



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:54 PM UTC

PDB ID : 9MTR / pdb\_00009mtr  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with mRNA, A-site GGS-mutant Release Factor 1, and P-site fMEAAA KC-peptidyl-tRNA<sub>cys</sub> at 2.80Å resolution  
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Basu, R.S.; Vassilevski, A.A.; Gagnon, M.G.; Polikanov, Y.S.  
Deposited on : 2025-01-12  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

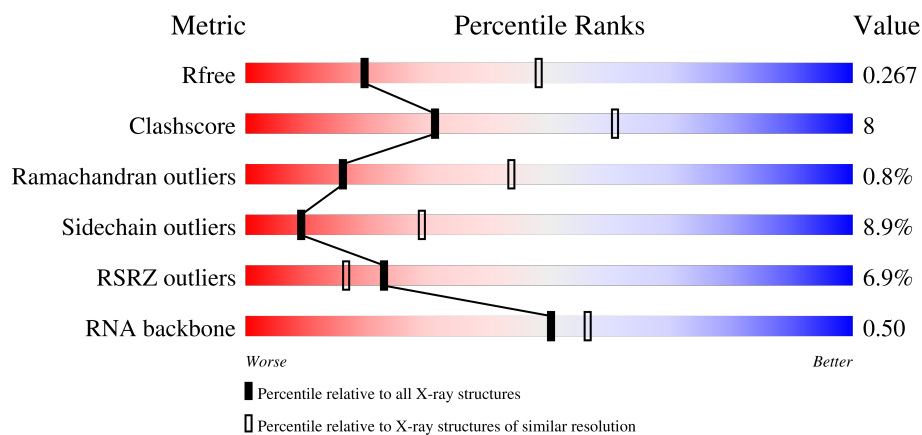
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



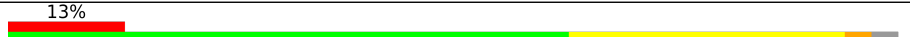
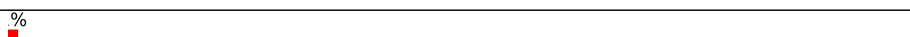
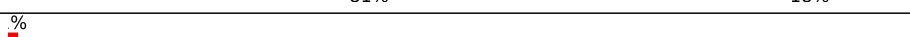
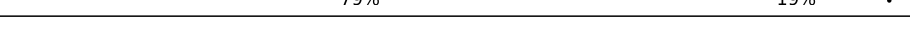
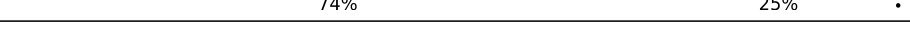
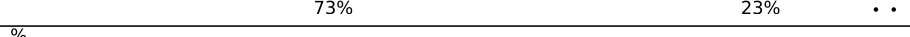
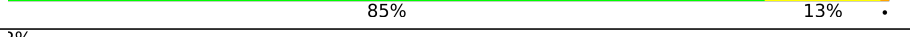
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |
| RNA backbone          | 3983                        | 1114 (3.00-2.60)                                      |

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   | <div> <div>6%</div> <div>65% 28% 6%</div> </div> |
| 1   | 2A    | 2915   | <div> <div>5%</div> <div>58% 32% 6%</div> </div> |
| 2   | 1B    | 121    | <div> <div>75% 20%</div> </div>                  |

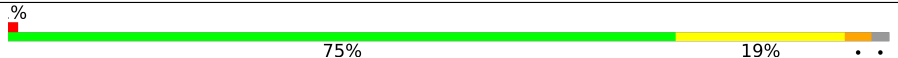
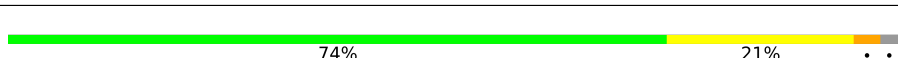
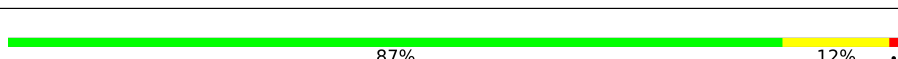
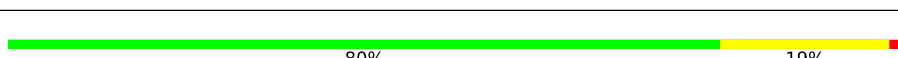
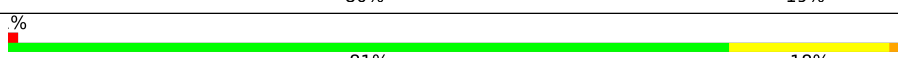
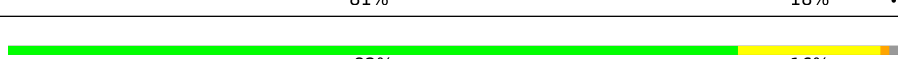
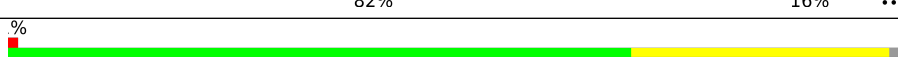
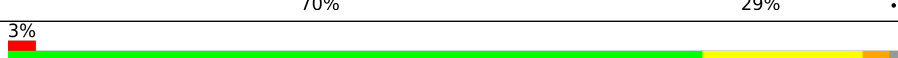
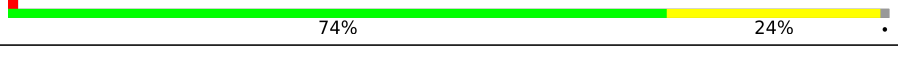
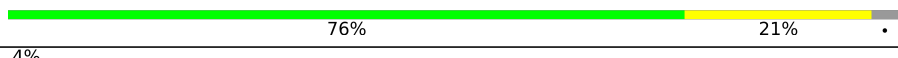
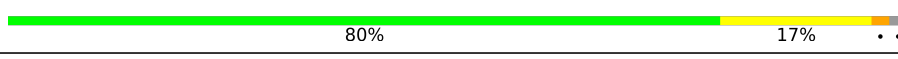
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | 2B    | 121    |    |
| 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    |    |
| 15  | 2T    | 146    |    |
| 16  | 1U    | 118    |    |
| 16  | 2U    | 118    |    |
| 17  | 1V    | 101    |    |
| 17  | 2V    | 101    |    |
| 18  | 1W    | 113    |    |
| 18  | 2W    | 113    |    |
| 19  | 1X    | 96     |    |
| 19  | 2X    | 96     |    |
| 20  | 1Y    | 110    |    |
| 20  | 2Y    | 110    |    |
| 21  | 1Z    | 206    |   |
| 21  | 2Z    | 206    |  |
| 22  | 10    | 85     |  |
| 22  | 20    | 85     |  |
| 23  | 11    | 98     |  |
| 23  | 21    | 98     |  |
| 24  | 12    | 72     |  |
| 24  | 22    | 72     |  |
| 25  | 13    | 60     |  |
| 25  | 23    | 60     |  |
| 26  | 14    | 71     |  |
| 26  | 24    | 71     |  |
| 27  | 15    | 60     |  |

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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    | 74     |                  |
| 55  | 2x    | 74     |                  |
| 56  | 1z    | 7      |                  |
| 56  | 2z    | 7      |                  |

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    | 4032 | -         | -        | -       | X                |
| 57  | MG   | 1U    | 212  | -         | -        | -       | X                |

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296656 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     |
|     |       |          | 2577  | 1146 | 476 | 835 | 120 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2575  | 1146 | 476 | 833 | 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     |
|     |       |          | 1423  | 913 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 913 | 258 | 253 | 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     |
|     |       |          | 1097  | 701 | 191 | 204 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 681 | 186 | 196 | 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     |
|     |       |          | 873   | 550 | 174 | 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     |
|     |       |          | 750   | 488 | 135 | 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     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1240  | 795 | 222 | 220 | 3 |         |         |       |
| 21  | 2Z    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1271  | 814 | 228 | 227 | 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    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 604   | 373 | 128 | 102 | 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     |
|     |       |          | 552   | 349 | 99 | 99 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 97 | 91 | 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     |
|     |       |          | 517   | 331 | 102 | 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     |
|     |       |          | 1548  | 973 | 301 | 273 | 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     |
|     |       |          | 1655  | 1038 | 326 | 284 | 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     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |

- 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   | 514 | 144 | 149 | 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    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 978   | 619 | 190 | 169 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | 1j    | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 709   | 440 | 138 | 131 |         |         |       |
| 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     |
|     |       |          | 919   | 566 | 190 | 161 | 2 |         |         |       |
| 44  | 2m    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 907   | 558 | 188 | 159 | 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     |
|     |       |          | 492   | 312 | 104 | 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     |
|     |       |          | 555   | 355 | 108 | 92 |  |         |         |       |

- 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 CYS-Stop mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 53  | 1v    | 9        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 191   | 86 | 34 | 62 | 9 |         |         |       |
| 53  | 2v    | 9        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 191   | 86 | 34 | 62 | 9 |         |         |       |

- 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     |
|     |       |          | 1935  | 1196 | 359 | 371 | 9 |         |         |       |
| 54  | 2w    | 253      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1953  | 1207 | 360 | 377 | 9 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| 1w    | 230     | SER      | GLN    | engineered mutation | UNP P96077 |
| 2w    | 230     | SER      | GLN    | engineered mutation | UNP P96077 |

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMEAAAKC-tRNA<sub>cys</sub> RNA-part.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 55  | 1x    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1577  | 704 | 281 | 517 | 74 | 1 |         |         |       |
| 55  | 2x    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1577  | 704 | 281 | 517 | 74 | 1 |         |         |       |

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMEAAAKC-tRNA<sub>cys</sub> Peptide-part.

| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---|---------|---------|-------|
| 56  | 1z    | 5        | Total | C  | N | O | S | 0       | 0       | 0     |
|     |       |          | 30    | 18 | 6 | 5 | 1 |         |         |       |
| 56  | 2z    | 4        | Total | C  | N | O | S | 0       | 0       | 0     |
|     |       |          | 25    | 15 | 5 | 4 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 57  | 1A    | 1084     | Total | Mg   | 0       | 0       |
|     |       |          | 1084  | 1084 |         |         |
| 57  | 1B    | 39       | Total | Mg   | 0       | 0       |
|     |       |          | 39    | 39   |         |         |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 57  | 1D    | 14       | Total<br>14 | Mg<br>14 | 0       | 0       |
| 57  | 1E    | 13       | Total<br>13 | Mg<br>13 | 0       | 0       |
| 57  | 1F    | 14       | Total<br>14 | Mg<br>14 | 0       | 0       |
| 57  | 1G    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 57  | 1H    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | 1I    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | 1N    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 57  | 1O    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 57  | 1P    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 57  | 1Q    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 57  | 1R    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 57  | 1S    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 57  | 1T    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 57  | 1U    | 12       | Total<br>12 | Mg<br>12 | 0       | 0       |
| 57  | 1V    | 8        | Total<br>8  | Mg<br>8  | 0       | 0       |
| 57  | 1W    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 57  | 1X    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 57  | 1Y    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 57  | 1Z    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 57  | 10    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 57  | 11    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | 12    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 13    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 15    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 57  | 16    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 17    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 57  | 18    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 57  | 19    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1a    | 221      | Total<br>221 | Mg<br>221 | 0       | 0       |
| 57  | 1b    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 1d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 1k    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1l    | 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  | 1p    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1v    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 1w    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 1x    | 13       | Total<br>13  | Mg<br>13  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | 2A    | 835      | Total<br>835 | Mg<br>835 | 0       | 0       |
| 57  | 2B    | 18       | Total<br>18  | Mg<br>18  | 0       | 0       |
| 57  | 2D    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | 2E    | 10       | Total<br>10  | Mg<br>10  | 0       | 0       |
| 57  | 2F    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 57  | 2G    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2O    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 2P    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2Q    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 2R    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2T    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 2U    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 2V    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2W    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 2Y    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2Z    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2I    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 23    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 25    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | 26    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 27    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | 28    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | 2a    | 178      | Total<br>178 | Mg<br>178 | 0       | 0       |
| 57  | 2d    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2g    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2i    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2j    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2k    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2q    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2r    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | 2v    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | 2x    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 58  | 1A    | 1        | Total<br>1 | K<br>1 | 0       | 0       |

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

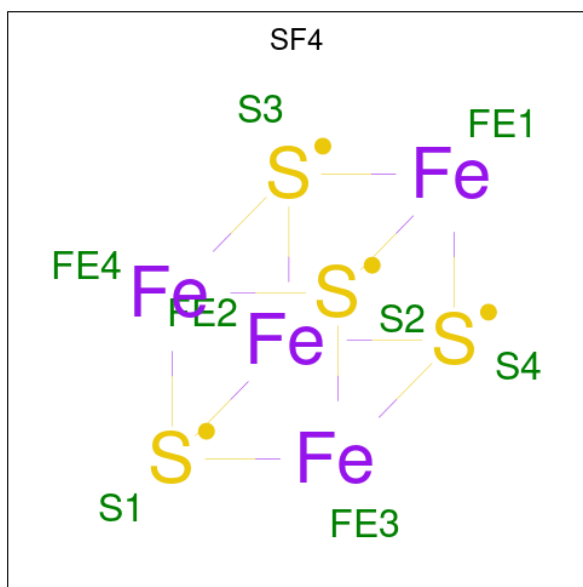
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59  | 1Y    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 29    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | 2n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms      |         |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 60  | 1d    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |
| 60  | 2d    | 1        | Total<br>8 | Fe<br>4 | S<br>4 | 0       | 0       |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61  | 1A    | 1897     | Total<br>1897 | O<br>1897 | 0       | 0       |
| 61  | 1B    | 61       | Total<br>61   | O<br>61   | 0       | 0       |
| 61  | 1D    | 30       | Total<br>30   | O<br>30   | 0       | 0       |
| 61  | 1E    | 27       | Total<br>27   | O<br>27   | 0       | 0       |
| 61  | 1F    | 18       | Total<br>18   | O<br>18   | 0       | 0       |
| 61  | 1G    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 61  | 1H    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 1I    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 1N    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 61  | 1O    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 61  | 1P    | 23       | Total<br>23   | O<br>23   | 0       | 0       |
| 61  | 1Q    | 11       | Total<br>11   | O<br>11   | 0       | 0       |
| 61  | 1R    | 11       | Total<br>11   | O<br>11   | 0       | 0       |
| 61  | 1S    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 1T    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 61  | 1U    | 13       | Total<br>13   | O<br>13   | 0       | 0       |
| 61  | 1V    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 61  | 1W    | 12       | Total<br>12   | O<br>12   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 1X    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 61  | 1Y    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 10    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 61  | 11    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 61  | 12    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 13    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 15    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 61  | 16    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 17    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 61  | 18    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 61  | 1a    | 259      | Total<br>259 | O<br>259 | 0       | 0       |
| 61  | 1b    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1d    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1j    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1l    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 1n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1q    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 1u    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1v    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 1w    | 3        | Total<br>3   | O<br>3   | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61  | 1x    | 25       | Total<br>25   | O<br>25   | 0       | 0       |
| 61  | 2A    | 1003     | Total<br>1003 | O<br>1003 | 0       | 0       |
| 61  | 2B    | 14       | Total<br>14   | O<br>14   | 0       | 0       |
| 61  | 2D    | 25       | Total<br>25   | O<br>25   | 0       | 0       |
| 61  | 2E    | 14       | Total<br>14   | O<br>14   | 0       | 0       |
| 61  | 2F    | 12       | Total<br>12   | O<br>12   | 0       | 0       |
| 61  | 2N    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2O    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | 2P    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 61  | 2Q    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | 2R    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 61  | 2T    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 61  | 2U    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | 2V    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2W    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | 2X    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 20    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 21    | 10       | Total<br>10   | O<br>10   | 0       | 0       |
| 61  | 25    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | 27    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | 28    | 4        | Total<br>4    | O<br>4    | 0       | 0       |

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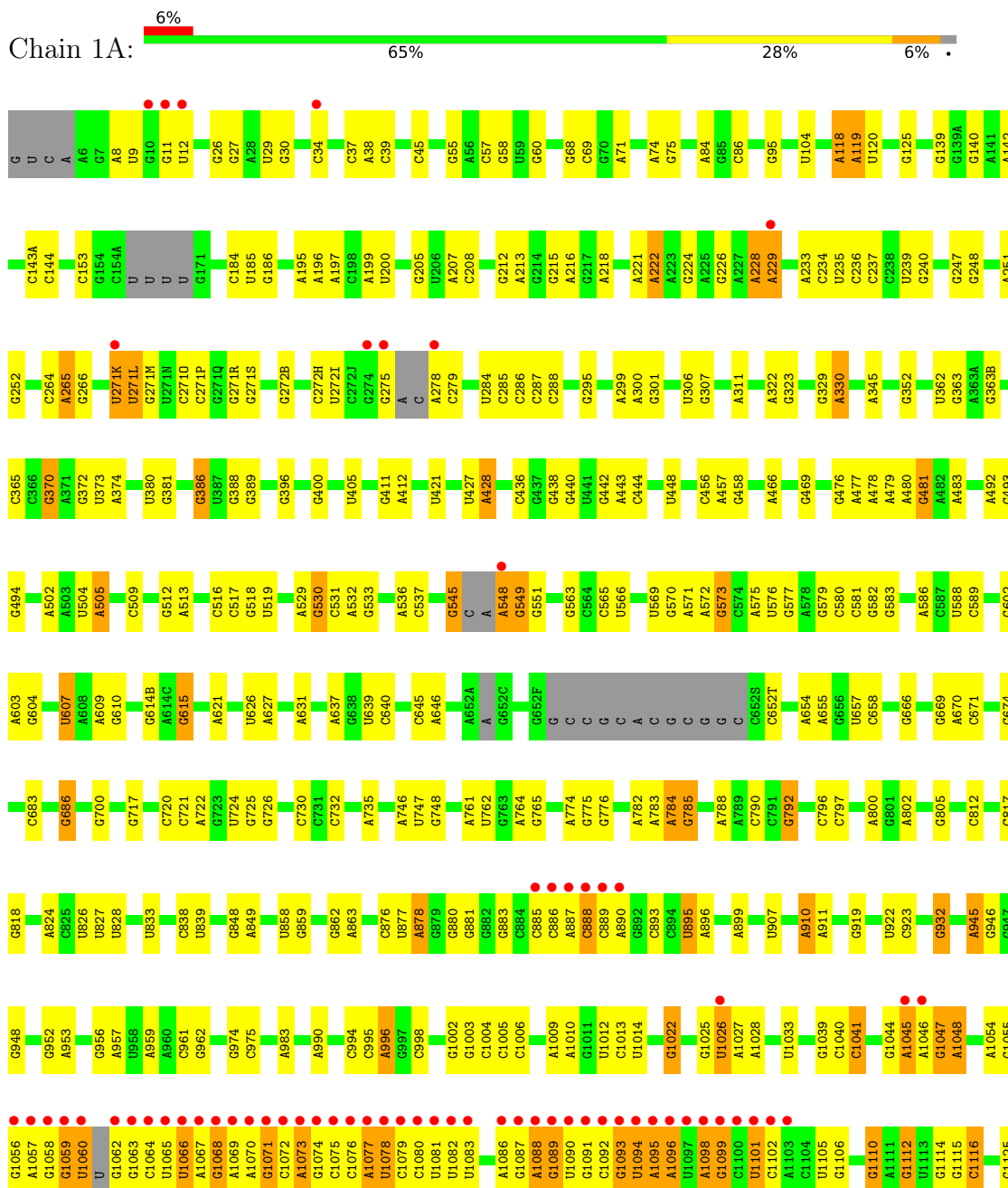
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 29    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2a    | 130      | Total<br>130 | O<br>130 | 0       | 0       |
| 61  | 2e    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2i    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2j    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2l    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 2n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2q    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2t    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2v    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2w    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2x    | 14       | Total<br>14  | O<br>14  | 0       | 0       |

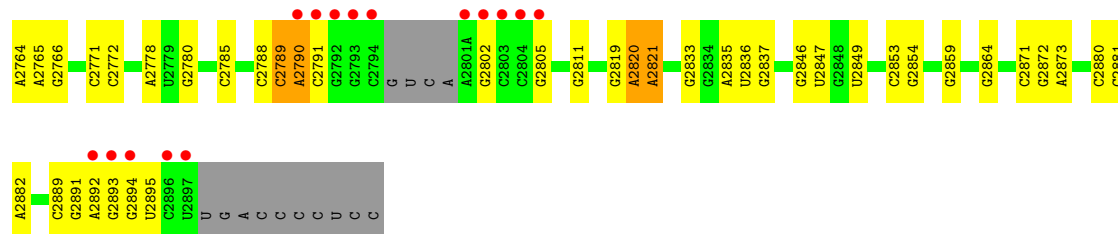
### 3 Residue-property plots

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

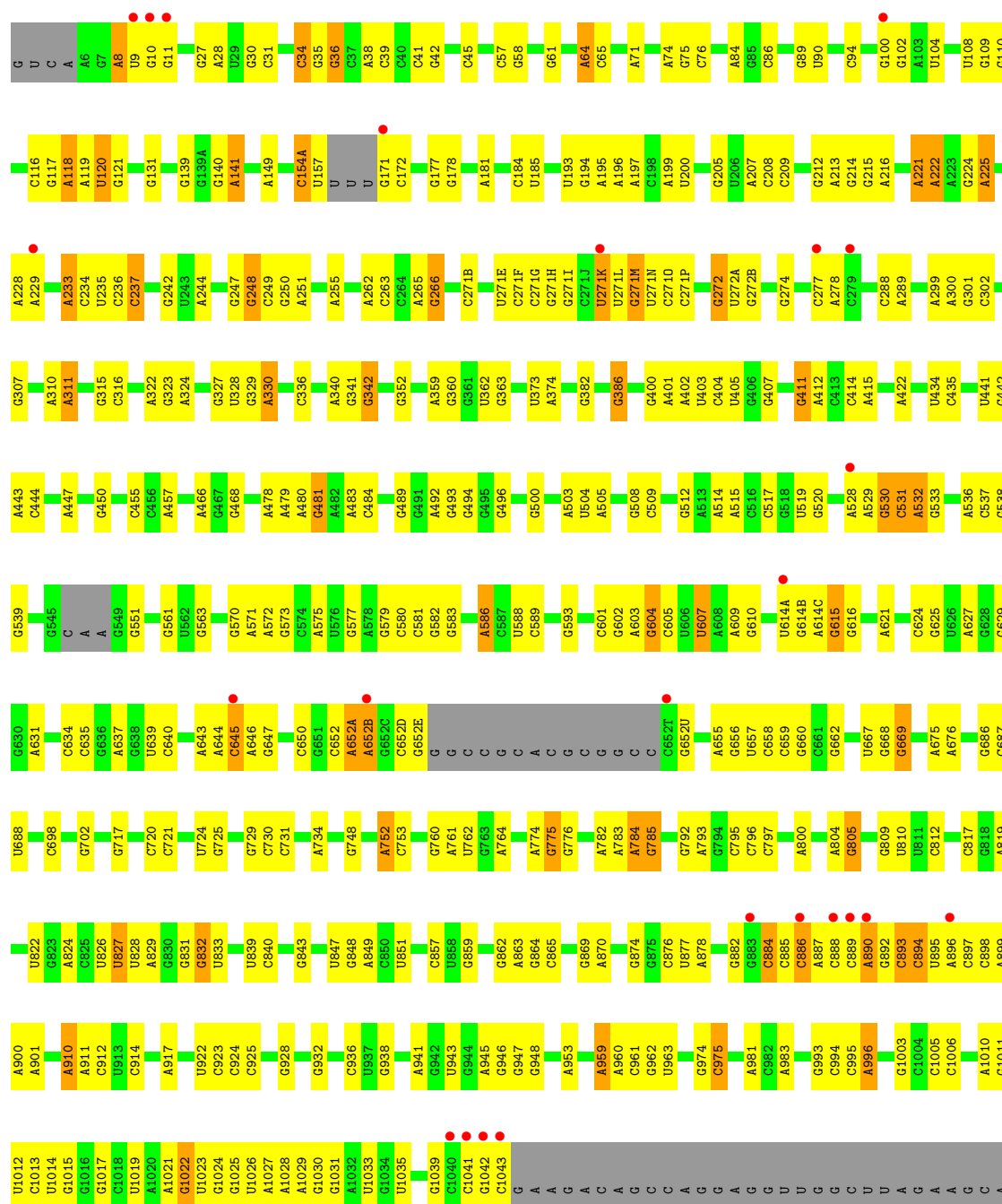
#### • Molecule 1: 23S Ribosomal RNA

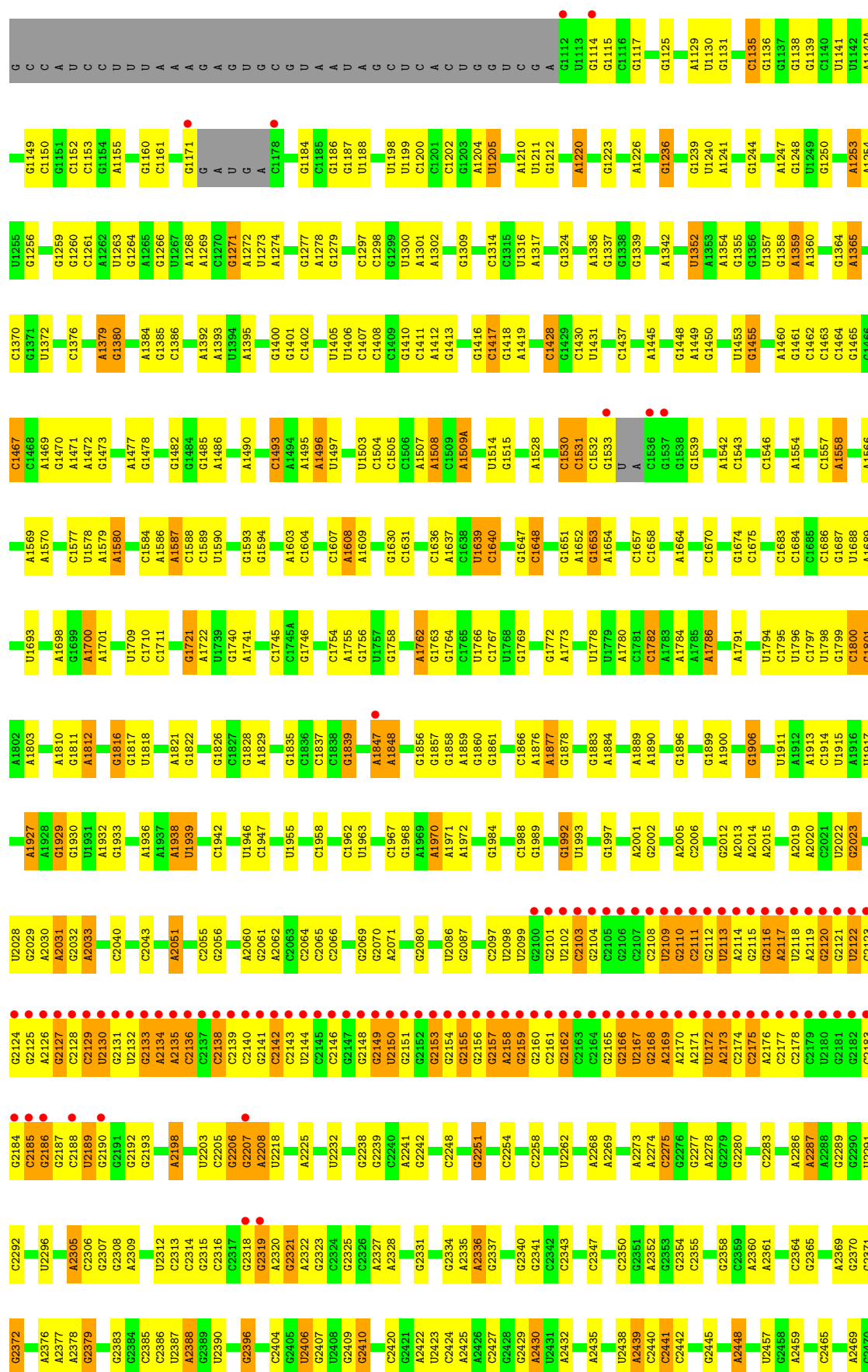


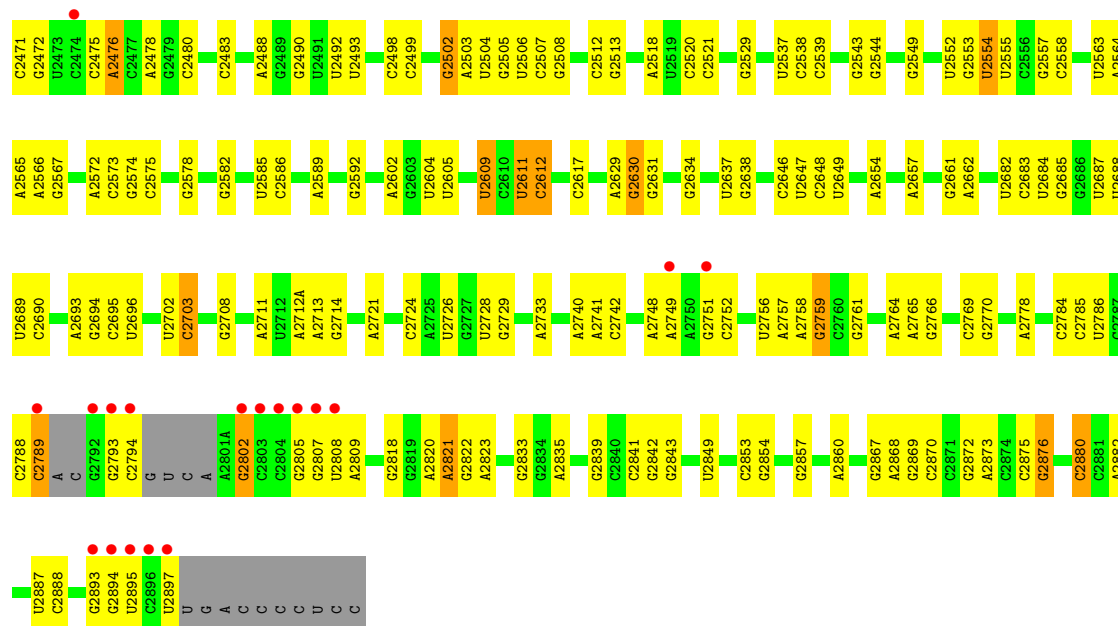




• Molecule 1: 23S Ribosomal RNA

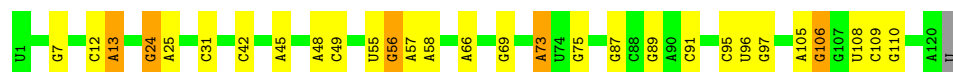






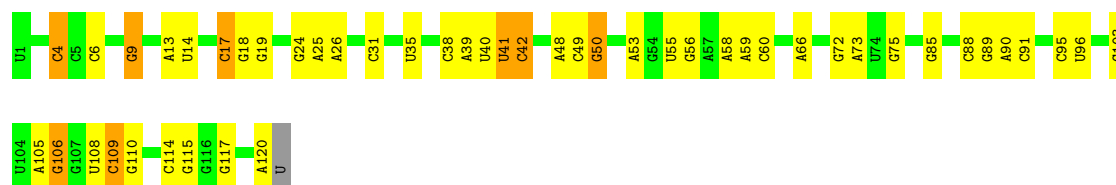
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 75% 20% . .



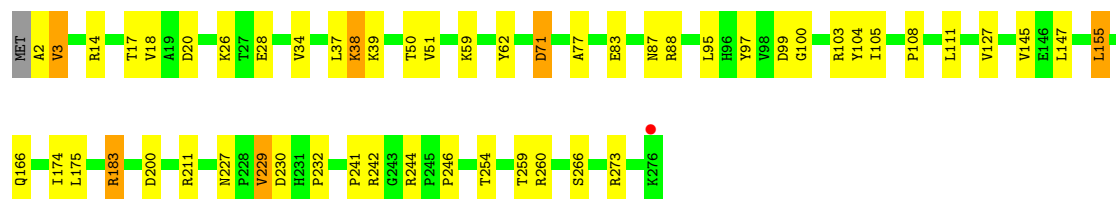
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 60% 33% 7% .



• Molecule 3: 50S ribosomal protein L2

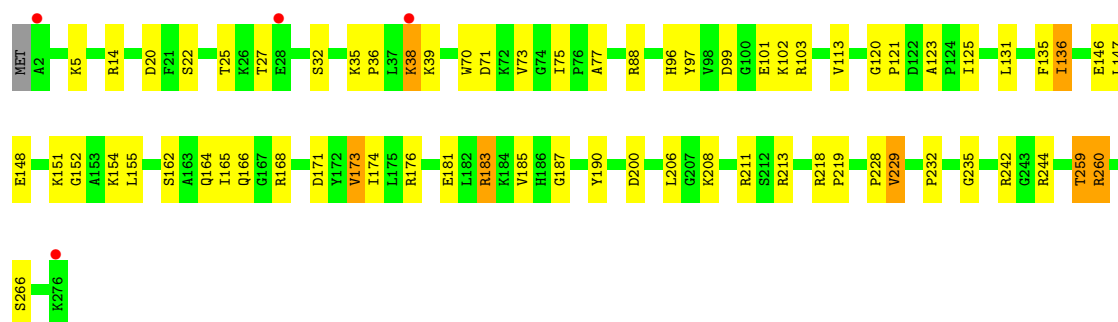
Chain 1D: 80% 17% .



• Molecule 3: 50S ribosomal protein L2

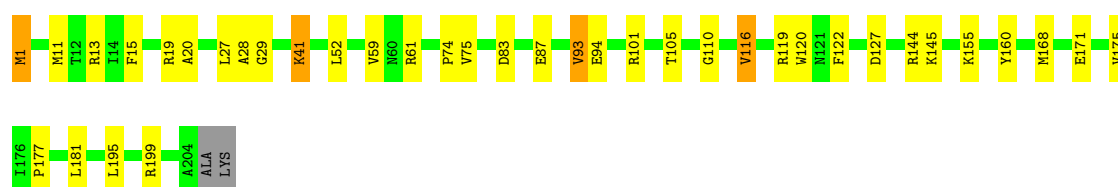
Chain 2D: 75% 22% .





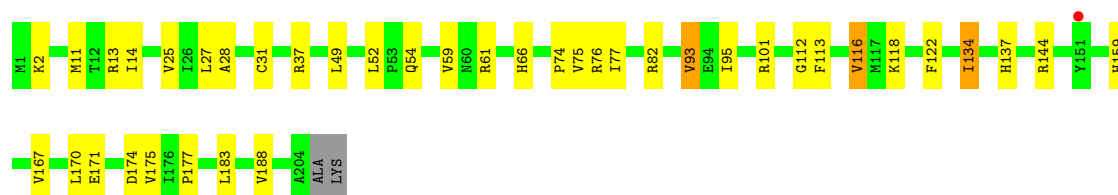
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 81% 17% ..



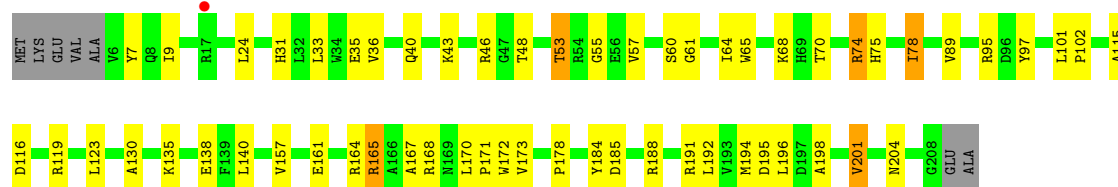
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 80% 18% ..



• Molecule 5: 50S ribosomal protein L4

Chain 1F: 69% 25% . .



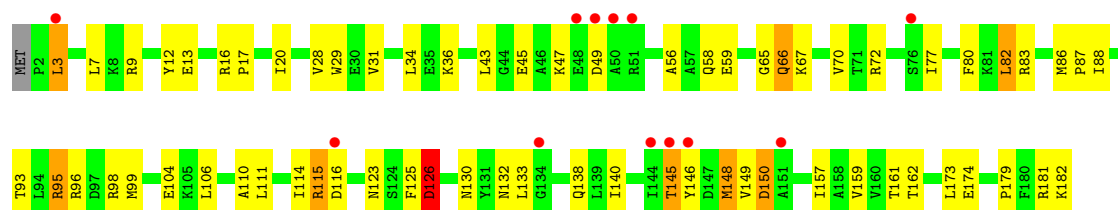
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 64% 28% 5% .

