    | 3030 | 1/1   | 0.89 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3621 | 1/1   | 0.89 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 1747 | 1/1   | 0.89 | 0.16 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1748 | 1/1   | 0.89 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3683 | 1/1   | 0.89 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3135 | 1/1   | 0.89 | 0.28 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3188 | 1/1   | 0.89 | 0.24 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3802 | 1/1   | 0.89 | 0.07 | 20,20,20,20                 | 0     |
| 57  | MG   | 2a    | 1760 | 1/1   | 0.89 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3355 | 1/1   | 0.89 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3288 | 1/1   | 0.89 | 0.40 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 1639 | 1/1   | 0.89 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 1768 | 1/1   | 0.89 | 0.20 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 1647 | 1/1   | 0.89 | 0.20 | 60,60,60,60                 | 0     |
| 57  | MG   | 1x    | 107  | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3493 | 1/1   | 0.89 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3322 | 1/1   | 0.89 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3514 | 1/1   | 0.89 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 2k    | 201  | 1/1   | 0.89 | 0.27 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3019 | 1/1   | 0.89 | 0.25 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3515 | 1/1   | 0.89 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3162 | 1/1   | 0.89 | 0.23 | 45,45,45,45                 | 0     |
| 57  | MG   | 2x    | 105  | 1/1   | 0.89 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2B    | 204  | 1/1   | 0.89 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1685 | 1/1   | 0.90 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3738 | 1/1   | 0.90 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3027 | 1/1   | 0.90 | 0.35 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3247 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3214 | 1/1   | 0.90 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3463 | 1/1   | 0.90 | 0.30 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3424 | 1/1   | 0.90 | 0.10 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 1609 | 1/1   | 0.90 | 0.20 | 65,65,65,65                 | 0     |
| 57  | MG   | 2B    | 202  | 1/1   | 0.90 | 0.19 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3470 | 1/1   | 0.90 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3431 | 1/1   | 0.90 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3452 | 1/1   | 0.90 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3474 | 1/1   | 0.90 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 2D    | 301  | 1/1   | 0.90 | 0.25 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 1614 | 1/1   | 0.90 | 0.12 | 74,74,74,74                 | 0     |
| 57  | MG   | 2A    | 3478 | 1/1   | 0.90 | 0.17 | 70,70,70,70                 | 0     |
| 57  | MG   | 2Q    | 201  | 1/1   | 0.90 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1711 | 1/1   | 0.90 | 0.16 | 76,76,76,76                 | 0     |
| 57  | MG   | 2R    | 201  | 1/1   | 0.90 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 2V    | 202  | 1/1   | 0.90 | 0.19 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3058 | 1/1   | 0.90 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1717 | 1/1   | 0.90 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3490 | 1/1   | 0.90 | 0.17 | 75,75,75,75                 | 0     |
| 57  | MG   | 1A    | 3750 | 1/1   | 0.90 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3495 | 1/1   | 0.90 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3261 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1724 | 1/1   | 0.90 | 0.21 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3278 | 1/1   | 0.90 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3504 | 1/1   | 0.90 | 0.16 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1613 | 1/1   | 0.90 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3279 | 1/1   | 0.90 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1622 | 1/1   | 0.90 | 0.26 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3642 | 1/1   | 0.90 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | 2a    | 1629 | 1/1   | 0.90 | 0.13 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3082 | 1/1   | 0.90 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 1730 | 1/1   | 0.90 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3528 | 1/1   | 0.90 | 0.12 | 68,68,68,68                 | 0     |
| 57  | MG   | 2a    | 1639 | 1/1   | 0.90 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3096 | 1/1   | 0.90 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3542 | 1/1   | 0.90 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1646 | 1/1   | 0.90 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3533 | 1/1   | 0.90 | 0.11 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3156 | 1/1   | 0.90 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3028 | 1/1   | 0.90 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3546 | 1/1   | 0.90 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3467 | 1/1   | 0.90 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3334 | 1/1   | 0.90 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3275 | 1/1   | 0.90 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3127 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3554 | 1/1   | 0.90 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 1743 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3131 | 1/1   | 0.90 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1675 | 1/1   | 0.90 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1646 | 1/1   | 0.90 | 0.18 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3566 | 1/1   | 0.90 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3568 | 1/1   | 0.90 | 0.09 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3583 | 1/1   | 0.90 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | 1a    | 1753 | 1/1   | 0.90 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 1691 | 1/1   | 0.90 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3279 | 1/1   | 0.90 | 0.26 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3361 | 1/1   | 0.90 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 1651 | 1/1   | 0.90 | 0.25 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1711 | 1/1   | 0.90 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3143 | 1/1   | 0.90 | 0.25 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1762 | 1/1   | 0.90 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3019 | 1/1   | 0.90 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3368 | 1/1   | 0.90 | 0.10 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3677 | 1/1   | 0.90 | 0.11 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3590 | 1/1   | 0.90 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3153 | 1/1   | 0.90 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1742 | 1/1   | 0.90 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3191 | 1/1   | 0.90 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 1775 | 1/1   | 0.90 | 0.12 | 71,71,71,71                 | 0     |
| 57  | MG   | 1a    | 1660 | 1/1   | 0.90 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3163 | 1/1   | 0.90 | 0.23 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 1754 | 1/1   | 0.90 | 0.23 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3287 | 1/1   | 0.90 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3709 | 1/1   | 0.90 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1E    | 303  | 1/1   | 0.90 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 1787 | 1/1   | 0.90 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3409 | 1/1   | 0.90 | 0.14 | 76,76,76,76                 | 0     |
| 57  | MG   | 1A    | 3103 | 1/1   | 0.90 | 0.25 | 53,53,53,53                 | 0     |
| 57  | MG   | 1N    | 203  | 1/1   | 0.90 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3191 | 1/1   | 0.90 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 1671 | 1/1   | 0.90 | 0.33 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3624 | 1/1   | 0.90 | 0.27 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3619 | 1/1   | 0.90 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 2e    | 202  | 1/1   | 0.90 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3731 | 1/1   | 0.90 | 0.26 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3632 | 1/1   | 0.90 | 0.24 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3633 | 1/1   | 0.90 | 0.08 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3077 | 1/1   | 0.90 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3200 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3002 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3645 | 1/1   | 0.90 | 0.41 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3433 | 1/1   | 0.90 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3636 | 1/1   | 0.91 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3157 | 1/1   | 0.91 | 0.24 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3068 | 1/1   | 0.91 | 0.30 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3640 | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 1642 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3003 | 1/1   | 0.91 | 0.07 | 21,21,21,21                 | 0     |
| 57  | MG   | 1a    | 1772 | 1/1   | 0.91 | 0.19 | 76,76,76,76                 | 0     |
| 57  | MG   | 2A    | 3420 | 1/1   | 0.91 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3224 | 1/1   | 0.91 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3461 | 1/1   | 0.91 | 0.07 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3364 | 1/1   | 0.91 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3657 | 1/1   | 0.91 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3658 | 1/1   | 0.91 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3659 | 1/1   | 0.91 | 0.25 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3230 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3176 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3177 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3438 | 1/1   | 0.91 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3178 | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3553 | 1/1   | 0.91 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3173 | 1/1   | 0.91 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3458 | 1/1   | 0.91 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2B    | 210  | 1/1   | 0.91 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3776 | 1/1   | 0.91 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3780 | 1/1   | 0.91 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3781 | 1/1   | 0.91 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1w    | 401  | 1/1   | 0.91 | 0.41 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3785 | 1/1   | 0.91 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3651 | 1/1   | 0.91 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 2U    | 201  | 1/1   | 0.91 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3580 | 1/1   | 0.91 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3253 | 1/1   | 0.91 | 0.10 | 73,73,73,73                 | 0     |
| 57  | MG   | 1A    | 3585 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3005 | 1/1   | 0.91 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3006 | 1/1   | 0.91 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | 23    | 101  | 1/1   | 0.91 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3668 | 1/1   | 0.91 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3484 | 1/1   | 0.91 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1604 | 1/1   | 0.91 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3216 | 1/1   | 0.91 | 0.24 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3221 | 1/1   | 0.91 | 0.32 | 66,66,66,66                 | 0     |
| 57  | MG   | 2a    | 1611 | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | 1B    | 209  | 1/1   | 0.91 | 0.23 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3026 | 1/1   | 0.91 | 0.25 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3259 | 1/1   | 0.91 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3671 | 1/1   | 0.91 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1625 | 1/1   | 0.91 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3032 | 1/1   | 0.91 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3245 | 1/1   | 0.91 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3592 | 1/1   | 0.91 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 1B    | 219  | 1/1   | 0.91 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 1634 | 1/1   | 0.91 | 0.22 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3377 | 1/1   | 0.91 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3514 | 1/1   | 0.91 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 1640 | 1/1   | 0.91 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1642 | 1/1   | 0.91 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 1692 | 1/1   | 0.91 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3678 | 1/1   | 0.91 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3266 | 1/1   | 0.91 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3529 | 1/1   | 0.91 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3051 | 1/1   | 0.91 | 0.21 | 67,67,67,67                 | 0     |
| 57  | MG   | 1N    | 202  | 1/1   | 0.91 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3393 | 1/1   | 0.91 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3689 | 1/1   | 0.91 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1706 | 1/1   | 0.91 | 0.13 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3285 | 1/1   | 0.91 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1663 | 1/1   | 0.91 | 0.31 | 54,54,54,54                 | 0     |
| 57  | MG   | 1P    | 204  | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1666 | 1/1   | 0.91 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3599 | 1/1   | 0.91 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 1712 | 1/1   | 0.91 | 0.25 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1673 | 1/1   | 0.91 | 0.14 | 80,80,80,80                 | 0     |
| 57  | MG   | 2A    | 3296 | 1/1   | 0.91 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3548 | 1/1   | 0.91 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3553 | 1/1   | 0.91 | 0.22 | 65,65,65,65                 | 0     |
| 57  | MG   | 2a    | 1679 | 1/1   | 0.91 | 0.13 | 73,73,73,73                 | 0     |
