



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:46 PM UTC

PDB ID : 8UD7 / pdb\_00008ud7  
Title : Crystal structure of the A2058-N6-dimethylated *Thermus thermophilus* 70S ribosome in complex with cresomycin, mRNA, deacylated A-site tRNA<sup>phe</sup>, aminoacylated P-site fMet-tRNA<sup>met</sup>, and deacylated E-site tRNA<sup>phe</sup> at 2.70Å resolution  
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Wu, K.J.Y.; Tresco, B.I.C.; Ramkissoon, A.; See, D.N.Y.; Liow, P.; Dittamore, G.A.; Yu, M.; Testolin, G.; Mitcheltree, M.J.; Liu, R.Y.; Svetlov, M.S.; Myers, A.G.; Polikanov, Y.S.  
Deposited on : 2023-09-28  
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                       |   |                                                                  |
|-----------------------|---|------------------------------------------------------------------|
| MolProbity            | : | 4-5-2 with Phenix2.0                                             |
| Mogul                 | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)      | : | 2.0                                                              |
| EDS                   | : | 3.0                                                              |
| Buster-report         | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                  | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness       | : | 1.0.12                                                           |

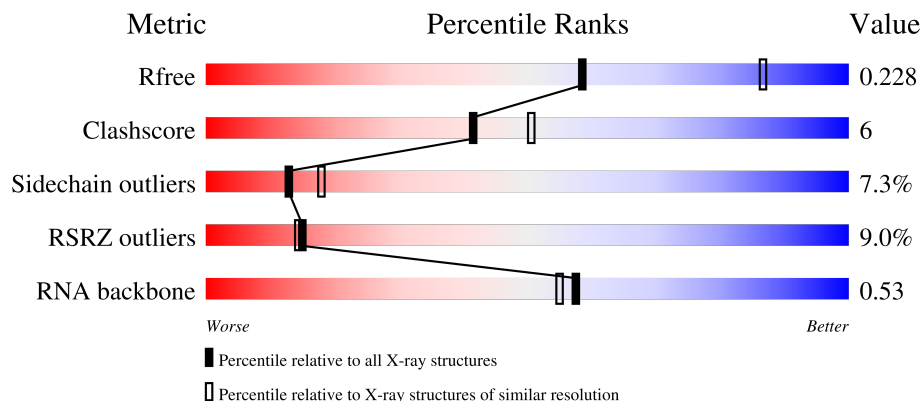
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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                      | 1091 (2.54-2.54)                                      |
| Clashscore         | 190562                      | 1120 (2.54-2.54)                                      |
| Sidechain outliers | 187428                      | 1106 (2.54-2.54)                                      |
| RSRZ outliers      | 180081                      | 1091 (2.54-2.54)                                      |
| RNA backbone       | 3983                        | 1112 (2.80-2.28)                                      |

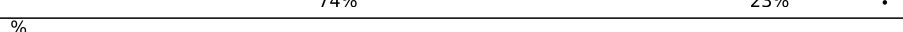
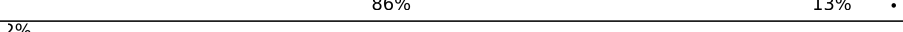
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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> <div></div> <div>71%</div> <div>22%</div> <div>6%</div> </div> </div> |
| 1   | 2A    | 2915   | <div> <div>5%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>5%</div> </div> </div> |

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Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | 1B    | 121    |    |
| 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    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14  | 2S    | 112    |                  |
| 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     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | 15    | 60     |                  |
| 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    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | 2h    | 138    |                  |
| 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    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | 1u    | 27     |                  |
| 52  | 2u    | 27     |                  |
| 53  | 1v    | 24     |                  |
| 53  | 2v    | 24     |                  |
| 54  | 1w    | 76     |                  |
| 54  | 1y    | 76     |                  |
| 54  | 2w    | 76     |                  |
| 54  | 2y    | 76     |                  |
| 55  | 1x    | 77     |                  |
| 55  | 2x    | 77     |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | PSU  | 2y    | 55   | -         | -        | X       | -                |
| 56  | MG   | 1A    | 3293 | -         | -        | -       | X                |
| 56  | MG   | 1A    | 3553 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3130 | -         | -        | -       | X                |
| 56  | MG   | 2A    | 3336 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1634 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1647 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1686 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1722 | -         | -        | -       | X                |
| 56  | MG   | 2a    | 1814 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 299373 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     |
|     |       |          | 61854 | 27533 | 11572 | 19878 | 2871 |         |         |       |
| 1   | 2A    | 2800     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60324 | 26850 | 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    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 608   | 375 | 129 | 103 | 1 |         |         |       |
| 22  | 20    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 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    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 958   | 592 | 198 | 166 | 2 |         |         |       |
| 44  | 2m    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 950   | 586 | 197 | 165 | 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 MF-mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 53  | 1v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 125 | 51 | 88 | 13 |         |         |       |
| 53  | 2v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 125 | 51 | 88 | 13 |         |         |       |