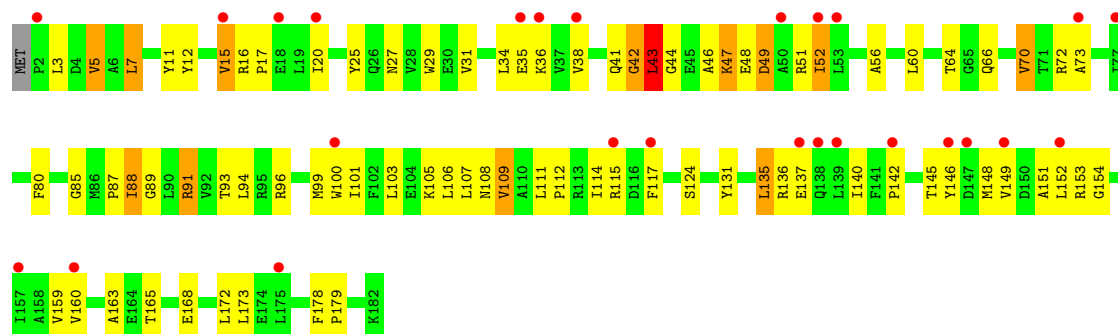




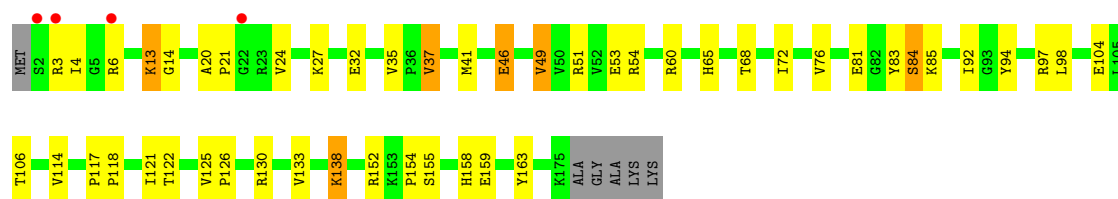
- Molecule 6: 50S ribosomal protein L5



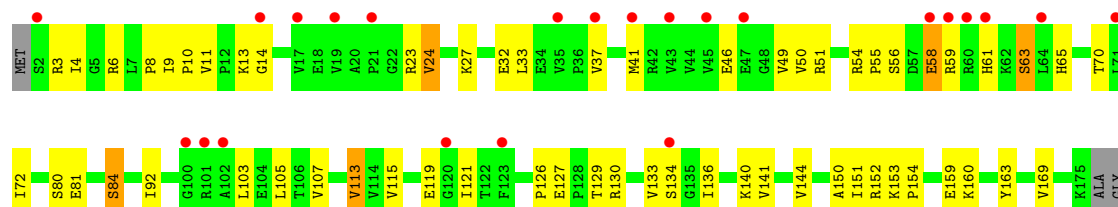
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



ALA  
LYS  
LYS

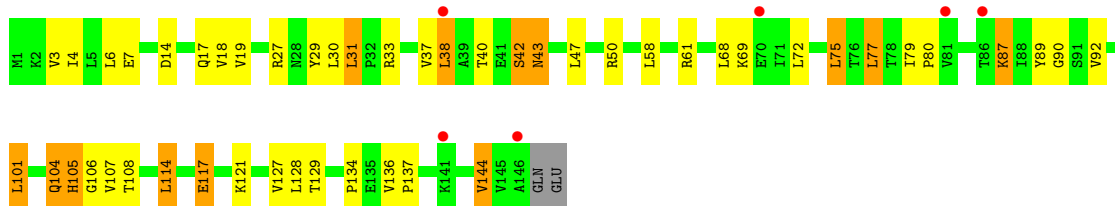
• Molecule 8: 50S ribosomal protein L9

Chain 1I:  2% 74% 23% ..



• Molecule 8: 50S ribosomal protein L9

Chain 2I:  4% 66% 24% 9% .



• Molecule 9: 50S ribosomal protein L13

Chain 1N:  % 81% 18% .



• Molecule 9: 50S ribosomal protein L13

Chain 2N:  % 79% 19% .



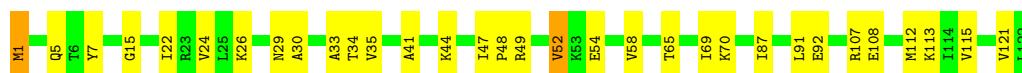
• Molecule 10: 50S ribosomal protein L14

Chain 1O:  75% 25%



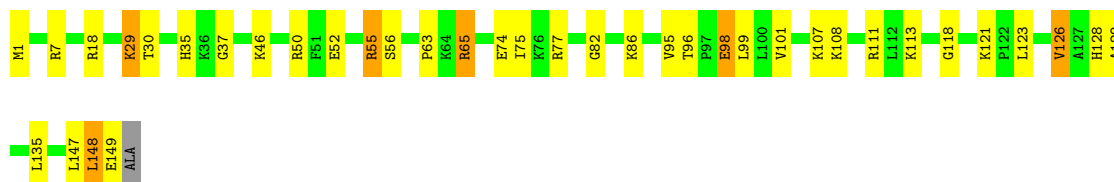
• Molecule 10: 50S ribosomal protein L14

Chain 2O:  74% 25% .



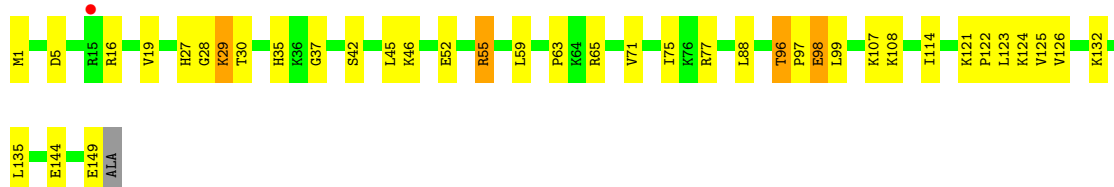
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 74% 21% ..



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 73% 23% ..



- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 85% 13% .



- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 79% 20% .



- Molecule 13: 50S ribosomal protein L17

Chain 1R: 86% 14% .

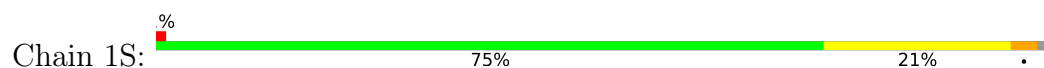


- Molecule 13: 50S ribosomal protein L17

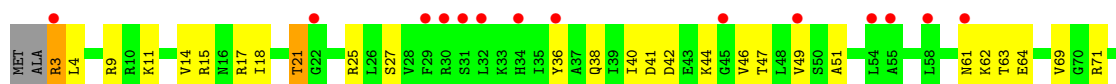
Chain 2R: 80% 20%



- Molecule 14: 50S ribosomal protein L18



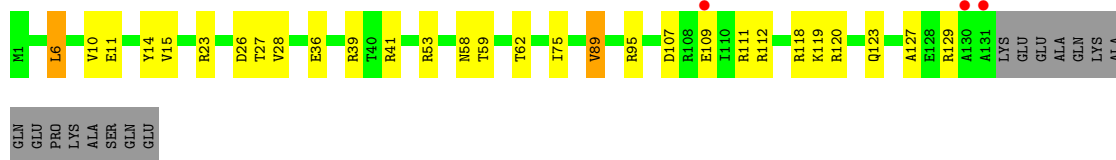
- Molecule 14: 50S ribosomal protein L18



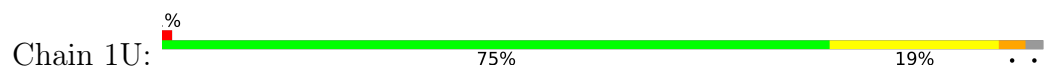
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

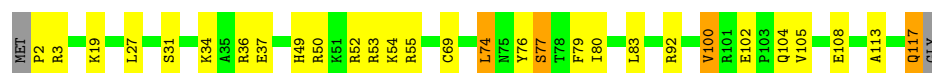


- Molecule 16: 50S ribosomal protein L20



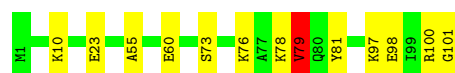
- Molecule 16: 50S ribosomal protein L20

Chain 2U:  74% 21% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  87% 12% .



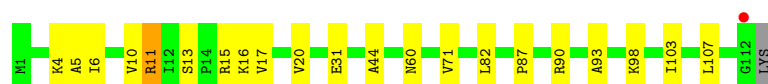
- Molecule 17: 50S ribosomal protein L21

Chain 2V:  80% 19% .



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  81% 18% ..



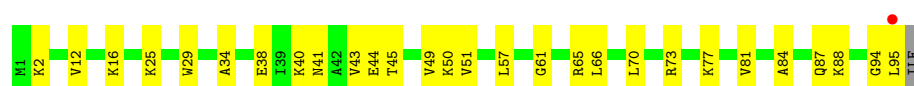
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  82% 16% ..



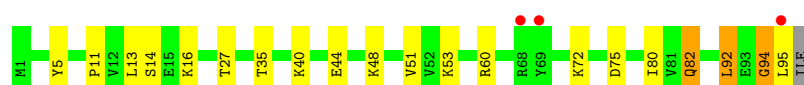
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  70% 29% .

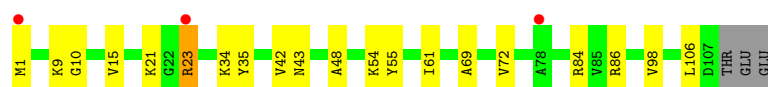
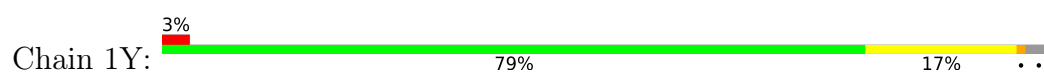


- Molecule 19: 50S ribosomal protein L23

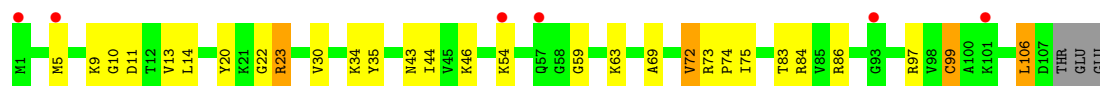
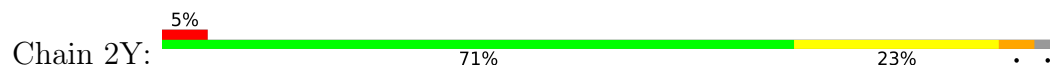
Chain 2X:  78% 18% ..



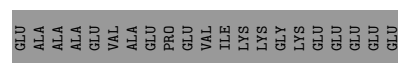
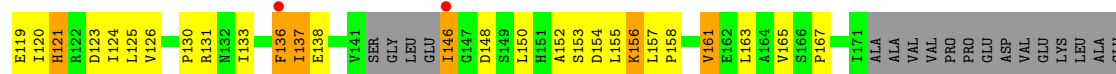
- Molecule 20: 50S ribosomal protein L24



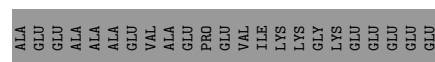
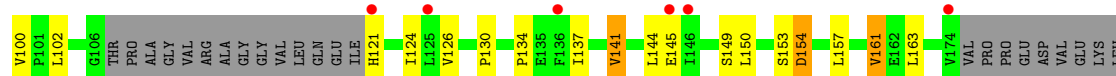
• Molecule 20: 50S ribosomal protein L24



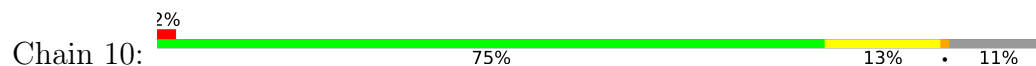
• Molecule 21: 50S ribosomal protein L25



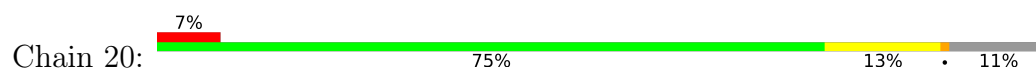
• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27

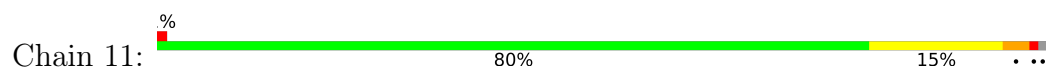


• Molecule 22: 50S ribosomal protein L27

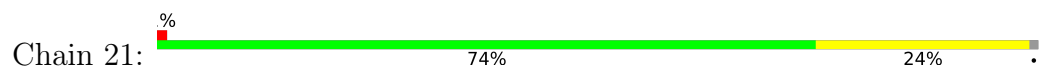




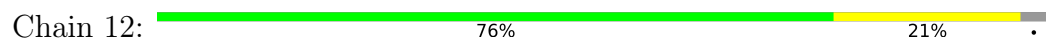
- Molecule 23: 50S ribosomal protein L28



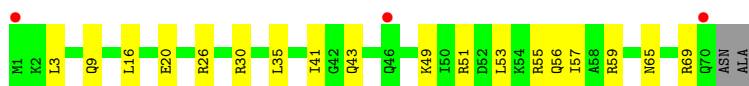
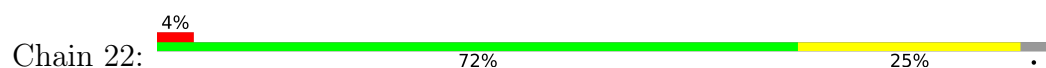
- Molecule 23: 50S ribosomal protein L28



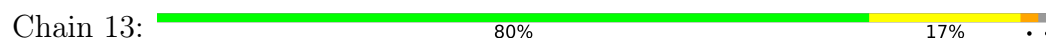
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



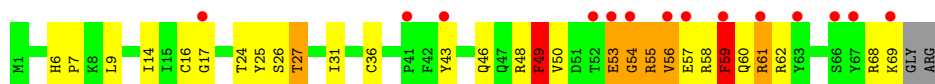
- Molecule 25: 50S ribosomal protein L30



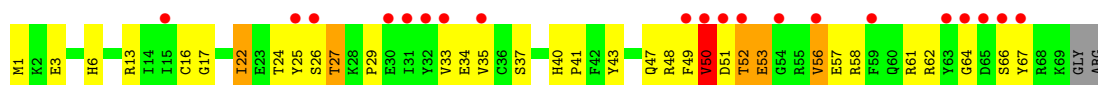
- Molecule 26: 50S ribosomal protein L31



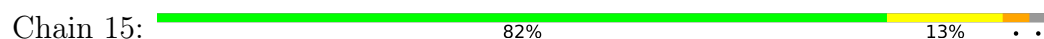




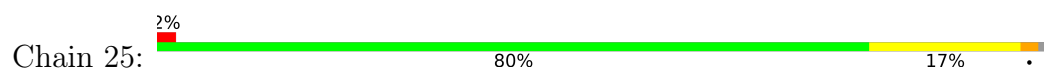
- Molecule 26: 50S ribosomal protein L31



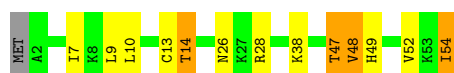
- Molecule 27: 50S ribosomal protein L32



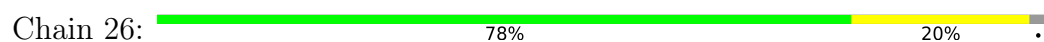
- Molecule 27: 50S ribosomal protein L32



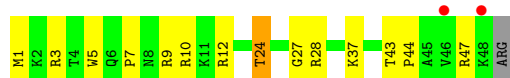
- Molecule 28: 50S ribosomal protein L33



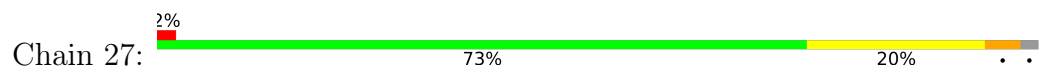
- Molecule 28: 50S ribosomal protein L33

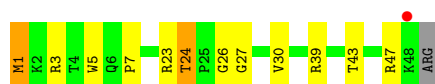


- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34





- Molecule 30: 50S ribosomal protein L35

Chain 18: 82% 17% .



- Molecule 30: 50S ribosomal protein L35

Chain 28: 74% 25% .



- Molecule 31: 50S ribosomal protein L36

Chain 19: 81% 19%



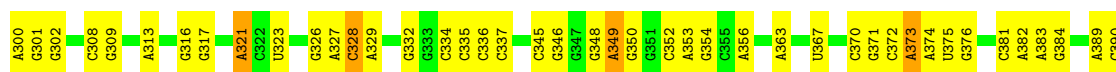
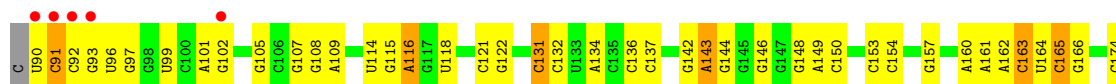
- Molecule 31: 50S ribosomal protein L36

Chain 29: 3% 68% 32%



- Molecule 32: 16S Ribosomal RNA

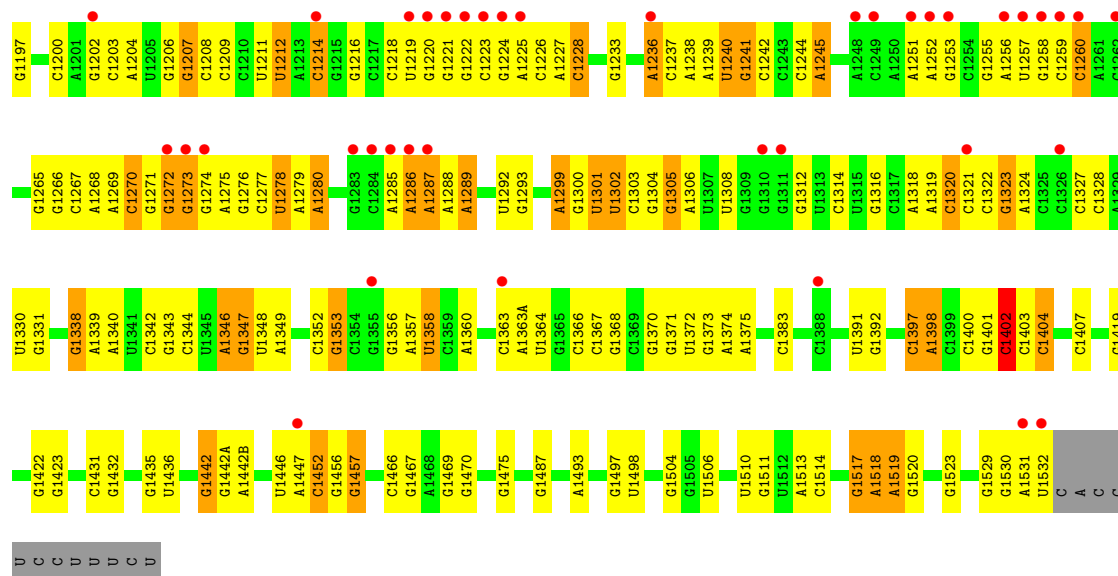
Chain 1a: 8% 52% 38% 9%



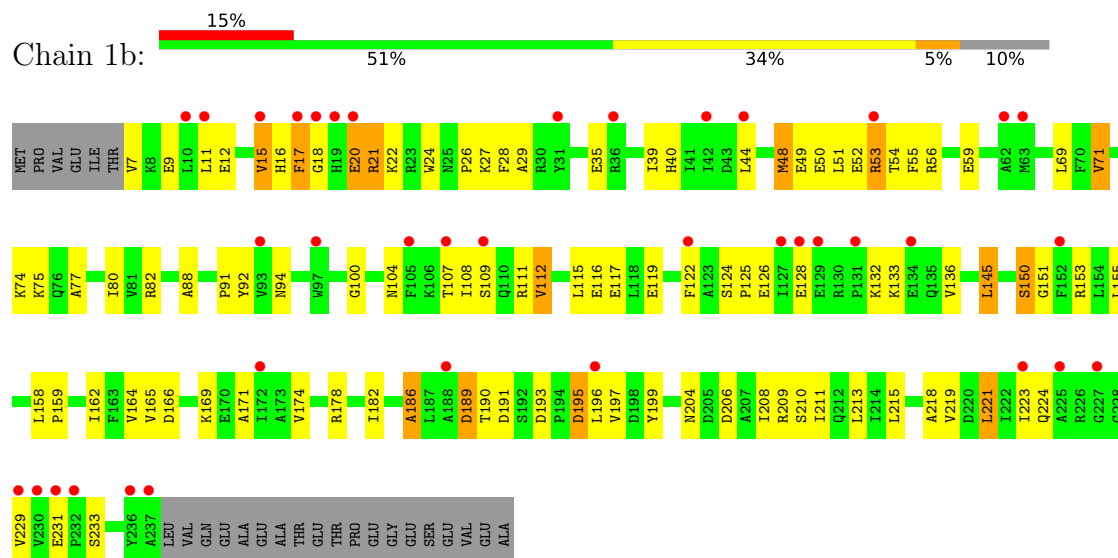


Chain 2a: 

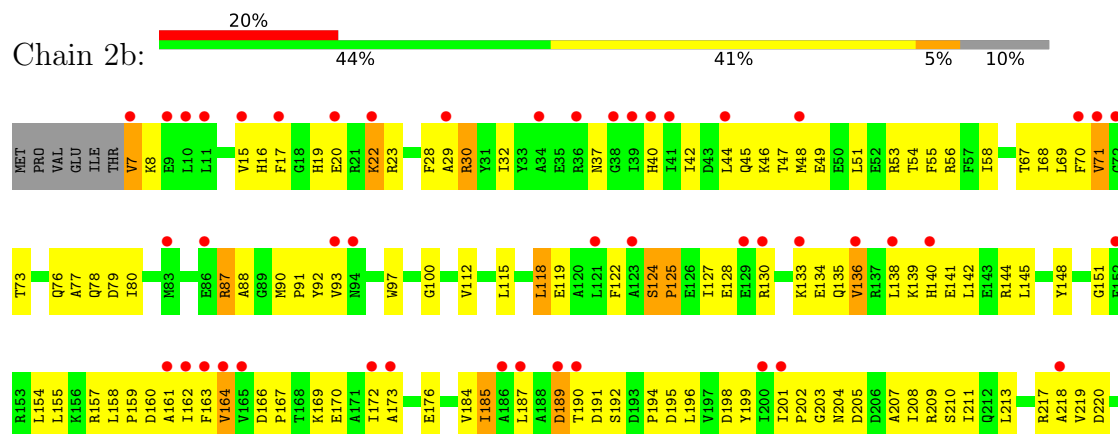




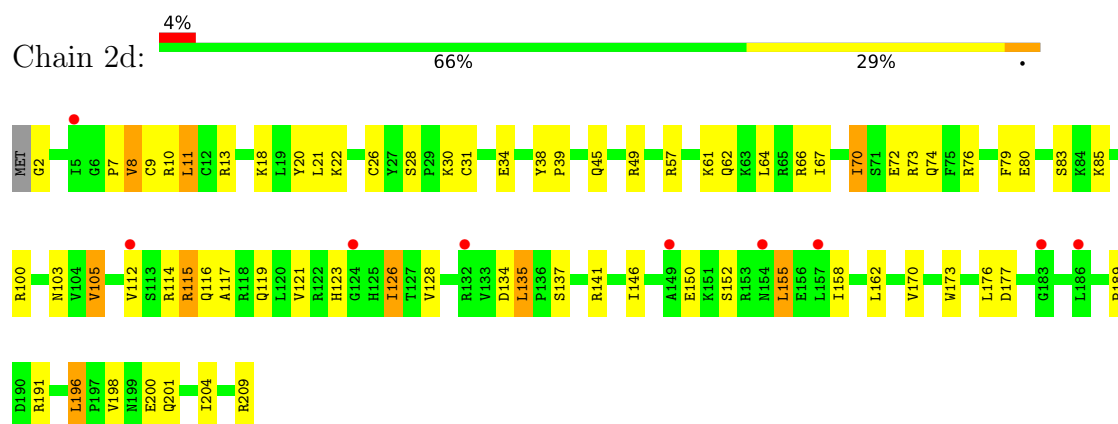
• Molecule 33: 30S ribosomal protein S2



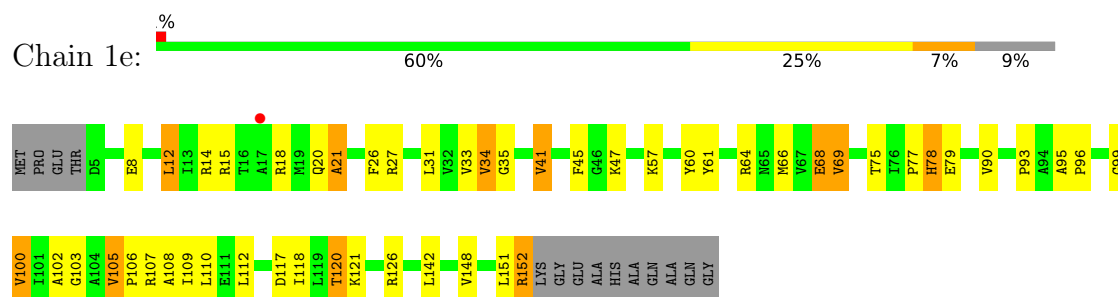
• Molecule 33: 30S ribosomal protein S2



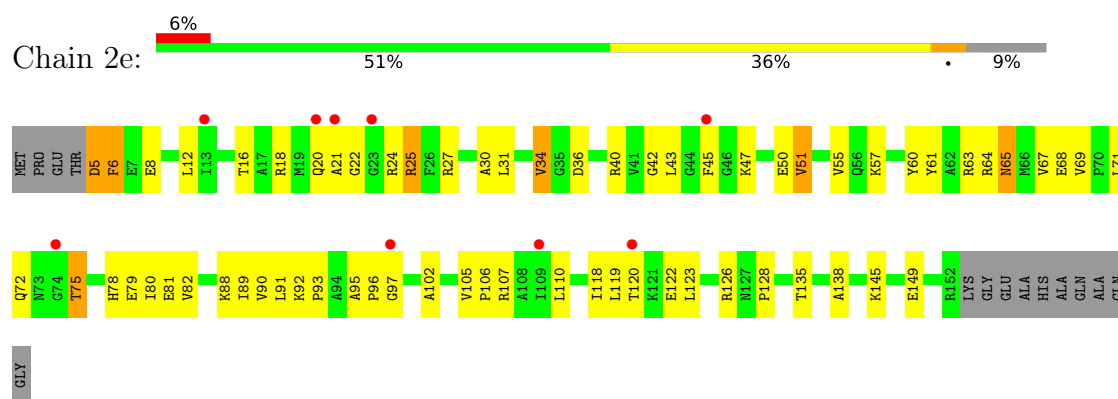




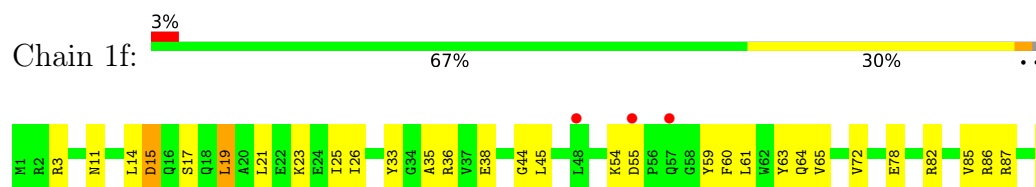
• Molecule 36: 30S ribosomal protein S5



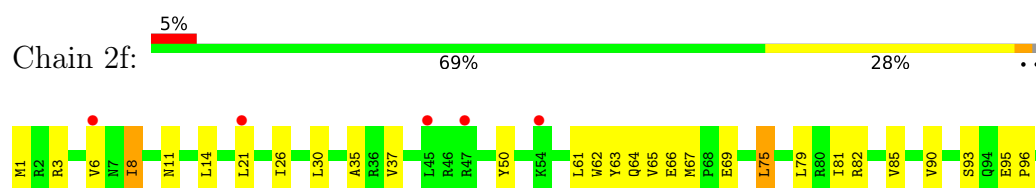
• Molecule 36: 30S ribosomal protein S5



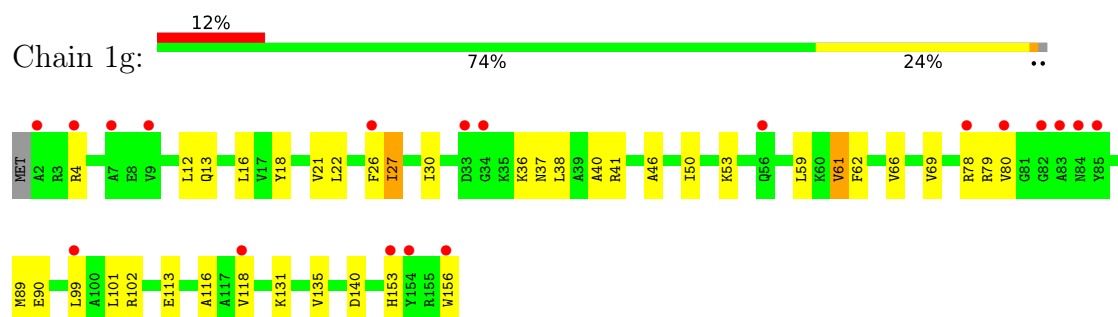
• Molecule 37: 30S ribosomal protein S6



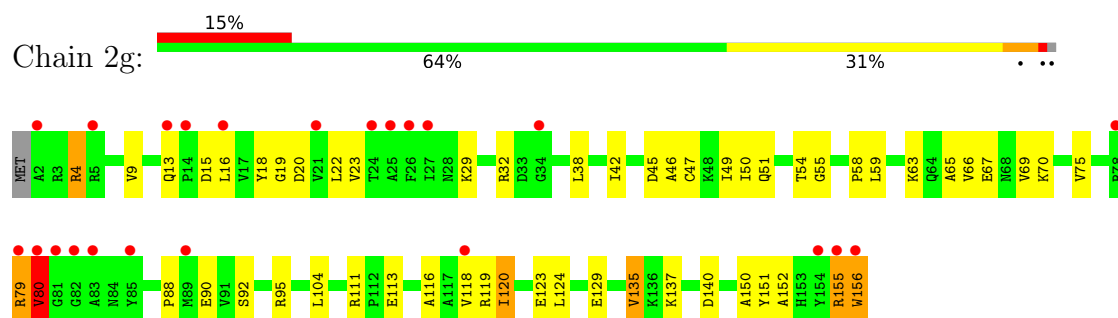
• Molecule 37: 30S ribosomal protein S6



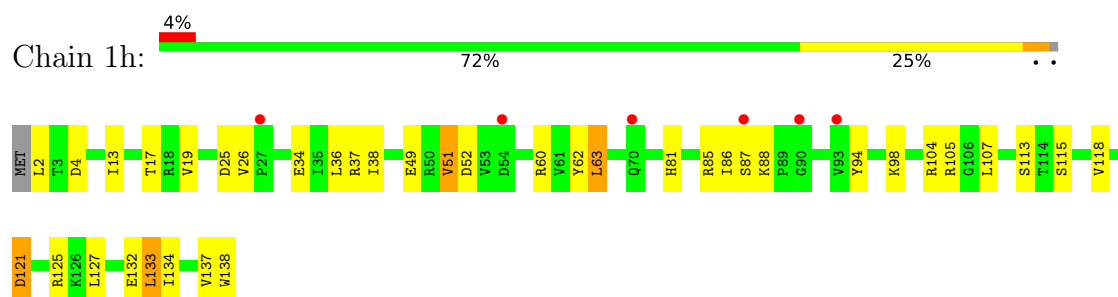
- Molecule 38: 30S ribosomal protein S7



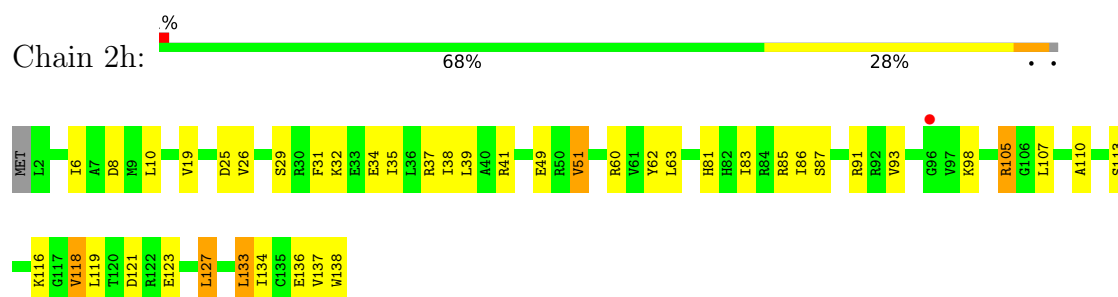
- Molecule 38: 30S ribosomal protein S7



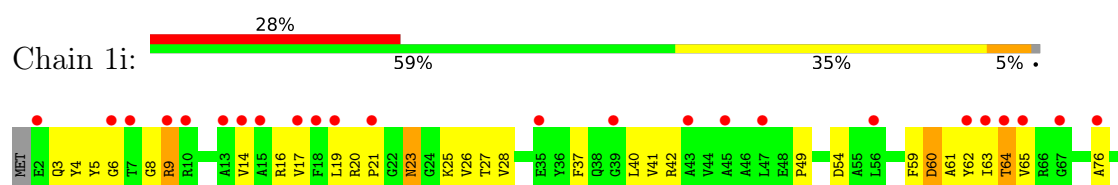
- Molecule 39: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S8



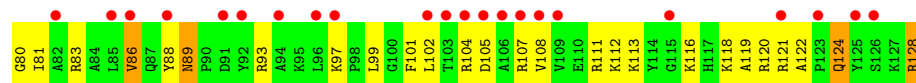
- Molecule 40: 30S ribosomal protein S9



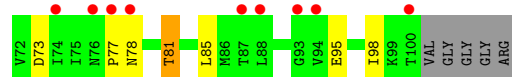
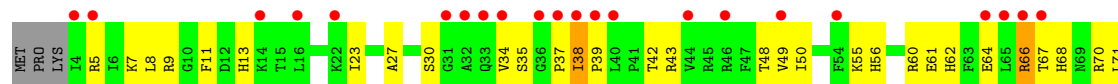




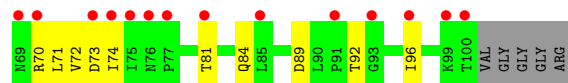
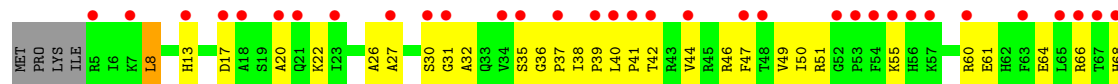
- Molecule 40: 30S ribosomal protein S9



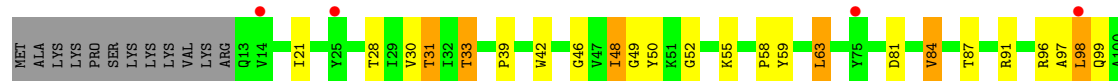
- Molecule 41: 30S ribosomal protein S10



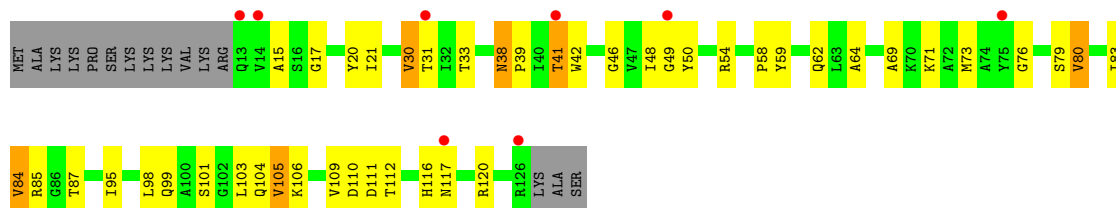
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11



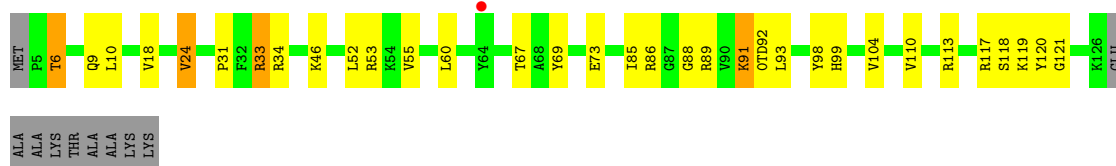
- Molecule 42: 30S ribosomal protein S11



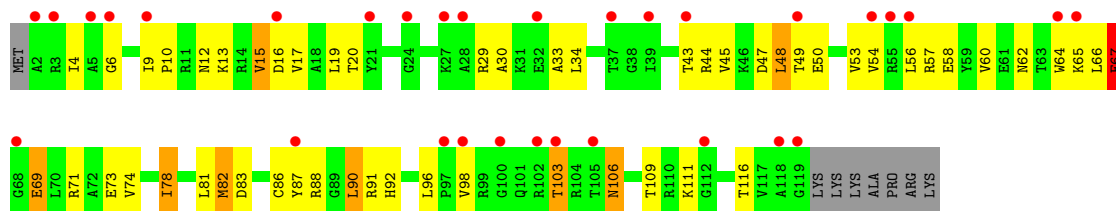
- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

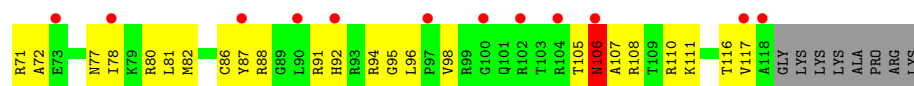


- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

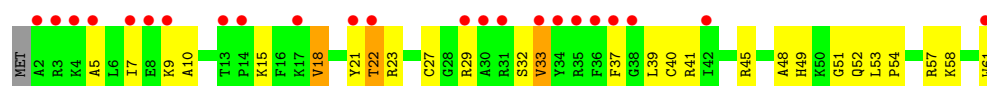
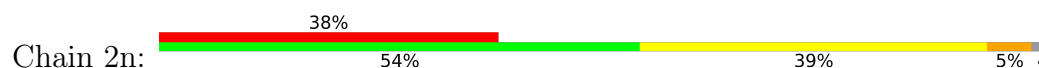




- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



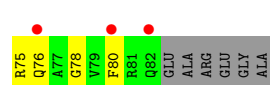
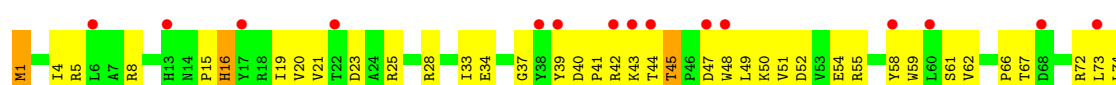
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

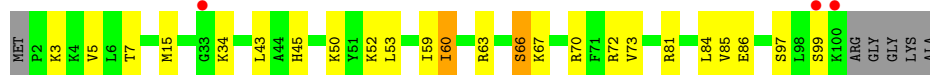
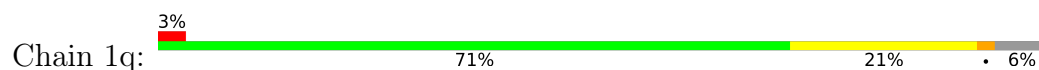


- Molecule 47: 30S ribosomal protein S16





- Molecule 48: 30S ribosomal protein S17



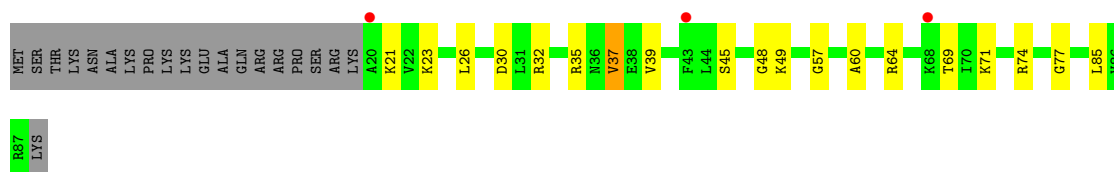
- Molecule 48: 30S ribosomal protein S17



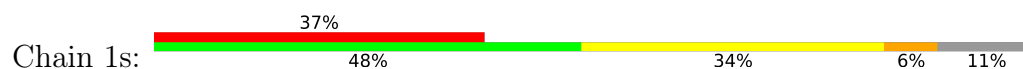
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

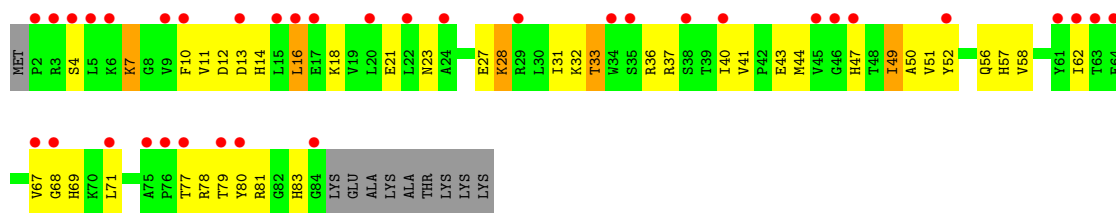


- Molecule 50: 30S ribosomal protein S19

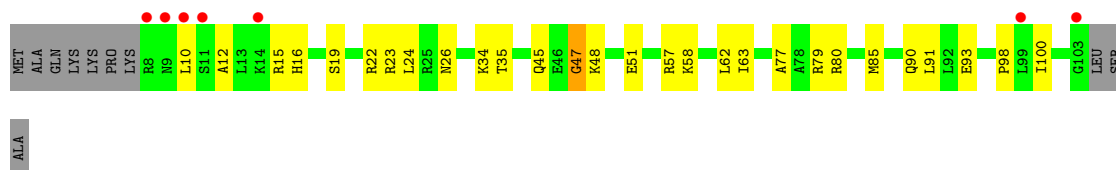


- Molecule 50: 30S ribosomal protein S19

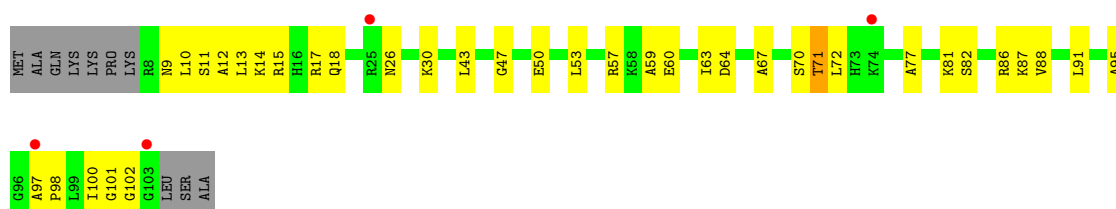




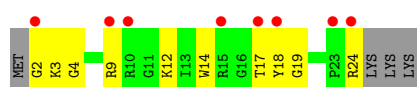
• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



• Molecule 52: 30S ribosomal protein Thx



• Molecule 53: CYS-Stop mRNA



Chain 2v: 



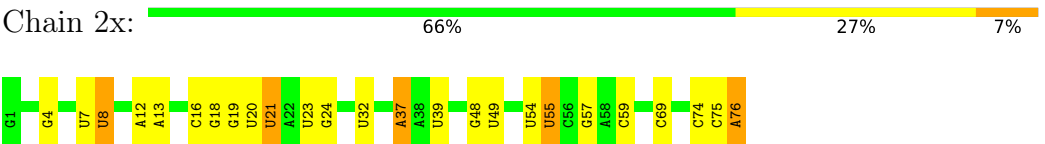
[illegible]

Chain 2w:

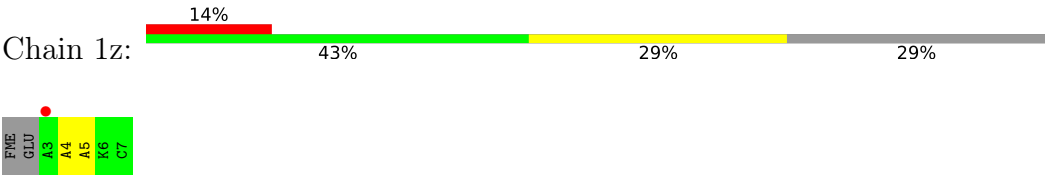
| Amino Acid | Percentage |
|------------|------------|
| MET        | 2%         |
| ASP        | 48%        |
| LEU        | 20%        |
| GLU        | 29%        |
| ALA        | 0%         |
| ARG        | 0%         |
| ASN        | 0%         |
| ASP        | 0%         |
| GLY        | 0%         |
| GLU        | 0%         |
| GLY        | 0%         |
| ILE        | 0%         |
| ILE        | 0%         |
| ARG        | 0%         |
| GLU        | 0%         |
| TRP        | 0%         |
| ARG        | 0%         |
| LYS        | 0%         |
| VAL        | 0%         |
| LEU        | 0%         |
| GLU        | 0%         |
| CYS        | 0%         |
| ALA        | 0%         |
| SER        | 0%         |
| LEU        | 0%         |
| LYS        | 0%         |
| LEU        | 0%         |
| ASP        | 0%         |
| ASP        | 0%         |
| ASP        | 0%         |
| PRO        | 0%         |
| GLU        | 0%         |
| GLU        | 0%         |
| LYS        | 0%         |
| GLU        | 0%         |
| ALA        | 0%         |
| GLU        | 0%         |
| ARG        | 0%         |
| GLU        | 0%         |
| ALA        | 0%         |
| SER        | 0%         |
| ASP        | 0%         |
| LEU        | 0%         |
| LEU        | 0%         |
| ALA        | 0%         |
| ARG        | 0%         |
| LYS        | 0%         |
| LYS        | 0%         |
| ALA        | 0%         |
| GLU        | 0%         |
| GLY        | 0%         |
| ARG        | 0%         |
| TRP        | 0%         |
| GLN        | 0%         |
| GLU        | 0%         |
| GLU        | 0%         |
| SER        | 0%         |
| LEU        | 0%         |
| SER        | 0%         |
| ARG        | 0%         |
| ARG        | 0%         |
| TRP        | 0%         |
| ALA        | 0%         |
| LYS        | 0%         |
| ASP        | 0%         |
| PRO        | 0%         |
| M102       | 0%         |
| D103       | 0%         |
| E104       | 0%         |
| R105       | 0%         |
| D106       | 0%         |
| V109       | 0%         |
| E110       | 0%         |
| I111       | 0%         |
| R112       | 0%         |
| T115       | 0%         |
| E119       | 0%         |
| R125       | 0%         |
| D126       | 0%         |
| N129       | 0%         |
| L132       | 0%         |
| R133       | 0%         |
| F134       | 0%         |
| M138       | 0%         |
| E143       | 0%         |
| V144       | 0%         |
| L145       | 0%         |
| V158       | 0%         |
| E161       | 0%         |
| V162       | 0%         |
| R163       | 0%         |
| G166       | 0%         |
| A167       | 0%         |
| Y168       | 0%         |
| G169       | 0%         |
| T170       | 0%         |
| F171       | 0%         |
| K172       | 0%         |
| Y173       | 0%         |
| E174       | 0%         |
| S175       | 0%         |
| G176       | 0%         |
| V177       | 0%         |
| H178       | 0%         |
| R179       | 0%         |
| V180       | 0%         |
| Q181       | 0%         |
| R182       | 0%         |
| K183       | 0%         |
| V183       | 0%         |
| P184       | 0%         |
| V185       | 0%         |
| T186       | 0%         |
| E187       | 0%         |
| T188       | 0%         |
| Q189       | 0%         |
| T191       | 0%         |
| G190       | 0%         |
| R191       | 0%         |
| T196       | 0%         |
| A197       | 0%         |
| T198       | 0%         |
| V201       | 0%         |
| I217       | 0%         |
| K204       | 0%         |
| A205       | 0%         |
| E208       | 0%         |
| D209       | 0%         |
| I218       | 0%         |
| R218       | 0%         |
| I219       | 0%         |
| R220       | 0%         |
| V221       | 0%         |
| M222       | 0%         |
| R223       | 0%         |
| A224       | 0%         |
| S225       | 0%         |
| G228       | 0%         |
| V232       | 0%         |
| A238       | 0%         |
| V239       | 0%         |
| R240       | 0%         |
| V241       | 0%         |
| V242       | 0%         |
| I248       | 0%         |
| M249       | 0%         |
| V250       | 0%         |
| T251       | 0%         |
| K260       | 0%         |
| M261       | 0%         |
| R262       | 0%         |
| M267       | 0%         |
| E283       | 0%         |
| I293       | 0%         |
| S299       | 0%         |
| E300       | 0%         |
| K301       | 0%         |
| I302       | 0%         |
| R303       | 0%         |
| V312       | 0%         |
| T320       | 0%         |
| T321       | 0%         |
| H322       | 0%         |
| D323       | 0%         |
| L324       | 0%         |
| V327       | 0%         |
| T333       | 0%         |
| P334       | 0%         |
| I335       | 0%         |
| L336       | 0%         |
| K340       | 0%         |
| Q347       | 0%         |
| A350       | 0%         |
| L351       | 0%         |
| V354       | 0%         |

Chain 1x: 

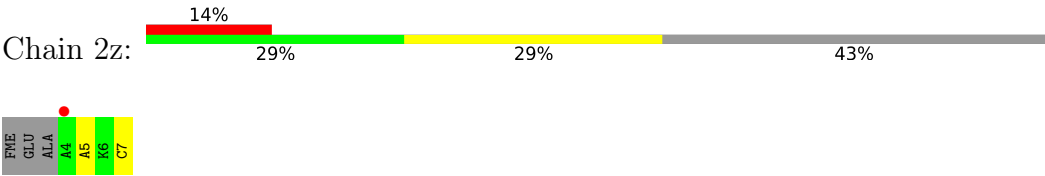




● Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part



● Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.01Å 450.19Å 622.19Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 69.56 – 2.80<br>69.56 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.5 (69.56-2.80)<br>97.5 (69.56-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.24                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.29 (at 2.82Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.2                                                | Depositor        |
| R, $R_{free}$                                                           | 0.217 , 0.264<br>0.222 , 0.267                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 69979 reflections (4.90%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.144                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 51.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 296656                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: K, M2G, 2MA, OMU, 8AN, OMG, H2U, SF4, MIA, 4SU, OMC, UR3, MG, 0TD, 5MU, G7M, PSU, ZN, 4OC, MA6, 5MC, 2MG

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 | 0.45        | 1/107720 (0.0%) |
| 1   | 2A    | 0.22         | 0/67295 | 0.40        | 1/105042 (0.0%) |
| 2   | 1B    | 0.22         | 0/2882  | 0.40        | 0/4494          |
| 2   | 2B    | 0.18         | 0/2879  | 0.33        | 0/4487          |
| 3   | 1D    | 0.27         | 0/2186  | 0.48        | 0/2944          |
| 3   | 2D    | 0.24         | 0/2186  | 0.47        | 0/2944          |
| 4   | 1E    | 0.27         | 0/1592  | 0.50        | 0/2149          |
| 4   | 2E    | 0.21         | 0/1592  | 0.45        | 0/2149          |
| 5   | 1F    | 0.27         | 0/1619  | 0.50        | 0/2193          |
| 5   | 2F    | 0.20         | 0/1615  | 0.41        | 0/2188          |
| 6   | 1G    | 0.21         | 0/1448  | 0.45        | 0/1957          |
| 6   | 2G    | 0.19         | 0/1453  | 0.42        | 0/1963          |
| 7   | 1H    | 0.23         | 0/1356  | 0.43        | 0/1834          |
| 7   | 2H    | 0.20         | 0/1356  | 0.38        | 0/1834          |
| 8   | 1I    | 0.21         | 0/1112  | 0.42        | 0/1514          |
| 8   | 2I    | 0.19         | 0/1079  | 0.43        | 0/1475          |
| 9   | 1N    | 0.26         | 0/1144  | 0.43        | 0/1543          |
| 9   | 2N    | 0.19         | 0/1144  | 0.38        | 0/1543          |
| 10  | 1O    | 0.26         | 0/943   | 0.47        | 0/1269          |
| 10  | 2O    | 0.22         | 0/943   | 0.46        | 0/1269          |
| 11  | 1P    | 0.28         | 0/1152  | 0.54        | 0/1533          |
| 11  | 2P    | 0.21         | 0/1152  | 0.44        | 0/1533          |
| 12  | 1Q    | 0.26         | 0/1143  | 0.48        | 0/1527          |
| 12  | 2Q    | 0.21         | 0/1143  | 0.42        | 0/1527          |
| 13  | 1R    | 0.27         | 0/982   | 0.50        | 0/1312          |
| 13  | 2R    | 0.21         | 0/982   | 0.46        | 0/1312          |
| 14  | 1S    | 0.21         | 0/883   | 0.44        | 0/1176          |
| 14  | 2S    | 0.21         | 0/880   | 0.44        | 0/1172          |
| 15  | 1T    | 0.25         | 0/1105  | 0.49        | 0/1477          |
| 15  | 2T    | 0.21         | 0/1097  | 0.45        | 0/1468          |
| 16  | 1U    | 0.30         | 0/977   | 0.48        | 0/1301          |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 16  | 2U    | 0.20         | 0/977          | 0.40        | 0/1301         |
| 17  | 1V    | 0.27         | 0/782          | 0.45        | 0/1049         |
| 17  | 2V    | 0.18         | 0/782          | 0.38        | 0/1049         |
| 18  | 1W    | 0.28         | 0/897          | 0.46        | 0/1205         |
| 18  | 2W    | 0.23         | 0/897          | 0.43        | 0/1205         |
| 19  | 1X    | 0.28         | 0/764          | 0.55        | 0/1025         |
| 19  | 2X    | 0.22         | 0/764          | 0.50        | 2/1025 (0.2%)  |
| 20  | 1Y    | 0.26         | 0/819          | 0.47        | 0/1095         |
| 20  | 2Y    | 0.22         | 0/819          | 0.47        | 0/1095         |
| 21  | 1Z    | 0.22         | 0/1267         | 0.49        | 0/1717         |
| 21  | 2Z    | 0.22         | 0/1299         | 0.47        | 0/1763         |
| 22  | 10    | 0.26         | 0/612          | 0.51        | 0/816          |
| 22  | 20    | 0.19         | 0/612          | 0.42        | 0/816          |
| 23  | 11    | 0.27         | 0/762          | 0.46        | 0/1014         |
| 23  | 21    | 0.22         | 0/762          | 0.39        | 0/1014         |
| 24  | 12    | 0.25         | 0/590          | 0.42        | 0/781          |
| 24  | 22    | 0.18         | 0/590          | 0.37        | 0/781          |
| 25  | 13    | 0.28         | 0/474          | 0.48        | 0/635          |
| 25  | 23    | 0.18         | 0/469          | 0.41        | 0/630          |
| 26  | 14    | 0.23         | 0/565          | 0.61        | 2/761 (0.3%)   |
| 26  | 24    | 0.24         | 0/545          | 0.49        | 0/737          |
| 27  | 15    | 0.28         | 0/469          | 0.53        | 0/635          |
| 27  | 25    | 0.23         | 0/469          | 0.47        | 0/635          |
| 28  | 16    | 0.25         | 0/460          | 0.49        | 0/613          |
| 28  | 26    | 0.21         | 0/456          | 0.46        | 0/608          |
| 29  | 17    | 0.32         | 0/426          | 0.52        | 0/561          |
| 29  | 27    | 0.25         | 0/426          | 0.49        | 0/561          |
| 30  | 18    | 0.26         | 0/525          | 0.50        | 0/691          |
| 30  | 28    | 0.22         | 0/525          | 0.42        | 0/691          |
| 31  | 19    | 0.28         | 0/310          | 0.47        | 0/407          |
| 31  | 29    | 0.22         | 0/310          | 0.42        | 0/407          |
| 32  | 1a    | 0.21         | 2/35795 (0.0%) | 0.39        | 0/55864        |
| 32  | 2a    | 0.20         | 1/35886 (0.0%) | 0.38        | 2/56005 (0.0%) |
| 33  | 1b    | 0.23         | 0/1881         | 0.51        | 0/2542         |
| 33  | 2b    | 0.24         | 0/1860         | 0.49        | 0/2518         |
| 34  | 1c    | 0.22         | 0/1572         | 0.43        | 0/2126         |
| 34  | 2c    | 0.20         | 0/1566         | 0.42        | 0/2119         |
| 35  | 1d    | 0.20         | 0/1685         | 0.43        | 0/2262         |
| 35  | 2d    | 0.20         | 0/1704         | 0.44        | 0/2284         |
| 36  | 1e    | 0.21         | 0/1145         | 0.48        | 0/1543         |
| 36  | 2e    | 0.22         | 0/1149         | 0.47        | 0/1548         |
| 37  | 1f    | 0.20         | 0/823          | 0.40        | 0/1115         |
| 37  | 2f    | 0.21         | 0/829          | 0.45        | 0/1123         |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 38  | 1g    | 0.21         | 0/1250          | 0.40        | 0/1679          |
| 38  | 2g    | 0.20         | 0/1254          | 0.41        | 0/1683          |
| 39  | 1h    | 0.22         | 0/1108          | 0.42        | 0/1494          |
| 39  | 2h    | 0.18         | 0/1108          | 0.45        | 1/1494 (0.1%)   |
| 40  | 1i    | 0.21         | 0/1002          | 0.48        | 0/1346          |
| 40  | 2i    | 0.21         | 0/997           | 0.45        | 0/1343          |
| 41  | 1j    | 0.22         | 0/722           | 0.43        | 0/982           |
| 41  | 2j    | 0.22         | 0/727           | 0.46        | 0/988           |
| 42  | 1k    | 0.19         | 0/844           | 0.41        | 0/1145          |
| 42  | 2k    | 0.19         | 0/848           | 0.39        | 0/1149          |
| 43  | 1l    | 0.21         | 0/937           | 0.45        | 0/1260          |
| 43  | 2l    | 0.20         | 0/937           | 0.44        | 0/1260          |
| 44  | 1m    | 0.21         | 0/929           | 0.46        | 0/1250          |
| 44  | 2m    | 0.21         | 0/917           | 0.45        | 0/1234          |
| 45  | 1n    | 0.20         | 0/501           | 0.44        | 0/664           |
| 45  | 2n    | 0.21         | 0/501           | 0.42        | 0/664           |
| 46  | 1o    | 0.21         | 0/739           | 0.43        | 0/985           |
| 46  | 2o    | 0.19         | 0/739           | 0.39        | 0/985           |
| 47  | 1p    | 0.20         | 0/697           | 0.49        | 0/939           |
| 47  | 2p    | 0.19         | 0/693           | 0.41        | 0/935           |
| 48  | 1q    | 0.20         | 0/836           | 0.42        | 0/1117          |
| 48  | 2q    | 0.20         | 0/836           | 0.46        | 0/1117          |
| 49  | 1r    | 0.21         | 0/560           | 0.45        | 0/746           |
| 49  | 2r    | 0.20         | 0/560           | 0.40        | 0/746           |
| 50  | 1s    | 0.21         | 0/667           | 0.49        | 0/900           |
| 50  | 2s    | 0.21         | 0/661           | 0.45        | 0/893           |
| 51  | 1t    | 0.19         | 0/730           | 0.46        | 0/965           |
| 51  | 2t    | 0.22         | 0/729           | 0.46        | 0/965           |
| 52  | 1u    | 0.21         | 0/203           | 0.44        | 0/266           |
| 52  | 2u    | 0.20         | 0/203           | 0.48        | 0/266           |
| 53  | 1v    | 0.25         | 0/213           | 0.48        | 0/329           |
| 53  | 2v    | 0.20         | 0/213           | 0.34        | 0/329           |
| 54  | 1w    | 0.22         | 0/1963          | 0.42        | 0/2645          |
| 54  | 2w    | 0.22         | 0/1981          | 0.43        | 0/2668          |
| 55  | 1x    | 0.25         | 1/1555 (0.1%)   | 0.37        | 0/2419          |
| 55  | 2x    | 0.23         | 0/1555          | 0.36        | 0/2419          |
| 56  | 1z    | 0.33         | 0/29            | 0.53        | 0/37            |
| 56  | 2z    | 0.21         | 0/24            | 0.38        | 0/30            |
| All | All   | 0.23         | 4/313618 (0.0%) | 0.42        | 9/468557 (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  | 1P    | 0                   | 1                   |
| 11  | 2P    | 0                   | 1                   |
| 21  | 1Z    | 0                   | 2                   |
| 33  | 1b    | 0                   | 3                   |
| 33  | 2b    | 0                   | 2                   |
| 56  | 1z    | 0                   | 1                   |
| All | All   | 0                   | 10                  |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 55  | 1x    | 8    | 4SU  | O3'-P | 5.57 | 1.61        | 1.56     |
| 32  | 2a    | 527  | G7M  | O3'-P | 5.28 | 1.61        | 1.56     |
| 32  | 1a    | 1498 | UR3  | O3'-P | 5.16 | 1.61        | 1.56     |
| 32  | 1a    | 527  | G7M  | O3'-P | 5.13 | 1.61        | 1.56     |

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

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 1992 | G    | C2'-C3'-O3' | 6.97  | 119.95      | 109.50   |
| 39  | 2h    | 19   | VAL  | N-CA-C      | -6.36 | 106.32      | 112.29   |
| 1   | 2A    | 1992 | G    | C2'-C3'-O3' | 6.34  | 119.00      | 109.50   |
| 26  | 14    | 54   | GLY  | CA-C-N      | 5.86  | 132.72      | 121.54   |
| 26  | 14    | 54   | GLY  | C-N-CA      | 5.86  | 132.72      | 121.54   |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 11  | 1P    | 35  | HIS  | Peptide |
| 21  | 1Z    | 136 | PHE  | Peptide |
| 21  | 1Z    | 146 | ILE  | Peptide |
| 33  | 1b    | 122 | PHE  | Peptide |
| 33  | 1b    | 9   | GLU  | 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    | 579     | 0            |
| 1   | 2A    | 60322 | 0        | 30427    | 655     | 0            |
| 2   | 1B    | 2577  | 0        | 1305     | 21      | 0            |
| 2   | 2B    | 2575  | 0        | 1303     | 27      | 0            |
| 3   | 1D    | 2136  | 0        | 2218     | 42      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 49      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 25      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 26      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 35      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 45      | 0            |
| 6   | 1G    | 1423  | 0        | 1436     | 36      | 0            |
| 6   | 2G    | 1428  | 0        | 1438     | 51      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 26      | 0            |
| 7   | 2H    | 1330  | 0        | 1407     | 37      | 0            |
| 8   | 1I    | 1097  | 0        | 1140     | 22      | 0            |
| 8   | 2I    | 1064  | 0        | 1082     | 25      | 0            |
| 9   | 1N    | 1117  | 0        | 1184     | 10      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 15      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 21      | 0            |
| 10  | 2O    | 933   | 0        | 996      | 20      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 25      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 26      | 0            |
| 12  | 1Q    | 1122  | 0        | 1179     | 13      | 0            |
| 12  | 2Q    | 1122  | 0        | 1179     | 16      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 12      | 0            |
| 13  | 2R    | 968   | 0        | 1033     | 15      | 0            |
| 14  | 1S    | 873   | 0        | 927      | 20      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 27      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 20      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 20      | 0            |
| 16  | 1U    | 959   | 0        | 1019     | 20      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 22      | 0            |
| 17  | 1V    | 771   | 0        | 830      | 8       | 0            |
| 17  | 2V    | 771   | 0        | 830      | 12      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 13      | 0            |
| 18  | 2W    | 886   | 0        | 940      | 10      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 17      | 0            |
| 19  | 2X    | 750   | 0        | 814      | 13      | 0            |
| 20  | 1Y    | 806   | 0        | 881      | 13      | 0            |
| 20  | 2Y    | 806   | 0        | 881      | 19      | 0            |
| 21  | 1Z    | 1240  | 0        | 1240     | 30      | 0            |
| 21  | 2Z    | 1271  | 0        | 1273     | 29      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | 10    | 604   | 0        | 619      | 11      | 0            |
| 22  | 20    | 604   | 0        | 619      | 11      | 0            |
| 23  | 11    | 755   | 0        | 826      | 16      | 0            |
| 23  | 21    | 755   | 0        | 826      | 18      | 0            |
| 24  | 12    | 588   | 0        | 643      | 6       | 0            |
| 24  | 22    | 588   | 0        | 643      | 8       | 0            |
| 25  | 13    | 469   | 0        | 518      | 3       | 0            |
| 25  | 23    | 464   | 0        | 514      | 13      | 0            |
| 26  | 14    | 552   | 0        | 533      | 22      | 0            |
| 26  | 24    | 532   | 0        | 503      | 23      | 0            |
| 27  | 15    | 455   | 0        | 465      | 9       | 0            |
| 27  | 25    | 455   | 0        | 465      | 8       | 0            |
| 28  | 16    | 453   | 0        | 473      | 6       | 0            |
| 28  | 26    | 449   | 0        | 469      | 8       | 0            |
| 29  | 17    | 418   | 0        | 467      | 12      | 0            |
| 29  | 27    | 418   | 0        | 467      | 10      | 0            |
| 30  | 18    | 517   | 0        | 582      | 8       | 0            |
| 30  | 28    | 517   | 0        | 582      | 13      | 0            |
| 31  | 19    | 307   | 0        | 335      | 4       | 0            |
| 31  | 29    | 307   | 0        | 335      | 6       | 0            |
| 32  | 1a    | 32246 | 0        | 16295    | 444     | 0            |
| 32  | 2a    | 32327 | 0        | 16338    | 453     | 0            |
| 33  | 1b    | 1846  | 0        | 1867     | 54      | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 66      | 0            |
| 34  | 1c    | 1548  | 0        | 1535     | 44      | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 64      | 0            |
| 35  | 1d    | 1655  | 0        | 1672     | 54      | 0            |
| 35  | 2d    | 1674  | 0        | 1713     | 48      | 0            |
| 36  | 1e    | 1129  | 0        | 1185     | 38      | 0            |
| 36  | 2e    | 1133  | 0        | 1191     | 43      | 0            |
| 37  | 1f    | 810   | 0        | 804      | 18      | 0            |
| 37  | 2f    | 816   | 0        | 808      | 21      | 0            |
| 38  | 1g    | 1231  | 0        | 1238     | 29      | 0            |
| 38  | 2g    | 1235  | 0        | 1249     | 32      | 0            |
| 39  | 1h    | 1088  | 0        | 1126     | 21      | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 25      | 0            |
| 40  | 1i    | 983   | 0        | 986      | 38      | 0            |
| 40  | 2i    | 978   | 0        | 966      | 50      | 0            |
| 41  | 1j    | 709   | 0        | 650      | 25      | 0            |
| 41  | 2j    | 714   | 0        | 672      | 33      | 0            |
| 42  | 1k    | 829   | 0        | 825      | 15      | 0            |
| 42  | 2k    | 833   | 0        | 836      | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | 1l    | 932   | 0        | 981      | 21      | 0            |
| 43  | 2l    | 932   | 0        | 981      | 20      | 0            |
| 44  | 1m    | 919   | 0        | 951      | 34      | 0            |
| 44  | 2m    | 907   | 0        | 934      | 43      | 0            |
| 45  | 1n    | 492   | 0        | 529      | 20      | 0            |
| 45  | 2n    | 492   | 0        | 529      | 26      | 0            |
| 46  | 1o    | 728   | 0        | 760      | 16      | 0            |
| 46  | 2o    | 728   | 0        | 760      | 16      | 0            |
| 47  | 1p    | 681   | 0        | 697      | 27      | 0            |
| 47  | 2p    | 677   | 0        | 686      | 14      | 0            |
| 48  | 1q    | 823   | 0        | 891      | 8       | 0            |
| 48  | 2q    | 823   | 0        | 891      | 14      | 0            |
| 49  | 1r    | 555   | 0        | 618      | 14      | 0            |
| 49  | 2r    | 555   | 0        | 618      | 16      | 0            |
| 50  | 1s    | 652   | 0        | 662      | 27      | 0            |
| 50  | 2s    | 646   | 0        | 644      | 29      | 0            |
| 51  | 1t    | 728   | 0        | 798      | 20      | 0            |
| 51  | 2t    | 727   | 0        | 796      | 25      | 0            |
| 52  | 1u    | 199   | 0        | 208      | 6       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 10      | 0            |
| 53  | 1v    | 191   | 0        | 97       | 2       | 0            |
| 53  | 2v    | 191   | 0        | 97       | 1       | 0            |
| 54  | 1w    | 1935  | 0        | 1920     | 32      | 0            |
| 54  | 2w    | 1953  | 0        | 1930     | 43      | 0            |
| 55  | 1x    | 1577  | 0        | 801      | 12      | 0            |
| 55  | 2x    | 1577  | 0        | 801      | 11      | 0            |
| 56  | 1z    | 30    | 0        | 32       | 2       | 0            |
| 56  | 2z    | 25    | 0        | 27       | 1       | 0            |
| 57  | 10    | 9     | 0        | 0        | 0       | 0            |
| 57  | 11    | 3     | 0        | 0        | 0       | 0            |
| 57  | 12    | 2     | 0        | 0        | 0       | 0            |
| 57  | 13    | 4     | 0        | 0        | 0       | 0            |
| 57  | 15    | 9     | 0        | 0        | 0       | 0            |
| 57  | 16    | 3     | 0        | 0        | 0       | 0            |
| 57  | 17    | 6     | 0        | 0        | 0       | 0            |
| 57  | 18    | 6     | 0        | 0        | 0       | 0            |
| 57  | 19    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1A    | 1084  | 0        | 0        | 0       | 0            |
| 57  | 1B    | 39    | 0        | 0        | 0       | 0            |
| 57  | 1D    | 14    | 0        | 0        | 0       | 0            |
| 57  | 1E    | 13    | 0        | 0        | 0       | 0            |
| 57  | 1F    | 14    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | 1G    | 5     | 0        | 0        | 0       | 0            |
| 57  | 1H    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1I    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1N    | 6     | 0        | 0        | 0       | 0            |
| 57  | 1O    | 5     | 0        | 0        | 0       | 0            |
| 57  | 1P    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1Q    | 6     | 0        | 0        | 0       | 0            |
| 57  | 1R    | 5     | 0        | 0        | 0       | 0            |
| 57  | 1S    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1T    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1U    | 12    | 0        | 0        | 0       | 0            |
| 57  | 1V    | 8     | 0        | 0        | 0       | 0            |
| 57  | 1W    | 5     | 0        | 0        | 0       | 0            |
| 57  | 1X    | 6     | 0        | 0        | 0       | 0            |
| 57  | 1Y    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1Z    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1a    | 221   | 0        | 0        | 0       | 0            |
| 57  | 1b    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1d    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1e    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1f    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1k    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1l    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1p    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1t    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1v    | 2     | 0        | 0        | 0       | 0            |
| 57  | 1w    | 1     | 0        | 0        | 0       | 0            |
| 57  | 1x    | 13    | 0        | 0        | 0       | 0            |
| 57  | 21    | 2     | 0        | 0        | 0       | 0            |
| 57  | 23    | 1     | 0        | 0        | 0       | 0            |
| 57  | 25    | 4     | 0        | 0        | 0       | 0            |
| 57  | 26    | 1     | 0        | 0        | 0       | 0            |
| 57  | 27    | 3     | 0        | 0        | 0       | 0            |
| 57  | 28    | 3     | 0        | 0        | 0       | 0            |
| 57  | 2A    | 835   | 0        | 0        | 0       | 0            |
| 57  | 2B    | 18    | 0        | 0        | 0       | 0            |
| 57  | 2D    | 5     | 0        | 0        | 0       | 0            |
| 57  | 2E    | 10    | 0        | 0        | 0       | 0            |
| 57  | 2F    | 7     | 0        | 0        | 0       | 0            |
| 57  | 2G    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | 2O    | 3     | 0        | 0        | 0       | 0            |
| 57  | 2P    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2Q    | 4     | 0        | 0        | 0       | 0            |
| 57  | 2R    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2T    | 4     | 0        | 0        | 0       | 0            |
| 57  | 2U    | 4     | 0        | 0        | 0       | 0            |
| 57  | 2V    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2W    | 3     | 0        | 0        | 0       | 0            |
| 57  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2Z    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2a    | 178   | 0        | 0        | 0       | 0            |
| 57  | 2d    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2e    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2f    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2g    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2i    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2j    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2k    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2l    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2q    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2r    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 57  | 2v    | 2     | 0        | 0        | 0       | 0            |
| 57  | 2x    | 8     | 0        | 0        | 0       | 0            |
| 58  | 1A    | 1     | 0        | 0        | 0       | 0            |
| 59  | 14    | 1     | 0        | 0        | 0       | 0            |
| 59  | 15    | 1     | 0        | 0        | 0       | 0            |
| 59  | 16    | 1     | 0        | 0        | 0       | 0            |
| 59  | 19    | 1     | 0        | 0        | 0       | 0            |
| 59  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 59  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 59  | 24    | 1     | 0        | 0        | 0       | 0            |
| 59  | 25    | 1     | 0        | 0        | 0       | 0            |
| 59  | 26    | 1     | 0        | 0        | 0       | 0            |
| 59  | 29    | 1     | 0        | 0        | 0       | 0            |
| 59  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 59  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1d    | 8     | 0        | 0        | 1       | 0            |
| 60  | 2d    | 8     | 0        | 0        | 0       | 0            |
| 61  | 10    | 9     | 0        | 0        | 0       | 0            |
| 61  | 11    | 8     | 0        | 0        | 0       | 0            |
| 61  | 12    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61  | 13    | 4     | 0        | 0        | 0       | 0            |
| 61  | 15    | 7     | 0        | 0        | 0       | 0            |
| 61  | 16    | 1     | 0        | 0        | 0       | 0            |
| 61  | 17    | 8     | 0        | 0        | 1       | 0            |
| 61  | 18    | 12    | 0        | 0        | 0       | 0            |
| 61  | 1A    | 1897  | 0        | 0        | 67      | 0            |
| 61  | 1B    | 61    | 0        | 0        | 2       | 0            |
| 61  | 1D    | 30    | 0        | 0        | 1       | 0            |
| 61  | 1E    | 27    | 0        | 0        | 3       | 0            |
| 61  | 1F    | 18    | 0        | 0        | 1       | 0            |
| 61  | 1G    | 5     | 0        | 0        | 3       | 0            |
| 61  | 1H    | 2     | 0        | 0        | 0       | 0            |
| 61  | 1I    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1N    | 8     | 0        | 0        | 0       | 0            |
| 61  | 1O    | 6     | 0        | 0        | 0       | 0            |
| 61  | 1P    | 23    | 0        | 0        | 0       | 0            |
| 61  | 1Q    | 11    | 0        | 0        | 1       | 0            |
| 61  | 1R    | 11    | 0        | 0        | 2       | 0            |
| 61  | 1S    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1T    | 7     | 0        | 0        | 1       | 0            |
| 61  | 1U    | 13    | 0        | 0        | 0       | 0            |
| 61  | 1V    | 6     | 0        | 0        | 0       | 0            |
| 61  | 1W    | 12    | 0        | 0        | 1       | 0            |
| 61  | 1X    | 10    | 0        | 0        | 0       | 0            |
| 61  | 1Y    | 2     | 0        | 0        | 0       | 0            |
| 61  | 1a    | 259   | 0        | 0        | 18      | 0            |
| 61  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1d    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1f    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1j    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1l    | 2     | 0        | 0        | 0       | 0            |
| 61  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1q    | 4     | 0        | 0        | 0       | 0            |
| 61  | 1u    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1v    | 3     | 0        | 0        | 0       | 0            |
| 61  | 1w    | 3     | 0        | 0        | 0       | 0            |
| 61  | 1x    | 25    | 0        | 0        | 3       | 0            |
| 61  | 20    | 2     | 0        | 0        | 0       | 0            |
| 61  | 21    | 10    | 0        | 0        | 1       | 0            |
| 61  | 25    | 3     | 0        | 0        | 0       | 0            |
| 61  | 27    | 2     | 0        | 0        | 0       | 0            |
| 61  | 28    | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61  | 29    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2A    | 1003   | 0        | 0        | 73      | 0            |
| 61  | 2B    | 14     | 0        | 0        | 0       | 0            |
| 61  | 2D    | 25     | 0        | 0        | 1       | 0            |
| 61  | 2E    | 14     | 0        | 0        | 0       | 0            |
| 61  | 2F    | 12     | 0        | 0        | 0       | 0            |
| 61  | 2N    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2O    | 3      | 0        | 0        | 1       | 0            |
| 61  | 2P    | 7      | 0        | 0        | 0       | 0            |
| 61  | 2Q    | 3      | 0        | 0        | 0       | 0            |
| 61  | 2R    | 4      | 0        | 0        | 1       | 0            |
| 61  | 2T    | 5      | 0        | 0        | 0       | 0            |
| 61  | 2U    | 3      | 0        | 0        | 0       | 0            |
| 61  | 2V    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2W    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2X    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2a    | 130    | 0        | 0        | 5       | 0            |
| 61  | 2e    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2i    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2j    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2l    | 4      | 0        | 0        | 1       | 0            |
| 61  | 2n    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2q    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2t    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2v    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2w    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2x    | 14     | 0        | 0        | 2       | 0            |
| All | All   | 296656 | 0        | 197040   | 3915    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 3915 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:2A:2129:C:N4   | 1:2A:2159:G:H1   | 1.55                     | 1.03              |
| 32:1a:1035:A:H2' | 32:1a:1036:G:H21 | 1.24                     | 1.02              |
| 1:1A:1082:U:C4   | 1:1A:1086:A:N1   | 2.34                     | 0.96              |
| 41:2j:30:SER:HB3 | 41:2j:81:THR:HB  | 1.46                     | 0.95              |
| 1:2A:784:A:OP2   | 61:2A:3903:HOH:O | 1.83                     | 0.94              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 260 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 3   | 2D    | 273/276 (99%) | 256 (94%) | 17 (6%)  | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 192 (95%) | 9 (4%)   | 1 (0%)   | 24          | 55  |
| 4   | 2E    | 202/206 (98%) | 193 (96%) | 8 (4%)   | 1 (0%)   | 24          | 55  |
| 5   | 1F    | 201/210 (96%) | 194 (96%) | 6 (3%)   | 1 (0%)   | 24          | 55  |
| 5   | 2F    | 201/210 (96%) | 186 (92%) | 14 (7%)  | 1 (0%)   | 24          | 55  |
| 6   | 1G    | 179/182 (98%) | 154 (86%) | 22 (12%) | 3 (2%)   | 7           | 25  |
| 6   | 2G    | 179/182 (98%) | 160 (89%) | 14 (8%)  | 5 (3%)   | 4           | 14  |
| 7   | 1H    | 172/180 (96%) | 163 (95%) | 7 (4%)   | 2 (1%)   | 10          | 34  |
| 7   | 2H    | 172/180 (96%) | 156 (91%) | 15 (9%)  | 1 (1%)   | 21          | 51  |
| 8   | 1I    | 144/148 (97%) | 126 (88%) | 18 (12%) | 0        | 100         | 100 |
| 8   | 2I    | 144/148 (97%) | 118 (82%) | 21 (15%) | 5 (4%)   | 3           | 10  |
| 9   | 1N    | 138/140 (99%) | 134 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 135 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 10  | 1O    | 120/122 (98%) | 113 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 10  | 2O    | 120/122 (98%) | 111 (92%) | 8 (7%)   | 1 (1%)   | 16          | 44  |
| 11  | 1P    | 147/150 (98%) | 139 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 11  | 2P    | 147/150 (98%) | 137 (93%) | 9 (6%)   | 1 (1%)   | 18          | 47  |
| 12  | 1Q    | 139/141 (99%) | 131 (94%) | 6 (4%)   | 2 (1%)   | 9           | 30  |
| 12  | 2Q    | 139/141 (99%) | 127 (91%) | 10 (7%)  | 2 (1%)   | 9           | 30  |
| 13  | 1R    | 116/118 (98%) | 110 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 13  | 2R    | 116/118 (98%) | 108 (93%) | 8 (7%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 14  | 1S    | 108/112 (96%) | 101 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 14  | 2S    | 108/112 (96%) | 97 (90%)   | 10 (9%)  | 1 (1%)   | 14          | 41  |
| 15  | 1T    | 129/146 (88%) | 120 (93%)  | 8 (6%)   | 1 (1%)   | 16          | 44  |
| 15  | 2T    | 129/146 (88%) | 120 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 16  | 1U    | 114/118 (97%) | 113 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 114 (100%) | 0        | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 94 (95%)   | 3 (3%)   | 2 (2%)   | 6           | 21  |
| 17  | 2V    | 99/101 (98%)  | 92 (93%)   | 6 (6%)   | 1 (1%)   | 12          | 38  |
| 18  | 1W    | 110/113 (97%) | 108 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 108 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 19  | 2X    | 93/96 (97%)   | 88 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 20  | 1Y    | 105/110 (96%) | 99 (94%)   | 5 (5%)   | 1 (1%)   | 12          | 38  |
| 20  | 2Y    | 105/110 (96%) | 91 (87%)   | 13 (12%) | 1 (1%)   | 12          | 38  |
| 21  | 1Z    | 148/206 (72%) | 130 (88%)  | 13 (9%)  | 5 (3%)   | 3           | 11  |
| 21  | 2Z    | 156/206 (76%) | 138 (88%)  | 15 (10%) | 3 (2%)   | 6           | 22  |
| 22  | 10    | 74/85 (87%)   | 73 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 22  | 20    | 74/85 (87%)   | 70 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 23  | 11    | 95/98 (97%)   | 92 (97%)   | 2 (2%)   | 1 (1%)   | 11          | 36  |
| 23  | 21    | 95/98 (97%)   | 93 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 24  | 12    | 68/72 (94%)   | 68 (100%)  | 0        | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 66 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 54 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 25  | 23    | 57/60 (95%)   | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 26  | 14    | 67/71 (94%)   | 51 (76%)   | 13 (19%) | 3 (4%)   | 2           | 7   |
| 26  | 24    | 67/71 (94%)   | 54 (81%)   | 8 (12%)  | 5 (8%)   | 1           | 2   |
| 27  | 15    | 57/60 (95%)   | 54 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 54 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 50 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 48 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 29  | 17    | 46/49 (94%)   | 46 (100%)  | 0        | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29  | 27    | 46/49 (94%)   | 46 (100%) | 0        | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 190 (83%) | 32 (14%) | 7 (3%)   | 3           | 12  |
| 33  | 2b    | 229/256 (90%) | 193 (84%) | 32 (14%) | 4 (2%)   | 7           | 25  |
| 34  | 1c    | 204/239 (85%) | 174 (85%) | 26 (13%) | 4 (2%)   | 6           | 21  |
| 34  | 2c    | 204/239 (85%) | 176 (86%) | 28 (14%) | 0        | 100         | 100 |
| 35  | 1d    | 206/209 (99%) | 186 (90%) | 19 (9%)  | 1 (0%)   | 24          | 55  |
| 35  | 2d    | 206/209 (99%) | 191 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 36  | 1e    | 146/162 (90%) | 130 (89%) | 14 (10%) | 2 (1%)   | 9           | 30  |
| 36  | 2e    | 146/162 (90%) | 133 (91%) | 10 (7%)  | 3 (2%)   | 5           | 20  |
| 37  | 1f    | 98/101 (97%)  | 92 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 37  | 2f    | 98/101 (97%)  | 92 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/156 (98%) | 131 (86%) | 20 (13%) | 2 (1%)   | 9           | 31  |
| 38  | 2g    | 153/156 (98%) | 138 (90%) | 12 (8%)  | 3 (2%)   | 6           | 21  |
| 39  | 1h    | 135/138 (98%) | 125 (93%) | 9 (7%)   | 1 (1%)   | 18          | 47  |
| 39  | 2h    | 135/138 (98%) | 130 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | 1i    | 125/128 (98%) | 106 (85%) | 18 (14%) | 1 (1%)   | 16          | 44  |
| 40  | 2i    | 125/128 (98%) | 108 (86%) | 16 (13%) | 1 (1%)   | 16          | 44  |
| 41  | 1j    | 95/105 (90%)  | 84 (88%)  | 9 (10%)  | 2 (2%)   | 5           | 20  |
| 41  | 2j    | 94/105 (90%)  | 81 (86%)  | 12 (13%) | 1 (1%)   | 11          | 36  |
| 42  | 1k    | 112/129 (87%) | 102 (91%) | 9 (8%)   | 1 (1%)   | 14          | 41  |
| 42  | 2k    | 112/129 (87%) | 99 (88%)  | 11 (10%) | 2 (2%)   | 6           | 23  |
| 43  | 1l    | 119/132 (90%) | 107 (90%) | 12 (10%) | 0        | 100         | 100 |
| 43  | 2l    | 119/132 (90%) | 113 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 44  | 1m    | 116/126 (92%) | 106 (91%) | 9 (8%)   | 1 (1%)   | 14          | 41  |
| 44  | 2m    | 114/126 (90%) | 98 (86%)  | 14 (12%) | 2 (2%)   | 6           | 23  |
| 45  | 1n    | 58/61 (95%)   | 51 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 45  | 2n    | 58/61 (95%)   | 51 (88%)  | 7 (12%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 46  | 1o    | 86/89 (97%)       | 83 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 46  | 2o    | 86/89 (97%)       | 82 (95%)    | 4 (5%)   | 0        | 100         | 100 |
| 47  | 1p    | 80/88 (91%)       | 67 (84%)    | 13 (16%) | 0        | 100         | 100 |
| 47  | 2p    | 80/88 (91%)       | 71 (89%)    | 9 (11%)  | 0        | 100         | 100 |
| 48  | 1q    | 97/105 (92%)      | 90 (93%)    | 7 (7%)   | 0        | 100         | 100 |
| 48  | 2q    | 97/105 (92%)      | 88 (91%)    | 8 (8%)   | 1 (1%)   | 12          | 38  |
| 49  | 1r    | 66/88 (75%)       | 62 (94%)    | 4 (6%)   | 0        | 100         | 100 |
| 49  | 2r    | 66/88 (75%)       | 63 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 50  | 1s    | 81/93 (87%)       | 64 (79%)    | 17 (21%) | 0        | 100         | 100 |
| 50  | 2s    | 81/93 (87%)       | 68 (84%)    | 12 (15%) | 1 (1%)   | 10          | 34  |
| 51  | 1t    | 94/106 (89%)      | 87 (93%)    | 5 (5%)   | 2 (2%)   | 5           | 20  |
| 51  | 2t    | 94/106 (89%)      | 85 (90%)    | 7 (7%)   | 2 (2%)   | 5           | 20  |
| 52  | 1u    | 21/27 (78%)       | 20 (95%)    | 1 (5%)   | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| 54  | 1w    | 247/354 (70%)     | 227 (92%)   | 17 (7%)  | 3 (1%)   | 10          | 34  |
| 54  | 2w    | 251/354 (71%)     | 232 (92%)   | 17 (7%)  | 2 (1%)   | 16          | 44  |
| 56  | 1z    | 3/7 (43%)         | 2 (67%)     | 1 (33%)  | 0        | 100         | 100 |
| 56  | 2z    | 2/7 (29%)         | 2 (100%)    | 0        | 0        | 100         | 100 |
| All | All   | 11848/12850 (92%) | 10869 (92%) | 880 (7%) | 99 (1%)  | 16          | 44  |