| 57  | MG   | 1A    | 3695 | 1/1   | 0.91 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3303 | 1/1   | 0.91 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | 12    | 101  | 1/1   | 0.91 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3557 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3307 | 1/1   | 0.91 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3565 | 1/1   | 0.91 | 0.20 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 1698 | 1/1   | 0.91 | 0.21 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 1720 | 1/1   | 0.91 | 0.22 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3084 | 1/1   | 0.91 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3320 | 1/1   | 0.91 | 0.09 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3086 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3092 | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3706 | 1/1   | 0.91 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3104 | 1/1   | 0.91 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | 15    | 101  | 1/1   | 0.91 | 0.20 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3108 | 1/1   | 0.91 | 0.33 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 1734 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3585 | 1/1   | 0.91 | 0.09 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1736 | 1/1   | 0.91 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1738 | 1/1   | 0.91 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3707 | 1/1   | 0.91 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3603 | 1/1   | 0.91 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 1607 | 1/1   | 0.91 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3710 | 1/1   | 0.91 | 0.09 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3120 | 1/1   | 0.91 | 0.24 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3395 | 1/1   | 0.91 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3358 | 1/1   | 0.91 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3401 | 1/1   | 0.91 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3730 | 1/1   | 0.91 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3606 | 1/1   | 0.91 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3608 | 1/1   | 0.91 | 0.08 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3368 | 1/1   | 0.91 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3061 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 1766 | 1/1   | 0.91 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 1618 | 1/1   | 0.91 | 0.25 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 1741 | 1/1   | 0.91 | 0.14 | 71,71,71,71                 | 0     |
| 57  | MG   | 1A    | 3504 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3508 | 1/1   | 0.91 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3406 | 1/1   | 0.91 | 0.07 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3395 | 1/1   | 0.91 | 0.18 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3086 | 1/1   | 0.91 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 1754 | 1/1   | 0.91 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3031 | 1/1   | 0.91 | 0.34 | 38,38,38,38                 | 0     |
| 57  | MG   | 2v    | 101  | 1/1   | 0.91 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3194 | 1/1   | 0.91 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3635 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3441 | 1/1   | 0.91 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | 1a    | 1763 | 1/1   | 0.91 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3192 | 1/1   | 0.92 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3618 | 1/1   | 0.92 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3021 | 1/1   | 0.92 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3196 | 1/1   | 0.92 | 0.12 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1E    | 306  | 1/1   | 0.92 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3278 | 1/1   | 0.92 | 0.32 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3450 | 1/1   | 0.92 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3199 | 1/1   | 0.92 | 0.20 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 1687 | 1/1   | 0.92 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3622 | 1/1   | 0.92 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 1691 | 1/1   | 0.92 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3466 | 1/1   | 0.92 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3159 | 1/1   | 0.92 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3034 | 1/1   | 0.92 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3036 | 1/1   | 0.92 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3471 | 1/1   | 0.92 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3522 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 1698 | 1/1   | 0.92 | 0.19 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3220 | 1/1   | 0.92 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3040 | 1/1   | 0.92 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3225 | 1/1   | 0.92 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 2V    | 201  | 1/1   | 0.92 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3479 | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | 1P    | 201  | 1/1   | 0.92 | 0.27 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3433 | 1/1   | 0.92 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3236 | 1/1   | 0.92 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3049 | 1/1   | 0.92 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | 1Q    | 205  | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3491 | 1/1   | 0.92 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 29    | 101  | 1/1   | 0.92 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3241 | 1/1   | 0.92 | 0.09 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1603 | 1/1   | 0.92 | 0.19 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3052 | 1/1   | 0.92 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1U    | 201  | 1/1   | 0.92 | 0.16 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3537 | 1/1   | 0.92 | 0.10 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3360 | 1/1   | 0.92 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3060 | 1/1   | 0.92 | 0.18 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3257 | 1/1   | 0.92 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1614 | 1/1   | 0.92 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3509 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 1623 | 1/1   | 0.92 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3258 | 1/1   | 0.92 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3512 | 1/1   | 0.92 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3739 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3539 | 1/1   | 0.92 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3518 | 1/1   | 0.92 | 0.16 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3519 | 1/1   | 0.92 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3442 | 1/1   | 0.92 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3267 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3052 | 1/1   | 0.92 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3076 | 1/1   | 0.92 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1603 | 1/1   | 0.92 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3282 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3076 | 1/1   | 0.92 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3248 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3286 | 1/1   | 0.92 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1649 | 1/1   | 0.92 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3287 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3540 | 1/1   | 0.92 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3187 | 1/1   | 0.92 | 0.28 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3754 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3555 | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3007 | 1/1   | 0.92 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1660 | 1/1   | 0.92 | 0.18 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1661 | 1/1   | 0.92 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3763 | 1/1   | 0.92 | 0.18 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 1664 | 1/1   | 0.92 | 0.24 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3552 | 1/1   | 0.92 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3129 | 1/1   | 0.92 | 0.28 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1667 | 1/1   | 0.92 | 0.14 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3315 | 1/1   | 0.92 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 1669 | 1/1   | 0.92 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3485 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3380 | 1/1   | 0.92 | 0.15 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3317 | 1/1   | 0.92 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3559 | 1/1   | 0.92 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 1676 | 1/1   | 0.92 | 0.39 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3591 | 1/1   | 0.92 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3118 | 1/1   | 0.92 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3321 | 1/1   | 0.92 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1683 | 1/1   | 0.92 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 1627 | 1/1   | 0.92 | 0.34 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3323 | 1/1   | 0.92 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 1687 | 1/1   | 0.92 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3121 | 1/1   | 0.92 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1689 | 1/1   | 0.92 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1628 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3669 | 1/1   | 0.92 | 0.28 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3778 | 1/1   | 0.92 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3130 | 1/1   | 0.92 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 1703 | 1/1   | 0.92 | 0.22 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1757 | 1/1   | 0.92 | 0.10 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 3386 | 1/1   | 0.92 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3325 | 1/1   | 0.92 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 1715 | 1/1   | 0.92 | 0.09 | 70,70,70,70                 | 0     |
| 57  | MG   | 1a    | 1760 | 1/1   | 0.92 | 0.18 | 71,71,71,71                 | 0     |
| 57  | MG   | 1a    | 1761 | 1/1   | 0.92 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | 2a    | 1722 | 1/1   | 0.92 | 0.22 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 1723 | 1/1   | 0.92 | 0.14 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3783 | 1/1   | 0.92 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3133 | 1/1   | 0.92 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1729 | 1/1   | 0.92 | 0.21 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3142 | 1/1   | 0.92 | 0.26 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3789 | 1/1   | 0.92 | 0.22 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3366 | 1/1   | 0.92 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3791 | 1/1   | 0.92 | 0.12 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3794 | 1/1   | 0.92 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 1741 | 1/1   | 0.92 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3370 | 1/1   | 0.92 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3399 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3329 | 1/1   | 0.92 | 0.06 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3152 | 1/1   | 0.92 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1653 | 1/1   | 0.92 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3615 | 1/1   | 0.92 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3066 | 1/1   | 0.92 | 0.30 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3337 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3396 | 1/1   | 0.92 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3160 | 1/1   | 0.92 | 0.20 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 1658 | 1/1   | 0.92 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 1762 | 1/1   | 0.92 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3411 | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1B    | 202  | 1/1   | 0.92 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 1B    | 205  | 1/1   | 0.92 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3107 | 1/1   | 0.92 | 0.23 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3700 | 1/1   | 0.92 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 1770 | 1/1   | 0.92 | 0.22 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3703 | 1/1   | 0.92 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3635 | 1/1   | 0.92 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3412 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3616 | 1/1   | 0.92 | 0.07 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 1670 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3617 | 1/1   | 0.92 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3641 | 1/1   | 0.92 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1D    | 305  | 1/1   | 0.92 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | 2v    | 102  | 1/1   | 0.92 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3183 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3184 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 1E    | 302  | 1/1   | 0.92 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 1680 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3523 | 1/1   | 0.93 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3095 | 1/1   | 0.93 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3172 | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 1784 | 1/1   | 0.93 | 0.20 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3174 | 1/1   | 0.93 | 0.16 | 71,71,71,71                 | 0     |
| 57  | MG   | 1A    | 3533 | 1/1   | 0.93 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 1a    | 1650 | 1/1   | 0.93 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3407 | 1/1   | 0.93 | 0.07 | 21,21,21,21                 | 0     |
| 57  | MG   | 1v    | 103  | 1/1   | 0.93 | 0.15 | 78,78,78,78                 | 0     |
| 57  | MG   | 2A    | 3424 | 1/1   | 0.93 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3426 | 1/1   | 0.93 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | 2B    | 201  | 1/1   | 0.93 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3250 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3100 | 1/1   | 0.93 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3341 | 1/1   | 0.93 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3344 | 1/1   | 0.93 | 0.21 | 43,43,43,43                 | 0     |
| 57  | MG   | 2B    | 208  | 1/1   | 0.93 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3432 | 1/1   | 0.93 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3193 | 1/1   | 0.93 | 0.10 | 68,68,68,68                 | 0     |