- Molecule 54 is a RNA chain called A- and E-site Deacylated tRNA<sup>phe</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 54  | 1w    | 72       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1550  | 694 | 277 | 505 | 72 | 2 |         |         |       |
| 54  | 1y    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1585  | 707 | 285 | 518 | 74 | 1 |         |         |       |
| 54  | 2w    | 69       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1482  | 662 | 267 | 482 | 69 | 2 |         |         |       |
| 54  | 2y    | 73       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1565  | 698 | 283 | 510 | 73 | 1 |         |         |       |

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-tRNA<sup>met</sup>.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 55  | 1x    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1635  | 731 | 296 | 530 | 76 | 2 |         |         |       |
| 55  | 2x    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1635  | 731 | 296 | 530 | 76 | 2 |         |         |       |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 56  | 1A    | 1097     | Total | Mg   | 0       | 0       |
|     |       |          | 1097  | 1097 |         |         |
| 56  | 1B    | 36       | Total | Mg   | 0       | 0       |
|     |       |          | 36    | 36   |         |         |
| 56  | 1D    | 11       | Total | Mg   | 0       | 0       |
|     |       |          | 11    | 11   |         |         |
| 56  | 1E    | 18       | Total | Mg   | 0       | 0       |
|     |       |          | 18    | 18   |         |         |
| 56  | 1F    | 13       | Total | Mg   | 0       | 0       |
|     |       |          | 13    | 13   |         |         |
| 56  | 1G    | 4        | Total | Mg   | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 56  | 1I    | 1        | Total | Mg   | 0       | 0       |
|     |       |          | 1     | 1    |         |         |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56  | 1N    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 56  | 1O    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 56  | 1P    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 56  | 1Q    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 56  | 1R    | 8        | Total<br>8  | Mg<br>8  | 0       | 0       |
| 56  | 1S    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 56  | 1T    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 1U    | 10       | Total<br>10 | Mg<br>10 | 0       | 0       |
| 56  | 1V    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 56  | 1W    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 56  | 1X    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 56  | 1Y    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 56  | 1Z    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 56  | 10    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 56  | 11    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 56  | 12    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | 13    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 56  | 14    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | 15    | 8        | Total<br>8  | Mg<br>8  | 0       | 0       |
| 56  | 16    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | 17    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 18    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 19    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1a    | 196      | Total<br>196 | Mg<br>196 | 0       | 0       |
| 56  | 1b    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1f    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1m    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1n    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 1r    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 1w    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | 1x    | 14       | Total<br>14  | Mg<br>14  | 0       | 0       |
| 56  | 1y    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2A    | 808      | Total<br>808 | Mg<br>808 | 0       | 0       |
| 56  | 2B    | 15       | Total<br>15  | Mg<br>15  | 0       | 0       |
| 56  | 2D    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 56  | 2E    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 56  | 2F    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 56  | 2G    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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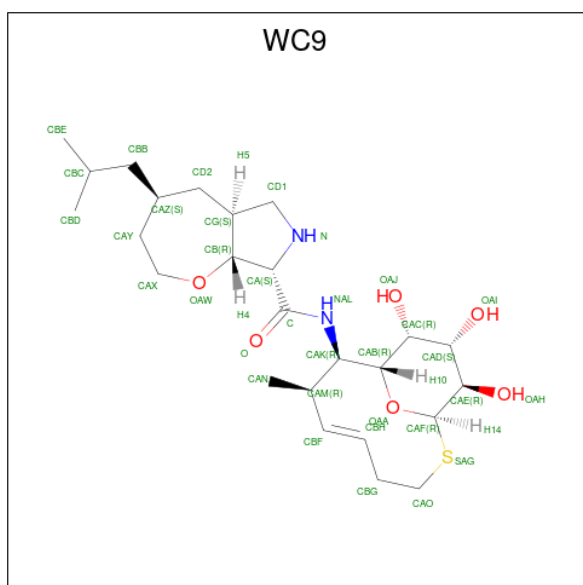
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | 2N    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2O    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2P    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2Q    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 2R    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 2T    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 2U    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2V    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2W    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | 2X    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 20    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 21    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 23    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 25    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 56  | 27    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 28    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | 2a    | 230      | Total<br>230 | Mg<br>230 | 0       | 0       |
| 56  | 2d    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | 2f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | 2j    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | 2l    | 4        | Total | Mg | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 56  | 2q    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | 2r    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | 2t    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | 2v    | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 56  | 2w    | 4        | Total | Mg | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 56  | 2x    | 5        | Total | Mg | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 56  | 2y    | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