5 of 99 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1F    | 130 | ALA  |
| 6   | 1G    | 96  | ARG  |
| 6   | 1G    | 126 | ASP  |
| 12  | 1Q    | 16  | ARG  |
| 21  | 1Z    | 53  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | 1D    | 215/218 (99%)  | 204 (95%) | 11 (5%)  | 21          | 54 |
| 3   | 2D    | 215/218 (99%)  | 203 (94%) | 12 (6%)  | 19          | 50 |
| 4   | 1E    | 164/166 (99%)  | 156 (95%) | 8 (5%)   | 22          | 55 |
| 4   | 2E    | 164/166 (99%)  | 157 (96%) | 7 (4%)   | 26          | 60 |
| 5   | 1F    | 160/166 (96%)  | 148 (92%) | 12 (8%)  | 12          | 37 |
| 5   | 2F    | 159/166 (96%)  | 143 (90%) | 16 (10%) | 7           | 23 |
| 6   | 1G    | 143/156 (92%)  | 123 (86%) | 20 (14%) | 3           | 12 |
| 6   | 2G    | 143/156 (92%)  | 126 (88%) | 17 (12%) | 5           | 17 |
| 7   | 1H    | 144/148 (97%)  | 131 (91%) | 13 (9%)  | 9           | 28 |
| 7   | 2H    | 144/148 (97%)  | 131 (91%) | 13 (9%)  | 9           | 28 |
| 8   | 1I    | 113/124 (91%)  | 105 (93%) | 8 (7%)   | 13          | 39 |
| 8   | 2I    | 105/124 (85%)  | 85 (81%)  | 20 (19%) | 1           | 5  |
| 9   | 1N    | 118/119 (99%)  | 108 (92%) | 10 (8%)  | 10          | 31 |
| 9   | 2N    | 118/119 (99%)  | 107 (91%) | 11 (9%)  | 8           | 27 |
| 10  | 1O    | 100/100 (100%) | 98 (98%)  | 2 (2%)   | 48          | 80 |
| 10  | 2O    | 100/100 (100%) | 96 (96%)  | 4 (4%)   | 28          | 63 |
| 11  | 1P    | 115/116 (99%)  | 100 (87%) | 15 (13%) | 4           | 14 |
| 11  | 2P    | 115/116 (99%)  | 103 (90%) | 12 (10%) | 7           | 22 |
| 12  | 1Q    | 111/111 (100%) | 106 (96%) | 5 (4%)   | 24          | 58 |
| 12  | 2Q    | 111/111 (100%) | 103 (93%) | 8 (7%)   | 13          | 39 |
| 13  | 1R    | 101/101 (100%) | 100 (99%) | 1 (1%)   | 68          | 88 |
| 13  | 2R    | 101/101 (100%) | 99 (98%)  | 2 (2%)   | 48          | 80 |
| 14  | 1S    | 86/88 (98%)    | 80 (93%)  | 6 (7%)   | 14          | 40 |
| 14  | 2S    | 85/88 (97%)    | 77 (91%)  | 8 (9%)   | 8           | 27 |
| 15  | 1T    | 115/127 (91%)  | 104 (90%) | 11 (10%) | 8           | 26 |
| 15  | 2T    | 113/127 (89%)  | 109 (96%) | 4 (4%)   | 32          | 67 |
| 16  | 1U    | 93/94 (99%)    | 88 (95%)  | 5 (5%)   | 20          | 51 |
| 16  | 2U    | 93/94 (99%)    | 86 (92%)  | 7 (8%)   | 12          | 37 |
| 17  | 1V    | 80/82 (98%)    | 78 (98%)  | 2 (2%)   | 42          | 76 |
| 17  | 2V    | 80/82 (98%)    | 76 (95%)  | 4 (5%)   | 22          | 54 |
| 18  | 1W    | 90/92 (98%)    | 87 (97%)  | 3 (3%)   | 33          | 69 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 18  | 2W    | 90/92 (98%)   | 85 (94%)  | 5 (6%)   | 19          | 50  |
| 19  | 1X    | 77/78 (99%)   | 74 (96%)  | 3 (4%)   | 28          | 64  |
| 19  | 2X    | 77/78 (99%)   | 73 (95%)  | 4 (5%)   | 21          | 53  |
| 20  | 1Y    | 85/91 (93%)   | 80 (94%)  | 5 (6%)   | 18          | 48  |
| 20  | 2Y    | 85/91 (93%)   | 78 (92%)  | 7 (8%)   | 10          | 33  |
| 21  | 1Z    | 135/179 (75%) | 117 (87%) | 18 (13%) | 4           | 14  |
| 21  | 2Z    | 137/179 (76%) | 116 (85%) | 21 (15%) | 3           | 10  |
| 22  | 10    | 61/67 (91%)   | 60 (98%)  | 1 (2%)   | 55          | 83  |
| 22  | 20    | 61/67 (91%)   | 59 (97%)  | 2 (3%)   | 33          | 69  |
| 23  | 11    | 80/83 (96%)   | 74 (92%)  | 6 (8%)   | 12          | 37  |
| 23  | 21    | 80/83 (96%)   | 77 (96%)  | 3 (4%)   | 29          | 64  |
| 24  | 12    | 65/67 (97%)   | 60 (92%)  | 5 (8%)   | 12          | 36  |
| 24  | 22    | 65/67 (97%)   | 62 (95%)  | 3 (5%)   | 24          | 58  |
| 25  | 13    | 51/52 (98%)   | 45 (88%)  | 6 (12%)  | 5           | 17  |
| 25  | 23    | 50/52 (96%)   | 45 (90%)  | 5 (10%)  | 7           | 24  |
| 26  | 14    | 59/63 (94%)   | 52 (88%)  | 7 (12%)  | 5           | 17  |
| 26  | 24    | 53/63 (84%)   | 45 (85%)  | 8 (15%)  | 3           | 10  |
| 27  | 15    | 50/52 (96%)   | 46 (92%)  | 4 (8%)   | 11          | 34  |
| 27  | 25    | 50/52 (96%)   | 46 (92%)  | 4 (8%)   | 11          | 34  |
| 28  | 16    | 51/52 (98%)   | 44 (86%)  | 7 (14%)  | 3           | 13  |
| 28  | 26    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 28          | 63  |
| 29  | 17    | 41/42 (98%)   | 39 (95%)  | 2 (5%)   | 22          | 55  |
| 29  | 27    | 41/42 (98%)   | 37 (90%)  | 4 (10%)  | 7           | 25  |
| 30  | 18    | 54/55 (98%)   | 52 (96%)  | 2 (4%)   | 30          | 65  |
| 30  | 28    | 54/55 (98%)   | 52 (96%)  | 2 (4%)   | 30          | 65  |
| 31  | 19    | 34/34 (100%)  | 34 (100%) | 0        | 100         | 100 |
| 31  | 29    | 34/34 (100%)  | 31 (91%)  | 3 (9%)   | 9           | 29  |
| 33  | 1b    | 192/220 (87%) | 166 (86%) | 26 (14%) | 4           | 13  |
| 33  | 2b    | 187/220 (85%) | 161 (86%) | 26 (14%) | 3           | 12  |
| 34  | 1c    | 142/188 (76%) | 124 (87%) | 18 (13%) | 4           | 15  |
| 34  | 2c    | 140/188 (74%) | 129 (92%) | 11 (8%)  | 11          | 35  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 35  | 1d    | 169/181 (93%) | 160 (95%) | 9 (5%)   | 20          | 52 |
| 35  | 2d    | 173/181 (96%) | 153 (88%) | 20 (12%) | 5           | 18 |
| 36  | 1e    | 113/123 (92%) | 100 (88%) | 13 (12%) | 5           | 18 |
| 36  | 2e    | 114/123 (93%) | 103 (90%) | 11 (10%) | 8           | 26 |
| 37  | 1f    | 84/90 (93%)   | 78 (93%)  | 6 (7%)   | 13          | 39 |
| 37  | 2f    | 85/90 (94%)   | 79 (93%)  | 6 (7%)   | 13          | 39 |
| 38  | 1g    | 119/127 (94%) | 109 (92%) | 10 (8%)  | 10          | 32 |
| 38  | 2g    | 120/127 (94%) | 109 (91%) | 11 (9%)  | 8           | 27 |
| 39  | 1h    | 114/119 (96%) | 102 (90%) | 12 (10%) | 6           | 22 |
| 39  | 2h    | 114/119 (96%) | 103 (90%) | 11 (10%) | 8           | 26 |
| 40  | 1i    | 90/99 (91%)   | 78 (87%)  | 12 (13%) | 4           | 14 |
| 40  | 2i    | 89/99 (90%)   | 77 (86%)  | 12 (14%) | 4           | 13 |
| 41  | 1j    | 66/92 (72%)   | 56 (85%)  | 10 (15%) | 3           | 10 |
| 41  | 2j    | 69/92 (75%)   | 65 (94%)  | 4 (6%)   | 18          | 49 |
| 42  | 1k    | 82/99 (83%)   | 70 (85%)  | 12 (15%) | 3           | 11 |
| 42  | 2k    | 83/99 (84%)   | 74 (89%)  | 9 (11%)  | 6           | 21 |
| 43  | 1l    | 96/108 (89%)  | 87 (91%)  | 9 (9%)   | 8           | 27 |
| 43  | 2l    | 96/108 (89%)  | 88 (92%)  | 8 (8%)   | 10          | 32 |
| 44  | 1m    | 89/101 (88%)  | 70 (79%)  | 19 (21%) | 1           | 4  |
| 44  | 2m    | 88/101 (87%)  | 81 (92%)  | 7 (8%)   | 11          | 34 |
| 45  | 1n    | 49/50 (98%)   | 40 (82%)  | 9 (18%)  | 1           | 6  |
| 45  | 2n    | 49/50 (98%)   | 45 (92%)  | 4 (8%)   | 10          | 33 |
| 46  | 1o    | 78/80 (98%)   | 71 (91%)  | 7 (9%)   | 9           | 28 |
| 46  | 2o    | 78/80 (98%)   | 69 (88%)  | 9 (12%)  | 5           | 18 |
| 47  | 1p    | 69/74 (93%)   | 56 (81%)  | 13 (19%) | 1           | 5  |
| 47  | 2p    | 68/74 (92%)   | 57 (84%)  | 11 (16%) | 2           | 8  |
| 48  | 1q    | 94/97 (97%)   | 82 (87%)  | 12 (13%) | 4           | 15 |
| 48  | 2q    | 94/97 (97%)   | 86 (92%)  | 8 (8%)   | 10          | 31 |
| 49  | 1r    | 59/77 (77%)   | 57 (97%)  | 2 (3%)   | 32          | 68 |
| 49  | 2r    | 59/77 (77%)   | 57 (97%)  | 2 (3%)   | 32          | 68 |
| 50  | 1s    | 69/80 (86%)   | 60 (87%)  | 9 (13%)  | 4           | 14 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 50  | 2s    | 67/80 (84%)      | 59 (88%)   | 8 (12%)  | 5           | 17  |
| 51  | 1t    | 70/82 (85%)      | 68 (97%)   | 2 (3%)   | 37          | 73  |
| 51  | 2t    | 70/82 (85%)      | 67 (96%)   | 3 (4%)   | 26          | 60  |
| 52  | 1u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)   | 19          | 50  |
| 52  | 2u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)   | 19          | 50  |
| 54  | 1w    | 204/299 (68%)    | 183 (90%)  | 21 (10%) | 7           | 23  |
| 54  | 2w    | 204/299 (68%)    | 171 (84%)  | 33 (16%) | 2           | 8   |
| 56  | 1z    | 2/3 (67%)        | 2 (100%)   | 0        | 100         | 100 |
| 56  | 2z    | 2/3 (67%)        | 2 (100%)   | 0        | 100         | 100 |
| All | All   | 9699/10668 (91%) | 8836 (91%) | 863 (9%) | 9           | 29  |

5 of 863 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 2F    | 190 | GLU  |
| 17  | 2V    | 73  | SER  |
| 47  | 2p    | 5   | ARG  |
| 6   | 2G    | 135 | LEU  |
| 5   | 2F    | 183 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | 2f    | 100 | ASN  |
| 40  | 2i    | 3   | GLN  |
| 44  | 2m    | 12  | ASN  |
| 35  | 1d    | 161 | ASN  |
| 35  | 1d    | 160 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2864/2915 (98%) | 449 (15%)         | 30 (1%)         |
| 1   | 2A    | 2791/2915 (95%) | 458 (16%)         | 19 (0%)         |
| 2   | 1B    | 119/121 (98%)   | 9 (7%)            | 0               |
| 2   | 2B    | 118/121 (97%)   | 18 (15%)          | 0               |
| 32  | 1a    | 1497/1521 (98%) | 295 (19%)         | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 32  | 2a    | 1501/1521 (98%) | 279 (18%)         | 0               |
| 53  | 1v    | 8/24 (33%)      | 1 (12%)           | 0               |
| 53  | 2v    | 8/24 (33%)      | 1 (12%)           | 0               |
| 55  | 1x    | 72/74 (97%)     | 12 (16%)          | 0               |
| 55  | 2x    | 72/74 (97%)     | 5 (6%)            | 0               |
| All | All   | 9050/9310 (97%) | 1527 (16%)        | 49 (0%)         |

5 of 1527 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 11  | G    |
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 34  | C    |
| 1   | 1A    | 45  | C    |
| 1   | 1A    | 55  | G    |

5 of 49 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2689 | U    |
| 1   | 2A    | 752  | A    |
| 1   | 1A    | 2756 | U    |
| 1   | 2A    | 277  | C    |
| 1   | 2A    | 893  | C    |

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

66 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 |
| 1   | 5MU  | 1A    | 1939 | 57,1 | 19,22,23     | 1.41 | 5 (26%)  | 27,32,35    | 2.06 | 5 (18%)  |
| 1   | OMC  | 2A    | 1920 | 1    | 19,22,23     | 0.81 | 0        | 25,31,34    | 0.82 | 0        |
| 1   | OMG  | 2A    | 2251 | 55,1 | 23,26,27     | 1.23 | 3 (13%)  | 32,38,41    | 1.99 | 6 (18%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | M2G  | 2a    | 966  | 32       | 24,27,28     | 1.26 | 3 (12%)  | 33,40,43    | 1.89 | 6 (18%)  |
| 55  | 4SU  | 1x    | 8    | 55       | 18,21,22     | 1.85 | 4 (22%)  | 25,30,33    | 1.78 | 4 (16%)  |
| 32  | PSU  | 1a    | 516  | 57,32    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 1   | 5MU  | 1A    | 1915 | 1        | 19,22,23     | 1.39 | 5 (26%)  | 27,32,35    | 2.29 | 6 (22%)  |
| 1   | PSU  | 1A    | 1911 | 1        | 18,21,22     | 1.41 | 3 (16%)  | 21,30,33    | 2.11 | 5 (23%)  |
| 32  | 5MC  | 1a    | 967  | 32       | 19,22,23     | 1.57 | 3 (15%)  | 26,32,35    | 1.16 | 2 (7%)   |
| 1   | OMU  | 1A    | 2552 | 57,1     | 19,22,23     | 1.25 | 3 (15%)  | 25,31,34    | 1.67 | 5 (20%)  |
| 1   | 5MU  | 2A    | 1915 | 57,1     | 19,22,23     | 1.46 | 6 (31%)  | 27,32,35    | 2.18 | 6 (22%)  |
| 32  | 5MC  | 2a    | 1407 | 32       | 19,22,23     | 1.50 | 3 (15%)  | 26,32,35    | 1.24 | 3 (11%)  |
| 43  | 0TD  | 2l    | 92   | 43       | 8,9,10       | 4.52 | 1 (12%)  | 6,11,13     | 8.81 | 3 (50%)  |
| 1   | PSU  | 2A    | 2605 | 1        | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.27 | 4 (19%)  |
| 55  | MIA  | 1x    | 37   | 55       | 21,24,32     | 1.59 | 4 (19%)  | 30,35,47    | 1.97 | 7 (23%)  |
| 32  | MA6  | 1a    | 1518 | 32       | 23,26,27     | 0.42 | 0        | 33,38,41    | 2.04 | 9 (27%)  |
| 32  | 2MG  | 1a    | 1207 | 57,32    | 23,26,27     | 1.25 | 4 (17%)  | 33,38,41    | 2.08 | 8 (24%)  |
| 55  | 5MU  | 1x    | 54   | 55       | 19,22,23     | 1.37 | 3 (15%)  | 27,32,35    | 1.81 | 5 (18%)  |
| 1   | PSU  | 2A    | 1911 | 1        | 18,21,22     | 1.38 | 3 (16%)  | 21,30,33    | 2.02 | 4 (19%)  |
| 32  | M2G  | 1a    | 966  | 32       | 24,27,28     | 1.30 | 3 (12%)  | 33,40,43    | 1.93 | 6 (18%)  |
| 1   | OMC  | 1A    | 1920 | 1        | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.88 | 0        |
| 32  | MA6  | 1a    | 1519 | 32       | 23,26,27     | 0.43 | 0        | 33,38,41    | 2.11 | 9 (27%)  |
| 32  | UR3  | 1a    | 1498 | 32       | 19,22,23     | 1.13 | 2 (10%)  | 26,32,35    | 1.74 | 5 (19%)  |
| 32  | PSU  | 2a    | 516  | 57,32    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.95 | 5 (23%)  |
| 32  | MA6  | 2a    | 1518 | 32       | 23,26,27     | 0.41 | 0        | 33,38,41    | 1.98 | 9 (27%)  |
| 32  | 5MC  | 1a    | 1407 | 32       | 19,22,23     | 1.53 | 3 (15%)  | 26,32,35    | 0.97 | 2 (7%)   |
| 55  | 4SU  | 2x    | 8    | 55       | 18,21,22     | 1.80 | 4 (22%)  | 25,30,33    | 2.12 | 5 (20%)  |
| 32  | 5MC  | 2a    | 1404 | 32       | 19,22,23     | 1.66 | 3 (15%)  | 26,32,35    | 1.18 | 2 (7%)   |
| 1   | PSU  | 1A    | 1917 | 1        | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 55  | H2U  | 1x    | 21   | 55       | 18,21,22     | 0.94 | 2 (11%)  | 19,30,33    | 0.93 | 1 (5%)   |
| 55  | H2U  | 2x    | 21   | 55       | 18,21,22     | 0.99 | 2 (11%)  | 19,30,33    | 0.88 | 1 (5%)   |
| 32  | 4OC  | 2a    | 1402 | 57,32    | 20,23,24     | 0.79 | 0        | 25,32,35    | 0.94 | 1 (4%)   |
| 55  | PSU  | 1x    | 32   | 55,57    | 18,21,22     | 1.30 | 2 (11%)  | 21,30,33    | 1.94 | 4 (19%)  |
| 55  | 8AN  | 1x    | 76   | 55,56,57 | 21,24,25     | 1.39 | 3 (14%)  | 26,35,38    | 2.16 | 9 (34%)  |
| 1   | 5MC  | 2A    | 1942 | 1        | 19,22,23     | 1.52 | 3 (15%)  | 26,32,35    | 1.19 | 2 (7%)   |
| 1   | 2MA  | 1A    | 2503 | 57,1     | 22,25,26     | 1.46 | 3 (13%)  | 32,37,40    | 2.34 | 8 (25%)  |
| 55  | H2U  | 2x    | 20   | 55       | 18,21,22     | 0.96 | 2 (11%)  | 19,30,33    | 0.95 | 1 (5%)   |
| 32  | G7M  | 1a    | 527  | 32       | 23,26,27     | 1.49 | 3 (13%)  | 34,39,42    | 1.76 | 5 (14%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 2MG  | 2a    | 1207 | 32       | 23,26,27     | 1.25 | 3 (13%)  | 33,38,41    | 2.12 | 5 (15%)  |
| 55  | H2U  | 1x    | 20   | 55       | 18,21,22     | 0.93 | 2 (11%)  | 19,30,33    | 1.01 | 1 (5%)   |
| 1   | 2MA  | 2A    | 2503 | 57,1     | 22,25,26     | 1.47 | 4 (18%)  | 32,37,40    | 2.39 | 8 (25%)  |
| 55  | PSU  | 2x    | 32   | 55       | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.02 | 4 (19%)  |
| 32  | G7M  | 2a    | 527  | 57,32    | 23,26,27     | 1.49 | 3 (13%)  | 34,39,42    | 1.70 | 5 (14%)  |
| 55  | PSU  | 1x    | 39   | 55       | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.89 | 4 (19%)  |
| 55  | PSU  | 1x    | 55   | 55       | 18,21,22     | 1.30 | 2 (11%)  | 21,30,33    | 2.03 | 4 (19%)  |
| 1   | 5MU  | 2A    | 1939 | 57,1     | 19,22,23     | 1.40 | 5 (26%)  | 27,32,35    | 2.22 | 6 (22%)  |
| 1   | PSU  | 2A    | 1917 | 1        | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 1.99 | 5 (23%)  |
| 1   | 5MC  | 1A    | 1942 | 1        | 19,22,23     | 1.60 | 3 (15%)  | 26,32,35    | 1.27 | 3 (11%)  |
| 32  | 5MC  | 2a    | 967  | 32       | 19,22,23     | 1.71 | 3 (15%)  | 26,32,35    | 1.10 | 3 (11%)  |
| 55  | MIA  | 2x    | 37   | 55       | 21,24,32     | 1.58 | 4 (19%)  | 30,35,47    | 2.06 | 9 (30%)  |
| 43  | 0TD  | 1l    | 92   | 43       | 8,9,10       | 4.74 | 2 (25%)  | 6,11,13     | 5.96 | 3 (50%)  |
| 55  | 5MU  | 2x    | 54   | 55       | 19,22,23     | 1.40 | 4 (21%)  | 27,32,35    | 2.05 | 6 (22%)  |
| 1   | OMU  | 2A    | 2552 | 57,1     | 19,22,23     | 1.21 | 3 (15%)  | 25,31,34    | 1.70 | 5 (20%)  |
| 55  | 8AN  | 2x    | 76   | 55,56,57 | 21,24,25     | 1.40 | 3 (14%)  | 26,35,38    | 2.31 | 10 (38%) |
| 32  | 5MC  | 1a    | 1404 | 32       | 19,22,23     | 1.73 | 3 (15%)  | 26,32,35    | 1.21 | 3 (11%)  |
| 32  | MA6  | 2a    | 1519 | 32       | 23,26,27     | 0.41 | 0        | 33,38,41    | 2.15 | 10 (30%) |
| 1   | 5MC  | 2A    | 1962 | 57,1     | 19,22,23     | 1.52 | 3 (15%)  | 26,32,35    | 1.16 | 2 (7%)   |
| 32  | 4OC  | 1a    | 1402 | 57,32    | 20,23,24     | 0.75 | 0        | 25,32,35    | 0.98 | 2 (8%)   |
| 1   | OMG  | 1A    | 2251 | 57,55,1  | 23,26,27     | 1.18 | 3 (13%)  | 32,38,41    | 1.98 | 7 (21%)  |
| 1   | 5MC  | 1A    | 1962 | 57,1     | 19,22,23     | 1.60 | 3 (15%)  | 26,32,35    | 1.06 | 2 (7%)   |
| 55  | PSU  | 2x    | 39   | 55       | 18,21,22     | 1.43 | 3 (16%)  | 21,30,33    | 1.71 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1400 | 32       | 19,22,23     | 1.48 | 3 (15%)  | 26,32,35    | 1.25 | 4 (15%)  |
| 32  | UR3  | 2a    | 1498 | 32       | 19,22,23     | 1.02 | 0        | 26,32,35    | 1.68 | 2 (7%)   |
| 55  | PSU  | 2x    | 55   | 55       | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 1   | PSU  | 1A    | 2605 | 57,1     | 18,21,22     | 1.32 | 2 (11%)  | 21,30,33    | 2.02 | 5 (23%)  |
| 32  | 5MC  | 1a    | 1400 | 32       | 19,22,23     | 1.62 | 3 (15%)  | 26,32,35    | 1.19 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 1   | 5MU  | 1A    | 1939 | 57,1 | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 1   | OMC  | 2A    | 1920 | 1        | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 55,1     | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | M2G  | 2a    | 966  | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 55  | 4SU  | 1x    | 8    | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | PSU  | 1a    | 516  | 57,32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1        | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1911 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 967  | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 1A    | 2552 | 57,1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1915 | 57,1     | -       | 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       | -       | 2/7/12/14  | -       |
| 1   | PSU  | 2A    | 2605 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | MIA  | 1x    | 37   | 55       | -       | 2/7/25/34  | 0/3/3/3 |
| 32  | MA6  | 1a    | 1518 | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 2MG  | 1a    | 1207 | 57,32    | -       | 0/9/27/28  | 0/3/3/3 |
| 55  | 5MU  | 1x    | 54   | 55       | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | OMC  | 1A    | 1920 | 1        | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1519 | 32       | -       | 3/11/29/30 | 0/3/3/3 |
| 32  | UR3  | 1a    | 1498 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 57,32    | -       | 1/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1518 | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1407 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 2x    | 8    | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1404 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | H2U  | 1x    | 21   | 55       | -       | 4/7/38/39  | 0/2/2/2 |
| 55  | H2U  | 2x    | 21   | 55       | -       | 2/7/38/39  | 0/2/2/2 |
| 32  | 4OC  | 2a    | 1402 | 57,32    | -       | 3/9/29/30  | 0/2/2/2 |
| 55  | PSU  | 1x    | 32   | 55,57    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 8AN  | 1x    | 76   | 55,56,57 | -       | 1/7/25/26  | 0/3/3/3 |
| 1   | 5MC  | 2A    | 1942 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2503 | 57,1     | -       | 1/7/25/26  | 0/3/3/3 |
| 55  | H2U  | 2x    | 20   | 55       | -       | 0/7/38/39  | 0/2/2/2 |
| 32  | G7M  | 1a    | 527  | 32       | -       | 2/7/25/26  | 0/3/3/3 |
| 32  | 2MG  | 2a    | 1207 | 32       | -       | 2/9/27/28  | 0/3/3/3 |
| 55  | H2U  | 1x    | 20   | 55       | -       | 2/7/38/39  | 0/2/2/2 |
| 1   | 2MA  | 2A    | 2503 | 57,1     | -       | 1/7/25/26  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 55  | PSU  | 2x    | 32   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | G7M  | 2a    | 527  | 57,32    | -       | 1/7/25/26  | 0/3/3/3 |
| 55  | PSU  | 1x    | 39   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 1x    | 55   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 57,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1917 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1942 | 1        | -       | 1/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 967  | 32       | -       | 1/7/25/26  | 0/2/2/2 |
| 55  | MIA  | 2x    | 37   | 55       | -       | 2/7/25/34  | 0/3/3/3 |
| 43  | 0TD  | 1l    | 92   | 43       | -       | 1/7/12/14  | -       |
| 55  | 5MU  | 2x    | 54   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2A    | 2552 | 57,1     | -       | 0/9/27/28  | 0/2/2/2 |
| 55  | 8AN  | 2x    | 76   | 55,56,57 | -       | 1/7/25/26  | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1404 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1519 | 32       | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | 5MC  | 2A    | 1962 | 57,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 4OC  | 1a    | 1402 | 57,32    | -       | 3/9/29/30  | 0/2/2/2 |
| 1   | OMG  | 1A    | 2251 | 57,55,1  | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1962 | 57,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 2x    | 39   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1400 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | UR3  | 2a    | 1498 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 2x    | 55   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2605 | 57,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1400 | 32       | -       | 0/7/25/26  | 0/2/2/2 |

The worst 5 of 168 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CB-SB | -12.57 | 1.69        | 1.82     |
| 43  | 2l    | 92   | 0TD  | CB-SB | -12.33 | 1.69        | 1.82     |
| 32  | 2a    | 967  | 5MC  | C5-C4 | 6.37   | 1.48        | 1.44     |
| 32  | 1a    | 1404 | 5MC  | C5-C4 | 6.36   | 1.48        | 1.44     |
| 32  | 2a    | 1404 | 5MC  | C5-C4 | 5.86   | 1.48        | 1.44     |

The worst 5 of 299 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB | -21.15 | 64.35       | 102.36   |
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB | -14.05 | 77.11       | 102.36   |
| 1   | 2A    | 2503 | 2MA  | C5-C4-N3  | -8.55  | 118.17      | 127.18   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3 | -8.21 | 118.54      | 127.18   |
| 1   | 2A    | 2605 | PSU  | N1-C2-N3 | 7.00  | 122.55      | 115.17   |

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 32  | 1a    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 32  | 2a    | 1207 | 2MG  | N1-C2-N2-CM2    |
| 32  | 2a    | 1207 | 2MG  | N3-C2-N2-CM2    |
| 32  | 2a    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 43  | 2l    | 92   | 0TD  | O-C-CA-CB       |

There are no ring outliers.