| 57  | MG   | 2B    | 211  | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 1y    | 102  | 1/1   | 0.93 | 0.12 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3001 | 1/1   | 0.93 | 0.18 | 59,59,59,59                 | 0     |
| 57  | MG   | 2D    | 307  | 1/1   | 0.93 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3451 | 1/1   | 0.93 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2F    | 304  | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3453 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3545 | 1/1   | 0.93 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3457 | 1/1   | 0.93 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3804 | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3806 | 1/1   | 0.93 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3007 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 2W    | 201  | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2X    | 101  | 1/1   | 0.93 | 0.18 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3013 | 1/1   | 0.93 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3181 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3205 | 1/1   | 0.93 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3469 | 1/1   | 0.93 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3435 | 1/1   | 0.93 | 0.16 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3209 | 1/1   | 0.93 | 0.11 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3024 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3123 | 1/1   | 0.93 | 0.06 | 32,32,32,32                 | 0     |
| 57  | MG   | 1B    | 203  | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3263 | 1/1   | 0.93 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3447 | 1/1   | 0.93 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3219 | 1/1   | 0.93 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3480 | 1/1   | 0.93 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3031 | 1/1   | 0.93 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 1672 | 1/1   | 0.93 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3449 | 1/1   | 0.93 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1615 | 1/1   | 0.93 | 0.15 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1675 | 1/1   | 0.93 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 1622 | 1/1   | 0.93 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3489 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3229 | 1/1   | 0.93 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3035 | 1/1   | 0.93 | 0.10 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3679 | 1/1   | 0.93 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3358 | 1/1   | 0.93 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3497 | 1/1   | 0.93 | 0.07 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1631 | 1/1   | 0.93 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3498 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 1681 | 1/1   | 0.93 | 0.18 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3359 | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1637 | 1/1   | 0.93 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3456 | 1/1   | 0.93 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3017 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3190 | 1/1   | 0.93 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3508 | 1/1   | 0.93 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1644 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3701 | 1/1   | 0.93 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3032 | 1/1   | 0.93 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3053 | 1/1   | 0.93 | 0.21 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3595 | 1/1   | 0.93 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3260 | 1/1   | 0.93 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3138 | 1/1   | 0.93 | 0.19 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3468 | 1/1   | 0.93 | 0.09 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3520 | 1/1   | 0.93 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3263 | 1/1   | 0.93 | 0.11 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3524 | 1/1   | 0.93 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3264 | 1/1   | 0.93 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3602 | 1/1   | 0.93 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3065 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3066 | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3276 | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3277 | 1/1   | 0.93 | 0.23 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3067 | 1/1   | 0.93 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1P    | 202  | 1/1   | 0.93 | 0.24 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3140 | 1/1   | 0.93 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3538 | 1/1   | 0.93 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3471 | 1/1   | 0.93 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3727 | 1/1   | 0.93 | 0.35 | 21,21,21,21                 | 0     |
| 57  | MG   | 1U    | 203  | 1/1   | 0.93 | 0.07 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3606 | 1/1   | 0.93 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 1714 | 1/1   | 0.93 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 10    | 102  | 1/1   | 0.93 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3474 | 1/1   | 0.93 | 0.07 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3733 | 1/1   | 0.93 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3196 | 1/1   | 0.93 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3093 | 1/1   | 0.93 | 0.07 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3095 | 1/1   | 0.93 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3152 | 1/1   | 0.93 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3221 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3316 | 1/1   | 0.93 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1693 | 1/1   | 0.93 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 1601 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3106 | 1/1   | 0.93 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1700 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3740 | 1/1   | 0.93 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3569 | 1/1   | 0.93 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 1706 | 1/1   | 0.93 | 0.25 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 1707 | 1/1   | 0.93 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 1604 | 1/1   | 0.93 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3011 | 1/1   | 0.93 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3378 | 1/1   | 0.93 | 0.06 | 23,23,23,23                 | 0     |
| 57  | MG   | 2a    | 1714 | 1/1   | 0.93 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3324 | 1/1   | 0.93 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 2a    | 1716 | 1/1   | 0.93 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3326 | 1/1   | 0.93 | 0.16 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3327 | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 1608 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1735 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1724 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1726 | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3119 | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3379 | 1/1   | 0.93 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3621 | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3343 | 1/1   | 0.93 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 1731 | 1/1   | 0.93 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3494 | 1/1   | 0.93 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3593 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3595 | 1/1   | 0.93 | 0.28 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3623 | 1/1   | 0.93 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 1740 | 1/1   | 0.93 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3600 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 1616 | 1/1   | 0.93 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 1748 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3227 | 1/1   | 0.93 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3293 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3757 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1753 | 1/1   | 0.93 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3388 | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3633 | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3229 | 1/1   | 0.93 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 1625 | 1/1   | 0.93 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3764 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3001 | 1/1   | 0.93 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3232 | 1/1   | 0.93 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1a    | 1632 | 1/1   | 0.93 | 0.26 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3380 | 1/1   | 0.93 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 1764 | 1/1   | 0.93 | 0.19 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 1767 | 1/1   | 0.93 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3623 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3384 | 1/1   | 0.93 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3387 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3627 | 1/1   | 0.93 | 0.09 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3637 | 1/1   | 0.93 | 0.24 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3638 | 1/1   | 0.93 | 0.32 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 1637 | 1/1   | 0.93 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3155 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3773 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3236 | 1/1   | 0.93 | 0.28 | 35,35,35,35                 | 0     |
| 57  | MG   | 2u    | 101  | 1/1   | 0.93 | 0.19 | 66,66,66,66                 | 0     |
| 57  | MG   | 1a    | 1774 | 1/1   | 0.93 | 0.08 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3404 | 1/1   | 0.93 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3402 | 1/1   | 0.93 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 1645 | 1/1   | 0.93 | 0.29 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3050 | 1/1   | 0.93 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 2x    | 106  | 1/1   | 0.93 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 1781 | 1/1   | 0.93 | 0.16 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3337 | 1/1   | 0.94 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3182 | 1/1   | 0.94 | 0.32 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3078 | 1/1   | 0.94 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3079 | 1/1   | 0.94 | 0.06 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3390 | 1/1   | 0.94 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3277 | 1/1   | 0.94 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1B    | 206  | 1/1   | 0.94 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3628 | 1/1   | 0.94 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 1689 | 1/1   | 0.94 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3631 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3085 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3667 | 1/1   | 0.94 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3090 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3394 | 1/1   | 0.94 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3117 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 1694 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3119 | 1/1   | 0.94 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3099 | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 1B    | 214  | 1/1   | 0.94 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 1B    | 215  | 1/1   | 0.94 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3189 | 1/1   | 0.94 | 0.25 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 1704 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3651 | 1/1   | 0.94 | 0.09 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3109 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3381 | 1/1   | 0.94 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3089 | 1/1   | 0.94 | 0.27 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3675 | 1/1   | 0.94 | 0.06 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3403 | 1/1   | 0.94 | 0.07 | 14,14,14,14                 | 0     |
| 57  | MG   | 2A    | 3389 | 1/1   | 0.94 | 0.08 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3283 | 1/1   | 0.94 | 0.24 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3284 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 57  | MG   | 1F    | 308  | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 1N    | 201  | 1/1   | 0.94 | 0.24 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3682 | 1/1   | 0.94 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3090 | 1/1   | 0.94 | 0.22 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 1722 | 1/1   | 0.94 | 0.16 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3128 | 1/1   | 0.94 | 0.28 | 53,53,53,53                 | 0     |
| 57  | MG   | 1N    | 204  | 1/1   | 0.94 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3687 | 1/1   | 0.94 | 0.21 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 1726 | 1/1   | 0.94 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3688 | 1/1   | 0.94 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3550 | 1/1   | 0.94 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3411 | 1/1   | 0.94 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | 2D    | 304  | 1/1   | 0.94 | 0.51 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3136 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3192 | 1/1   | 0.94 | 0.21 | 30,30,30,30                 | 0     |
| 57  | MG   | 2D    | 308  | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 2D    | 309  | 1/1   | 0.94 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3414 | 1/1   | 0.94 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1Q    | 201  | 1/1   | 0.94 | 0.21 | 38,38,38,38                 | 0     |
| 57  | MG   | 2O    | 3700 | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3193 | 1/1   | 0.94 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3699 | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3124 | 1/1   | 0.94 | 0.19 | 36,36,36,36                 | 0     |