- Molecule 57 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1R,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-13-oxa-2-thiabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: WC9) (formula: C<sub>25</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub>S) (labeled as "Ligand of Interest" by depositor).

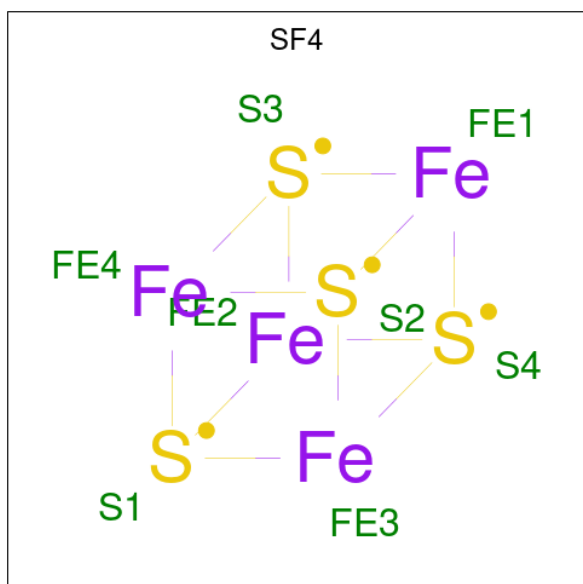


| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 57  | 1A    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 34    | 25 | 2 | 6 | 1 |         |         |
| 57  | 2A    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 34    | 25 | 2 | 6 | 1 |         |         |

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

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

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



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

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 60  | 1x    | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | 2x    | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 61  | 1A    | 1899     | Total | O    | 0       | 0       |
|     |       |          | 1899  | 1899 |         |         |
| 61  | 1B    | 59       | Total | O    | 0       | 0       |
|     |       |          | 59    | 59   |         |         |
| 61  | 1D    | 27       | Total | O    | 0       | 0       |
|     |       |          | 27    | 27   |         |         |
| 61  | 1E    | 26       | Total | O    | 0       | 0       |
|     |       |          | 26    | 26   |         |         |
| 61  | 1F    | 16       | Total | O    | 0       | 0       |
|     |       |          | 16    | 16   |         |         |
| 61  | 1G    | 1        | Total | O    | 0       | 0       |
|     |       |          | 1     | 1    |         |         |
| 61  | 1H    | 2        | Total | O    | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 61  | 1N    | 6        | Total | O    | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 61  | 1O    | 5        | Total | O    | 0       | 0       |
|     |       |          | 5     | 5    |         |         |
| 61  | 1P    | 22       | Total | O    | 0       | 0       |
|     |       |          | 22    | 22   |         |         |
| 61  | 1Q    | 8        | Total | O    | 0       | 0       |
|     |       |          | 8     | 8    |         |         |
| 61  | 1R    | 9        | Total | O    | 0       | 0       |
|     |       |          | 9     | 9    |         |         |
| 61  | 1S    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 61  | 1T    | 8        | Total | O    | 0       | 0       |
|     |       |          | 8     | 8    |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 1U    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 61  | 1V    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 61  | 1W    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 61  | 1X    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 1Y    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 1Z    | 1        | Total<br>1   | O<br>1   | 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    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 14    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 15    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 16    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 17    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 61  | 18    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 61  | 1a    | 263      | Total<br>263 | O<br>263 | 0       | 0       |
| 61  | 1b    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1d    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 1f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1g    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1l    | 3        | Total<br>3   | O<br>3   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 1n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 1q    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 1v    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | 1w    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 61  | 1x    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 61  | 1y    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2A    | 974      | Total<br>974 | O<br>974 | 0       | 0       |
| 61  | 2B    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 61  | 2D    | 19       | Total<br>19  | O<br>19  | 0       | 0       |
| 61  | 2E    | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 61  | 2F    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 61  | 2N    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2O    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2P    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 61  | 2Q    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2R    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 2T    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 2U    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 2X    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 20    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 21    | 7        | Total<br>7   | O<br>7   | 0       | 0       |