28 monomers are involved in 37 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1A    | 1939 | 5MU  | 1       | 0            |
| 1   | 2A    | 2251 | OMG  | 1       | 0            |
| 55  | 1x    | 8    | 4SU  | 1       | 0            |
| 32  | 1a    | 516  | PSU  | 1       | 0            |
| 1   | 1A    | 1915 | 5MU  | 2       | 0            |
| 1   | 1A    | 2552 | OMU  | 1       | 0            |
| 32  | 1a    | 1518 | MA6  | 2       | 0            |
| 32  | 1a    | 1207 | 2MG  | 2       | 0            |
| 32  | 1a    | 966  | M2G  | 1       | 0            |
| 1   | 1A    | 1920 | OMC  | 1       | 0            |
| 32  | 1a    | 1519 | MA6  | 2       | 0            |
| 32  | 2a    | 1518 | MA6  | 4       | 0            |
| 55  | 2x    | 8    | 4SU  | 1       | 0            |
| 32  | 2a    | 1404 | 5MC  | 1       | 0            |
| 55  | 1x    | 21   | H2U  | 1       | 0            |
| 32  | 2a    | 1402 | 4OC  | 2       | 0            |
| 55  | 1x    | 76   | 8AN  | 4       | 0            |
| 1   | 1A    | 2503 | 2MA  | 1       | 0            |
| 32  | 2a    | 1207 | 2MG  | 2       | 0            |
| 55  | 1x    | 20   | H2U  | 1       | 0            |
| 1   | 2A    | 1939 | 5MU  | 1       | 0            |
| 1   | 1A    | 1942 | 5MC  | 1       | 0            |
| 43  | 1l    | 92   | 0TD  | 1       | 0            |
| 55  | 2x    | 76   | 8AN  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32  | 1a    | 1404 | 5MC  | 1       | 0            |
| 32  | 2a    | 1519 | MA6  | 3       | 0            |
| 32  | 1a    | 1402 | 4OC  | 2       | 0            |
| 55  | 2x    | 55   | PSU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2664 ligands modelled in this entry, 2662 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 | $\# Z  > 2$ |
| 60  | SF4  | 2d    | 303 | 35   | 0,12,12      | -    | -           | -           |      |             |
| 60  | 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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 60  | SF4  | 2d    | 303 | 35   | -       | -        | 0/6/5/5 |
| 60  | 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.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 60  | 1d    | 302 | SF4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%) | -0.37  | 174 (6%) | 27  | 20  | 9, 24, 87, 101        | 0     |
| 1   | 2A    | 2789/2915 (95%) | 0.04   | 142 (5%) | 33  | 25  | 22, 43, 83, 100       | 0     |
| 2   | 1B    | 120/121 (99%)   | -0.28  | 0        | 100 | 100 | 20, 40, 53, 78        | 0     |
| 2   | 2B    | 120/121 (99%)   | 0.58   | 0        | 100 | 100 | 45, 64, 73, 84        | 0     |
| 3   | 1D    | 275/276 (99%)   | -0.41  | 1 (0%)   | 88  | 84  | 12, 24, 38, 68        | 0     |
| 3   | 2D    | 275/276 (99%)   | -0.07  | 4 (1%)   | 72  | 63  | 20, 36, 48, 68        | 0     |
| 4   | 1E    | 204/206 (99%)   | -0.40  | 0        | 100 | 100 | 10, 25, 46, 60        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.08   | 1 (0%)   | 87  | 82  | 23, 41, 57, 68        | 0     |
| 5   | 1F    | 203/210 (96%)   | -0.28  | 1 (0%)   | 87  | 82  | 10, 27, 57, 78        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.36   | 2 (0%)   | 79  | 72  | 22, 51, 66, 78        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.65   | 12 (6%)  | 24  | 18  | 34, 51, 66, 77        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.26   | 26 (14%) | 6   | 5   | 58, 66, 76, 84        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.15   | 4 (2%)   | 61  | 51  | 26, 39, 53, 60        | 0     |
| 7   | 2H    | 174/180 (96%)   | 1.13   | 23 (13%) | 7   | 6   | 53, 69, 79, 85        | 0     |
| 8   | 1I    | 146/148 (98%)   | 0.66   | 3 (2%)   | 63  | 54  | 31, 58, 68, 72        | 0     |
| 8   | 2I    | 146/148 (98%)   | 0.74   | 6 (4%)   | 41  | 33  | 42, 61, 68, 75        | 0     |
| 9   | 1N    | 140/140 (100%)  | -0.42  | 1 (0%)   | 84  | 77  | 15, 24, 45, 61        | 0     |
| 9   | 2N    | 140/140 (100%)  | 0.37   | 2 (1%)   | 73  | 64  | 30, 49, 63, 70        | 0     |
| 10  | 1O    | 122/122 (100%)  | -0.40  | 0        | 100 | 100 | 16, 26, 43, 47        | 0     |
| 10  | 2O    | 122/122 (100%)  | -0.01  | 0        | 100 | 100 | 30, 39, 54, 60        | 0     |
| 11  | 1P    | 149/150 (99%)   | -0.19  | 0        | 100 | 100 | 10, 32, 53, 66        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.47   | 1 (0%)   | 84  | 77  | 29, 53, 68, 75        | 0     |
| 12  | 1Q    | 141/141 (100%)  | -0.25  | 2 (1%)   | 73  | 64  | 16, 27, 42, 53        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 0.43   | 3 (2%)   | 63  | 54  | 32, 49, 60, 66        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | -0.51  | 0 100 100     | 15, 22, 35, 47        | 0     |
| 13  | 2R    | 118/118 (100%) | -0.03  | 1 (0%) 82 75  | 29, 38, 50, 59        | 0     |
| 14  | 1S    | 110/112 (98%)  | -0.01  | 1 (0%) 81 74  | 29, 40, 52, 58        | 0     |
| 14  | 2S    | 110/112 (98%)  | 1.07   | 16 (14%) 6 4  | 48, 59, 67, 71        | 0     |
| 15  | 1T    | 131/146 (89%)  | -0.19  | 2 (1%) 72 63  | 20, 30, 58, 65        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.21   | 3 (2%) 61 51  | 34, 43, 66, 71        | 0     |
| 16  | 1U    | 116/118 (98%)  | -0.54  | 1 (0%) 81 74  | 11, 17, 29, 47        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.18   | 0 100 100     | 29, 46, 58, 66        | 0     |
| 17  | 1V    | 101/101 (100%) | -0.45  | 0 100 100     | 11, 24, 42, 59        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.39   | 0 100 100     | 30, 54, 66, 73        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.50  | 1 (0%) 81 74  | 11, 18, 36, 68        | 0     |
| 18  | 2W    | 112/113 (99%)  | -0.05  | 0 100 100     | 27, 37, 52, 75        | 0     |
| 19  | 1X    | 95/96 (98%)    | -0.27  | 1 (1%) 78 70  | 15, 27, 51, 64        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.41   | 3 (3%) 50 40  | 37, 47, 62, 75        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.03   | 3 (2%) 55 45  | 22, 35, 53, 73        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 0.77   | 6 (5%) 30 23  | 45, 58, 70, 77        | 0     |
| 21  | 1Z    | 154/206 (74%)  | 0.31   | 4 (2%) 57 47  | 26, 44, 62, 66        | 0     |
| 21  | 2Z    | 160/206 (77%)  | 0.94   | 10 (6%) 26 19 | 49, 63, 73, 76        | 0     |
| 22  | 10    | 76/85 (89%)    | -0.34  | 2 (2%) 57 47  | 18, 25, 44, 58        | 0     |
| 22  | 20    | 76/85 (89%)    | 0.63   | 6 (7%) 18 13  | 38, 49, 62, 72        | 0     |
| 23  | 11    | 97/98 (98%)    | -0.10  | 1 (1%) 79 72  | 16, 31, 57, 63        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.23   | 1 (1%) 79 72  | 28, 44, 64, 68        | 0     |
| 24  | 12    | 70/72 (97%)    | -0.09  | 0 100 100     | 24, 36, 48, 64        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.54   | 3 (4%) 40 31  | 46, 56, 67, 71        | 0     |
| 25  | 13    | 59/60 (98%)    | -0.38  | 0 100 100     | 15, 21, 42, 59        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.24   | 0 100 100     | 39, 46, 63, 66        | 0     |
| 26  | 14    | 69/71 (97%)    | 1.22   | 14 (20%) 3 2  | 44, 68, 82, 86        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.67   | 20 (28%) 1 1  | 60, 74, 81, 88        | 0     |
| 27  | 15    | 59/60 (98%)    | -0.59  | 0 100 100     | 9, 19, 37, 44         | 0     |
| 27  | 25    | 59/60 (98%)    | -0.00  | 1 (1%) 69 60  | 22, 39, 53, 64        | 0     |
| 28  | 16    | 53/54 (98%)    | -0.32  | 0 100 100     | 23, 29, 38, 46        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.12   | 0 100 100      | 37, 46, 55, 60        | 0     |
| 29  | 17    | 48/49 (97%)     | -0.19  | 2 (4%) 40 32   | 12, 18, 43, 52        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.11   | 1 (2%) 63 54   | 23, 31, 51, 63        | 0     |
| 30  | 18    | 64/65 (98%)     | -0.56  | 0 100 100      | 15, 21, 28, 39        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.25   | 0 100 100      | 33, 42, 49, 55        | 0     |
| 31  | 19    | 37/37 (100%)    | -0.29  | 0 100 100      | 17, 27, 45, 45        | 0     |
| 31  | 29    | 37/37 (100%)    | 0.68   | 1 (2%) 56 46   | 44, 51, 59, 61        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.66   | 118 (7%) 18 13 | 21, 61, 84, 99        | 0     |
| 32  | 2a    | 1491/1521 (98%) | 0.65   | 121 (8%) 18 13 | 31, 61, 85, 98        | 0     |
| 33  | 1b    | 231/256 (90%)   | 1.28   | 38 (16%) 4 3   | 50, 67, 76, 83        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.42   | 52 (22%) 2 1   | 56, 71, 79, 86        | 0     |
| 34  | 1c    | 206/239 (86%)   | 1.38   | 36 (17%) 4 3   | 56, 69, 77, 80        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.36   | 37 (17%) 3 3   | 59, 70, 77, 84        | 0     |
| 35  | 1d    | 208/209 (99%)   | 1.07   | 23 (11%) 10 7  | 47, 61, 71, 78        | 0     |
| 35  | 2d    | 208/209 (99%)   | 0.77   | 9 (4%) 40 31   | 47, 57, 66, 71        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.50   | 1 (0%) 84 77   | 33, 54, 65, 75        | 0     |
| 36  | 2e    | 148/162 (91%)   | 0.73   | 9 (6%) 27 20   | 44, 57, 66, 76        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.62   | 3 (3%) 52 42   | 42, 56, 64, 68        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.76   | 5 (5%) 34 26   | 53, 61, 68, 71        | 0     |
| 38  | 1g    | 155/156 (99%)   | 1.02   | 19 (12%) 8 6   | 53, 64, 76, 80        | 0     |
| 38  | 2g    | 155/156 (99%)   | 1.23   | 23 (14%) 5 4   | 58, 68, 77, 82        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.62   | 6 (4%) 39 31   | 44, 55, 62, 68        | 0     |
| 39  | 2h    | 137/138 (99%)   | 0.57   | 1 (0%) 84 77   | 47, 58, 65, 73        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.68   | 36 (28%) 1 1   | 51, 69, 74, 80        | 0     |
| 40  | 2i    | 127/128 (99%)   | 1.82   | 46 (36%) 1 0   | 61, 73, 77, 82        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.71   | 31 (31%) 1 1   | 56, 72, 80, 83        | 0     |
| 41  | 2j    | 96/105 (91%)    | 2.10   | 47 (48%) 0 0   | 61, 74, 81, 84        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.49   | 5 (4%) 39 31   | 28, 54, 66, 73        | 0     |
| 42  | 2k    | 114/129 (88%)   | 0.67   | 8 (7%) 22 16   | 45, 59, 70, 80        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.58   | 6 (4%) 34 26   | 35, 48, 60, 67        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.30   | 1 (0%) 82 75   | 40, 47, 57, 68        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 118/126 (93%)     | 1.53   | 31 (26%) 1 1    | 56, 68, 74, 78        | 0     |
| 44  | 2m    | 116/126 (92%)     | 1.69   | 39 (33%) 1 1    | 60, 71, 76, 77        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.71   | 15 (25%) 2 1    | 57, 69, 74, 76        | 0     |
| 45  | 2n    | 60/61 (98%)       | 1.87   | 23 (38%) 1 0    | 63, 72, 77, 78        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.50   | 2 (2%) 61 51    | 35, 53, 64, 68        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.82   | 8 (9%) 15 11    | 45, 58, 67, 73        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.40   | 18 (21%) 2 2    | 52, 61, 71, 79        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.81   | 5 (6%) 27 20    | 46, 56, 63, 70        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.66   | 3 (3%) 52 42    | 43, 53, 65, 68        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.40   | 2 (2%) 65 56    | 43, 54, 63, 69        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.41   | 0 100 100       | 41, 52, 67, 71        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.86   | 3 (4%) 39 31    | 52, 60, 69, 76        | 0     |
| 50  | 1s    | 83/93 (89%)       | 1.94   | 34 (40%) 0 0    | 63, 72, 79, 81        | 0     |
| 50  | 2s    | 83/93 (89%)       | 1.97   | 36 (43%) 0 0    | 67, 76, 82, 84        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.77   | 7 (7%) 21 15    | 47, 58, 67, 78        | 0     |
| 51  | 2t    | 96/106 (90%)      | 0.80   | 4 (4%) 40 32    | 44, 55, 67, 70        | 0     |
| 52  | 1u    | 23/27 (85%)       | 2.06   | 8 (34%) 1 0     | 56, 68, 71, 75        | 0     |
| 52  | 2u    | 23/27 (85%)       | 1.54   | 6 (26%) 1 1     | 64, 69, 74, 78        | 0     |
| 53  | 1v    | 9/24 (37%)        | 0.55   | 2 (22%) 2 1     | 39, 41, 73, 83        | 0     |
| 53  | 2v    | 9/24 (37%)        | 1.12   | 3 (33%) 1 1     | 49, 53, 80, 87        | 0     |
| 54  | 1w    | 249/354 (70%)     | 0.33   | 6 (2%) 59 49    | 15, 48, 66, 80        | 0     |
| 54  | 2w    | 253/354 (71%)     | 0.54   | 6 (2%) 59 49    | 32, 55, 72, 82        | 0     |
| 55  | 1x    | 65/74 (87%)       | 0.06   | 0 100 100       | 16, 50, 66, 71        | 0     |
| 55  | 2x    | 65/74 (87%)       | 0.35   | 0 100 100       | 32, 60, 73, 79        | 0     |
| 56  | 1z    | 5/7 (71%)         | 0.95   | 1 (20%) 3 2     | 16, 20, 34, 50        | 0     |
| 56  | 2z    | 4/7 (57%)         | 0.71   | 1 (25%) 2 1     | 33, 35, 36, 40        | 0     |
| All | All   | 21074/22160 (95%) | 0.35   | 1456 (6%) 23 16 | 9, 50, 77, 101        | 0     |