| 57  | MG   | 1V    | 204  | 1/1   | 0.94 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | 1W    | 202  | 1/1   | 0.94 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3094 | 1/1   | 0.94 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3303 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3581 | 1/1   | 0.94 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3430 | 1/1   | 0.94 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 1746 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 2Y    | 201  | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 1747 | 1/1   | 0.94 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3582 | 1/1   | 0.94 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | 12    | 102  | 1/1   | 0.94 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3440 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3441 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3442 | 1/1   | 0.94 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 1752 | 1/1   | 0.94 | 0.10 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3310 | 1/1   | 0.94 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3132 | 1/1   | 0.94 | 0.22 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 1606 | 1/1   | 0.94 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1608 | 1/1   | 0.94 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | 15    | 102  | 1/1   | 0.94 | 0.20 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3452 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 15    | 103  | 1/1   | 0.94 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 15    | 104  | 1/1   | 0.94 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3456 | 1/1   | 0.94 | 0.09 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3165 | 1/1   | 0.94 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1616 | 1/1   | 0.94 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 1618 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 16    | 101  | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1621 | 1/1   | 0.94 | 0.25 | 50,50,50,50                 | 0     |
| 57  | MG   | 17    | 105  | 1/1   | 0.94 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3712 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3464 | 1/1   | 0.94 | 0.25 | 58,58,58,58                 | 0     |
| 57  | MG   | 18    | 102  | 1/1   | 0.94 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3715 | 1/1   | 0.94 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3587 | 1/1   | 0.94 | 0.06 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3717 | 1/1   | 0.94 | 0.20 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3720 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 1770 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3723 | 1/1   | 0.94 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1635 | 1/1   | 0.94 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3724 | 1/1   | 0.94 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3185 | 1/1   | 0.94 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3439 | 1/1   | 0.94 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3477 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1641 | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3189 | 1/1   | 0.94 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3590 | 1/1   | 0.94 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3198 | 1/1   | 0.94 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 1776 | 1/1   | 0.94 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 1777 | 1/1   | 0.94 | 0.15 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 1647 | 1/1   | 0.94 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 1613 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3485 | 1/1   | 0.94 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3317 | 1/1   | 0.94 | 0.18 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1780 | 1/1   | 0.94 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3593 | 1/1   | 0.94 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 2a    | 1656 | 1/1   | 0.94 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3324 | 1/1   | 0.94 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3211 | 1/1   | 0.94 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3212 | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3454 | 1/1   | 0.94 | 0.07 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3206 | 1/1   | 0.94 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1662 | 1/1   | 0.94 | 0.08 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3499 | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3048 | 1/1   | 0.94 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1n    | 101  | 1/1   | 0.94 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3502 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3335 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1v    | 102  | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3457 | 1/1   | 0.94 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3458 | 1/1   | 0.94 | 0.08 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3607 | 1/1   | 0.94 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3218 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3036 | 1/1   | 0.94 | 0.33 | 30,30,30,30                 | 0     |
| 57  | MG   | 1x    | 103  | 1/1   | 0.94 | 0.12 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 1630 | 1/1   | 0.94 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3752 | 1/1   | 0.94 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3222 | 1/1   | 0.94 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1681 | 1/1   | 0.94 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3101 | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3230 | 1/1   | 0.94 | 0.52 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3232 | 1/1   | 0.94 | 0.32 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3525 | 1/1   | 0.94 | 0.07 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 1636 | 1/1   | 0.94 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3756 | 1/1   | 0.94 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3237 | 1/1   | 0.94 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3530 | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3141 | 1/1   | 0.94 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 1697 | 1/1   | 0.94 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3142 | 1/1   | 0.94 | 0.28 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3009 | 1/1   | 0.94 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3011 | 1/1   | 0.94 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 1641 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3016 | 1/1   | 0.94 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3017 | 1/1   | 0.94 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3253 | 1/1   | 0.94 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1709 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3469 | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 1644 | 1/1   | 0.94 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3023 | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3259 | 1/1   | 0.94 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3145 | 1/1   | 0.94 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3551 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3620 | 1/1   | 0.94 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3149 | 1/1   | 0.94 | 0.23 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3472 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3151 | 1/1   | 0.94 | 0.05 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 1725 | 1/1   | 0.94 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3475 | 1/1   | 0.94 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3772 | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3244 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3038 | 1/1   | 0.94 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 1655 | 1/1   | 0.94 | 0.31 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3070 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1733 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3777 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3154 | 1/1   | 0.94 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3044 | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3045 | 1/1   | 0.94 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3573 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3574 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3576 | 1/1   | 0.94 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1743 | 1/1   | 0.94 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3257 | 1/1   | 0.94 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 1746 | 1/1   | 0.94 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3047 | 1/1   | 0.94 | 0.20 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3258 | 1/1   | 0.94 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1750 | 1/1   | 0.94 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1751 | 1/1   | 0.94 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3582 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3004 | 1/1   | 0.94 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3293 | 1/1   | 0.94 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1755 | 1/1   | 0.94 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3050 | 1/1   | 0.94 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 1666 | 1/1   | 0.94 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3788 | 1/1   | 0.94 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3299 | 1/1   | 0.94 | 0.06 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3640 | 1/1   | 0.94 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3054 | 1/1   | 0.94 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3592 | 1/1   | 0.94 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3372 | 1/1   | 0.94 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 1765 | 1/1   | 0.94 | 0.14 | 72,72,72,72                 | 0     |
| 57  | MG   | 2A    | 3056 | 1/1   | 0.94 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3057 | 1/1   | 0.94 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3599 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3792 | 1/1   | 0.94 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3046 | 1/1   | 0.94 | 0.13 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3063 | 1/1   | 0.94 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3512 | 1/1   | 0.94 | 0.06 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3604 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3264 | 1/1   | 0.94 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3607 | 1/1   | 0.94 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 1677 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3177 | 1/1   | 0.94 | 0.30 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3271 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3073 | 1/1   | 0.94 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3328 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 2w    | 402  | 1/1   | 0.94 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3614 | 1/1   | 0.94 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3332 | 1/1   | 0.94 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2x    | 103  | 1/1   | 0.94 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3112 | 1/1   | 0.94 | 0.19 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3520 | 1/1   | 0.94 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3619 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3438 | 1/1   | 0.95 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2B    | 203  | 1/1   | 0.95 | 0.21 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3427 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3179 | 1/1   | 0.95 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3005 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2B    | 207  | 1/1   | 0.95 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1x    | 102  | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3799 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3340 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3436 | 1/1   | 0.95 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3803 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3187 | 1/1   | 0.95 | 0.31 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3033 | 1/1   | 0.95 | 0.08 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3805 | 1/1   | 0.95 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3444 | 1/1   | 0.95 | 0.06 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3445 | 1/1   | 0.95 | 0.07 | 22,22,22,22                 | 0     |
| 57  | MG   | 2E    | 301  | 1/1   | 0.95 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2E    | 303  | 1/1   | 0.95 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3557 | 1/1   | 0.95 | 0.07 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3558 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3561 | 1/1   | 0.95 | 0.05 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3568 | 1/1   | 0.95 | 0.06 | 22,22,22,22                 | 0     |
| 57  | MG   | 1a    | 1662 | 1/1   | 0.95 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3015 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3680 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1B    | 207  | 1/1   | 0.95 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3203 | 1/1   | 0.95 | 0.23 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3342 | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3579 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3465 | 1/1   | 0.95 | 0.15 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3686 | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3208 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3072 | 1/1   | 0.95 | 0.28 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3266 | 1/1   | 0.95 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3205 | 1/1   | 0.95 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 25    | 101  | 1/1   | 0.95 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3206 | 1/1   | 0.95 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | 28    | 103  | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3028 | 1/1   | 0.95 | 0.15 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3215 | 1/1   | 0.95 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 1B    | 220  | 1/1   | 0.95 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3691 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3693 | 1/1   | 0.95 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3272 | 1/1   | 0.95 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3697 | 1/1   | 0.95 | 0.23 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 1609 | 1/1   | 0.95 | 0.22 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3273 | 1/1   | 0.95 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3226 | 1/1   | 0.95 | 0.25 | 43,43,43,43                 | 0     |