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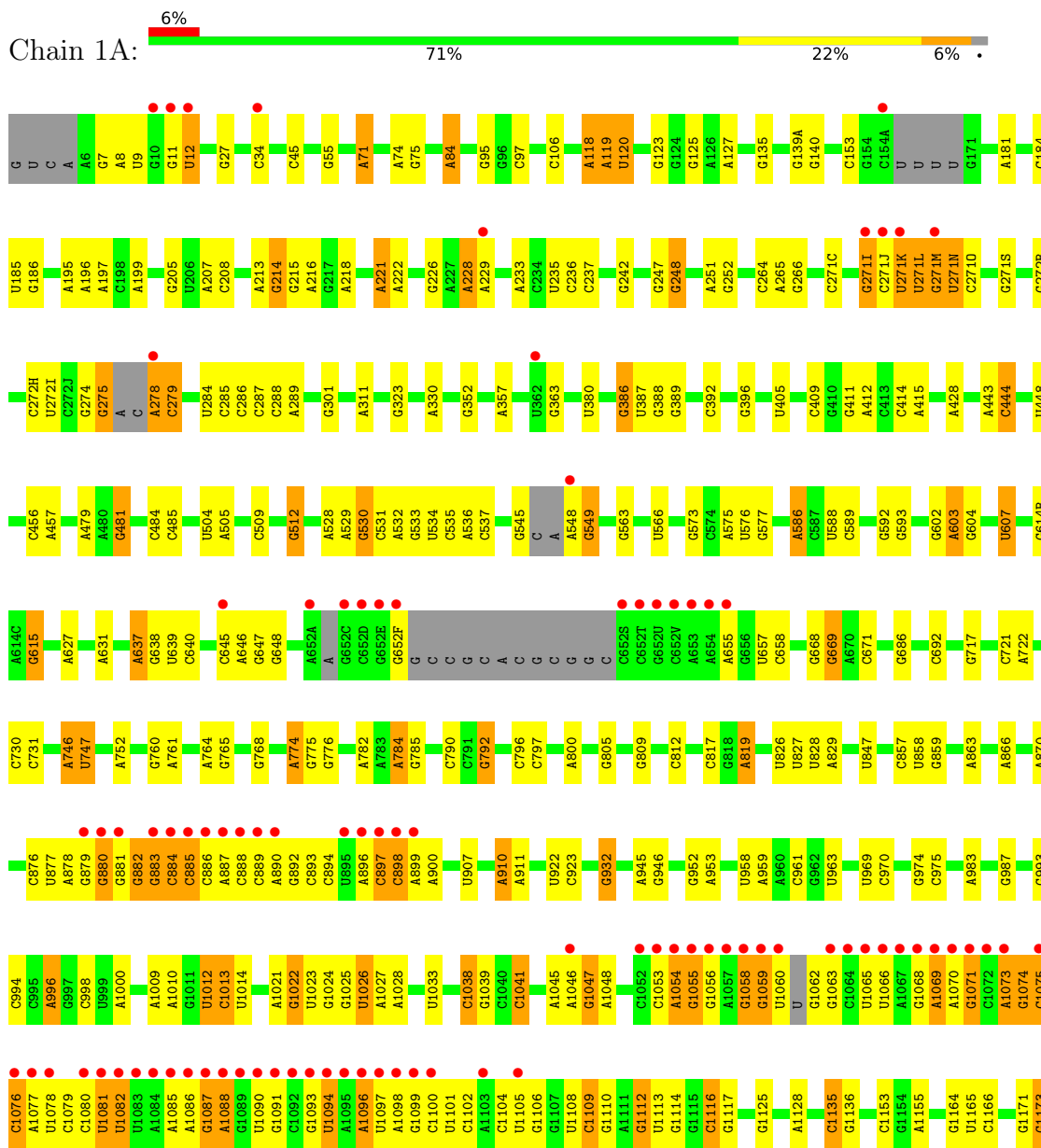
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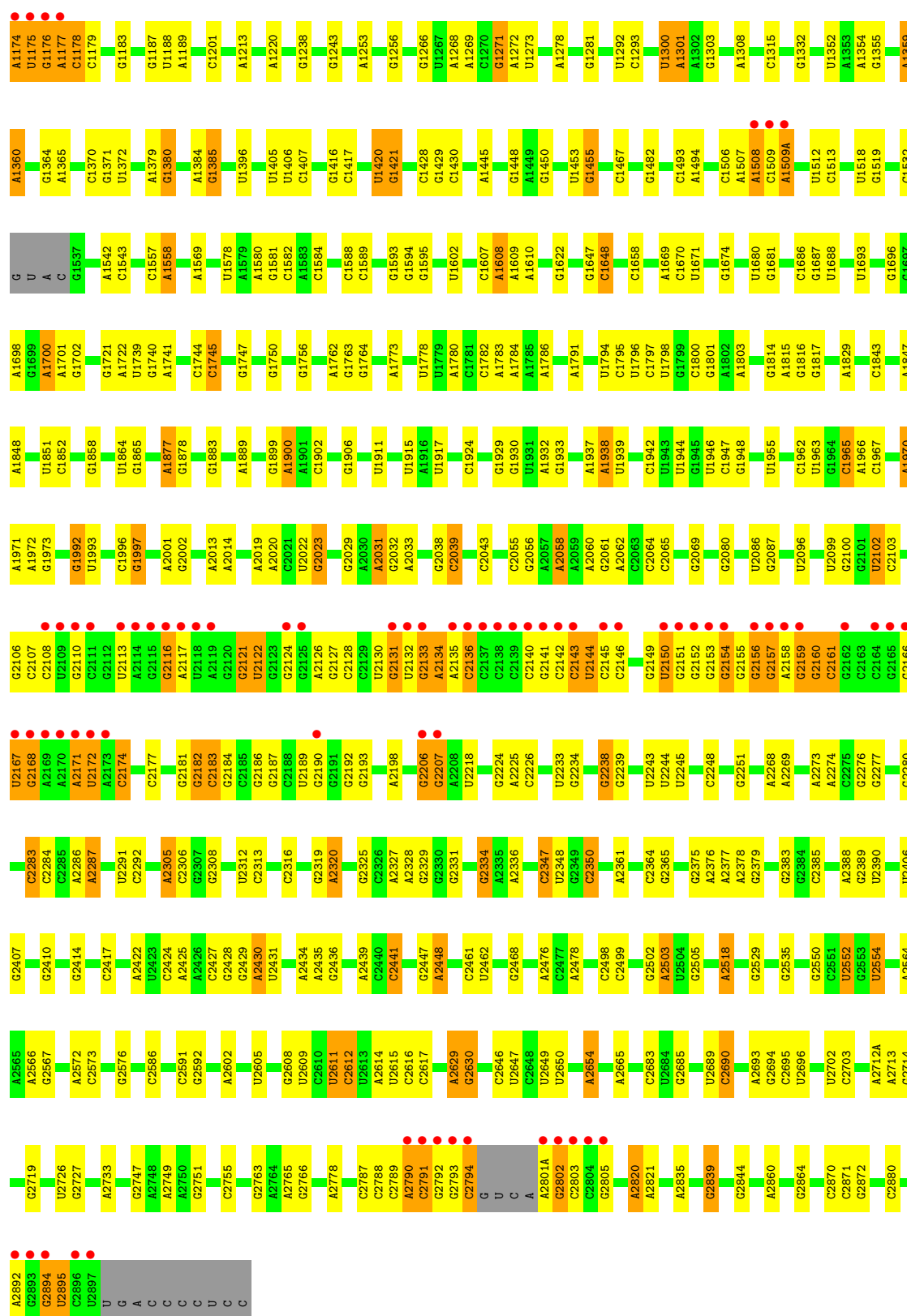
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | 23    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | 27    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 28    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 29    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2a    | 184      | Total<br>184 | O<br>184 | 0       | 0       |
| 61  | 2e    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2g    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2j    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 2l    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | 2t    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2v    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | 2x    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | 2y    | 2        | Total<br>2   | O<br>2   | 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.