The worst 5 of 1456 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 2112 | G    | 8.7  |
| 1   | 2A    | 2147 | G    | 8.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 2146 | C    | 8.5  |
| 1   | 2A    | 2145 | C    | 8.5  |
| 1   | 1A    | 2117 | A    | 8.2  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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  | H2U  | 1x    | 21   | 20/21 | 0.74 | 0.16 | 66,85,89,106               | 0     |
| 55  | H2U  | 2x    | 21   | 20/21 | 0.74 | 0.17 | 76,84,91,98                | 0     |
| 55  | H2U  | 2x    | 20   | 20/21 | 0.75 | 0.14 | 68,78,83,86                | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.82 | 0.16 | 65,74,83,85                | 0     |
| 55  | PSU  | 2x    | 55   | 20/21 | 0.82 | 0.12 | 62,69,77,82                | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.84 | 0.15 | 61,71,77,79                | 0     |
| 55  | PSU  | 2x    | 32   | 20/21 | 0.87 | 0.12 | 54,62,67,68                | 0     |
| 55  | 5MU  | 2x    | 54   | 21/22 | 0.88 | 0.11 | 62,68,75,80                | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.88 | 0.13 | 44,49,53,68                | 0     |
| 55  | MIA  | 2x    | 37   | 22/30 | 0.89 | 0.11 | 53,62,64,66                | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.90 | 0.11 | 54,61,65,66                | 0     |
| 55  | 5MU  | 1x    | 54   | 21/22 | 0.90 | 0.13 | 51,61,69,73                | 0     |
| 55  | H2U  | 1x    | 20   | 20/21 | 0.90 | 0.10 | 52,67,79,79                | 0     |
| 55  | PSU  | 1x    | 55   | 20/21 | 0.90 | 0.11 | 52,59,69,71                | 0     |
| 32  | G7M  | 2a    | 527  | 24/25 | 0.90 | 0.12 | 47,56,60,65                | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.91 | 0.11 | 41,49,55,60                | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.91 | 0.13 | 46,56,67,71                | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.91 | 0.12 | 47,60,66,67                | 0     |
| 55  | PSU  | 2x    | 39   | 20/21 | 0.91 | 0.10 | 43,60,64,66                | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.92 | 0.10 | 43,48,51,59                | 0     |
| 55  | PSU  | 1x    | 32   | 20/21 | 0.92 | 0.11 | 50,54,63,66                | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.92 | 0.11 | 40,49,55,57                | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.93 | 0.12 | 52,56,65,68                | 0     |
| 55  | MIA  | 1x    | 37   | 22/30 | 0.94 | 0.09 | 41,51,55,60                | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.94 | 0.12 | 45,55,60,62                | 0     |
| 55  | PSU  | 1x    | 39   | 20/21 | 0.94 | 0.10 | 35,44,51,55                | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.94 | 0.10 | 42,48,59,64                | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.95 | 0.10 | 39,44,48,49                | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.95 | 0.09 | 38,43,47,53                | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.95 | 0.10 | 34,45,51,52                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.95 | 0.11 | 39,43,50,51                 | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.95 | 0.08 | 36,44,48,53                 | 0     |
| 55  | 4SU  | 2x    | 8    | 20/21 | 0.95 | 0.09 | 45,63,67,68                 | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.95 | 0.09 | 40,47,49,51                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.95 | 0.08 | 25,38,41,42                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.95 | 0.09 | 39,47,54,57                 | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.95 | 0.09 | 35,47,52,54                 | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.96 | 0.09 | 30,36,39,43                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.96 | 0.09 | 29,37,42,48                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.96 | 0.08 | 29,37,41,44                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.96 | 0.11 | 20,30,37,39                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.96 | 0.09 | 23,29,36,40                 | 0     |
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.96 | 0.09 | 31,40,44,45                 | 0     |
| 55  | 4SU  | 1x    | 8    | 20/21 | 0.96 | 0.08 | 29,40,45,45                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.96 | 0.10 | 39,46,49,50                 | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.96 | 0.08 | 32,37,40,43                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.96 | 0.08 | 27,31,34,38                 | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.96 | 0.08 | 41,45,50,51                 | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.97 | 0.08 | 28,34,41,42                 | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.07 | 14,24,29,31                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.97 | 0.09 | 16,24,26,32                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.97 | 0.07 | 22,28,34,35                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.07 | 20,23,27,30                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.07 | 20,25,29,31                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.97 | 0.07 | 26,32,34,37                 | 0     |
| 55  | 8AN  | 2x    | 76   | 22/23 | 0.97 | 0.08 | 27,32,34,43                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.06 | 11,16,20,22                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.98 | 0.07 | 26,30,36,40                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.07 | 9,12,14,19                  | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.06 | 8,11,13,14                  | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.98 | 0.08 | 19,25,29,31                 | 0     |
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.98 | 0.06 | 11,16,19,20                 | 0     |
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.98 | 0.07 | 13,15,19,22                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.98 | 0.07 | 21,29,31,34                 | 0     |
| 55  | 8AN  | 1x    | 76   | 22/23 | 0.98 | 0.06 | 10,14,18,21                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.98 | 0.07 | 22,25,28,33                 | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 57  | MG   | 1X    | 105  | 1/1   | 0.52 | 0.26 | 58,58,58,58                | 0     |
| 57  | MG   | 2A    | 3835 | 1/1   | 0.56 | 0.16 | 58,58,58,58                | 0     |
| 57  | MG   | 2a    | 1731 | 1/1   | 0.61 | 0.20 | 57,57,57,57                | 0     |
| 57  | MG   | 2A    | 3593 | 1/1   | 0.62 | 0.26 | 65,65,65,65                | 0     |
| 57  | MG   | 1A    | 3524 | 1/1   | 0.63 | 0.24 | 57,57,57,57                | 0     |
| 57  | MG   | 2A    | 3049 | 1/1   | 0.63 | 0.30 | 55,55,55,55                | 0     |
| 57  | MG   | 2A    | 3490 | 1/1   | 0.63 | 0.26 | 54,54,54,54                | 0     |
| 57  | MG   | 1A    | 3848 | 1/1   | 0.63 | 0.24 | 42,42,42,42                | 0     |
| 57  | MG   | 1A    | 4032 | 1/1   | 0.63 | 0.43 | 75,75,75,75                | 0     |
| 57  | MG   | 1B    | 233  | 1/1   | 0.63 | 0.22 | 74,74,74,74                | 0     |
| 57  | MG   | 2A    | 3094 | 1/1   | 0.64 | 0.37 | 71,71,71,71                | 0     |
| 57  | MG   | 1A    | 3917 | 1/1   | 0.65 | 0.15 | 20,20,20,20                | 0     |
| 57  | MG   | 2B    | 207  | 1/1   | 0.66 | 0.21 | 64,64,64,64                | 0     |
| 57  | MG   | 2A    | 3808 | 1/1   | 0.66 | 0.20 | 62,62,62,62                | 0     |
| 57  | MG   | 1a    | 3675 | 1/1   | 0.67 | 0.34 | 65,65,65,65                | 0     |
| 57  | MG   | 2A    | 3335 | 1/1   | 0.67 | 0.24 | 47,47,47,47                | 0     |
| 57  | MG   | 2A    | 3118 | 1/1   | 0.68 | 0.19 | 65,65,65,65                | 0     |
| 57  | MG   | 1A    | 3949 | 1/1   | 0.68 | 0.19 | 59,59,59,59                | 0     |
| 57  | MG   | 1a    | 3681 | 1/1   | 0.69 | 0.31 | 57,57,57,57                | 0     |
| 57  | MG   | 2A    | 3694 | 1/1   | 0.69 | 0.18 | 53,53,53,53                | 0     |
| 57  | MG   | 2A    | 3263 | 1/1   | 0.69 | 0.14 | 51,51,51,51                | 0     |
| 57  | MG   | 2a    | 1740 | 1/1   | 0.69 | 0.29 | 68,68,68,68                | 0     |
| 57  | MG   | 2A    | 3083 | 1/1   | 0.70 | 0.18 | 77,77,77,77                | 0     |
| 57  | MG   | 1B    | 236  | 1/1   | 0.70 | 0.27 | 58,58,58,58                | 0     |
| 57  | MG   | 1A    | 4077 | 1/1   | 0.70 | 0.20 | 39,39,39,39                | 0     |
| 57  | MG   | 2A    | 3626 | 1/1   | 0.70 | 0.22 | 66,66,66,66                | 0     |
| 57  | MG   | 1a    | 3563 | 1/1   | 0.70 | 0.28 | 65,65,65,65                | 0     |
| 57  | MG   | 2a    | 1747 | 1/1   | 0.70 | 0.27 | 69,69,69,69                | 0     |
| 57  | MG   | 2A    | 3816 | 1/1   | 0.71 | 0.14 | 50,50,50,50                | 0     |
| 57  | MG   | 2A    | 3622 | 1/1   | 0.71 | 0.15 | 55,55,55,55                | 0     |
| 57  | MG   | 1a    | 3613 | 1/1   | 0.71 | 0.23 | 46,46,46,46                | 0     |
| 57  | MG   | 1A    | 3496 | 1/1   | 0.71 | 0.11 | 55,55,55,55                | 0     |
| 57  | MG   | 2A    | 3700 | 1/1   | 0.71 | 0.18 | 40,40,40,40                | 0     |
| 57  | MG   | 2A    | 3295 | 1/1   | 0.71 | 0.22 | 55,55,55,55                | 0     |
| 57  | MG   | 1A    | 3773 | 1/1   | 0.72 | 0.17 | 53,53,53,53                | 0     |
| 57  | MG   | 1A    | 3970 | 1/1   | 0.72 | 0.22 | 67,67,67,67                | 0     |
| 57  | MG   | 1B    | 219  | 1/1   | 0.72 | 0.15 | 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    | 3383 | 1/1   | 0.73 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3808 | 1/1   | 0.73 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 2f    | 201  | 1/1   | 0.73 | 0.22 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3655 | 1/1   | 0.74 | 0.25 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 4031 | 1/1   | 0.74 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3969 | 1/1   | 0.74 | 0.28 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3803 | 1/1   | 0.74 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3162 | 1/1   | 0.74 | 0.24 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3804 | 1/1   | 0.74 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2i    | 201  | 1/1   | 0.74 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3334 | 1/1   | 0.75 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3033 | 1/1   | 0.75 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1B    | 222  | 1/1   | 0.75 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3519 | 1/1   | 0.75 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3163 | 1/1   | 0.75 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2R    | 201  | 1/1   | 0.75 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3246 | 1/1   | 0.75 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3685 | 1/1   | 0.75 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3866 | 1/1   | 0.75 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1757 | 1/1   | 0.75 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3326 | 1/1   | 0.75 | 0.28 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3746 | 1/1   | 0.75 | 0.28 | 80,80,80,80                 | 0     |
| 57  | MG   | 2A    | 3396 | 1/1   | 0.76 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 4064 | 1/1   | 0.76 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1732 | 1/1   | 0.76 | 0.28 | 75,75,75,75                 | 0     |
| 57  | MG   | 1a    | 3624 | 1/1   | 0.76 | 0.38 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3344 | 1/1   | 0.76 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3854 | 1/1   | 0.76 | 0.13 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3464 | 1/1   | 0.76 | 0.21 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3595 | 1/1   | 0.76 | 0.26 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3514 | 1/1   | 0.77 | 0.28 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3810 | 1/1   | 0.77 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3499 | 1/1   | 0.77 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1I    | 201  | 1/1   | 0.77 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 1U    | 212  | 1/1   | 0.77 | 0.55 | 53,53,53,53                 | 0     |
| 57  | MG   | 1x    | 108  | 1/1   | 0.77 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3770 | 1/1   | 0.77 | 0.16 | 8,8,8,8                     | 0     |
| 57  | MG   | 2A    | 3310 | 1/1   | 0.77 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 4081 | 1/1   | 0.77 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3430 | 1/1   | 0.77 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3611 | 1/1   | 0.77 | 0.12 | 13,13,13,13                 | 0     |
| 57  | MG   | 2A    | 3804 | 1/1   | 0.77 | 0.15 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3712 | 1/1   | 0.78 | 0.18 | 66,66,66,66                 | 0     |
| 57  | MG   | 1x    | 106  | 1/1   | 0.78 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | 2B    | 202  | 1/1   | 0.78 | 0.22 | 61,61,61,61                 | 0     |
| 57  | MG   | 2B    | 203  | 1/1   | 0.78 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3999 | 1/1   | 0.78 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 2B    | 210  | 1/1   | 0.78 | 0.23 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3520 | 1/1   | 0.78 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1655 | 1/1   | 0.78 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3633 | 1/1   | 0.78 | 0.21 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3244 | 1/1   | 0.78 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3352 | 1/1   | 0.78 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3247 | 1/1   | 0.78 | 0.22 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3742 | 1/1   | 0.78 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | 2a    | 1759 | 1/1   | 0.78 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3275 | 1/1   | 0.78 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 2g    | 201  | 1/1   | 0.78 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3515 | 1/1   | 0.78 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1B    | 232  | 1/1   | 0.79 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3282 | 1/1   | 0.79 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3676 | 1/1   | 0.79 | 0.21 | 74,74,74,74                 | 0     |
| 57  | MG   | 1a    | 3679 | 1/1   | 0.79 | 0.21 | 66,66,66,66                 | 0     |
| 57  | MG   | 1B    | 235  | 1/1   | 0.79 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3409 | 1/1   | 0.79 | 0.26 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3892 | 1/1   | 0.79 | 0.18 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3348 | 1/1   | 0.79 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 4034 | 1/1   | 0.79 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3030 | 1/1   | 0.79 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3507 | 1/1   | 0.79 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1610 | 1/1   | 0.79 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3506 | 1/1   | 0.79 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 3533 | 1/1   | 0.79 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3541 | 1/1   | 0.79 | 0.26 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3630 | 1/1   | 0.79 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3144 | 1/1   | 0.79 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3510 | 1/1   | 0.79 | 0.33 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3381 | 1/1   | 0.79 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3646 | 1/1   | 0.79 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3972 | 1/1   | 0.79 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3646 | 1/1   | 0.79 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3977 | 1/1   | 0.80 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3564 | 1/1   | 0.80 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3361 | 1/1   | 0.80 | 0.24 | 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    | 3791 | 1/1   | 0.80 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3602 | 1/1   | 0.80 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3719 | 1/1   | 0.80 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 4004 | 1/1   | 0.80 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3503 | 1/1   | 0.80 | 0.26 | 74,74,74,74                 | 0     |
| 57  | MG   | 2A    | 3548 | 1/1   | 0.80 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3630 | 1/1   | 0.80 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3602 | 1/1   | 0.80 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 26    | 101  | 1/1   | 0.80 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3276 | 1/1   | 0.80 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3919 | 1/1   | 0.80 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1667 | 1/1   | 0.80 | 0.32 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 1690 | 1/1   | 0.80 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1714 | 1/1   | 0.80 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3900 | 1/1   | 0.80 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3643 | 1/1   | 0.80 | 0.28 | 68,68,68,68                 | 0     |
| 57  | MG   | 1a    | 3659 | 1/1   | 0.80 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3663 | 1/1   | 0.80 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3669 | 1/1   | 0.80 | 0.13 | 59,59,59,59                 | 0     |
| 57  | MG   | 1E    | 311  | 1/1   | 0.80 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3117 | 1/1   | 0.80 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3703 | 1/1   | 0.80 | 0.21 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3728 | 1/1   | 0.80 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 2j    | 202  | 1/1   | 0.80 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3500 | 1/1   | 0.81 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3810 | 1/1   | 0.81 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3664 | 1/1   | 0.81 | 0.37 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3673 | 1/1   | 0.81 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1B    | 214  | 1/1   | 0.81 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3557 | 1/1   | 0.81 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3246 | 1/1   | 0.81 | 0.47 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3594 | 1/1   | 0.81 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3442 | 1/1   | 0.81 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4009 | 1/1   | 0.81 | 0.16 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3702 | 1/1   | 0.81 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3629 | 1/1   | 0.81 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 4027 | 1/1   | 0.81 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1668 | 1/1   | 0.81 | 0.39 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3641 | 1/1   | 0.81 | 0.20 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3817 | 1/1   | 0.81 | 0.19 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3446 | 1/1   | 0.81 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 1B    | 237  | 1/1   | 0.81 | 0.15 | 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    | 3613 | 1/1   | 0.81 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3201 | 1/1   | 0.81 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1750 | 1/1   | 0.81 | 0.25 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3871 | 1/1   | 0.81 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3075 | 1/1   | 0.81 | 0.29 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1769 | 1/1   | 0.81 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3662 | 1/1   | 0.81 | 0.12 | 10,10,10,10                 | 0     |
| 57  | MG   | 1a    | 3647 | 1/1   | 0.81 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 1Y    | 202  | 1/1   | 0.81 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 18    | 104  | 1/1   | 0.81 | 0.19 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3715 | 1/1   | 0.82 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3340 | 1/1   | 0.82 | 0.21 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3615 | 1/1   | 0.82 | 0.27 | 59,59,59,59                 | 0     |
| 57  | MG   | 15    | 3209 | 1/1   | 0.82 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3031 | 1/1   | 0.82 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3385 | 1/1   | 0.82 | 0.30 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3628 | 1/1   | 0.82 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3807 | 1/1   | 0.82 | 0.10 | 22,22,22,22                 | 0     |
| 57  | MG   | 1a    | 3631 | 1/1   | 0.82 | 0.24 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3450 | 1/1   | 0.82 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3502 | 1/1   | 0.82 | 0.22 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3756 | 1/1   | 0.82 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3098 | 1/1   | 0.82 | 0.30 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3518 | 1/1   | 0.82 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3097 | 1/1   | 0.82 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3540 | 1/1   | 0.82 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1631 | 1/1   | 0.82 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 1635 | 1/1   | 0.82 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 1636 | 1/1   | 0.82 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3656 | 1/1   | 0.82 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3785 | 1/1   | 0.82 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3621 | 1/1   | 0.82 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3188 | 1/1   | 0.82 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3588 | 1/1   | 0.82 | 0.08 | 6,6,6,6                     | 0     |
| 57  | MG   | 1a    | 3574 | 1/1   | 0.82 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3579 | 1/1   | 0.82 | 0.25 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3640 | 1/1   | 0.82 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3269 | 1/1   | 0.82 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3682 | 1/1   | 0.82 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1751 | 1/1   | 0.82 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 3699 | 1/1   | 0.82 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3660 | 1/1   | 0.82 | 0.12 | 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    | 1760 | 1/1   | 0.82 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3793 | 1/1   | 0.82 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 1774 | 1/1   | 0.82 | 0.29 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3794 | 1/1   | 0.82 | 0.21 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 3607 | 1/1   | 0.82 | 0.30 | 75,75,75,75                 | 0     |
| 57  | MG   | 1l    | 201  | 1/1   | 0.82 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3087 | 1/1   | 0.82 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3758 | 1/1   | 0.83 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3783 | 1/1   | 0.83 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3364 | 1/1   | 0.83 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 1B    | 223  | 1/1   | 0.83 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3093 | 1/1   | 0.83 | 0.27 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3403 | 1/1   | 0.83 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | 1B    | 231  | 1/1   | 0.83 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3719 | 1/1   | 0.83 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3114 | 1/1   | 0.83 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3350 | 1/1   | 0.83 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3367 | 1/1   | 0.83 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3283 | 1/1   | 0.83 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 2D    | 304  | 1/1   | 0.83 | 0.23 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3570 | 1/1   | 0.83 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3549 | 1/1   | 0.83 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3936 | 1/1   | 0.83 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1625 | 1/1   | 0.83 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 1630 | 1/1   | 0.83 | 0.26 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3585 | 1/1   | 0.83 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 1634 | 1/1   | 0.83 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3449 | 1/1   | 0.83 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3689 | 1/1   | 0.83 | 0.24 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3696 | 1/1   | 0.83 | 0.26 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1661 | 1/1   | 0.83 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | 1F    | 310  | 1/1   | 0.83 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3266 | 1/1   | 0.83 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 1677 | 1/1   | 0.83 | 0.25 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 1688 | 1/1   | 0.83 | 0.31 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3832 | 1/1   | 0.83 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1710 | 1/1   | 0.83 | 0.27 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3273 | 1/1   | 0.83 | 0.28 | 60,60,60,60                 | 0     |
| 57  | MG   | 1S    | 203  | 1/1   | 0.83 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 4075 | 1/1   | 0.83 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4076 | 1/1   | 0.83 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3301 | 1/1   | 0.83 | 0.12 | 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    | 3315 | 1/1   | 0.83 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3625 | 1/1   | 0.83 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3331 | 1/1   | 0.83 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1x    | 111  | 1/1   | 0.83 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 13    | 102  | 1/1   | 0.83 | 0.17 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3119 | 1/1   | 0.83 | 0.27 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3568 | 1/1   | 0.83 | 0.27 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3690 | 1/1   | 0.83 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3357 | 1/1   | 0.83 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 4002 | 1/1   | 0.83 | 0.14 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3748 | 1/1   | 0.83 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3628 | 1/1   | 0.84 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3503 | 1/1   | 0.84 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3387 | 1/1   | 0.84 | 0.24 | 38,38,38,38                 | 0     |
| 57  | MG   | 1B    | 227  | 1/1   | 0.84 | 0.20 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 3668 | 1/1   | 0.84 | 0.23 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3421 | 1/1   | 0.84 | 0.29 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3440 | 1/1   | 0.84 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3458 | 1/1   | 0.84 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3476 | 1/1   | 0.84 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 1v    | 101  | 1/1   | 0.84 | 0.27 | 77,77,77,77                 | 0     |
| 57  | MG   | 2A    | 3681 | 1/1   | 0.84 | 0.23 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3907 | 1/1   | 0.84 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3122 | 1/1   | 0.84 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3393 | 1/1   | 0.84 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3559 | 1/1   | 0.84 | 0.19 | 70,70,70,70                 | 0     |
| 57  | MG   | 2a    | 1683 | 1/1   | 0.84 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3593 | 1/1   | 0.84 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3729 | 1/1   | 0.84 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3177 | 1/1   | 0.84 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3788 | 1/1   | 0.84 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3757 | 1/1   | 0.84 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3343 | 1/1   | 0.84 | 0.33 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3581 | 1/1   | 0.84 | 0.22 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1743 | 1/1   | 0.84 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3584 | 1/1   | 0.84 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3347 | 1/1   | 0.84 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3941 | 1/1   | 0.84 | 0.12 | 21,21,21,21                 | 0     |
| 57  | MG   | 2a    | 1753 | 1/1   | 0.84 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3439 | 1/1   | 0.84 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3355 | 1/1   | 0.84 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3830 | 1/1   | 0.84 | 0.21 | 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    | 3606 | 1/1   | 0.84 | 0.16 | 19,19,19,19                 | 0     |
| 57  | MG   | 2a    | 1772 | 1/1   | 0.84 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3610 | 1/1   | 0.84 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3577 | 1/1   | 0.84 | 0.29 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3889 | 1/1   | 0.84 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3669 | 1/1   | 0.84 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | 2j    | 201  | 1/1   | 0.84 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 2B    | 215  | 1/1   | 0.84 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3590 | 1/1   | 0.85 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3780 | 1/1   | 0.85 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1F    | 311  | 1/1   | 0.85 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3698 | 1/1   | 0.85 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 2B    | 211  | 1/1   | 0.85 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3605 | 1/1   | 0.85 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3061 | 1/1   | 0.85 | 0.28 | 49,49,49,49                 | 0     |
| 57  | MG   | 2D    | 305  | 1/1   | 0.85 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 2G    | 201  | 1/1   | 0.85 | 0.22 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3349 | 1/1   | 0.85 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3479 | 1/1   | 0.85 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3918 | 1/1   | 0.85 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3692 | 1/1   | 0.85 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 10    | 101  | 1/1   | 0.85 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3345 | 1/1   | 0.85 | 0.26 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3174 | 1/1   | 0.85 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 1B    | 224  | 1/1   | 0.85 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3797 | 1/1   | 0.85 | 0.09 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 3716 | 1/1   | 0.85 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3405 | 1/1   | 0.85 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3416 | 1/1   | 0.85 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3668 | 1/1   | 0.85 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3798 | 1/1   | 0.85 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3436 | 1/1   | 0.85 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3693 | 1/1   | 0.85 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3254 | 1/1   | 0.85 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1692 | 1/1   | 0.85 | 0.23 | 67,67,67,67                 | 0     |
| 57  | MG   | 2a    | 1695 | 1/1   | 0.85 | 0.30 | 54,54,54,54                 | 0     |
| 57  | MG   | 1b    | 302  | 1/1   | 0.85 | 0.15 | 75,75,75,75                 | 0     |
| 57  | MG   | 2A    | 3464 | 1/1   | 0.85 | 0.24 | 66,66,66,66                 | 0     |
| 57  | MG   | 2a    | 1719 | 1/1   | 0.85 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1724 | 1/1   | 0.85 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3704 | 1/1   | 0.85 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3709 | 1/1   | 0.85 | 0.17 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3467 | 1/1   | 0.85 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3942 | 1/1   | 0.85 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3484 | 1/1   | 0.85 | 0.19 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3734 | 1/1   | 0.85 | 0.14 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3947 | 1/1   | 0.85 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3272 | 1/1   | 0.85 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3520 | 1/1   | 0.85 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3638 | 1/1   | 0.85 | 0.16 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3523 | 1/1   | 0.85 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 1762 | 1/1   | 0.85 | 0.26 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3654 | 1/1   | 0.85 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4055 | 1/1   | 0.85 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3806 | 1/1   | 0.85 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1777 | 1/1   | 0.85 | 0.29 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3951 | 1/1   | 0.85 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3321 | 1/1   | 0.85 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3958 | 1/1   | 0.85 | 0.11 | 63,63,63,63                 | 0     |
| 57  | MG   | 1F    | 304  | 1/1   | 0.85 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | 1a    | 3672 | 1/1   | 0.85 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3209 | 1/1   | 0.86 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3606 | 1/1   | 0.86 | 0.25 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3538 | 1/1   | 0.86 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3314 | 1/1   | 0.86 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3824 | 1/1   | 0.86 | 0.12 | 20,20,20,20                 | 0     |
| 57  | MG   | 1F    | 305  | 1/1   | 0.86 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3507 | 1/1   | 0.86 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3511 | 1/1   | 0.86 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3515 | 1/1   | 0.86 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 1v    | 102  | 1/1   | 0.86 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 1x    | 101  | 1/1   | 0.86 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 1x    | 105  | 1/1   | 0.86 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3282 | 1/1   | 0.86 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3586 | 1/1   | 0.86 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3298 | 1/1   | 0.86 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | 2E    | 301  | 1/1   | 0.86 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 2E    | 304  | 1/1   | 0.86 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3635 | 1/1   | 0.86 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 2Q    | 203  | 1/1   | 0.86 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2Q    | 204  | 1/1   | 0.86 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4036 | 1/1   | 0.86 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2U    | 201  | 1/1   | 0.86 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 2W    | 201  | 1/1   | 0.86 | 0.39 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3314 | 1/1   | 0.86 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1602 | 1/1   | 0.86 | 0.11 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1607 | 1/1   | 0.86 | 0.25 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3316 | 1/1   | 0.86 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1617 | 1/1   | 0.86 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4038 | 1/1   | 0.86 | 0.15 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3324 | 1/1   | 0.86 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3325 | 1/1   | 0.86 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3624 | 1/1   | 0.86 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1T    | 202  | 1/1   | 0.86 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1U    | 202  | 1/1   | 0.86 | 0.29 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3039 | 1/1   | 0.86 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3657 | 1/1   | 0.86 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3056 | 1/1   | 0.86 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3550 | 1/1   | 0.86 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3551 | 1/1   | 0.86 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 1681 | 1/1   | 0.86 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3090 | 1/1   | 0.86 | 0.21 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3653 | 1/1   | 0.86 | 0.29 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1689 | 1/1   | 0.86 | 0.32 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3557 | 1/1   | 0.86 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 1U    | 204  | 1/1   | 0.86 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3382 | 1/1   | 0.86 | 0.26 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3109 | 1/1   | 0.86 | 0.33 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 1711 | 1/1   | 0.86 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3110 | 1/1   | 0.86 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3692 | 1/1   | 0.86 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3592 | 1/1   | 0.86 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 1730 | 1/1   | 0.86 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3759 | 1/1   | 0.86 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3763 | 1/1   | 0.86 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1736 | 1/1   | 0.86 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3392 | 1/1   | 0.86 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 10    | 107  | 1/1   | 0.86 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3142 | 1/1   | 0.86 | 0.25 | 48,48,48,48                 | 0     |
| 57  | MG   | 11    | 102  | 1/1   | 0.86 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3723 | 1/1   | 0.86 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3412 | 1/1   | 0.86 | 0.22 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3160 | 1/1   | 0.86 | 0.08 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3733 | 1/1   | 0.86 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3590 | 1/1   | 0.86 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1761 | 1/1   | 0.86 | 0.17 | 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   | 2A    | 3740 | 1/1   | 0.86 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3591 | 1/1   | 0.86 | 0.23 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3168 | 1/1   | 0.86 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3453 | 1/1   | 0.86 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3693 | 1/1   | 0.86 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3766 | 1/1   | 0.86 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3776 | 1/1   | 0.86 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3088 | 1/1   | 0.86 | 0.24 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3207 | 1/1   | 0.86 | 0.14 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3199 | 1/1   | 0.86 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 2x    | 108  | 1/1   | 0.86 | 0.27 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3555 | 1/1   | 0.87 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3356 | 1/1   | 0.87 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3864 | 1/1   | 0.87 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 1a    | 3695 | 1/1   | 0.87 | 0.25 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3201 | 1/1   | 0.87 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3488 | 1/1   | 0.87 | 0.23 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 4010 | 1/1   | 0.87 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3820 | 1/1   | 0.87 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3235 | 1/1   | 0.87 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3238 | 1/1   | 0.87 | 0.35 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3831 | 1/1   | 0.87 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3251 | 1/1   | 0.87 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3508 | 1/1   | 0.87 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3701 | 1/1   | 0.87 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3470 | 1/1   | 0.87 | 0.42 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3525 | 1/1   | 0.87 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3528 | 1/1   | 0.87 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3546 | 1/1   | 0.87 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3705 | 1/1   | 0.87 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3707 | 1/1   | 0.87 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3268 | 1/1   | 0.87 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3571 | 1/1   | 0.87 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 2F    | 304  | 1/1   | 0.87 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3573 | 1/1   | 0.87 | 0.31 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3574 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | 1P    | 203  | 1/1   | 0.87 | 0.23 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3765 | 1/1   | 0.87 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3600 | 1/1   | 0.87 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | 1T    | 203  | 1/1   | 0.87 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3591 | 1/1   | 0.87 | 0.24 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3473 | 1/1   | 0.87 | 0.12 | 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    | 1603 | 1/1   | 0.87 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4037 | 1/1   | 0.87 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3598 | 1/1   | 0.87 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3610 | 1/1   | 0.87 | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | 1V    | 203  | 1/1   | 0.87 | 0.32 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 4040 | 1/1   | 0.87 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4052 | 1/1   | 0.87 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3167 | 1/1   | 0.87 | 0.27 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3004 | 1/1   | 0.87 | 0.30 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3019 | 1/1   | 0.87 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3787 | 1/1   | 0.87 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3630 | 1/1   | 0.87 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1662 | 1/1   | 0.87 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 1663 | 1/1   | 0.87 | 0.18 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3632 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3178 | 1/1   | 0.87 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3635 | 1/1   | 0.87 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3627 | 1/1   | 0.87 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 12    | 101  | 1/1   | 0.87 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3923 | 1/1   | 0.87 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3644 | 1/1   | 0.87 | 0.27 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3928 | 1/1   | 0.87 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3636 | 1/1   | 0.87 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3346 | 1/1   | 0.87 | 0.24 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1700 | 1/1   | 0.87 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3076 | 1/1   | 0.87 | 0.16 | 33,33,33,33                 | 0     |
| 57  | MG   | 17    | 103  | 1/1   | 0.87 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3931 | 1/1   | 0.87 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3676 | 1/1   | 0.87 | 0.23 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3677 | 1/1   | 0.87 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3091 | 1/1   | 0.87 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3614 | 1/1   | 0.87 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3499 | 1/1   | 0.87 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3500 | 1/1   | 0.87 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3362 | 1/1   | 0.87 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3284 | 1/1   | 0.87 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3187 | 1/1   | 0.87 | 0.20 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3137 | 1/1   | 0.87 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3711 | 1/1   | 0.87 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3714 | 1/1   | 0.87 | 0.24 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3317 | 1/1   | 0.87 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3146 | 1/1   | 0.87 | 0.28 | 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    | 3153 | 1/1   | 0.87 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3123 | 1/1   | 0.87 | 0.20 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3408 | 1/1   | 0.87 | 0.24 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3445 | 1/1   | 0.87 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1770 | 1/1   | 0.87 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3677 | 1/1   | 0.87 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3418 | 1/1   | 0.87 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3822 | 1/1   | 0.87 | 0.25 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3754 | 1/1   | 0.87 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3155 | 1/1   | 0.87 | 0.10 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3352 | 1/1   | 0.87 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3445 | 1/1   | 0.87 | 0.28 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3684 | 1/1   | 0.87 | 0.13 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3778 | 1/1   | 0.87 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3890 | 1/1   | 0.88 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3304 | 1/1   | 0.88 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3084 | 1/1   | 0.88 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3833 | 1/1   | 0.88 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3086 | 1/1   | 0.88 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3089 | 1/1   | 0.88 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3319 | 1/1   | 0.88 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2B    | 206  | 1/1   | 0.88 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3891 | 1/1   | 0.88 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3743 | 1/1   | 0.88 | 0.11 | 8,8,8,8                     | 0     |
| 57  | MG   | 10    | 109  | 1/1   | 0.88 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3685 | 1/1   | 0.88 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3899 | 1/1   | 0.88 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3108 | 1/1   | 0.88 | 0.35 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3596 | 1/1   | 0.88 | 0.37 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3615 | 1/1   | 0.88 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 2E    | 305  | 1/1   | 0.88 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | 2E    | 308  | 1/1   | 0.88 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3619 | 1/1   | 0.88 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3651 | 1/1   | 0.88 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 2O    | 201  | 1/1   | 0.88 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3800 | 1/1   | 0.88 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3623 | 1/1   | 0.88 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3596 | 1/1   | 0.88 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4020 | 1/1   | 0.88 | 0.29 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3627 | 1/1   | 0.88 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3609 | 1/1   | 0.88 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 28    | 101  | 1/1   | 0.88 | 0.15 | 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   | 1A    | 3080 | 1/1   | 0.88 | 0.27 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3351 | 1/1   | 0.88 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3131 | 1/1   | 0.88 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3136 | 1/1   | 0.88 | 0.19 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1614 | 1/1   | 0.88 | 0.25 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3414 | 1/1   | 0.88 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3618 | 1/1   | 0.88 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 3710 | 1/1   | 0.88 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3668 | 1/1   | 0.88 | 0.14 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3370 | 1/1   | 0.88 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3715 | 1/1   | 0.88 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 1D    | 311  | 1/1   | 0.88 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3388 | 1/1   | 0.88 | 0.21 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3390 | 1/1   | 0.88 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3169 | 1/1   | 0.88 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3171 | 1/1   | 0.88 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 1E    | 306  | 1/1   | 0.88 | 0.21 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3269 | 1/1   | 0.88 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 1669 | 1/1   | 0.88 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1671 | 1/1   | 0.88 | 0.22 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3180 | 1/1   | 0.88 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3690 | 1/1   | 0.88 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1f    | 201  | 1/1   | 0.88 | 0.22 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3819 | 1/1   | 0.88 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3779 | 1/1   | 0.88 | 0.34 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 3632 | 1/1   | 0.88 | 0.31 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 1691 | 1/1   | 0.88 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3210 | 1/1   | 0.88 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3212 | 1/1   | 0.88 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3705 | 1/1   | 0.88 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3451 | 1/1   | 0.88 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3236 | 1/1   | 0.88 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3325 | 1/1   | 0.88 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3459 | 1/1   | 0.88 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 1723 | 1/1   | 0.88 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3239 | 1/1   | 0.88 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 1G    | 203  | 1/1   | 0.88 | 0.06 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3944 | 1/1   | 0.88 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3649 | 1/1   | 0.88 | 0.20 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3255 | 1/1   | 0.88 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3384 | 1/1   | 0.88 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3265 | 1/1   | 0.88 | 0.23 | 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    | 3747 | 1/1   | 0.88 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3377 | 1/1   | 0.88 | 0.25 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3752 | 1/1   | 0.88 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3733 | 1/1   | 0.88 | 0.12 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3954 | 1/1   | 0.88 | 0.15 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3509 | 1/1   | 0.88 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3739 | 1/1   | 0.88 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3874 | 1/1   | 0.88 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 4084 | 1/1   | 0.88 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3052 | 1/1   | 0.88 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3789 | 1/1   | 0.88 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3802 | 1/1   | 0.88 | 0.14 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 1773 | 1/1   | 0.88 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3530 | 1/1   | 0.88 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3533 | 1/1   | 0.88 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2a    | 1778 | 1/1   | 0.88 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3535 | 1/1   | 0.88 | 0.13 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3569 | 1/1   | 0.88 | 0.22 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3292 | 1/1   | 0.88 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3813 | 1/1   | 0.88 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 1B    | 208  | 1/1   | 0.88 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 2l    | 202  | 1/1   | 0.88 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 2r    | 101  | 1/1   | 0.88 | 0.28 | 62,62,62,62                 | 0     |
| 57  | MG   | 2v    | 101  | 1/1   | 0.88 | 0.35 | 46,46,46,46                 | 0     |
| 57  | MG   | 2x    | 104  | 1/1   | 0.88 | 0.26 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3477 | 1/1   | 0.88 | 0.19 | 46,46,46,46                 | 0     |
| 58  | K    | 1A    | 3537 | 1/1   | 0.88 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 3717 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3821 | 1/1   | 0.89 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3720 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3229 | 1/1   | 0.89 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3369 | 1/1   | 0.89 | 0.26 | 31,31,31,31                 | 0     |
| 57  | MG   | 2F    | 301  | 1/1   | 0.89 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2F    | 302  | 1/1   | 0.89 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3631 | 1/1   | 0.89 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | 1B    | 201  | 1/1   | 0.89 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3178 | 1/1   | 0.89 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1f    | 202  | 1/1   | 0.89 | 0.28 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3638 | 1/1   | 0.89 | 0.26 | 33,33,33,33                 | 0     |
| 57  | MG   | 1B    | 207  | 1/1   | 0.89 | 0.24 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3518 | 1/1   | 0.89 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 1B    | 209  | 1/1   | 0.89 | 0.21 | 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   | 2Z    | 301  | 1/1   | 0.89 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3205 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3142 | 1/1   | 0.89 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3651 | 1/1   | 0.89 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3194 | 1/1   | 0.89 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3654 | 1/1   | 0.89 | 0.10 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3858 | 1/1   | 0.89 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1611 | 1/1   | 0.89 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3410 | 1/1   | 0.89 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3228 | 1/1   | 0.89 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3386 | 1/1   | 0.89 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3769 | 1/1   | 0.89 | 0.13 | 14,14,14,14                 | 0     |
| 57  | MG   | 2A    | 3002 | 1/1   | 0.89 | 0.29 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3973 | 1/1   | 0.89 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3682 | 1/1   | 0.89 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3685 | 1/1   | 0.89 | 0.19 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 1649 | 1/1   | 0.89 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3687 | 1/1   | 0.89 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1656 | 1/1   | 0.89 | 0.21 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3565 | 1/1   | 0.89 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3979 | 1/1   | 0.89 | 0.22 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3249 | 1/1   | 0.89 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3636 | 1/1   | 0.89 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3480 | 1/1   | 0.89 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3528 | 1/1   | 0.89 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1670 | 1/1   | 0.89 | 0.23 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3570 | 1/1   | 0.89 | 0.28 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4007 | 1/1   | 0.89 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3573 | 1/1   | 0.89 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3542 | 1/1   | 0.89 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3575 | 1/1   | 0.89 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 4019 | 1/1   | 0.89 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3718 | 1/1   | 0.89 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3492 | 1/1   | 0.89 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 4021 | 1/1   | 0.89 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3277 | 1/1   | 0.89 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3730 | 1/1   | 0.89 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1706 | 1/1   | 0.89 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3247 | 1/1   | 0.89 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3290 | 1/1   | 0.89 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3672 | 1/1   | 0.89 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1716 | 1/1   | 0.89 | 0.27 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3916 | 1/1   | 0.89 | 0.22 | 18,18,18,18                 | 0     |
| 57  | MG   | 1a    | 3567 | 1/1   | 0.89 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3299 | 1/1   | 0.89 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1728 | 1/1   | 0.89 | 0.29 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3590 | 1/1   | 0.89 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3591 | 1/1   | 0.89 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3541 | 1/1   | 0.89 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3102 | 1/1   | 0.89 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3086 | 1/1   | 0.89 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3705 | 1/1   | 0.89 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3551 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3554 | 1/1   | 0.89 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3706 | 1/1   | 0.89 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1752 | 1/1   | 0.89 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3566 | 1/1   | 0.89 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1754 | 1/1   | 0.89 | 0.17 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3580 | 1/1   | 0.89 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3584 | 1/1   | 0.89 | 0.21 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3206 | 1/1   | 0.89 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3933 | 1/1   | 0.89 | 0.08 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3592 | 1/1   | 0.89 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1768 | 1/1   | 0.89 | 0.27 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3332 | 1/1   | 0.89 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3127 | 1/1   | 0.89 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3817 | 1/1   | 0.89 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3593 | 1/1   | 0.89 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3339 | 1/1   | 0.89 | 0.29 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 1775 | 1/1   | 0.89 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3829 | 1/1   | 0.89 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3723 | 1/1   | 0.89 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3137 | 1/1   | 0.89 | 0.23 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3345 | 1/1   | 0.89 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3607 | 1/1   | 0.89 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3141 | 1/1   | 0.89 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3611 | 1/1   | 0.89 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 4067 | 1/1   | 0.89 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3143 | 1/1   | 0.89 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3458 | 1/1   | 0.89 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 2x    | 103  | 1/1   | 0.89 | 0.15 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3460 | 1/1   | 0.89 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3604 | 1/1   | 0.89 | 0.29 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3060 | 1/1   | 0.89 | 0.15 | 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   | 2A    | 3146 | 1/1   | 0.90 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3153 | 1/1   | 0.90 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3158 | 1/1   | 0.90 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3159 | 1/1   | 0.90 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 2E    | 302  | 1/1   | 0.90 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3368 | 1/1   | 0.90 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3594 | 1/1   | 0.90 | 0.25 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3343 | 1/1   | 0.90 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1Z    | 302  | 1/1   | 0.90 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3432 | 1/1   | 0.90 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 10    | 106  | 1/1   | 0.90 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 2F    | 305  | 1/1   | 0.90 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3721 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3952 | 1/1   | 0.90 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3383 | 1/1   | 0.90 | 0.23 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3784 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3434 | 1/1   | 0.90 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3961 | 1/1   | 0.90 | 0.10 | 15,15,15,15                 | 0     |
| 57  | MG   | 2V    | 202  | 1/1   | 0.90 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3642 | 1/1   | 0.90 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 2Y    | 201  | 1/1   | 0.90 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3868 | 1/1   | 0.90 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 25    | 103  | 1/1   | 0.90 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3686 | 1/1   | 0.90 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 16    | 102  | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3649 | 1/1   | 0.90 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1B    | 210  | 1/1   | 0.90 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3519 | 1/1   | 0.90 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 1x    | 107  | 1/1   | 0.90 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3655 | 1/1   | 0.90 | 0.10 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3656 | 1/1   | 0.90 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3217 | 1/1   | 0.90 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3223 | 1/1   | 0.90 | 0.30 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1628 | 1/1   | 0.90 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 19    | 101  | 1/1   | 0.90 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3879 | 1/1   | 0.90 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3419 | 1/1   | 0.90 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3886 | 1/1   | 0.90 | 0.10 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3679 | 1/1   | 0.90 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 1641 | 1/1   | 0.90 | 0.24 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3430 | 1/1   | 0.90 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 1651 | 1/1   | 0.90 | 0.25 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3433 | 1/1   | 0.90 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3307 | 1/1   | 0.90 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3005 | 1/1   | 0.90 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3441 | 1/1   | 0.90 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3444 | 1/1   | 0.90 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1665 | 1/1   | 0.90 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3012 | 1/1   | 0.90 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3981 | 1/1   | 0.90 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3987 | 1/1   | 0.90 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3253 | 1/1   | 0.90 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3249 | 1/1   | 0.90 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3607 | 1/1   | 0.90 | 0.08 | 15,15,15,15                 | 0     |
| 57  | MG   | 2a    | 1678 | 1/1   | 0.90 | 0.24 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3469 | 1/1   | 0.90 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3475 | 1/1   | 0.90 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3795 | 1/1   | 0.90 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3264 | 1/1   | 0.90 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3046 | 1/1   | 0.90 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3719 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3527 | 1/1   | 0.90 | 0.38 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1694 | 1/1   | 0.90 | 0.27 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3493 | 1/1   | 0.90 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3653 | 1/1   | 0.90 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3654 | 1/1   | 0.90 | 0.11 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3531 | 1/1   | 0.90 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3507 | 1/1   | 0.90 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1712 | 1/1   | 0.90 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3739 | 1/1   | 0.90 | 0.17 | 71,71,71,71                 | 0     |
| 57  | MG   | 1A    | 3039 | 1/1   | 0.90 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | 2a    | 1717 | 1/1   | 0.90 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3742 | 1/1   | 0.90 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3743 | 1/1   | 0.90 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 3538 | 1/1   | 0.90 | 0.23 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3562 | 1/1   | 0.90 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1B    | 238  | 1/1   | 0.90 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3278 | 1/1   | 0.90 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3280 | 1/1   | 0.90 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3529 | 1/1   | 0.90 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 4018 | 1/1   | 0.90 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3761 | 1/1   | 0.90 | 0.27 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3915 | 1/1   | 0.90 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3217 | 1/1   | 0.90 | 0.17 | 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    | 3294 | 1/1   | 0.90 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3447 | 1/1   | 0.90 | 0.25 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3296 | 1/1   | 0.90 | 0.29 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4022 | 1/1   | 0.90 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 1755 | 1/1   | 0.90 | 0.23 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3631 | 1/1   | 0.90 | 0.08 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 3680 | 1/1   | 0.90 | 0.22 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3805 | 1/1   | 0.90 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3560 | 1/1   | 0.90 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3355 | 1/1   | 0.90 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 1763 | 1/1   | 0.90 | 0.21 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 1764 | 1/1   | 0.90 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1767 | 1/1   | 0.90 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3311 | 1/1   | 0.90 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 1F    | 312  | 1/1   | 0.90 | 0.22 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3498 | 1/1   | 0.90 | 0.26 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3291 | 1/1   | 0.90 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3819 | 1/1   | 0.90 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3691 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3821 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 1N    | 201  | 1/1   | 0.90 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3827 | 1/1   | 0.90 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3828 | 1/1   | 0.90 | 0.20 | 38,38,38,38                 | 0     |