| 57  | MG   | 1F    | 304  | 1/1   | 0.95 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3483 | 1/1   | 0.95 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3155 | 1/1   | 0.95 | 0.10 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3038 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1G    | 201  | 1/1   | 0.95 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3488 | 1/1   | 0.95 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3073 | 1/1   | 0.95 | 0.29 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3042 | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3214 | 1/1   | 0.95 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3492 | 1/1   | 0.95 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3704 | 1/1   | 0.95 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3463 | 1/1   | 0.95 | 0.09 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3496 | 1/1   | 0.95 | 0.19 | 29,29,29,29                 | 0     |
| 57  | MG   | 2a    | 1628 | 1/1   | 0.95 | 0.19 | 39,39,39,39                 | 0     |
| 57  | MG   | 1O    | 201  | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3216 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3365 | 1/1   | 0.95 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3060 | 1/1   | 0.95 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | 1P    | 203  | 1/1   | 0.95 | 0.25 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3280 | 1/1   | 0.95 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3254 | 1/1   | 0.95 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3597 | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 1638 | 1/1   | 0.95 | 0.14 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 1705 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1Q    | 203  | 1/1   | 0.95 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 1Q    | 204  | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 1709 | 1/1   | 0.95 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3598 | 1/1   | 0.95 | 0.06 | 45,45,45,45                 | 0     |
| 57  | MG   | 1T    | 201  | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3062 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3516 | 1/1   | 0.95 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3517 | 1/1   | 0.95 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3063 | 1/1   | 0.95 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3220 | 1/1   | 0.95 | 0.23 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 1716 | 1/1   | 0.95 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3270 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3272 | 1/1   | 0.95 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 1654 | 1/1   | 0.95 | 0.30 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3601 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3275 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1U    | 204  | 1/1   | 0.95 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3721 | 1/1   | 0.95 | 0.07 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3722 | 1/1   | 0.95 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 1X    | 101  | 1/1   | 0.95 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3280 | 1/1   | 0.95 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1723 | 1/1   | 0.95 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3171 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 1Z    | 302  | 1/1   | 0.95 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 10    | 101  | 1/1   | 0.95 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3080 | 1/1   | 0.95 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 1728 | 1/1   | 0.95 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3022 | 1/1   | 0.95 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 1670 | 1/1   | 0.95 | 0.20 | 61,61,61,61                 | 0     |
| 57  | MG   | 10    | 103  | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3082 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3285 | 1/1   | 0.95 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3297 | 1/1   | 0.95 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3226 | 1/1   | 0.95 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3089 | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3300 | 1/1   | 0.95 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3609 | 1/1   | 0.95 | 0.08 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3304 | 1/1   | 0.95 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 1682 | 1/1   | 0.95 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3479 | 1/1   | 0.95 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3480 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3309 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3562 | 1/1   | 0.95 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3310 | 1/1   | 0.95 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 1739 | 1/1   | 0.95 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3483 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1692 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3135 | 1/1   | 0.95 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3101 | 1/1   | 0.95 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1695 | 1/1   | 0.95 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 1696 | 1/1   | 0.95 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3103 | 1/1   | 0.95 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3179 | 1/1   | 0.95 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1699 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3387 | 1/1   | 0.95 | 0.07 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 1745 | 1/1   | 0.95 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3742 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1705 | 1/1   | 0.95 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3325 | 1/1   | 0.95 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3136 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3296 | 1/1   | 0.95 | 0.20 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 1749 | 1/1   | 0.95 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 1602 | 1/1   | 0.95 | 0.22 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 1712 | 1/1   | 0.95 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 1751 | 1/1   | 0.95 | 0.12 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3299 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3084 | 1/1   | 0.95 | 0.23 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3498 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 1755 | 1/1   | 0.95 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1718 | 1/1   | 0.95 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3124 | 1/1   | 0.95 | 0.20 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3342 | 1/1   | 0.95 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3125 | 1/1   | 0.95 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3184 | 1/1   | 0.95 | 0.06 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3594 | 1/1   | 0.95 | 0.06 | 74,74,74,74                 | 0     |
| 57  | MG   | 1A    | 3308 | 1/1   | 0.95 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3507 | 1/1   | 0.95 | 0.06 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3350 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3351 | 1/1   | 0.95 | 0.11 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3630 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3400 | 1/1   | 0.95 | 0.05 | 18,18,18,18                 | 0     |
| 57  | MG   | 2a    | 1732 | 1/1   | 0.95 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3511 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3132 | 1/1   | 0.95 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3759 | 1/1   | 0.95 | 0.08 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3360 | 1/1   | 0.95 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3139 | 1/1   | 0.95 | 0.14 | 23,23,23,23                 | 0     |
| 57  | MG   | 2a    | 1739 | 1/1   | 0.95 | 0.12 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3364 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3245 | 1/1   | 0.95 | 0.04 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3037 | 1/1   | 0.95 | 0.17 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3109 | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3139 | 1/1   | 0.95 | 0.26 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3639 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3375 | 1/1   | 0.95 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3378 | 1/1   | 0.95 | 0.05 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3769 | 1/1   | 0.95 | 0.24 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3322 | 1/1   | 0.95 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3023 | 1/1   | 0.95 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3408 | 1/1   | 0.95 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3145 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3386 | 1/1   | 0.95 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3146 | 1/1   | 0.95 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3065 | 1/1   | 0.95 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3416 | 1/1   | 0.95 | 0.07 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3391 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3150 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3394 | 1/1   | 0.95 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3532 | 1/1   | 0.95 | 0.14 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3420 | 1/1   | 0.95 | 0.08 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3146 | 1/1   | 0.95 | 0.24 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3154 | 1/1   | 0.95 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3637 | 1/1   | 0.95 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3113 | 1/1   | 0.95 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3402 | 1/1   | 0.95 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3330 | 1/1   | 0.95 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3782 | 1/1   | 0.95 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3334 | 1/1   | 0.95 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3659 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 1786 | 1/1   | 0.95 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3650 | 1/1   | 0.95 | 0.07 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3787 | 1/1   | 0.95 | 0.06 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3040 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1d    | 301  | 1/1   | 0.95 | 0.23 | 37,37,37,37                 | 0     |
| 57  | MG   | 1f    | 201  | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3170 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1m    | 3001 | 1/1   | 0.95 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 1643 | 1/1   | 0.95 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3663 | 1/1   | 0.95 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3260 | 1/1   | 0.95 | 0.27 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3175 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3665 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3666 | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3408 | 1/1   | 0.96 | 0.05 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3161 | 1/1   | 0.96 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3486 | 1/1   | 0.96 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3162 | 1/1   | 0.96 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 1a    | 1619 | 1/1   | 0.96 | 0.05 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 1785 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3489 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3415 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 1621 | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3417 | 1/1   | 0.96 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3760 | 1/1   | 0.96 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3170 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3382 | 1/1   | 0.96 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1k    | 201  | 1/1   | 0.96 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3385 | 1/1   | 0.96 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3627 | 1/1   | 0.96 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3766 | 1/1   | 0.96 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3223 | 1/1   | 0.96 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 1629 | 1/1   | 0.96 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3768 | 1/1   | 0.96 | 0.14 | 15,15,15,15                 | 0     |
| 57  | MG   | 1a    | 1631 | 1/1   | 0.96 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3432 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 2D    | 303  | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1w    | 403  | 1/1   | 0.96 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 2D    | 305  | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3098 | 1/1   | 0.96 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3497 | 1/1   | 0.96 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3437 | 1/1   | 0.96 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3225 | 1/1   | 0.96 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1x    | 104  | 1/1   | 0.96 | 0.05 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1x    | 106  | 1/1   | 0.96 | 0.04 | 40,40,40,40                 | 0     |
| 57  | MG   | 2F    | 302  | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3126 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3174 | 1/1   | 0.96 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 2F    | 306  | 1/1   | 0.96 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 2N    | 201  | 1/1   | 0.96 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3444 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3445 | 1/1   | 0.96 | 0.05 | 60,60,60,60                 | 0     |
| 57  | MG   | 2Q    | 202  | 1/1   | 0.96 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3446 | 1/1   | 0.96 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3447 | 1/1   | 0.96 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3774 | 1/1   | 0.96 | 0.22 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3449 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3055 | 1/1   | 0.96 | 0.16 | 14,14,14,14                 | 0     |
| 57  | MG   | 1a    | 1640 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3300 | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3396 | 1/1   | 0.96 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3398 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3008 | 1/1   | 0.96 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3779 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | 20    | 102  | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3010 | 1/1   | 0.96 | 0.06 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3460 | 1/1   | 0.96 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | 23    | 102  | 1/1   | 0.96 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3513 | 1/1   | 0.96 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3012 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 28    | 102  | 1/1   | 0.96 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3130 | 1/1   | 0.96 | 0.32 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3643 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1601 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3178 | 1/1   | 0.96 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3304 | 1/1   | 0.96 | 0.30 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3217 | 1/1   | 0.96 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3234 | 1/1   | 0.96 | 0.23 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3519 | 1/1   | 0.96 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3022 | 1/1   | 0.96 | 0.04 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3309 | 1/1   | 0.96 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3235 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 1654 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3475 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3405 | 1/1   | 0.96 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3652 | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3655 | 1/1   | 0.96 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3797 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3312 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1619 | 1/1   | 0.96 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3235 | 1/1   | 0.96 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3525 | 1/1   | 0.96 | 0.04 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3660 | 1/1   | 0.96 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3238 | 1/1   | 0.96 | 0.05 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3313 | 1/1   | 0.96 | 0.06 | 18,18,18,18                 | 0     |
| 57  | MG   | 1a    | 1663 | 1/1   | 0.96 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3662 | 1/1   | 0.96 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3242 | 1/1   | 0.96 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3014 | 1/1   | 0.96 | 0.07 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3534 | 1/1   | 0.96 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3246 | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3247 | 1/1   | 0.96 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3494 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3238 | 1/1   | 0.96 | 0.36 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3412 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3413 | 1/1   | 0.96 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3044 | 1/1   | 0.96 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3316 | 1/1   | 0.96 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 1B    | 204  | 1/1   | 0.96 | 0.08 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3417 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 1674 | 1/1   | 0.96 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3418 | 1/1   | 0.96 | 0.06 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 1676 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3239 | 1/1   | 0.96 | 0.05 | 34,34,34,34                 | 0     |
| 57  | MG   | 1B    | 208  | 1/1   | 0.96 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3673 | 1/1   | 0.96 | 0.08 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3422 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3549 | 1/1   | 0.96 | 0.13 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3269 | 1/1   | 0.96 | 0.04 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 1684 | 1/1   | 0.96 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3271 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3676 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1655 | 1/1   | 0.96 | 0.27 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3273 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3319 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3024 | 1/1   | 0.96 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3522 | 1/1   | 0.96 | 0.08 | 63,63,63,63                 | 0     |
| 57  | MG   | 1B    | 218  | 1/1   | 0.96 | 0.04 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3027 | 1/1   | 0.96 | 0.18 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3246 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3064 | 1/1   | 0.96 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3527 | 1/1   | 0.96 | 0.06 | 62,62,62,62                 | 0     |
| 57  | MG   | 1D    | 301  | 1/1   | 0.96 | 0.26 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3327 | 1/1   | 0.96 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3282 | 1/1   | 0.96 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3283 | 1/1   | 0.96 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1E    | 301  | 1/1   | 0.96 | 0.24 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3070 | 1/1   | 0.96 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3434 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 1672 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3685 | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3560 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3289 | 1/1   | 0.96 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3015 | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 1F    | 301  | 1/1   | 0.96 | 0.17 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 1678 | 1/1   | 0.96 | 0.08 | 70,70,70,70                 | 0     |
| 57  | MG   | 1F    | 302  | 1/1   | 0.96 | 0.25 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3077 | 1/1   | 0.96 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3545 | 1/1   | 0.96 | 0.10 | 90,90,90,90                 | 0     |
| 57  | MG   | 1A    | 3562 | 1/1   | 0.96 | 0.05 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3547 | 1/1   | 0.96 | 0.05 | 51,51,51,51                 | 0     |
| 57  | MG   | 1F    | 306  | 1/1   | 0.96 | 0.05 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3550 | 1/1   | 0.96 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3564 | 1/1   | 0.96 | 0.06 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3565 | 1/1   | 0.96 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3301 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1G    | 203  | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 1713 | 1/1   | 0.96 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3009 | 1/1   | 0.96 | 0.05 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3306 | 1/1   | 0.96 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3692 | 1/1   | 0.96 | 0.12 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3560 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3561 | 1/1   | 0.96 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3569 | 1/1   | 0.96 | 0.05 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3563 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3087 | 1/1   | 0.96 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3039 | 1/1   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3696 | 1/1   | 0.96 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 1704 | 1/1   | 0.96 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3567 | 1/1   | 0.96 | 0.06 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3572 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3573 | 1/1   | 0.96 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3575 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3251 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3702 | 1/1   | 0.96 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3051 | 1/1   | 0.96 | 0.12 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 1727 | 1/1   | 0.96 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3443 | 1/1   | 0.96 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3255 | 1/1   | 0.96 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3256 | 1/1   | 0.96 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3708 | 1/1   | 0.96 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3584 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3087 | 1/1   | 0.96 | 0.05 | 20,20,20,20                 | 0     |
| 57  | MG   | 2a    | 1721 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3111 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3586 | 1/1   | 0.96 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3336 | 1/1   | 0.96 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3586 | 1/1   | 0.96 | 0.05 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3338 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3113 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1U    | 206  | 1/1   | 0.96 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 1736 | 1/1   | 0.96 | 0.05 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3117 | 1/1   | 0.96 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 1737 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1V    | 202  | 1/1   | 0.96 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3596 | 1/1   | 0.96 | 0.06 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3713 | 1/1   | 0.96 | 0.05 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3714 | 1/1   | 0.96 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3448 | 1/1   | 0.96 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3088 | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3143 | 1/1   | 0.96 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3006 | 1/1   | 0.96 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3115 | 1/1   | 0.96 | 0.16 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3605 | 1/1   | 0.96 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3116 | 1/1   | 0.96 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 10    | 104  | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1745 | 1/1   | 0.96 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | 10    | 105  | 1/1   | 0.96 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3609 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 11    | 102  | 1/1   | 0.96 | 0.38 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1749 | 1/1   | 0.96 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3353 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3365 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 1l    | 104  | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3150 | 1/1   | 0.96 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3725 | 1/1   | 0.96 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3616 | 1/1   | 0.96 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3357 | 1/1   | 0.96 | 0.07 | 20,20,20,20                 | 0     |
| 57  | MG   | 2a    | 1757 | 1/1   | 0.96 | 0.04 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3069 | 1/1   | 0.96 | 0.08 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3199 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3376 | 1/1   | 0.96 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3202 | 1/1   | 0.96 | 0.40 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3600 | 1/1   | 0.96 | 0.05 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3118 | 1/1   | 0.96 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 17    | 103  | 1/1   | 0.96 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3737 | 1/1   | 0.96 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3054 | 1/1   | 0.96 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3207 | 1/1   | 0.96 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 1766 | 1/1   | 0.96 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3630 | 1/1   | 0.96 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3149 | 1/1   | 0.96 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3120 | 1/1   | 0.96 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1772 | 1/1   | 0.96 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 2d    | 301  | 1/1   | 0.96 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 1768 | 1/1   | 0.96 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3121 | 1/1   | 0.96 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3369 | 1/1   | 0.96 | 0.06 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3743 | 1/1   | 0.96 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3608 | 1/1   | 0.96 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 2k    | 202  | 1/1   | 0.96 | 0.06 | 72,72,72,72                 | 0     |
| 57  | MG   | 1a    | 1606 | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3213 | 1/1   | 0.96 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3400 | 1/1   | 0.96 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3071 | 1/1   | 0.96 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 2w    | 401  | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3643 | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3644 | 1/1   | 0.96 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3157 | 1/1   | 0.96 | 0.04 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3478 | 1/1   | 0.96 | 0.08 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3373 | 1/1   | 0.96 | 0.12 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3217 | 1/1   | 0.96 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3096 | 1/1   | 0.96 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | 2x    | 109  | 1/1   | 0.96 | 0.08 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3499 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3163 | 1/1   | 0.97 | 0.17 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3165 | 1/1   | 0.97 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3318 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3625 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3265 | 1/1   | 0.97 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3166 | 1/1   | 0.97 | 0.05 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3509 | 1/1   | 0.97 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3268 | 1/1   | 0.97 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3320 | 1/1   | 0.97 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3208 | 1/1   | 0.97 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 13    | 101  | 1/1   | 0.97 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3487 | 1/1   | 0.97 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3631 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3088 | 1/1   | 0.97 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3323 | 1/1   | 0.97 | 0.04 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3755 | 1/1   | 0.97 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3091 | 1/1   | 0.97 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3137 | 1/1   | 0.97 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3053 | 1/1   | 0.97 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3094 | 1/1   | 0.97 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3409 | 1/1   | 0.97 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3326 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3097 | 1/1   | 0.97 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3172 | 1/1   | 0.97 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3100 | 1/1   | 0.97 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 17    | 106  | 1/1   | 0.97 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3102 