| 57  | MG   | 2f    | 202  | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3580 | 1/1   | 0.90 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3335 | 1/1   | 0.90 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3578 | 1/1   | 0.90 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3934 | 1/1   | 0.90 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3825 | 1/1   | 0.90 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3139 | 1/1   | 0.90 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3140 | 1/1   | 0.90 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2x    | 101  | 1/1   | 0.90 | 0.25 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3829 | 1/1   | 0.90 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3456 | 1/1   | 0.90 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3844 | 1/1   | 0.90 | 0.17 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3946 | 1/1   | 0.90 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4043 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3295 | 1/1   | 0.91 | 0.24 | 43,43,43,43                 | 0     |
| 57  | MG   | 1V    | 208  | 1/1   | 0.91 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3243 | 1/1   | 0.91 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3245 | 1/1   | 0.91 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3503 | 1/1   | 0.91 | 0.12 | 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   | 1a    | 3599 | 1/1   | 0.91 | 0.22 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3601 | 1/1   | 0.91 | 0.27 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3823 | 1/1   | 0.91 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 4053 | 1/1   | 0.91 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3511 | 1/1   | 0.91 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3514 | 1/1   | 0.91 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3692 | 1/1   | 0.91 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3605 | 1/1   | 0.91 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3361 | 1/1   | 0.91 | 0.28 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3256 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3834 | 1/1   | 0.91 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3259 | 1/1   | 0.91 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3306 | 1/1   | 0.91 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3608 | 1/1   | 0.91 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 4069 | 1/1   | 0.91 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3536 | 1/1   | 0.91 | 0.15 | 38,38,38,38                 | 0     |
| 57  | MG   | 2B    | 208  | 1/1   | 0.91 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3014 | 1/1   | 0.91 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3015 | 1/1   | 0.91 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 2B    | 212  | 1/1   | 0.91 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3818 | 1/1   | 0.91 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 2B    | 216  | 1/1   | 0.91 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3022 | 1/1   | 0.91 | 0.26 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3024 | 1/1   | 0.91 | 0.28 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3110 | 1/1   | 0.91 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3555 | 1/1   | 0.91 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | 2E    | 303  | 1/1   | 0.91 | 0.23 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3371 | 1/1   | 0.91 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3565 | 1/1   | 0.91 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3623 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3568 | 1/1   | 0.91 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3570 | 1/1   | 0.91 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3721 | 1/1   | 0.91 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3279 | 1/1   | 0.91 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3028 | 1/1   | 0.91 | 0.15 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3577 | 1/1   | 0.91 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3281 | 1/1   | 0.91 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3728 | 1/1   | 0.91 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3288 | 1/1   | 0.91 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 2T    | 201  | 1/1   | 0.91 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3587 | 1/1   | 0.91 | 0.21 | 43,43,43,43                 | 0     |
| 57  | MG   | 2U    | 204  | 1/1   | 0.91 | 0.12 | 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   | 1B    | 203  | 1/1   | 0.91 | 0.23 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3511 | 1/1   | 0.91 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3057 | 1/1   | 0.91 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3069 | 1/1   | 0.91 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3836 | 1/1   | 0.91 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3837 | 1/1   | 0.91 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3955 | 1/1   | 0.91 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3608 | 1/1   | 0.91 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3609 | 1/1   | 0.91 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3838 | 1/1   | 0.91 | 0.10 | 13,13,13,13                 | 0     |
| 57  | MG   | 2A    | 3303 | 1/1   | 0.91 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3640 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3642 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3960 | 1/1   | 0.91 | 0.15 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 1618 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1623 | 1/1   | 0.91 | 0.24 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3204 | 1/1   | 0.91 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3845 | 1/1   | 0.91 | 0.17 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3517 | 1/1   | 0.91 | 0.23 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3095 | 1/1   | 0.91 | 0.22 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1633 | 1/1   | 0.91 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3322 | 1/1   | 0.91 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3454 | 1/1   | 0.91 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3099 | 1/1   | 0.91 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3165 | 1/1   | 0.91 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 2a    | 1645 | 1/1   | 0.91 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 1648 | 1/1   | 0.91 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3107 | 1/1   | 0.91 | 0.29 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3521 | 1/1   | 0.91 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 1B    | 230  | 1/1   | 0.91 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3660 | 1/1   | 0.91 | 0.20 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 1659 | 1/1   | 0.91 | 0.37 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3336 | 1/1   | 0.91 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3337 | 1/1   | 0.91 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3338 | 1/1   | 0.91 | 0.23 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1664 | 1/1   | 0.91 | 0.27 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3322 | 1/1   | 0.91 | 0.22 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3523 | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3261 | 1/1   | 0.91 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3536 | 1/1   | 0.91 | 0.16 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3647 | 1/1   | 0.91 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3623 | 1/1   | 0.91 | 0.12 | 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   | 2a    | 1672 | 1/1   | 0.91 | 0.38 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1673 | 1/1   | 0.91 | 0.24 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3869 | 1/1   | 0.91 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3333 | 1/1   | 0.91 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3535 | 1/1   | 0.91 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3350 | 1/1   | 0.91 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3543 | 1/1   | 0.91 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3658 | 1/1   | 0.91 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3548 | 1/1   | 0.91 | 0.32 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3353 | 1/1   | 0.91 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1B    | 239  | 1/1   | 0.91 | 0.07 | 25,25,25,25                 | 0     |
| 57  | MG   | 2a    | 1693 | 1/1   | 0.91 | 0.26 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3632 | 1/1   | 0.91 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3670 | 1/1   | 0.91 | 0.19 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3675 | 1/1   | 0.91 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3360 | 1/1   | 0.91 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3553 | 1/1   | 0.91 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3038 | 1/1   | 0.91 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3888 | 1/1   | 0.91 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3367 | 1/1   | 0.91 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3683 | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3145 | 1/1   | 0.91 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3547 | 1/1   | 0.91 | 0.24 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1721 | 1/1   | 0.91 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3373 | 1/1   | 0.91 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3150 | 1/1   | 0.91 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1726 | 1/1   | 0.91 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3638 | 1/1   | 0.91 | 0.09 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3386 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3646 | 1/1   | 0.91 | 0.07 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3275 | 1/1   | 0.91 | 0.39 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 3565 | 1/1   | 0.91 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 1a    | 3566 | 1/1   | 0.91 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3707 | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1745 | 1/1   | 0.91 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3395 | 1/1   | 0.91 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3072 | 1/1   | 0.91 | 0.21 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3164 | 1/1   | 0.91 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1F    | 313  | 1/1   | 0.91 | 0.22 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3407 | 1/1   | 0.91 | 0.42 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3566 | 1/1   | 0.91 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3708 | 1/1   | 0.91 | 0.10 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3792 | 1/1   | 0.91 | 0.07 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3222 | 1/1   | 0.91 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1O    | 204  | 1/1   | 0.91 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3732 | 1/1   | 0.91 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3182 | 1/1   | 0.91 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3420 | 1/1   | 0.91 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3182 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3187 | 1/1   | 0.91 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1Q    | 206  | 1/1   | 0.91 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3191 | 1/1   | 0.91 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3194 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3718 | 1/1   | 0.91 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3442 | 1/1   | 0.91 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1S    | 202  | 1/1   | 0.91 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3204 | 1/1   | 0.91 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 1776 | 1/1   | 0.91 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3589 | 1/1   | 0.91 | 0.26 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3208 | 1/1   | 0.91 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3759 | 1/1   | 0.91 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3484 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3463 | 1/1   | 0.91 | 0.33 | 42,42,42,42                 | 0     |
| 57  | MG   | 1b    | 301  | 1/1   | 0.91 | 0.09 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3002 | 1/1   | 0.91 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3215 | 1/1   | 0.91 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 1e    | 201  | 1/1   | 0.91 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3793 | 1/1   | 0.91 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3794 | 1/1   | 0.91 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3494 | 1/1   | 0.91 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3477 | 1/1   | 0.91 | 0.11 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3482 | 1/1   | 0.91 | 0.10 | 13,13,13,13                 | 0     |
| 57  | MG   | 1A    | 3292 | 1/1   | 0.91 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3688 | 1/1   | 0.91 | 0.17 | 48,48,48,48                 | 0     |
| 59  | ZN   | 24    | 501  | 1/1   | 0.91 | 0.10 | 120,120,120,120             | 0     |
| 57  | MG   | 1A    | 3553 | 1/1   | 0.92 | 0.21 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3797 | 1/1   | 0.92 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3800 | 1/1   | 0.92 | 0.33 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3549 | 1/1   | 0.92 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3665 | 1/1   | 0.92 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3266 | 1/1   | 0.92 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3471 | 1/1   | 0.92 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3213 | 1/1   | 0.92 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3331 | 1/1   | 0.92 | 0.09 | 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    | 3943 | 1/1   | 0.92 | 0.21 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3812 | 1/1   | 0.92 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3218 | 1/1   | 0.92 | 0.19 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3220 | 1/1   | 0.92 | 0.14 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3487 | 1/1   | 0.92 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3801 | 1/1   | 0.92 | 0.18 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3093 | 1/1   | 0.92 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3231 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3497 | 1/1   | 0.92 | 0.11 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3232 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3673 | 1/1   | 0.92 | 0.11 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3677 | 1/1   | 0.92 | 0.08 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3027 | 1/1   | 0.92 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3504 | 1/1   | 0.92 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3506 | 1/1   | 0.92 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3813 | 1/1   | 0.92 | 0.21 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3815 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3478 | 1/1   | 0.92 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3401 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1k    | 201  | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1D    | 314  | 1/1   | 0.92 | 0.19 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3573 | 1/1   | 0.92 | 0.22 | 53,53,53,53                 | 0     |
| 57  | MG   | 1E    | 305  | 1/1   | 0.92 | 0.23 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 3575 | 1/1   | 0.92 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 1x    | 103  | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3258 | 1/1   | 0.92 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3405 | 1/1   | 0.92 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3260 | 1/1   | 0.92 | 0.24 | 43,43,43,43                 | 0     |
| 57  | MG   | 2B    | 218  | 1/1   | 0.92 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3483 | 1/1   | 0.92 | 0.30 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3539 | 1/1   | 0.92 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3693 | 1/1   | 0.92 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3544 | 1/1   | 0.92 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3583 | 1/1   | 0.92 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | 1x    | 110  | 1/1   | 0.92 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3267 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3827 | 1/1   | 0.92 | 0.13 | 8,8,8,8                     | 0     |
| 57  | MG   | 2E    | 309  | 1/1   | 0.92 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 2E    | 310  | 1/1   | 0.92 | 0.17 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3552 | 1/1   | 0.92 | 0.24 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3585 | 1/1   | 0.92 | 0.28 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3408 | 1/1   | 0.92 | 0.13 | 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   | 1A    | 3485 | 1/1   | 0.92 | 0.22 | 49,49,49,49                 | 0     |
| 57  | MG   | 2F    | 306  | 1/1   | 0.92 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3707 | 1/1   | 0.92 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3710 | 1/1   | 0.92 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3567 | 1/1   | 0.92 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3711 | 1/1   | 0.92 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3988 | 1/1   | 0.92 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 1N    | 203  | 1/1   | 0.92 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2T    | 202  | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3023 | 1/1   | 0.92 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1O    | 201  | 1/1   | 0.92 | 0.06 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3841 | 1/1   | 0.92 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3283 | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3285 | 1/1   | 0.92 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3286 | 1/1   | 0.92 | 0.19 | 42,42,42,42                 | 0     |
| 57  | MG   | 25    | 102  | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3287 | 1/1   | 0.92 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3488 | 1/1   | 0.92 | 0.32 | 45,45,45,45                 | 0     |
| 57  | MG   | 27    | 102  | 1/1   | 0.92 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 27    | 103  | 1/1   | 0.92 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3600 | 1/1   | 0.92 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3291 | 1/1   | 0.92 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3037 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3596 | 1/1   | 0.92 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3599 | 1/1   | 0.92 | 0.10 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3601 | 1/1   | 0.92 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3336 | 1/1   | 0.92 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1615 | 1/1   | 0.92 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 4006 | 1/1   | 0.92 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3047 | 1/1   | 0.92 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3603 | 1/1   | 0.92 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3493 | 1/1   | 0.92 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3300 | 1/1   | 0.92 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3853 | 1/1   | 0.92 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3276 | 1/1   | 0.92 | 0.24 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3064 | 1/1   | 0.92 | 0.21 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3065 | 1/1   | 0.92 | 0.21 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 4014 | 1/1   | 0.92 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3312 | 1/1   | 0.92 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3428 | 1/1   | 0.92 | 0.19 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3738 | 1/1   | 0.92 | 0.10 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 1647 | 1/1   | 0.92 | 0.17 | 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    | 3317 | 1/1   | 0.92 | 0.31 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3080 | 1/1   | 0.92 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3865 | 1/1   | 0.92 | 0.14 | 14,14,14,14                 | 0     |
| 57  | MG   | 1a    | 3614 | 1/1   | 0.92 | 0.28 | 61,61,61,61                 | 0     |
| 57  | MG   | 1V    | 207  | 1/1   | 0.92 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 1658 | 1/1   | 0.92 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3088 | 1/1   | 0.92 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3616 | 1/1   | 0.92 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3634 | 1/1   | 0.92 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3330 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3617 | 1/1   | 0.92 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3597 | 1/1   | 0.92 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 1666 | 1/1   | 0.92 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3333 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3621 | 1/1   | 0.92 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3622 | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3098 | 1/1   | 0.92 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 1Y    | 201  | 1/1   | 0.92 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4025 | 1/1   | 0.92 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3209 | 1/1   | 0.92 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3103 | 1/1   | 0.92 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3105 | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3870 | 1/1   | 0.92 | 0.12 | 18,18,18,18                 | 0     |
| 57  | MG   | 10    | 102  | 1/1   | 0.92 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3752 | 1/1   | 0.92 | 0.15 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3872 | 1/1   | 0.92 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3635 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3661 | 1/1   | 0.92 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3115 | 1/1   | 0.92 | 0.22 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3213 | 1/1   | 0.92 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3875 | 1/1   | 0.92 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3119 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 1696 | 1/1   | 0.92 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3354 | 1/1   | 0.92 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3290 | 1/1   | 0.92 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3883 | 1/1   | 0.92 | 0.33 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3678 | 1/1   | 0.92 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | 15    | 3202 | 1/1   | 0.92 | 0.17 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3440 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4048 | 1/1   | 0.92 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 4050 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3612 | 1/1   | 0.92 | 0.18 | 6,6,6,6                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3074 | 1/1   | 0.92 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3112 | 1/1   | 0.92 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3371 | 1/1   | 0.92 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3504 | 1/1   | 0.92 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3380 | 1/1   | 0.92 | 0.20 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3696 | 1/1   | 0.92 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3698 | 1/1   | 0.92 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3381 | 1/1   | 0.92 | 0.30 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1733 | 1/1   | 0.92 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3359 | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3775 | 1/1   | 0.92 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3508 | 1/1   | 0.92 | 0.27 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3670 | 1/1   | 0.92 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3671 | 1/1   | 0.92 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3389 | 1/1   | 0.92 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3510 | 1/1   | 0.92 | 0.22 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3113 | 1/1   | 0.92 | 0.26 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3513 | 1/1   | 0.92 | 0.08 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 4073 | 1/1   | 0.92 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 4074 | 1/1   | 0.92 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3116 | 1/1   | 0.92 | 0.16 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3901 | 1/1   | 0.92 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3783 | 1/1   | 0.92 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3052 | 1/1   | 0.92 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3525 | 1/1   | 0.92 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3527 | 1/1   | 0.92 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3176 | 1/1   | 0.92 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1765 | 1/1   | 0.92 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3129 | 1/1   | 0.92 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3690 | 1/1   | 0.92 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3529 | 1/1   | 0.92 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3786 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 1771 | 1/1   | 0.92 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3432 | 1/1   | 0.92 | 0.20 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3453 | 1/1   | 0.92 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3750 | 1/1   | 0.92 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3525 | 1/1   | 0.92 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3089 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3755 | 1/1   | 0.92 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3193 | 1/1   | 0.92 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3924 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3196 | 1/1   | 0.92 | 0.09 | 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    | 3380 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3764 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3450 | 1/1   | 0.92 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3768 | 1/1   | 0.92 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3770 | 1/1   | 0.92 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | 2q    | 201  | 1/1   | 0.92 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3771 | 1/1   | 0.92 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3774 | 1/1   | 0.92 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3452 | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3200 | 1/1   | 0.92 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3141 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3544 | 1/1   | 0.92 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3792 | 1/1   | 0.92 | 0.15 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3460 | 1/1   | 0.92 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3351 | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3779 | 1/1   | 0.93 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3781 | 1/1   | 0.93 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3782 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3812 | 1/1   | 0.93 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3784 | 1/1   | 0.93 | 0.12 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3268 | 1/1   | 0.93 | 0.17 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3192 | 1/1   | 0.93 | 0.09 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3353 | 1/1   | 0.93 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3455 | 1/1   | 0.93 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3354 | 1/1   | 0.93 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3798 | 1/1   | 0.93 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3688 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3198 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3461 | 1/1   | 0.93 | 0.23 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3463 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3166 | 1/1   | 0.93 | 0.28 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3202 | 1/1   | 0.93 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3270 | 1/1   | 0.93 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3629 | 1/1   | 0.93 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3474 | 1/1   | 0.93 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3206 | 1/1   | 0.93 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3077 | 1/1   | 0.93 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3826 | 1/1   | 0.93 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3479 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3481 | 1/1   | 0.93 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3475 | 1/1   | 0.93 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3698 | 1/1   | 0.93 | 0.07 | 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   | 1A    | 3476 | 1/1   | 0.93 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3830 | 1/1   | 0.93 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3489 | 1/1   | 0.93 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3831 | 1/1   | 0.93 | 0.31 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3491 | 1/1   | 0.93 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3524 | 1/1   | 0.93 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3360 | 1/1   | 0.93 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3498 | 1/1   | 0.93 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3221 | 1/1   | 0.93 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 2B    | 201  | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3526 | 1/1   | 0.93 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3226 | 1/1   | 0.93 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3835 | 1/1   | 0.93 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3711 | 1/1   | 0.93 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3174 | 1/1   | 0.93 | 0.09 | 25,25,25,25                 | 0     |
| 57  | MG   | 2B    | 209  | 1/1   | 0.93 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3363 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3364 | 1/1   | 0.93 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3237 | 1/1   | 0.93 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2B    | 213  | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3840 | 1/1   | 0.93 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3482 | 1/1   | 0.93 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 4058 | 1/1   | 0.93 | 0.12 | 13,13,13,13                 | 0     |
| 57  | MG   | 1a    | 3539 | 1/1   | 0.93 | 0.36 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3210 | 1/1   | 0.93 | 0.26 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3212 | 1/1   | 0.93 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 4068 | 1/1   | 0.93 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3049 | 1/1   | 0.93 | 0.12 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 4071 | 1/1   | 0.93 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3852 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2E    | 307  | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3215 | 1/1   | 0.93 | 0.26 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3181 | 1/1   | 0.93 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 1n    | 101  | 1/1   | 0.93 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3542 | 1/1   | 0.93 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3221 | 1/1   | 0.93 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3671 | 1/1   | 0.93 | 0.15 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3047 | 1/1   | 0.93 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3296 | 1/1   | 0.93 | 0.23 | 21,21,21,21                 | 0     |
| 57  | MG   | 2F    | 307  | 1/1   | 0.93 | 0.25 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3497 | 1/1   | 0.93 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3298 | 1/1   | 0.93 | 0.07 | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3561 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1B    | 205  | 1/1   | 0.93 | 0.28 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3227 | 1/1   | 0.93 | 0.24 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3389 | 1/1   | 0.93 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3274 | 1/1   | 0.93 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3183 | 1/1   | 0.93 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 2U    | 203  | 1/1   | 0.93 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3394 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2V    | 201  | 1/1   | 0.93 | 0.27 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3509 | 1/1   | 0.93 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3006 | 1/1   | 0.93 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 2W    | 202  | 1/1   | 0.93 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | 2W    | 203  | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3397 | 1/1   | 0.93 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3700 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3702 | 1/1   | 0.93 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3398 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3311 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3517 | 1/1   | 0.93 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3402 | 1/1   | 0.93 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3588 | 1/1   | 0.93 | 0.11 | 17,17,17,17                 | 0     |
| 57  | MG   | 28    | 102  | 1/1   | 0.93 | 0.19 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1601 | 1/1   | 0.93 | 0.21 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3028 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3231 | 1/1   | 0.93 | 0.28 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1605 | 1/1   | 0.93 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3714 | 1/1   | 0.93 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3406 | 1/1   | 0.93 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3235 | 1/1   | 0.93 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3243 | 1/1   | 0.93 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3041 | 1/1   | 0.93 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3727 | 1/1   | 0.93 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3410 | 1/1   | 0.93 | 0.25 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1622 | 1/1   | 0.93 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3729 | 1/1   | 0.93 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1624 | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1D    | 313  | 1/1   | 0.93 | 0.20 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3053 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3302 | 1/1   | 0.93 | 0.22 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3054 | 1/1   | 0.93 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3613 | 1/1   | 0.93 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3055 | 1/1   | 0.93 | 0.14 | 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   | 2A    | 3308 | 1/1   | 0.93 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3731 | 1/1   | 0.93 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3411 | 1/1   | 0.93 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3062 | 1/1   | 0.93 | 0.24 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3529 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 1E    | 307  | 1/1   | 0.93 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3530 | 1/1   | 0.93 | 0.28 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 1650 | 1/1   | 0.93 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3072 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3073 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3074 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1E    | 313  | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1F    | 303  | 1/1   | 0.93 | 0.17 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 1660 | 1/1   | 0.93 | 0.34 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3532 | 1/1   | 0.93 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3328 | 1/1   | 0.93 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3413 | 1/1   | 0.93 | 0.09 | 21,21,21,21                 | 0     |
| 57  | MG   | 1F    | 309  | 1/1   | 0.93 | 0.04 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3745 | 1/1   | 0.93 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3186 | 1/1   | 0.93 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3540 | 1/1   | 0.93 | 0.30 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3940 | 1/1   | 0.93 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3610 | 1/1   | 0.93 | 0.23 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3092 | 1/1   | 0.93 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3611 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | 1F    | 314  | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3415 | 1/1   | 0.93 | 0.29 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1676 | 1/1   | 0.93 | 0.22 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3342 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3096 | 1/1   | 0.93 | 0.15 | 20,20,20,20                 | 0     |
| 57  | MG   | 1G    | 204  | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3417 | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 1686 | 1/1   | 0.93 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3558 | 1/1   | 0.93 | 0.25 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3559 | 1/1   | 0.93 | 0.25 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3424 | 1/1   | 0.93 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3662 | 1/1   | 0.93 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3106 | 1/1   | 0.93 | 0.28 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3150 | 1/1   | 0.93 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3948 | 1/1   | 0.93 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3099 | 1/1   | 0.93 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3674 | 1/1   | 0.93 | 0.09 | 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    | 1699 | 1/1   | 0.93 | 0.21 | 37,37,37,37                 | 0     |
| 57  | MG   | 1R    | 205  | 1/1   | 0.93 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3113 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3626 | 1/1   | 0.93 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3359 | 1/1   | 0.93 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3950 | 1/1   | 0.93 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3567 | 1/1   | 0.93 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3629 | 1/1   | 0.93 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3332 | 1/1   | 0.93 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3684 | 1/1   | 0.93 | 0.11 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 1720 | 1/1   | 0.93 | 0.25 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3569 | 1/1   | 0.93 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3196 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3126 | 1/1   | 0.93 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1725 | 1/1   | 0.93 | 0.16 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3691 | 1/1   | 0.93 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3634 | 1/1   | 0.93 | 0.33 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3436 | 1/1   | 0.93 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3377 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3695 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3378 | 1/1   | 0.93 | 0.27 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1734 | 1/1   | 0.93 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 1735 | 1/1   | 0.93 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3959 | 1/1   | 0.93 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1737 | 1/1   | 0.93 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1739 | 1/1   | 0.93 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3637 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1742 | 1/1   | 0.93 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3702 | 1/1   | 0.93 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 1744 | 1/1   | 0.93 | 0.29 | 45,45,45,45                 | 0     |
| 57  | MG   | 1V    | 202  | 1/1   | 0.93 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3384 | 1/1   | 0.93 | 0.21 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3639 | 1/1   | 0.93 | 0.25 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3438 | 1/1   | 0.93 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3579 | 1/1   | 0.93 | 0.10 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3963 | 1/1   | 0.93 | 0.08 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3965 | 1/1   | 0.93 | 0.09 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3648 | 1/1   | 0.93 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3966 | 1/1   | 0.93 | 0.06 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3394 | 1/1   | 0.93 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3720 | 1/1   | 0.93 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3721 | 1/1   | 0.93 | 0.10 | 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   | 1A    | 3334 | 1/1   | 0.93 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3789 | 1/1   | 0.93 | 0.51 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3398 | 1/1   | 0.93 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3154 | 1/1   | 0.93 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3404 | 1/1   | 0.93 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3581 | 1/1   | 0.93 | 0.13 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3406 | 1/1   | 0.93 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3736 | 1/1   | 0.93 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3092 | 1/1   | 0.93 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3658 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3741 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3409 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 10    | 105  | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3744 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3411 | 1/1   | 0.93 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3253 | 1/1   | 0.93 | 0.07 | 24,24,24,24                 | 0     |
| 57  | MG   | 2d    | 301  | 1/1   | 0.93 | 0.25 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3415 | 1/1   | 0.93 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3444 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3340 | 1/1   | 0.93 | 0.19 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3254 | 1/1   | 0.93 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3259 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3448 | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3426 | 1/1   | 0.93 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3160 | 1/1   | 0.93 | 0.27 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3346 | 1/1   | 0.93 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3805 | 1/1   | 0.93 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3434 | 1/1   | 0.93 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3347 | 1/1   | 0.93 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3111 | 1/1   | 0.93 | 0.06 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3183 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3186 | 1/1   | 0.93 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3443 | 1/1   | 0.93 | 0.29 | 52,52,52,52                 | 0     |
| 57  | MG   | 17    | 105  | 1/1   | 0.94 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 18    | 101  | 1/1   | 0.94 | 0.24 | 47,47,47,47                 | 0     |
| 57  | MG   | 18    | 102  | 1/1   | 0.94 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3087 | 1/1   | 0.94 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3013 | 1/1   | 0.94 | 0.12 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 3643 | 1/1   | 0.94 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 4057 | 1/1   | 0.94 | 0.09 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3543 | 1/1   | 0.94 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3617 | 1/1   | 0.94 | 0.06 | 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    | 4060 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2B    | 204  | 1/1   | 0.94 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3547 | 1/1   | 0.94 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3505 | 1/1   | 0.94 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4062 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3776 | 1/1   | 0.94 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3094 | 1/1   | 0.94 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3893 | 1/1   | 0.94 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3898 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3556 | 1/1   | 0.94 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2B    | 214  | 1/1   | 0.94 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3100 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3563 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3625 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 2D    | 301  | 1/1   | 0.94 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3306 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3781 | 1/1   | 0.94 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3663 | 1/1   | 0.94 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3188 | 1/1   | 0.94 | 0.37 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3190 | 1/1   | 0.94 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3572 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3313 | 1/1   | 0.94 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3669 | 1/1   | 0.94 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3519 | 1/1   | 0.94 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3580 | 1/1   | 0.94 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3909 | 1/1   | 0.94 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3318 | 1/1   | 0.94 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3111 | 1/1   | 0.94 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3320 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3913 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3118 | 1/1   | 0.94 | 0.31 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3674 | 1/1   | 0.94 | 0.26 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3156 | 1/1   | 0.94 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3521 | 1/1   | 0.94 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3388 | 1/1   | 0.94 | 0.30 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3329 | 1/1   | 0.94 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3280 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3642 | 1/1   | 0.94 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3605 | 1/1   | 0.94 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 2T    | 204  | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3124 | 1/1   | 0.94 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3390 | 1/1   | 0.94 | 0.06 | 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   | 1A    | 3926 | 1/1   | 0.94 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3130 | 1/1   | 0.94 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3391 | 1/1   | 0.94 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3133 | 1/1   | 0.94 | 0.20 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3135 | 1/1   | 0.94 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3342 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3687 | 1/1   | 0.94 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3620 | 1/1   | 0.94 | 0.28 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3138 | 1/1   | 0.94 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3932 | 1/1   | 0.94 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3232 | 1/1   | 0.94 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3395 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3625 | 1/1   | 0.94 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3663 | 1/1   | 0.94 | 0.12 | 6,6,6,6                     | 0     |
| 57  | MG   | 1A    | 3533 | 1/1   | 0.94 | 0.26 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3534 | 1/1   | 0.94 | 0.18 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3802 | 1/1   | 0.94 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3396 | 1/1   | 0.94 | 0.20 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3149 | 1/1   | 0.94 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3021 | 1/1   | 0.94 | 0.17 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 1608 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3462 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3064 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 1612 | 1/1   | 0.94 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3356 | 1/1   | 0.94 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3156 | 1/1   | 0.94 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3358 | 1/1   | 0.94 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3552 | 1/1   | 0.94 | 0.13 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 1621 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3554 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3706 | 1/1   | 0.94 | 0.06 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3678 | 1/1   | 0.94 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3679 | 1/1   | 0.94 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1626 | 1/1   | 0.94 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3709 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3167 | 1/1   | 0.94 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3650 | 1/1   | 0.94 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3558 | 1/1   | 0.94 | 0.32 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3652 | 1/1   | 0.94 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 1D    | 301  | 1/1   | 0.94 | 0.18 | 24,24,24,24                 | 0     |
| 57  | MG   | 1D    | 302  | 1/1   | 0.94 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 2a    | 1637 | 1/1   | 0.94 | 0.34 | 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    | 1640 | 1/1   | 0.94 | 0.26 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3375 | 1/1   | 0.94 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 1644 | 1/1   | 0.94 | 0.29 | 40,40,40,40                 | 0     |
| 57  | MG   | 1D    | 305  | 1/1   | 0.94 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3175 | 1/1   | 0.94 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3379 | 1/1   | 0.94 | 0.24 | 35,35,35,35                 | 0     |
| 57  | MG   | 1D    | 309  | 1/1   | 0.94 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3682 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3285 | 1/1   | 0.94 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1652 | 1/1   | 0.94 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3179 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3469 | 1/1   | 0.94 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 1657 | 1/1   | 0.94 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3289 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3561 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3471 | 1/1   | 0.94 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3404 | 1/1   | 0.94 | 0.19 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3694 | 1/1   | 0.94 | 0.06 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3190 | 1/1   | 0.94 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3393 | 1/1   | 0.94 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3348 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3135 | 1/1   | 0.94 | 0.35 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3044 | 1/1   | 0.94 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3397 | 1/1   | 0.94 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3169 | 1/1   | 0.94 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3401 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3195 | 1/1   | 0.94 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3140 | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 1p    | 101  | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1674 | 1/1   | 0.94 | 0.24 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 1675 | 1/1   | 0.94 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3055 | 1/1   | 0.94 | 0.20 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3200 | 1/1   | 0.94 | 0.10 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3412 | 1/1   | 0.94 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1679 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3588 | 1/1   | 0.94 | 0.06 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3975 | 1/1   | 0.94 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3578 | 1/1   | 0.94 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1687 | 1/1   | 0.94 | 0.29 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3252 | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3091 | 1/1   | 0.94 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3984 | 1/1   | 0.94 | 0.09 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1x    | 109  | 1/1   | 0.94 | 0.16 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3706 | 1/1   | 0.94 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3211 | 1/1   | 0.94 | 0.29 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3358 | 1/1   | 0.94 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3710 | 1/1   | 0.94 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3842 | 1/1   | 0.94 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 1697 | 1/1   | 0.94 | 0.26 | 55,55,55,55                 | 0     |
| 57  | MG   | 1x    | 113  | 1/1   | 0.94 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3428 | 1/1   | 0.94 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 1704 | 1/1   | 0.94 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 1N    | 206  | 1/1   | 0.94 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 1709 | 1/1   | 0.94 | 0.22 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3003 | 1/1   | 0.94 | 0.25 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3219 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3992 | 1/1   | 0.94 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3994 | 1/1   | 0.94 | 0.05 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3725 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3727 | 1/1   | 0.94 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3437 | 1/1   | 0.94 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3438 | 1/1   | 0.94 | 0.34 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3439 | 1/1   | 0.94 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3731 | 1/1   | 0.94 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3222 | 1/1   | 0.94 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | 1P    | 202  | 1/1   | 0.94 | 0.51 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3995 | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3997 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 1729 | 1/1   | 0.94 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3229 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3843 | 1/1   | 0.94 | 0.08 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3145 | 1/1   | 0.94 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3233 | 1/1   | 0.94 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3418 | 1/1   | 0.94 | 0.15 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3420 | 1/1   | 0.94 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3456 | 1/1   | 0.94 | 0.27 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3849 | 1/1   | 0.94 | 0.15 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3851 | 1/1   | 0.94 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3309 | 1/1   | 0.94 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3751 | 1/1   | 0.94 | 0.23 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3240 | 1/1   | 0.94 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3495 | 1/1   | 0.94 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3426 | 1/1   | 0.94 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 1746 | 1/1   | 0.94 | 0.23 | 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    | 3036 | 1/1   | 0.94 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3737 | 1/1   | 0.94 | 0.09 | 9,9,9,9                     | 0     |
| 57  | MG   | 2A    | 3248 | 1/1   | 0.94 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3473 | 1/1   | 0.94 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3762 | 1/1   | 0.94 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3861 | 1/1   | 0.94 | 0.11 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3765 | 1/1   | 0.94 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3040 | 1/1   | 0.94 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1758 | 1/1   | 0.94 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3255 | 1/1   | 0.94 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3042 | 1/1   | 0.94 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3045 | 1/1   | 0.94 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3257 | 1/1   | 0.94 | 0.21 | 45,45,45,45                 | 0     |
| 57  | MG   | 1W    | 204  | 1/1   | 0.94 | 0.17 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3595 | 1/1   | 0.94 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3485 | 1/1   | 0.94 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4023 | 1/1   | 0.94 | 0.12 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3261 | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3050 | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3740 | 1/1   | 0.94 | 0.10 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3256 | 1/1   | 0.94 | 0.25 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3258 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3433 | 1/1   | 0.94 | 0.26 | 54,54,54,54                 | 0     |
| 57  | MG   | 10    | 103  | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3601 | 1/1   | 0.94 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3270 | 1/1   | 0.94 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3271 | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3058 | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3873 | 1/1   | 0.94 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3505 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3506 | 1/1   | 0.94 | 0.27 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 4041 | 1/1   | 0.94 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3877 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3809 | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3319 | 1/1   | 0.94 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3216 | 1/1   | 0.94 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3263 | 1/1   | 0.94 | 0.21 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3516 | 1/1   | 0.94 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3517 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3771 | 1/1   | 0.94 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3520 | 1/1   | 0.94 | 0.07 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3081 | 1/1   | 0.94 | 0.22 | 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   | 2A    | 3526 | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3082 | 1/1   | 0.94 | 0.05 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3284 | 1/1   | 0.94 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 18    | 105  | 1/1   | 0.95 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3462 | 1/1   | 0.95 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3154 | 1/1   | 0.95 | 0.21 | 22,22,22,22                 | 0     |
| 57  | MG   | 1a    | 3713 | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3465 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3067 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3105 | 1/1   | 0.95 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 4024 | 1/1   | 0.95 | 0.08 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3224 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3225 | 1/1   | 0.95 | 0.04 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3681 | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3227 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4026 | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3478 | 1/1   | 0.95 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3441 | 1/1   | 0.95 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3230 | 1/1   | 0.95 | 0.22 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 4028 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3683 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3814 | 1/1   | 0.95 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3512 | 1/1   | 0.95 | 0.13 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3486 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3818 | 1/1   | 0.95 | 0.15 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3684 | 1/1   | 0.95 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3286 | 1/1   | 0.95 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3516 | 1/1   | 0.95 | 0.08 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 4035 | 1/1   | 0.95 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3846 | 1/1   | 0.95 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3825 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3287 | 1/1   | 0.95 | 0.17 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3241 | 1/1   | 0.95 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3242 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3106 | 1/1   | 0.95 | 0.15 | 13,13,13,13                 | 0     |
| 57  | MG   | 2A    | 3244 | 1/1   | 0.95 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1t    | 201  | 1/1   | 0.95 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3161 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3522 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3366 | 1/1   | 0.95 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3548 | 1/1   | 0.95 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3250 | 1/1   | 0.95 | 0.16 | 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    | 3251 | 1/1   | 0.95 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 2B    | 205  | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 1x    | 104  | 1/1   | 0.95 | 0.30 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 4045 | 1/1   | 0.95 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 4046 | 1/1   | 0.95 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3162 | 1/1   | 0.95 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3695 | 1/1   | 0.95 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4051 | 1/1   | 0.95 | 0.12 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3163 | 1/1   | 0.95 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3522 | 1/1   | 0.95 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3555 | 1/1   | 0.95 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3556 | 1/1   | 0.95 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3370 | 1/1   | 0.95 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3293 | 1/1   | 0.95 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3452 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3532 | 1/1   | 0.95 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3373 | 1/1   | 0.95 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3534 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3375 | 1/1   | 0.95 | 0.21 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3009 | 1/1   | 0.95 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3455 | 1/1   | 0.95 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3715 | 1/1   | 0.95 | 0.08 | 8,8,8,8                     | 0     |
| 57  | MG   | 2E    | 306  | 1/1   | 0.95 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 3545 | 1/1   | 0.95 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3546 | 1/1   | 0.95 | 0.24 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3547 | 1/1   | 0.95 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3545 | 1/1   | 0.95 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3716 | 1/1   | 0.95 | 0.10 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 4070 | 1/1   | 0.95 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3027 | 1/1   | 0.95 | 0.20 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3718 | 1/1   | 0.95 | 0.05 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3550 | 1/1   | 0.95 | 0.08 | 13,13,13,13                 | 0     |
| 57  | MG   | 2A    | 3029 | 1/1   | 0.95 | 0.19 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3223 | 1/1   | 0.95 | 0.23 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3457 | 1/1   | 0.95 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 2Q    | 202  | 1/1   | 0.95 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3032 | 1/1   | 0.95 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3880 | 1/1   | 0.95 | 0.15 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3224 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3226 | 1/1   | 0.95 | 0.14 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 4078 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 4079 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3887 | 1/1   | 0.95 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3300 | 1/1   | 0.95 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3569 | 1/1   | 0.95 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3289 | 1/1   | 0.95 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3043 | 1/1   | 0.95 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3044 | 1/1   | 0.95 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3301 | 1/1   | 0.95 | 0.22 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3293 | 1/1   | 0.95 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 1B    | 202  | 1/1   | 0.95 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3730 | 1/1   | 0.95 | 0.08 | 9,9,9,9                     | 0     |
| 57  | MG   | 2I    | 102  | 1/1   | 0.95 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 23    | 101  | 1/1   | 0.95 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3576 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3577 | 1/1   | 0.95 | 0.10 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3304 | 1/1   | 0.95 | 0.17 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3895 | 1/1   | 0.95 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3571 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3897 | 1/1   | 0.95 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 1B    | 211  | 1/1   | 0.95 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3592 | 1/1   | 0.95 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3040 | 1/1   | 0.95 | 0.18 | 20,20,20,20                 | 0     |
| 57  | MG   | 1B    | 216  | 1/1   | 0.95 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 2a    | 1604 | 1/1   | 0.95 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3307 | 1/1   | 0.95 | 0.09 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3598 | 1/1   | 0.95 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3387 | 1/1   | 0.95 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3600 | 1/1   | 0.95 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3309 | 1/1   | 0.95 | 0.17 | 40,40,40,40                 | 0     |