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 17    | 107  | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3008 | 1/1   | 0.97 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3414 | 1/1   | 0.97 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3506 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 1607 | 1/1   | 0.97 | 0.23 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3507 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3291 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | 19    | 101  | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3265 | 1/1   | 0.97 | 0.13 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3079 | 1/1   | 0.97 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3331 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3526 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3515 | 1/1   | 0.97 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3530 | 1/1   | 0.97 | 0.14 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 1617 | 1/1   | 0.97 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3332 | 1/1   | 0.97 | 0.14 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3114 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3080 | 1/1   | 0.97 | 0.11 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3268 | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3521 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3649 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 1610 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3536 | 1/1   | 0.97 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3269 | 1/1   | 0.97 | 0.23 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 1627 | 1/1   | 0.97 | 0.26 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3308 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3428 | 1/1   | 0.97 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3122 | 1/1   | 0.97 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3312 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3123 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1633 | 1/1   | 0.97 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3653 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3654 | 1/1   | 0.97 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3429 | 1/1   | 0.97 | 0.05 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3656 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3657 | 1/1   | 0.97 | 0.03 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3540 | 1/1   | 0.97 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3218 | 1/1   | 0.97 | 0.19 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3338 | 1/1   | 0.97 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3784 | 1/1   | 0.97 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3176 | 1/1   | 0.97 | 0.30 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3081 | 1/1   | 0.97 | 0.30 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3002 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3329 | 1/1   | 0.97 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3330 | 1/1   | 0.97 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3331 | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3547 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3790 | 1/1   | 0.97 | 0.05 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 1651 | 1/1   | 0.97 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3343 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3144 | 1/1   | 0.97 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3793 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3551 | 1/1   | 0.97 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3180 | 1/1   | 0.97 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3348 | 1/1   | 0.97 | 0.05 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3554 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3349 | 1/1   | 0.97 | 0.06 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3672 | 1/1   | 0.97 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3344 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3345 | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3067 | 1/1   | 0.97 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3352 | 1/1   | 0.97 | 0.06 | 13,13,13,13                 | 0     |
| 57  | MG   | 1A    | 3104 | 1/1   | 0.97 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3349 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3183 | 1/1   | 0.97 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3147 | 1/1   | 0.97 | 0.26 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3563 | 1/1   | 0.97 | 0.06 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3450 | 1/1   | 0.97 | 0.05 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3355 | 1/1   | 0.97 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3451 | 1/1   | 0.97 | 0.04 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3357 | 1/1   | 0.97 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3577 | 1/1   | 0.97 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3156 | 1/1   | 0.97 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3681 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3158 | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3581 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3361 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3566 | 1/1   | 0.97 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 1x    | 101  | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3567 | 1/1   | 0.97 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3684 | 1/1   | 0.97 | 0.06 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3228 | 1/1   | 0.97 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3453 | 1/1   | 0.97 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3057 | 1/1   | 0.97 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3166 | 1/1   | 0.97 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3167 | 1/1   | 0.97 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1690 | 1/1   | 0.97 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3125 | 1/1   | 0.97 | 0.04 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3377 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3169 | 1/1   | 0.97 | 0.24 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3018 | 1/1   | 0.97 | 0.04 | 20,20,20,20                 | 0     |
| 57  | MG   | 1B    | 213  | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3597 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3127 | 1/1   | 0.97 | 0.03 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3004 | 1/1   | 0.97 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3578 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3385 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3043 | 1/1   | 0.97 | 0.28 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 1702 | 1/1   | 0.97 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3029 | 1/1   | 0.97 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3460 | 1/1   | 0.97 | 0.08 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3366 | 1/1   | 0.97 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1D    | 302  | 1/1   | 0.97 | 0.04 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3180 | 1/1   | 0.97 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 1D    | 303  | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3290 | 1/1   | 0.97 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | 2a    | 1710 | 1/1   | 0.97 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1D    | 306  | 1/1   | 0.97 | 0.17 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3014 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3398 | 1/1   | 0.97 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3464 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3465 | 1/1   | 0.97 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3188 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3292 | 1/1   | 0.97 | 0.10 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3403 | 1/1   | 0.97 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1719 | 1/1   | 0.97 | 0.09 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3018 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 1E    | 305  | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3020 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3131 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3295 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3062 | 1/1   | 0.97 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3297 | 1/1   | 0.97 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3625 | 1/1   | 0.97 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1F    | 303  | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3298 | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 1678 | 1/1   | 0.97 | 0.04 | 47,47,47,47                 | 0     |
| 57  | MG   | 1F    | 305  | 1/1   | 0.97 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3202 | 1/1   | 0.97 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3240 | 1/1   | 0.97 | 0.10 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3204 | 1/1   | 0.97 | 0.10 | 69,69,69,69                 | 0     |
| 57  | MG   | 1F    | 307  | 1/1   | 0.97 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 1682 | 1/1   | 0.97 | 0.04 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1737 | 1/1   | 0.97 | 0.24 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3473 | 1/1   | 0.97 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3010 | 1/1   | 0.97 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 1G    | 202  | 1/1   | 0.97 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3711 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3301 | 1/1   | 0.97 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3158 | 1/1   | 0.97 | 0.14 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3197 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3642 | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3383 | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3134 | 1/1   | 0.97 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3481 | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3718 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 1695 | 1/1   | 0.97 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3482 | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3305 | 1/1   | 0.97 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3224 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3484 | 1/1   | 0.97 | 0.07 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3605 | 1/1   | 0.97 | 0.04 | 25,25,25,25                 | 0     |
| 57  | MG   | 1Q    | 202  | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3228 | 1/1   | 0.97 | 0.33 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3306 | 1/1   | 0.97 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3307 | 1/1   | 0.97 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3231 | 1/1   | 0.97 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3389 | 1/1   | 0.97 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3663 | 1/1   | 0.97 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3664 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 1R    | 201  | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 1R    | 202  | 1/1   | 0.97 | 0.28 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3091 | 1/1   | 0.97 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3392 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3200 | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3732 | 1/1   | 0.97 | 0.30 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3061 | 1/1   | 0.97 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1U    | 205  | 1/1   | 0.97 | 0.19 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3075 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 1719 | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3734 | 1/1   | 0.97 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3735 | 1/1   | 0.97 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1W    | 201  | 1/1   | 0.97 | 0.23 | 41,41,41,41                 | 0     |
| 57  | MG   | 2D    | 302  | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3068 | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3249 | 1/1   | 0.97 | 0.19 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3252 | 1/1   | 0.97 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3251 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1W    | 203  | 1/1   | 0.97 | 0.17 | 27,27,27,27                 | 0     |
| 57  | MG   | 1W    | 204  | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3255 | 1/1   | 0.97 | 0.05 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3495 | 1/1   | 0.97 | 0.05 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2E    | 302  | 1/1   | 0.97 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3203 | 1/1   | 0.97 | 0.17 | 26,26,26,26                 | 0     |
| 57  | MG   | 2E    | 304  | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 2x    | 104  | 1/1   | 0.97 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 2E    | 305  | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 2F    | 301  | 1/1   | 0.97 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3254 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3204 | 1/1   | 0.97 | 0.12 | 22,22,22,22                 | 0     |
| 58  | ZN   | 1n    | 102  | 1/1   | 0.97 | 0.04 | 97,97,97,97                 | 0     |
| 58  | ZN   | 2n    | 501  | 1/1   | 0.97 | 0.06 | 86,86,86,86                 | 0     |
| 57  | MG   | 2A    | 3223 | 1/1   | 0.98 | 0.04 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3110 | 1/1   | 0.98 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3160 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 1715 | 1/1   | 0.98 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3462 | 1/1   | 0.98 | 0.06 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 3528 | 1/1   | 0.98 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3529 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3353 | 1/1   | 0.98 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3074 | 1/1   | 0.98 | 0.15 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3531 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3351 | 1/1   | 0.98 | 0.04 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3270 | 1/1   | 0.98 | 0.08 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3234 | 1/1   | 0.98 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3237 | 1/1   | 0.98 | 0.08 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3762 | 1/1   | 0.98 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3535 | 1/1   | 0.98 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3128 | 1/1   | 0.98 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3311 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3611 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3210 | 1/1   | 0.98 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3646 | 1/1   | 0.98 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3614 | 1/1   | 0.98 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3243 | 1/1   | 0.98 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3649 | 1/1   | 0.98 | 0.03 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3185 | 1/1   | 0.98 | 0.03 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3373 | 1/1   | 0.98 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3241 | 1/1   | 0.98 | 0.06 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3653 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3510 | 1/1   | 0.98 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3276 | 1/1   | 0.98 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3133 | 1/1   | 0.98 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 1635 | 1/1   | 0.98 | 0.10 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3242 | 1/1   | 0.98 | 0.03 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3363 | 1/1   | 0.98 | 0.06 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3660 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3243 | 1/1   | 0.98 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 1686 | 1/1   | 0.98 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3252 | 1/1   | 0.98 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3382 | 1/1   | 0.98 | 0.10 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3030 | 1/1   | 0.98 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3476 | 1/1   | 0.98 | 0.06 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3694 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3186 | 1/1   | 0.98 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3548 | 1/1   | 0.98 | 0.07 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3388 | 1/1   | 0.98 | 0.05 | 66,66,66,66                 | 0     |
| 57  | MG   | 1a    | 1742 | 1/1   | 0.98 | 0.12 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3097 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3698 | 1/1   | 0.98 | 0.09 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3392 | 1/1   | 0.98 | 0.04 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3367 | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3421 | 1/1   | 0.98 | 0.10 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3164 | 1/1   | 0.98 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3041 | 1/1   | 0.98 | 0.21 | 32,32,32,32                 | 0     |
| 57  | MG   | 1U    | 202  | 1/1   | 0.98 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3534 | 1/1   | 0.98 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3628 | 1/1   | 0.98 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3321 | 1/1   | 0.98 | 0.05 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3786 | 1/1   | 0.98 | 0.05 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3215 | 1/1   | 0.98 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 1V    | 201  | 1/1   | 0.98 | 0.25 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3541 | 1/1   | 0.98 | 0.07 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3705 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 57  | MG   | 1V    | 203  | 1/1   | 0.98 | 0.36 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3427 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1V    | 205  | 1/1   | 0.98 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3632 | 1/1   | 0.98 | 0.05 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3556 | 1/1   | 0.98 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3058 | 1/1   | 0.98 | 0.03 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3549 | 1/1   | 0.98 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3249 | 1/1   | 0.98 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | 2F    | 305  | 1/1   | 0.98 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3559 | 1/1   | 0.98 | 0.06 | 14,14,14,14                 | 0     |
| 57  | MG   | 1X    | 103  | 1/1   | 0.98 | 0.07 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 1664 | 1/1   | 0.98 | 0.04 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 1765 | 1/1   | 0.98 | 0.05 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3430 | 1/1   | 0.98 | 0.03 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3099 | 1/1   | 0.98 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3167 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3376 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3800 | 1/1   | 0.98 | 0.07 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3168 | 1/1   | 0.98 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3493 | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3290 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3148 | 1/1   | 0.98 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 2X    | 103  | 1/1   | 0.98 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3425 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3069 | 1/1   | 0.98 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3719 | 1/1   | 0.98 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3294 | 1/1   | 0.98 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3429 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3436 | 1/1   | 0.98 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3571 | 1/1   | 0.98 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3042 | 1/1   | 0.98 | 0.18 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3291 | 1/1   | 0.98 | 0.06 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3181 | 1/1   | 0.98 | 0.23 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3575 | 1/1   | 0.98 | 0.05 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3381 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3435 | 1/1   | 0.98 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3025 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3500 | 1/1   | 0.98 | 0.05 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3302 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3439 | 1/1   | 0.98 | 0.05 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3502 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3576 | 1/1   | 0.98 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3729 | 1/1   | 0.98 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3026 | 1/1   | 0.98 | 0.04 | 15,15,15,15                 | 0     |
| 57  | MG   | 17    | 101  | 1/1   | 0.98 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3190 | 1/1   | 0.98 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 17    | 102  | 1/1   | 0.98 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3294 | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3311 | 1/1   | 0.98 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3505 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3313 | 1/1   | 0.98 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3506 | 1/1   | 0.98 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3315 | 1/1   | 0.98 | 0.04 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3013 | 1/1   | 0.98 | 0.08 | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3454 | 1/1   | 0.98 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 1690 | 1/1   | 0.98 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3318 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3034 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3092 | 1/1   | 0.98 | 0.07 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3106 | 1/1   | 0.98 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 1B    | 217  | 1/1   | 0.98 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3462 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3339 | 1/1   | 0.98 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 1696 | 1/1   | 0.98 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 1697 | 1/1   | 0.98 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3391 | 1/1   | 0.98 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 1700 | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3201 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3098 | 1/1   | 0.98 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3262 | 1/1   | 0.98 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3093 | 1/1   | 0.98 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3517 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1x    | 105  | 1/1   | 0.98 | 0.06 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3035 | 1/1   | 0.98 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3213 | 1/1   | 0.98 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3231 | 1/1   | 0.98 | 0.19 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3747 | 1/1   | 0.98 | 0.06 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3397 | 1/1   | 0.98 | 0.04 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3107 | 1/1   | 0.98 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 1710 | 1/1   | 0.98 | 0.06 | 29,29,29,29                 | 0     |
| 57  | MG   | 2x    | 107  | 1/1   | 0.98 | 0.05 | 76,76,76,76                 | 0     |
| 57  | MG   | 1A    | 3345 | 1/1   | 0.98 | 0.04 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3003 | 1/1   | 0.98 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3041 | 1/1   | 0.98 | 0.10 | 19,19,19,19                 | 0     |
| 58  | ZN   | 2Y    | 202  | 1/1   | 0.98 | 0.04 | 89,89,89,89                 | 0     |
| 58  | ZN   | 24    | 501  | 1/1   | 0.98 | 0.09 | 125,125,125,125             | 0     |
| 57  | MG   | 2A    | 3222 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 59  | SF4  | 2d    | 302  | 8/8   | 0.98 | 0.04 | 55,65,83,89                 | 0     |
| 57  | MG   | 1B    | 216  | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |
| 57  | MG   | 1x    | 108  | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3384 | 1/1   | 0.99 | 0.03 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3539 | 1/1   | 0.99 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3114 | 1/1   | 0.99 | 0.22 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3487 | 1/1   | 0.99 | 0.03 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3356 | 1/1   | 0.99 | 0.07 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3169 | 1/1   | 0.99 | 0.08 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3333 | 1/1   | 0.99 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3541 | 1/1   | 0.99 | 0.09 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3333 | 1/1   | 0.99 | 0.03 | 23,23,23,23                 | 0     |
| 57  | MG   | 17    | 104  | 1/1   | 0.99 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | 1D    | 304  | 1/1   | 0.99 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3570 | 1/1   | 0.99 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3795 | 1/1   | 0.99 | 0.04 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3446 | 1/1   | 0.99 | 0.08 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3728 | 1/1   | 0.99 | 0.03 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3012 | 1/1   | 0.99 | 0.03 | 22,22,22,22                 | 0     |
| 57  | MG   | 1E    | 304  | 1/1   | 0.99 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3425 | 1/1   | 0.99 | 0.02 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3574 | 1/1   | 0.99 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3801 | 1/1   | 0.99 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3558 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3426 | 1/1   | 0.99 | 0.04 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3374 | 1/1   | 0.99 | 0.04 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3577 | 1/1   | 0.99 | 0.04 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3521 | 1/1   | 0.99 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3047 | 1/1   | 0.99 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3347 | 1/1   | 0.99 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 1X    | 102  | 1/1   | 0.99 | 0.03 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3056 | 1/1   | 0.99 | 0.09 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3459 | 1/1   | 0.99 | 0.03 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 1699 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3410 | 1/1   | 0.99 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3078 | 1/1   | 0.99 | 0.06 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 1615 | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3527 | 1/1   | 0.99 | 0.03 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3501 | 1/1   | 0.99 | 0.03 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3233 | 1/1   | 0.99 | 0.36 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3209 | 1/1   | 0.99 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3745 | 1/1   | 0.99 | 0.06 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 1708 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 11    | 101  | 1/1   | 0.99 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3367 | 1/1   | 0.99 | 0.04 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3588 | 1/1   | 0.99 | 0.03 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3289 | 1/1   | 0.99 | 0.07 | 14,14,14,14                 | 0     |
| 57  | MG   | 2A    | 3421 | 1/1   | 0.99 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3748 | 1/1   | 0.99 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3371 | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3372 | 1/1   | 0.99 | 0.04 | 38,38,38,38                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | ZN   | 1Y    | 501  | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |
| 58  | ZN   | 14    | 501  | 1/1   | 0.99 | 0.08 | 107,107,107,107             | 0     |
| 58  | ZN   | 15    | 105  | 1/1   | 0.99 | 0.02 | 38,38,38,38                 | 0     |
| 58  | ZN   | 16    | 102  | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3415 | 1/1   | 0.99 | 0.08 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3437 | 1/1   | 0.99 | 0.03 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3083 | 1/1   | 0.99 | 0.03 | 12,12,12,12                 | 0     |
| 58  | ZN   | 25    | 102  | 1/1   | 0.99 | 0.05 | 52,52,52,52                 | 0     |
| 58  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.02 | 55,55,55,55                 | 0     |
| 58  | ZN   | 29    | 102  | 1/1   | 0.99 | 0.04 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3354 | 1/1   | 0.99 | 0.07 | 13,13,13,13                 | 0     |
| 59  | SF4  | 1d    | 302  | 8/8   | 0.99 | 0.04 | 61,72,77,81                 | 0     |
| 57  | MG   | 2A    | 3043 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3363 | 1/1   | 1.00 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3440 | 1/1   | 1.00 | 0.07 | 17,17,17,17                 | 0     |
| 58  | ZN   | 19    | 102  | 1/1   | 1.00 | 0.02 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3419 | 1/1   | 1.00 | 0.01 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3612 | 1/1   | 1.00 | 0.01 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3510 | 1/1   | 1.00 | 0.03 | 52,52,52,52                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.