| 57  | MG   | 1B    | 220  | 1/1   | 0.95 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 1613 | 1/1   | 0.95 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 1B    | 221  | 1/1   | 0.95 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3582 | 1/1   | 0.95 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 1616 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3583 | 1/1   | 0.95 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3043 | 1/1   | 0.95 | 0.07 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3582 | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3586 | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3079 | 1/1   | 0.95 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3587 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3614 | 1/1   | 0.95 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3902 | 1/1   | 0.95 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3617 | 1/1   | 0.95 | 0.17 | 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    | 1629 | 1/1   | 0.95 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3618 | 1/1   | 0.95 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 1B    | 225  | 1/1   | 0.95 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1B    | 226  | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3323 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3308 | 1/1   | 0.95 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3474 | 1/1   | 0.95 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3750 | 1/1   | 0.95 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | 2a    | 1638 | 1/1   | 0.95 | 0.22 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3327 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3015 | 1/1   | 0.95 | 0.19 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3755 | 1/1   | 0.95 | 0.05 | 11,11,11,11                 | 0     |
| 57  | MG   | 1B    | 234  | 1/1   | 0.95 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3310 | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3168 | 1/1   | 0.95 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3046 | 1/1   | 0.95 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3920 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3922 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3764 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1654 | 1/1   | 0.95 | 0.28 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3114 | 1/1   | 0.95 | 0.20 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3636 | 1/1   | 0.95 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1D    | 303  | 1/1   | 0.95 | 0.22 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3766 | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3594 | 1/1   | 0.95 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3929 | 1/1   | 0.95 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3085 | 1/1   | 0.95 | 0.20 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3344 | 1/1   | 0.95 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3318 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3245 | 1/1   | 0.95 | 0.21 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3774 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3935 | 1/1   | 0.95 | 0.09 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3179 | 1/1   | 0.95 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3937 | 1/1   | 0.95 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3324 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3602 | 1/1   | 0.95 | 0.08 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3403 | 1/1   | 0.95 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1F    | 307  | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3490 | 1/1   | 0.95 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3659 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3782 | 1/1   | 0.95 | 0.06 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3608 | 1/1   | 0.95 | 0.07 | 20,20,20,20                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3609 | 1/1   | 0.95 | 0.09 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3180 | 1/1   | 0.95 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3664 | 1/1   | 0.95 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1680 | 1/1   | 0.95 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3666 | 1/1   | 0.95 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 1682 | 1/1   | 0.95 | 0.27 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3667 | 1/1   | 0.95 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | 2a    | 1684 | 1/1   | 0.95 | 0.25 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3327 | 1/1   | 0.95 | 0.22 | 40,40,40,40                 | 0     |
| 57  | MG   | 1G    | 201  | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3129 | 1/1   | 0.95 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | 1G    | 202  | 1/1   | 0.95 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3117 | 1/1   | 0.95 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3368 | 1/1   | 0.95 | 0.26 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3407 | 1/1   | 0.95 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3633 | 1/1   | 0.95 | 0.24 | 36,36,36,36                 | 0     |
| 57  | MG   | 1G    | 205  | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 1H    | 201  | 1/1   | 0.95 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3374 | 1/1   | 0.95 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3016 | 1/1   | 0.95 | 0.24 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 1698 | 1/1   | 0.95 | 0.19 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3376 | 1/1   | 0.95 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3615 | 1/1   | 0.95 | 0.12 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 1701 | 1/1   | 0.95 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 1N    | 202  | 1/1   | 0.95 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | 2a    | 1705 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3616 | 1/1   | 0.95 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 2a    | 1707 | 1/1   | 0.95 | 0.15 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 1708 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3019 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3618 | 1/1   | 0.95 | 0.07 | 14,14,14,14                 | 0     |
| 57  | MG   | 2A    | 3382 | 1/1   | 0.95 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1O    | 203  | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3185 | 1/1   | 0.95 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3796 | 1/1   | 0.95 | 0.08 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3148 | 1/1   | 0.95 | 0.29 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 1718 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3699 | 1/1   | 0.95 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3127 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3701 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3051 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1R    | 201  | 1/1   | 0.95 | 0.09 | 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   | 1R    | 202  | 1/1   | 0.95 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3799 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1727 | 1/1   | 0.95 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3132 | 1/1   | 0.95 | 0.07 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3004 | 1/1   | 0.95 | 0.08 | 11,11,11,11                 | 0     |
| 57  | MG   | 1T    | 201  | 1/1   | 0.95 | 0.19 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3971 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3023 | 1/1   | 0.95 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3712 | 1/1   | 0.95 | 0.08 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3633 | 1/1   | 0.95 | 0.08 | 9,9,9,9                     | 0     |
| 57  | MG   | 2A    | 3165 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3717 | 1/1   | 0.95 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3402 | 1/1   | 0.95 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 2a    | 1738 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3665 | 1/1   | 0.95 | 0.07 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3974 | 1/1   | 0.95 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3634 | 1/1   | 0.95 | 0.07 | 14,14,14,14                 | 0     |
| 57  | MG   | 2A    | 3722 | 1/1   | 0.95 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3195 | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3262 | 1/1   | 0.95 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3980 | 1/1   | 0.95 | 0.08 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3419 | 1/1   | 0.95 | 0.19 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 1748 | 1/1   | 0.95 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 1749 | 1/1   | 0.95 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 1W    | 201  | 1/1   | 0.95 | 0.13 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3983 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3009 | 1/1   | 0.95 | 0.05 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3413 | 1/1   | 0.95 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3643 | 1/1   | 0.95 | 0.08 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 3678 | 1/1   | 0.95 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3012 | 1/1   | 0.95 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3738 | 1/1   | 0.95 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3647 | 1/1   | 0.95 | 0.12 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3516 | 1/1   | 0.95 | 0.09 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3001 | 1/1   | 0.95 | 0.07 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3202 | 1/1   | 0.95 | 0.08 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3427 | 1/1   | 0.95 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3661 | 1/1   | 0.95 | 0.10 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3429 | 1/1   | 0.95 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3431 | 1/1   | 0.95 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3095 | 1/1   | 0.95 | 0.15 | 11,11,11,11                 | 0     |
| 57  | MG   | 10    | 108  | 1/1   | 0.95 | 0.09 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4005 | 1/1   | 0.95 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3431 | 1/1   | 0.95 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3666 | 1/1   | 0.95 | 0.07 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 4008 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3756 | 1/1   | 0.95 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3694 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 13    | 103  | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 13    | 104  | 1/1   | 0.95 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3760 | 1/1   | 0.95 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3096 | 1/1   | 0.95 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 2d    | 302  | 1/1   | 0.95 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 15    | 3208 | 1/1   | 0.95 | 0.11 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3763 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3700 | 1/1   | 0.95 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3147 | 1/1   | 0.95 | 0.13 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3447 | 1/1   | 0.95 | 0.20 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3449 | 1/1   | 0.95 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 2k    | 201  | 1/1   | 0.95 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4011 | 1/1   | 0.95 | 0.08 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3451 | 1/1   | 0.95 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 16    | 103  | 1/1   | 0.95 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 2t    | 201  | 1/1   | 0.95 | 0.27 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3775 | 1/1   | 0.95 | 0.10 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3014 | 1/1   | 0.95 | 0.06 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 4017 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3834 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2x    | 107  | 1/1   | 0.95 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3066 | 1/1   | 0.95 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3216 | 1/1   | 0.95 | 0.23 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3528 | 1/1   | 0.95 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3170 | 1/1   | 0.96 | 0.21 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3329 | 1/1   | 0.96 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3203 | 1/1   | 0.96 | 0.06 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3363 | 1/1   | 0.96 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3385 | 1/1   | 0.96 | 0.16 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 3537 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3032 | 1/1   | 0.96 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3712 | 1/1   | 0.96 | 0.05 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3714 | 1/1   | 0.96 | 0.25 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3288 | 1/1   | 0.96 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3372 | 1/1   | 0.96 | 0.27 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3968 | 1/1   | 0.96 | 0.09 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3512 | 1/1   | 0.96 | 0.19 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3185 | 1/1   | 0.96 | 0.24 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3143 | 1/1   | 0.96 | 0.33 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3717 | 1/1   | 0.96 | 0.09 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3839 | 1/1   | 0.96 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3603 | 1/1   | 0.96 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 2O    | 203  | 1/1   | 0.96 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | 2P    | 201  | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3053 | 1/1   | 0.96 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3041 | 1/1   | 0.96 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3337 | 1/1   | 0.96 | 0.16 | 33,33,33,33                 | 0     |
| 57  | MG   | 1D    | 310  | 1/1   | 0.96 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3057 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3341 | 1/1   | 0.96 | 0.29 | 33,33,33,33                 | 0     |
| 57  | MG   | 2T    | 203  | 1/1   | 0.96 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3120 | 1/1   | 0.96 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 1E    | 304  | 1/1   | 0.96 | 0.13 | 14,14,14,14                 | 0     |
| 57  | MG   | 2U    | 202  | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3294 | 1/1   | 0.96 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3121 | 1/1   | 0.96 | 0.35 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3122 | 1/1   | 0.96 | 0.28 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3391 | 1/1   | 0.96 | 0.26 | 40,40,40,40                 | 0     |
| 57  | MG   | 1E    | 310  | 1/1   | 0.96 | 0.12 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3736 | 1/1   | 0.96 | 0.09 | 25,25,25,25                 | 0     |
| 57  | MG   | 1x    | 102  | 1/1   | 0.96 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3207 | 1/1   | 0.96 | 0.24 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3639 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 2I    | 101  | 1/1   | 0.96 | 0.41 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3990 | 1/1   | 0.96 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3991 | 1/1   | 0.96 | 0.09 | 20,20,20,20                 | 0     |
| 57  | MG   | 25    | 101  | 1/1   | 0.96 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3526 | 1/1   | 0.96 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3993 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1F    | 306  | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3399 | 1/1   | 0.96 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3214 | 1/1   | 0.96 | 0.09 | 28,28,28,28                 | 0     |
| 57  | MG   | 1F    | 308  | 1/1   | 0.96 | 0.05 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3855 | 1/1   | 0.96 | 0.04 | 11,11,11,11                 | 0     |
| 57  | MG   | 28    | 103  | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3572 | 1/1   | 0.96 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3124 | 1/1   | 0.96 | 0.34 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3299 | 1/1   | 0.96 | 0.12 | 16,16,16,16                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3862 | 1/1   | 0.96 | 0.07 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 4003 | 1/1   | 0.96 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3620 | 1/1   | 0.96 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3621 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3744 | 1/1   | 0.96 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3581 | 1/1   | 0.96 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3417 | 1/1   | 0.96 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3013 | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3257 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3531 | 1/1   | 0.96 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3665 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3751 | 1/1   | 0.96 | 0.06 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3422 | 1/1   | 0.96 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 1620 | 1/1   | 0.96 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3627 | 1/1   | 0.96 | 0.07 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3753 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 4013 | 1/1   | 0.96 | 0.04 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3671 | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3026 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3234 | 1/1   | 0.96 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3628 | 1/1   | 0.96 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 4016 | 1/1   | 0.96 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1N    | 204  | 1/1   | 0.96 | 0.05 | 29,29,29,29                 | 0     |
| 57  | MG   | 1N    | 205  | 1/1   | 0.96 | 0.15 | 25,25,25,25                 | 0     |
| 57  | MG   | 2a    | 1632 | 1/1   | 0.96 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3349 | 1/1   | 0.96 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3461 | 1/1   | 0.96 | 0.27 | 27,27,27,27                 | 0     |
| 57  | MG   | 1O    | 202  | 1/1   | 0.96 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3876 | 1/1   | 0.96 | 0.23 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3761 | 1/1   | 0.96 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 1P    | 201  | 1/1   | 0.96 | 0.21 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 1639 | 1/1   | 0.96 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3126 | 1/1   | 0.96 | 0.11 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3302 | 1/1   | 0.96 | 0.04 | 23,23,23,23                 | 0     |
| 57  | MG   | 2a    | 1642 | 1/1   | 0.96 | 0.15 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1643 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 1Q    | 202  | 1/1   | 0.96 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 1Q    | 203  | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1646 | 1/1   | 0.96 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3448 | 1/1   | 0.96 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | 1Q    | 204  | 1/1   | 0.96 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3881 | 1/1   | 0.96 | 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   | 1A    | 3882 | 1/1   | 0.96 | 0.20 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3303 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3048 | 1/1   | 0.96 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3454 | 1/1   | 0.96 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3539 | 1/1   | 0.96 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3466 | 1/1   | 0.96 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3544 | 1/1   | 0.96 | 0.11 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3467 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3639 | 1/1   | 0.96 | 0.05 | 13,13,13,13                 | 0     |
| 57  | MG   | 1A    | 3640 | 1/1   | 0.96 | 0.06 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3158 | 1/1   | 0.96 | 0.19 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3262 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3549 | 1/1   | 0.96 | 0.07 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3060 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3713 | 1/1   | 0.96 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3061 | 1/1   | 0.96 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | 1U    | 205  | 1/1   | 0.96 | 0.24 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3716 | 1/1   | 0.96 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3470 | 1/1   | 0.96 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | 1U    | 206  | 1/1   | 0.96 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3472 | 1/1   | 0.96 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1U    | 210  | 1/1   | 0.96 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3067 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3619 | 1/1   | 0.96 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3551 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3896 | 1/1   | 0.96 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3726 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 4039 | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 1V    | 204  | 1/1   | 0.96 | 0.16 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3480 | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3048 | 1/1   | 0.96 | 0.09 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3077 | 1/1   | 0.96 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3649 | 1/1   | 0.96 | 0.07 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3107 | 1/1   | 0.96 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 4044 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 1W    | 205  | 1/1   | 0.96 | 0.09 | 12,12,12,12                 | 0     |
| 57  | MG   | 1X    | 103  | 1/1   | 0.96 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3554 | 1/1   | 0.96 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3085 | 1/1   | 0.96 | 0.28 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3193 | 1/1   | 0.96 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3492 | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3658 | 1/1   | 0.96 | 0.19 | 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    | 3495 | 1/1   | 0.96 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3745 | 1/1   | 0.96 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3496 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1Y    | 203  | 1/1   | 0.96 | 0.29 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3904 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3749 | 1/1   | 0.96 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3265 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3557 | 1/1   | 0.96 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 1702 | 1/1   | 0.96 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3501 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3753 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3911 | 1/1   | 0.96 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3076 | 1/1   | 0.96 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3010 | 1/1   | 0.96 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3505 | 1/1   | 0.96 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3312 | 1/1   | 0.96 | 0.20 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3362 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3644 | 1/1   | 0.96 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 4061 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 1715 | 1/1   | 0.96 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3510 | 1/1   | 0.96 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3313 | 1/1   | 0.96 | 0.13 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3513 | 1/1   | 0.96 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 4063 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 13    | 101  | 1/1   | 0.96 | 0.15 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3767 | 1/1   | 0.96 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 1722 | 1/1   | 0.96 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3136 | 1/1   | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 4065 | 1/1   | 0.96 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 4066 | 1/1   | 0.96 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 3656 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3305 | 1/1   | 0.96 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3481 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3777 | 1/1   | 0.96 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 15    | 3204 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 15    | 3205 | 1/1   | 0.96 | 0.15 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3112 | 1/1   | 0.96 | 0.16 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3921 | 1/1   | 0.96 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3661 | 1/1   | 0.96 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3230 | 1/1   | 0.96 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3786 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3787 | 1/1   | 0.96 | 0.08 | 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   | 16    | 101  | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3791 | 1/1   | 0.96 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3674 | 1/1   | 0.96 | 0.05 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3315 | 1/1   | 0.96 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3538 | 1/1   | 0.96 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3795 | 1/1   | 0.96 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3796 | 1/1   | 0.96 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3666 | 1/1   | 0.96 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3540 | 1/1   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3121 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3667 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3421 | 1/1   | 0.96 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3422 | 1/1   | 0.96 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3927 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3572 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3680 | 1/1   | 0.96 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3197 | 1/1   | 0.96 | 0.04 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3487 | 1/1   | 0.96 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3132 | 1/1   | 0.96 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3425 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3502 | 1/1   | 0.96 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3806 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3198 | 1/1   | 0.96 | 0.19 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 4085 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3427 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3559 | 1/1   | 0.96 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 1766 | 1/1   | 0.96 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3561 | 1/1   | 0.96 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3809 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3233 | 1/1   | 0.96 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3320 | 1/1   | 0.96 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3826 | 1/1   | 0.96 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3372 | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3814 | 1/1   | 0.96 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3079 | 1/1   | 0.96 | 0.24 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3945 | 1/1   | 0.96 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3241 | 1/1   | 0.96 | 0.08 | 27,27,27,27                 | 0     |
| 57  | MG   | 1B    | 212  | 1/1   | 0.96 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1B    | 213  | 1/1   | 0.96 | 0.14 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3152 | 1/1   | 0.96 | 0.35 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3576 | 1/1   | 0.96 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2e    | 201  | 1/1   | 0.96 | 0.05 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3025 | 1/1   | 0.96 | 0.25 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3578 | 1/1   | 0.96 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3579 | 1/1   | 0.96 | 0.07 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3326 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3155 | 1/1   | 0.96 | 0.31 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3583 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3820 | 1/1   | 0.96 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 2l    | 201  | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3062 | 1/1   | 0.96 | 0.20 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3502 | 1/1   | 0.96 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2q    | 202  | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3823 | 1/1   | 0.96 | 0.07 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3953 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3701 | 1/1   | 0.96 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | 2v    | 102  | 1/1   | 0.96 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3437 | 1/1   | 0.96 | 0.14 | 24,24,24,24                 | 0     |
| 57  | MG   | 2x    | 102  | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3703 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3166 | 1/1   | 0.96 | 0.13 | 24,24,24,24                 | 0     |
| 57  | MG   | 2x    | 106  | 1/1   | 0.96 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3956 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3597 | 1/1   | 0.96 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3328 | 1/1   | 0.96 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3530 | 1/1   | 0.96 | 0.22 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3762 | 1/1   | 0.97 | 0.08 | 7,7,7,7                     | 0     |
| 57  | MG   | 1A    | 3102 | 1/1   | 0.97 | 0.18 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3197 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3641 | 1/1   | 0.97 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 2O    | 202  | 1/1   | 0.97 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3472 | 1/1   | 0.97 | 0.20 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3103 | 1/1   | 0.97 | 0.10 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3767 | 1/1   | 0.97 | 0.07 | 9,9,9,9                     | 0     |
| 57  | MG   | 2A    | 3399 | 1/1   | 0.97 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3236 | 1/1   | 0.97 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3203 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3237 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3104 | 1/1   | 0.97 | 0.35 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3297 | 1/1   | 0.97 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 1x    | 112  | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3652 | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3576 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 4029 | 1/1   | 0.97 | 0.04 | 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    | 4030 | 1/1   | 0.97 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3242 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | 1O    | 205  | 1/1   | 0.97 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3007 | 1/1   | 0.97 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3645 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3655 | 1/1   | 0.97 | 0.06 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3010 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 4033 | 1/1   | 0.97 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3037 | 1/1   | 0.97 | 0.24 | 22,22,22,22                 | 0     |
| 57  | MG   | 1Q    | 201  | 1/1   | 0.97 | 0.14 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3005 | 1/1   | 0.97 | 0.08 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3017 | 1/1   | 0.97 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3018 | 1/1   | 0.97 | 0.06 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3424 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 25    | 104  | 1/1   | 0.97 | 0.05 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3425 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3657 | 1/1   | 0.97 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3416 | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3021 | 1/1   | 0.97 | 0.25 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3563 | 1/1   | 0.97 | 0.08 | 13,13,13,13                 | 0     |
| 57  | MG   | 2A    | 3429 | 1/1   | 0.97 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3192 | 1/1   | 0.97 | 0.29 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3664 | 1/1   | 0.97 | 0.07 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3025 | 1/1   | 0.97 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3144 | 1/1   | 0.97 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3024 | 1/1   | 0.97 | 0.27 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 1606 | 1/1   | 0.97 | 0.11 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3435 | 1/1   | 0.97 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1S    | 201  | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 1609 | 1/1   | 0.97 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3905 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3108 | 1/1   | 0.97 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3305 | 1/1   | 0.97 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3250 | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 4047 | 1/1   | 0.97 | 0.05 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3034 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3035 | 1/1   | 0.97 | 0.25 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3790 | 1/1   | 0.97 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3489 | 1/1   | 0.97 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | 2a    | 1619 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3446 | 1/1   | 0.97 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3038 | 1/1   | 0.97 | 0.25 | 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    | 3423 | 1/1   | 0.97 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3109 | 1/1   | 0.97 | 0.07 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3675 | 1/1   | 0.97 | 0.11 | 6,6,6,6                     | 0     |
| 57  | MG   | 1A    | 3676 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3688 | 1/1   | 0.97 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 1627 | 1/1   | 0.97 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3148 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3365 | 1/1   | 0.97 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3149 | 1/1   | 0.97 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 1V    | 206  | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3054 | 1/1   | 0.97 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3457 | 1/1   | 0.97 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3006 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3925 | 1/1   | 0.97 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3612 | 1/1   | 0.97 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1W    | 202  | 1/1   | 0.97 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3369 | 1/1   | 0.97 | 0.20 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3083 | 1/1   | 0.97 | 0.11 | 13,13,13,13                 | 0     |
| 57  | MG   | 1A    | 3084 | 1/1   | 0.97 | 0.23 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3585 | 1/1   | 0.97 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3930 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3058 | 1/1   | 0.97 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3059 | 1/1   | 0.97 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3708 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3501 | 1/1   | 0.97 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3620 | 1/1   | 0.97 | 0.21 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3587 | 1/1   | 0.97 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3063 | 1/1   | 0.97 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | 1Z    | 301  | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3689 | 1/1   | 0.97 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3066 | 1/1   | 0.97 | 0.04 | 36,36,36,36                 | 0     |
| 57  | MG   | 1Z    | 303  | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3068 | 1/1   | 0.97 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3026 | 1/1   | 0.97 | 0.09 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3070 | 1/1   | 0.97 | 0.04 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3071 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3205 | 1/1   | 0.97 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3435 | 1/1   | 0.97 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | 10    | 104  | 1/1   | 0.97 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3011 | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3938 | 1/1   | 0.97 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3939 | 1/1   | 0.97 | 0.07 | 14,14,14,14                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3078 | 1/1   | 0.97 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3376 | 1/1   | 0.97 | 0.14 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 4080 | 1/1   | 0.97 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3696 | 1/1   | 0.97 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3494 | 1/1   | 0.97 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1I    | 103  | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3816 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3735 | 1/1   | 0.97 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3697 | 1/1   | 0.97 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3737 | 1/1   | 0.97 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3508 | 1/1   | 0.97 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3699 | 1/1   | 0.97 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3059 | 1/1   | 0.97 | 0.08 | 25,25,25,25                 | 0     |
| 57  | MG   | 15    | 3201 | 1/1   | 0.97 | 0.37 | 27,27,27,27                 | 0     |
| 57  | MG   | 1B    | 204  | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 15    | 3203 | 1/1   | 0.97 | 0.35 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3378 | 1/1   | 0.97 | 0.42 | 29,29,29,29                 | 0     |
| 57  | MG   | 1B    | 206  | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 15    | 3206 | 1/1   | 0.97 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3297 | 1/1   | 0.97 | 0.10 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 1685 | 1/1   | 0.97 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 15    | 3207 | 1/1   | 0.97 | 0.17 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 3650 | 1/1   | 0.97 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3379 | 1/1   | 0.97 | 0.22 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3097 | 1/1   | 0.97 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3007 | 1/1   | 0.97 | 0.04 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3824 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3513 | 1/1   | 0.97 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3264 | 1/1   | 0.97 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 17    | 102  | 1/1   | 0.97 | 0.06 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3518 | 1/1   | 0.97 | 0.11 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3104 | 1/1   | 0.97 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3708 | 1/1   | 0.97 | 0.07 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3521 | 1/1   | 0.97 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | 17    | 104  | 1/1   | 0.97 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3523 | 1/1   | 0.97 | 0.07 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3828 | 1/1   | 0.97 | 0.11 | 12,12,12,12                 | 0     |
| 57  | MG   | 1a    | 3662 | 1/1   | 0.97 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3045 | 1/1   | 0.97 | 0.10 | 21,21,21,21                 | 0     |
| 57  | MG   | 1B    | 215  | 1/1   | 0.97 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3323 | 1/1   | 0.97 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3531 | 1/1   | 0.97 | 0.08 | 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   | 1A    | 3606 | 1/1   | 0.97 | 0.07 | 16,16,16,16                 | 0     |
| 57  | MG   | 18    | 106  | 1/1   | 0.97 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3772 | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3773 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3713 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3501 | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3116 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3537 | 1/1   | 0.97 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3833 | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3211 | 1/1   | 0.97 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3780 | 1/1   | 0.97 | 0.08 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3962 | 1/1   | 0.97 | 0.07 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3120 | 1/1   | 0.97 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3267 | 1/1   | 0.97 | 0.07 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3030 | 1/1   | 0.97 | 0.20 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3008 | 1/1   | 0.97 | 0.05 | 6,6,6,6                     | 0     |
| 57  | MG   | 1A    | 3065 | 1/1   | 0.97 | 0.10 | 15,15,15,15                 | 0     |
| 57  | MG   | 1a    | 3509 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3790 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | 1B    | 228  | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3033 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3330 | 1/1   | 0.97 | 0.07 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3125 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3514 | 1/1   | 0.97 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3683 | 1/1   | 0.97 | 0.05 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3553 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3725 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3392 | 1/1   | 0.97 | 0.17 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3686 | 1/1   | 0.97 | 0.18 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3279 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3035 | 1/1   | 0.97 | 0.07 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 3281 | 1/1   | 0.97 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1741 | 1/1   | 0.97 | 0.31 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3562 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3341 | 1/1   | 0.97 | 0.04 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3564 | 1/1   | 0.97 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3847 | 1/1   | 0.97 | 0.26 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3170 | 1/1   | 0.97 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3732 | 1/1   | 0.97 | 0.12 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3850 | 1/1   | 0.97 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3172 | 1/1   | 0.97 | 0.26 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3986 | 1/1   | 0.97 | 0.06 | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3147 | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1D    | 307  | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3735 | 1/1   | 0.97 | 0.06 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3622 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3822 | 1/1   | 0.97 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 1756 | 1/1   | 0.97 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3575 | 1/1   | 0.97 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3068 | 1/1   | 0.97 | 0.14 | 10,10,10,10                 | 0     |
| 57  | MG   | 1D    | 312  | 1/1   | 0.97 | 0.12 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3624 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3532 | 1/1   | 0.97 | 0.29 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3704 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3857 | 1/1   | 0.97 | 0.11 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3582 | 1/1   | 0.97 | 0.06 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3534 | 1/1   | 0.97 | 0.12 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3832 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3535 | 1/1   | 0.97 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1E    | 302  | 1/1   | 0.97 | 0.11 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3225 | 1/1   | 0.97 | 0.13 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3860 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3589 | 1/1   | 0.97 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3626 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3741 | 1/1   | 0.97 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3366 | 1/1   | 0.97 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | 1E    | 309  | 1/1   | 0.97 | 0.03 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3998 | 1/1   | 0.97 | 0.07 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3595 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3069 | 1/1   | 0.97 | 0.05 | 5,5,5,5                     | 0     |
| 57  | MG   | 1A    | 4000 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | 1F    | 302  | 1/1   | 0.97 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 4001 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3536 | 1/1   | 0.97 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3130 | 1/1   | 0.97 | 0.28 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3465 | 1/1   | 0.97 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3603 | 1/1   | 0.97 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3604 | 1/1   | 0.97 | 0.13 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3070 | 1/1   | 0.97 | 0.15 | 23,23,23,23                 | 0     |
| 57  | MG   | 2D    | 302  | 1/1   | 0.97 | 0.12 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3543 | 1/1   | 0.97 | 0.17 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3134 | 1/1   | 0.97 | 0.07 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3181 | 1/1   | 0.97 | 0.21 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3545 | 1/1   | 0.97 | 0.23 | 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    | 3754 | 1/1   | 0.97 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3184 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3612 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3556 | 1/1   | 0.97 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3468 | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 57  | MG   | 1m    | 3001 | 1/1   | 0.97 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3050 | 1/1   | 0.97 | 0.14 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3758 | 1/1   | 0.97 | 0.05 | 17,17,17,17                 | 0     |
| 57  | MG   | 2x    | 105  | 1/1   | 0.97 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3100 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3878 | 1/1   | 0.97 | 0.10 | 19,19,19,19                 | 0     |
| 57  | MG   | 2F    | 303  | 1/1   | 0.97 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3562 | 1/1   | 0.97 | 0.07 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3550 | 1/1   | 0.97 | 0.10 | 22,22,22,22                 | 0     |
| 59  | ZN   | 2n    | 501  | 1/1   | 0.97 | 0.04 | 89,89,89,89                 | 0     |
| 60  | SF4  | 1d    | 302  | 8/8   | 0.97 | 0.05 | 56,62,66,68                 | 0     |
| 57  | MG   | 1E    | 303  | 1/1   | 0.98 | 0.08 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3274 | 1/1   | 0.98 | 0.12 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3151 | 1/1   | 0.98 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3486 | 1/1   | 0.98 | 0.28 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3746 | 1/1   | 0.98 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3011 | 1/1   | 0.98 | 0.05 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3748 | 1/1   | 0.98 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | 1E    | 308  | 1/1   | 0.98 | 0.11 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3157 | 1/1   | 0.98 | 0.16 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3667 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3240 | 1/1   | 0.98 | 0.23 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3016 | 1/1   | 0.98 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3616 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3785 | 1/1   | 0.98 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3161 | 1/1   | 0.98 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3598 | 1/1   | 0.98 | 0.10 | 9,9,9,9                     | 0     |
| 57  | MG   | 2A    | 3788 | 1/1   | 0.98 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1E    | 312  | 1/1   | 0.98 | 0.27 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3670 | 1/1   | 0.98 | 0.07 | 11,11,11,11                 | 0     |
| 57  | MG   | 1F    | 301  | 1/1   | 0.98 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 1653 | 1/1   | 0.98 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3599 | 1/1   | 0.98 | 0.07 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3208 | 1/1   | 0.98 | 0.06 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3277 | 1/1   | 0.98 | 0.19 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3466 | 1/1   | 0.98 | 0.17 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3443 | 1/1   | 0.98 | 0.14 | 25,25,25,25                 | 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   | 0.98 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3491 | 1/1   | 0.98 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 4042 | 1/1   | 0.98 | 0.04 | 7,7,7,7                     | 0     |
| 57  | MG   | 2A    | 3801 | 1/1   | 0.98 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3173 | 1/1   | 0.98 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3760 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3604 | 1/1   | 0.98 | 0.06 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 3278 | 1/1   | 0.98 | 0.29 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3546 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3807 | 1/1   | 0.98 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 3641 | 1/1   | 0.98 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3400 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3637 | 1/1   | 0.98 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3811 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3357 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 4049 | 1/1   | 0.98 | 0.08 | 14,14,14,14                 | 0     |
| 57  | MG   | 1a    | 3645 | 1/1   | 0.98 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3815 | 1/1   | 0.98 | 0.06 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3316 | 1/1   | 0.98 | 0.11 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3131 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3483 | 1/1   | 0.98 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3164 | 1/1   | 0.98 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3101 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 4054 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 3652 | 1/1   | 0.98 | 0.08 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3648 | 1/1   | 0.98 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3189 | 1/1   | 0.98 | 0.04 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3036 | 1/1   | 0.98 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3772 | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3859 | 1/1   | 0.98 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4059 | 1/1   | 0.98 | 0.07 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3321 | 1/1   | 0.98 | 0.19 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3687 | 1/1   | 0.98 | 0.07 | 6,6,6,6                     | 0     |
| 57  | MG   | 1A    | 3189 | 1/1   | 0.98 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3957 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3051 | 1/1   | 0.98 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3075 | 1/1   | 0.98 | 0.11 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3248 | 1/1   | 0.98 | 0.19 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3691 | 1/1   | 0.98 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3867 | 1/1   | 0.98 | 0.07 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3504 | 1/1   | 0.98 | 0.21 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3619 | 1/1   | 0.98 | 0.04 | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3191 | 1/1   | 0.98 | 0.13 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3560 | 1/1   | 0.98 | 0.04 | 21,21,21,21                 | 0     |
| 57  | MG   | 2a    | 1703 | 1/1   | 0.98 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 4072 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3967 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3123 | 1/1   | 0.98 | 0.26 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3152 | 1/1   | 0.98 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | 1Q    | 205  | 1/1   | 0.98 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3672 | 1/1   | 0.98 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3063 | 1/1   | 0.98 | 0.13 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3564 | 1/1   | 0.98 | 0.11 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3171 | 1/1   | 0.98 | 0.08 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 1713 | 1/1   | 0.98 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1R    | 203  | 1/1   | 0.98 | 0.15 | 20,20,20,20                 | 0     |
| 57  | MG   | 2B    | 217  | 1/1   | 0.98 | 0.22 | 47,47,47,47                 | 0     |
| 57  | MG   | 1R    | 204  | 1/1   | 0.98 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3138 | 1/1   | 0.98 | 0.15 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3173 | 1/1   | 0.98 | 0.15 | 19,19,19,19                 | 0     |
| 57  | MG   | 2D    | 303  | 1/1   | 0.98 | 0.29 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3365 | 1/1   | 0.98 | 0.18 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3374 | 1/1   | 0.98 | 0.24 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 4082 | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 4083 | 1/1   | 0.98 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3686 | 1/1   | 0.98 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3552 | 1/1   | 0.98 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3524 | 1/1   | 0.98 | 0.09 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3976 | 1/1   | 0.98 | 0.05 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3018 | 1/1   | 0.98 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3527 | 1/1   | 0.98 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3199 | 1/1   | 0.98 | 0.09 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3571 | 1/1   | 0.98 | 0.14 | 7,7,7,7                     | 0     |
| 57  | MG   | 1A    | 3709 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3982 | 1/1   | 0.98 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | 1U    | 207  | 1/1   | 0.98 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | 1U    | 208  | 1/1   | 0.98 | 0.29 | 28,28,28,28                 | 0     |
| 57  | MG   | 1U    | 209  | 1/1   | 0.98 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3884 | 1/1   | 0.98 | 0.09 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3515 | 1/1   | 0.98 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3985 | 1/1   | 0.98 | 0.08 | 8,8,8,8                     | 0     |
| 57  | MG   | 1a    | 3697 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3228 | 1/1   | 0.98 | 0.21 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3574 | 1/1   | 0.98 | 0.07 | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1V    | 205  | 1/1   | 0.98 | 0.22 | 20,20,20,20                 | 0     |
| 57  | MG   | 2Q    | 201  | 1/1   | 0.98 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3568 | 1/1   | 0.98 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3177 | 1/1   | 0.98 | 0.04 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3260 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3078 | 1/1   | 0.98 | 0.06 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3803 | 1/1   | 0.98 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3338 | 1/1   | 0.98 | 0.19 | 15,15,15,15                 | 0     |
| 57  | MG   | 1W    | 203  | 1/1   | 0.98 | 0.20 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3339 | 1/1   | 0.98 | 0.25 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3522 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3101 | 1/1   | 0.98 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | 1X    | 101  | 1/1   | 0.98 | 0.29 | 24,24,24,24                 | 0     |
| 57  | MG   | 1B    | 217  | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 1X    | 104  | 1/1   | 0.98 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3252 | 1/1   | 0.98 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3400 | 1/1   | 0.98 | 0.29 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3996 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3724 | 1/1   | 0.98 | 0.06 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3558 | 1/1   | 0.98 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3157 | 1/1   | 0.98 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3560 | 1/1   | 0.98 | 0.20 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3720 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3645 | 1/1   | 0.98 | 0.09 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3722 | 1/1   | 0.98 | 0.05 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3029 | 1/1   | 0.98 | 0.19 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3724 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3903 | 1/1   | 0.98 | 0.06 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3128 | 1/1   | 0.98 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3726 | 1/1   | 0.98 | 0.10 | 11,11,11,11                 | 0     |
| 57  | MG   | 1B    | 229  | 1/1   | 0.98 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 1d    | 301  | 1/1   | 0.98 | 0.19 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3906 | 1/1   | 0.98 | 0.04 | 6,6,6,6                     | 0     |
| 57  | MG   | 1A    | 3648 | 1/1   | 0.98 | 0.05 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3584 | 1/1   | 0.98 | 0.06 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3910 | 1/1   | 0.98 | 0.04 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3650 | 1/1   | 0.98 | 0.04 | 15,15,15,15                 | 0     |
| 57  | MG   | 1l    | 101  | 1/1   | 0.98 | 0.26 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3597 | 1/1   | 0.98 | 0.22 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3912 | 1/1   | 0.98 | 0.06 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3125 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3423 | 1/1   | 0.98 | 0.11 | 14,14,14,14                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4012 | 1/1   | 0.98 | 0.06 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3234 | 1/1   | 0.98 | 0.08 | 10,10,10,10                 | 0     |
| 57  | MG   | 12    | 102  | 1/1   | 0.98 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3914 | 1/1   | 0.98 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3020 | 1/1   | 0.98 | 0.04 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3586 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3653 | 1/1   | 0.98 | 0.07 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3073 | 1/1   | 0.98 | 0.08 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3134 | 1/1   | 0.98 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3734 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 1D    | 304  | 1/1   | 0.98 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3184 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3589 | 1/1   | 0.98 | 0.08 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3657 | 1/1   | 0.98 | 0.05 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3238 | 1/1   | 0.98 | 0.38 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3659 | 1/1   | 0.98 | 0.04 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3239 | 1/1   | 0.98 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3271 | 1/1   | 0.98 | 0.10 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3001 | 1/1   | 0.98 | 0.26 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3272 | 1/1   | 0.98 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | 1E    | 301  | 1/1   | 0.98 | 0.29 | 21,21,21,21                 | 0     |
| 59  | ZN   | 14    | 501  | 1/1   | 0.98 | 0.06 | 98,98,98,98                 | 0     |
| 59  | ZN   | 1n    | 102  | 1/1   | 0.98 | 0.04 | 72,72,72,72                 | 0     |
| 59  | ZN   | 2Y    | 202  | 1/1   | 0.98 | 0.04 | 75,75,75,75                 | 0     |
| 57  | MG   | 2A    | 3769 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 59  | ZN   | 29    | 501  | 1/1   | 0.98 | 0.04 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3273 | 1/1   | 0.98 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | 17    | 101  | 1/1   | 0.98 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3017 | 1/1   | 0.99 | 0.07 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3031 | 1/1   | 0.99 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3459 | 1/1   | 0.99 | 0.03 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3042 | 1/1   | 0.99 | 0.10 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3218 | 1/1   | 0.99 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1w    | 401  | 1/1   | 0.99 | 0.10 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3811 | 1/1   | 0.99 | 0.05 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3964 | 1/1   | 0.99 | 0.07 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3777 | 1/1   | 0.99 | 0.04 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3885 | 1/1   | 0.99 | 0.04 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3414 | 1/1   | 0.99 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3799 | 1/1   | 0.99 | 0.09 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3778 | 1/1   | 0.99 | 0.03 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3219 | 1/1   | 0.99 | 0.04 | 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    | 3172 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3660 | 1/1   | 0.99 | 0.06 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3747 | 1/1   | 0.99 | 0.02 | 11,11,11,11                 | 0     |
| 57  | MG   | 1B    | 218  | 1/1   | 0.99 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3220 | 1/1   | 0.99 | 0.04 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 4015 | 1/1   | 0.99 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3749 | 1/1   | 0.99 | 0.03 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3133 | 1/1   | 0.99 | 0.03 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3022 | 1/1   | 0.99 | 0.11 | 6,6,6,6                     | 0     |
| 57  | MG   | 1A    | 3894 | 1/1   | 0.99 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1U    | 201  | 1/1   | 0.99 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3680 | 1/1   | 0.99 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3856 | 1/1   | 0.99 | 0.08 | 16,16,16,16                 | 0     |
| 57  | MG   | 1U    | 203  | 1/1   | 0.99 | 0.20 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3056 | 1/1   | 0.99 | 0.09 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3978 | 1/1   | 0.99 | 0.07 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3008 | 1/1   | 0.99 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3637 | 1/1   | 0.99 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3128 | 1/1   | 0.99 | 0.35 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3071 | 1/1   | 0.99 | 0.19 | 6,6,6,6                     | 0     |
| 57  | MG   | 2A    | 3689 | 1/1   | 0.99 | 0.02 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3151 | 1/1   | 0.99 | 0.06 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3090 | 1/1   | 0.99 | 0.15 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3757 | 1/1   | 0.99 | 0.04 | 17,17,17,17                 | 0     |
| 57  | MG   | 1U    | 211  | 1/1   | 0.99 | 0.13 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3863 | 1/1   | 0.99 | 0.10 | 10,10,10,10                 | 0     |
| 57  | MG   | 1a    | 3651 | 1/1   | 0.99 | 0.02 | 27,27,27,27                 | 0     |
| 57  | MG   | 1V    | 201  | 1/1   | 0.99 | 0.12 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3697 | 1/1   | 0.99 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3003 | 1/1   | 0.99 | 0.04 | 11,11,11,11                 | 0     |
| 57  | MG   | 1A    | 3541 | 1/1   | 0.99 | 0.08 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3020 | 1/1   | 0.99 | 0.03 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3542 | 1/1   | 0.99 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3644 | 1/1   | 0.99 | 0.06 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3989 | 1/1   | 0.99 | 0.03 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3139 | 1/1   | 0.99 | 0.06 | 9,9,9,9                     | 0     |
| 57  | MG   | 2A    | 3512 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 57  | MG   | 17    | 106  | 1/1   | 0.99 | 0.05 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3908 | 1/1   | 0.99 | 0.05 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3081 | 1/1   | 0.99 | 0.08 | 24,24,24,24                 | 0     |
| 57  | MG   | 27    | 101  | 1/1   | 0.99 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 18    | 103  | 1/1   | 0.99 | 0.18 | 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    | 3115 | 1/1   | 0.99 | 0.26 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3082 | 1/1   | 0.99 | 0.08 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3034 | 1/1   | 0.99 | 0.11 | 25,25,25,25                 | 0     |
| 57  | MG   | 1D    | 306  | 1/1   | 0.99 | 0.03 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3175 | 1/1   | 0.99 | 0.10 | 17,17,17,17                 | 0     |
| 59  | ZN   | 1Y    | 204  | 1/1   | 0.99 | 0.03 | 54,54,54,54                 | 0     |
| 57  | MG   | 1X    | 102  | 1/1   | 0.99 | 0.09 | 33,33,33,33                 | 0     |
| 59  | ZN   | 15    | 3210 | 1/1   | 0.99 | 0.07 | 43,43,43,43                 | 0     |
| 59  | ZN   | 16    | 104  | 1/1   | 0.99 | 0.03 | 31,31,31,31                 | 0     |
| 57  | MG   | 1D    | 308  | 1/1   | 0.99 | 0.11 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3768 | 1/1   | 0.99 | 0.03 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 3176 | 1/1   | 0.99 | 0.08 | 15,15,15,15                 | 0     |
| 59  | ZN   | 25    | 105  | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 59  | ZN   | 26    | 102  | 1/1   | 0.99 | 0.03 | 47,47,47,47                 | 0     |
| 57  | MG   | 1X    | 106  | 1/1   | 0.99 | 0.10 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3159 | 1/1   | 0.99 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3214 | 1/1   | 0.99 | 0.23 | 23,23,23,23                 | 0     |
| 60  | SF4  | 2d    | 303  | 8/8   | 0.99 | 0.04 | 51,58,65,70                 | 0     |
| 59  | ZN   | 19    | 102  | 1/1   | 1.00 | 0.03 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3703 | 1/1   | 1.00 | 0.06 | 5,5,5,5                     | 0     |
| 57  | MG   | 2A    | 3673 | 1/1   | 1.00 | 0.01 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 4056 | 1/1   | 1.00 | 0.03 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3704 | 1/1   | 1.00 | 0.02 | 6,6,6,6                     | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.