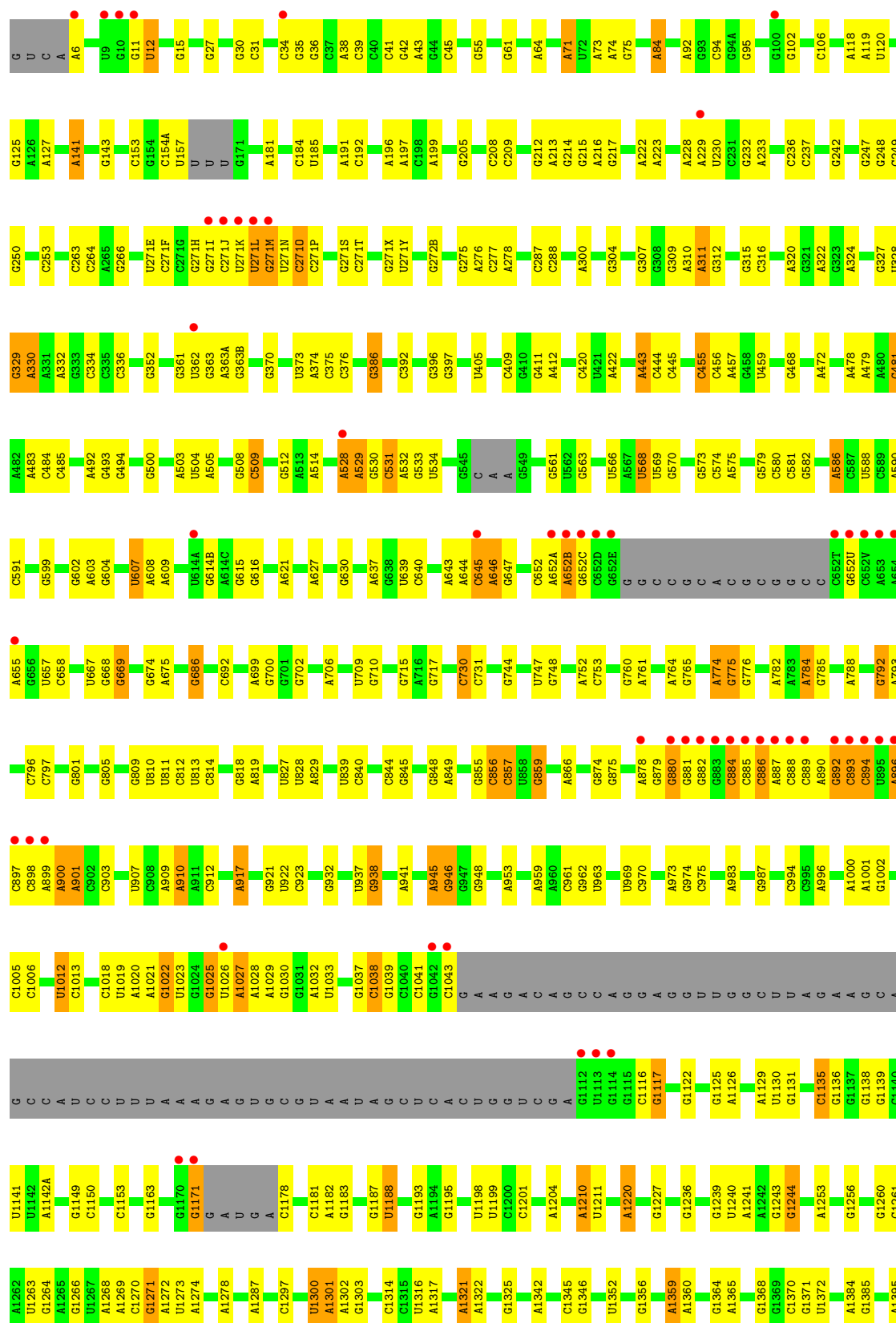
#### • Molecule 1: 23S Ribosomal RNA

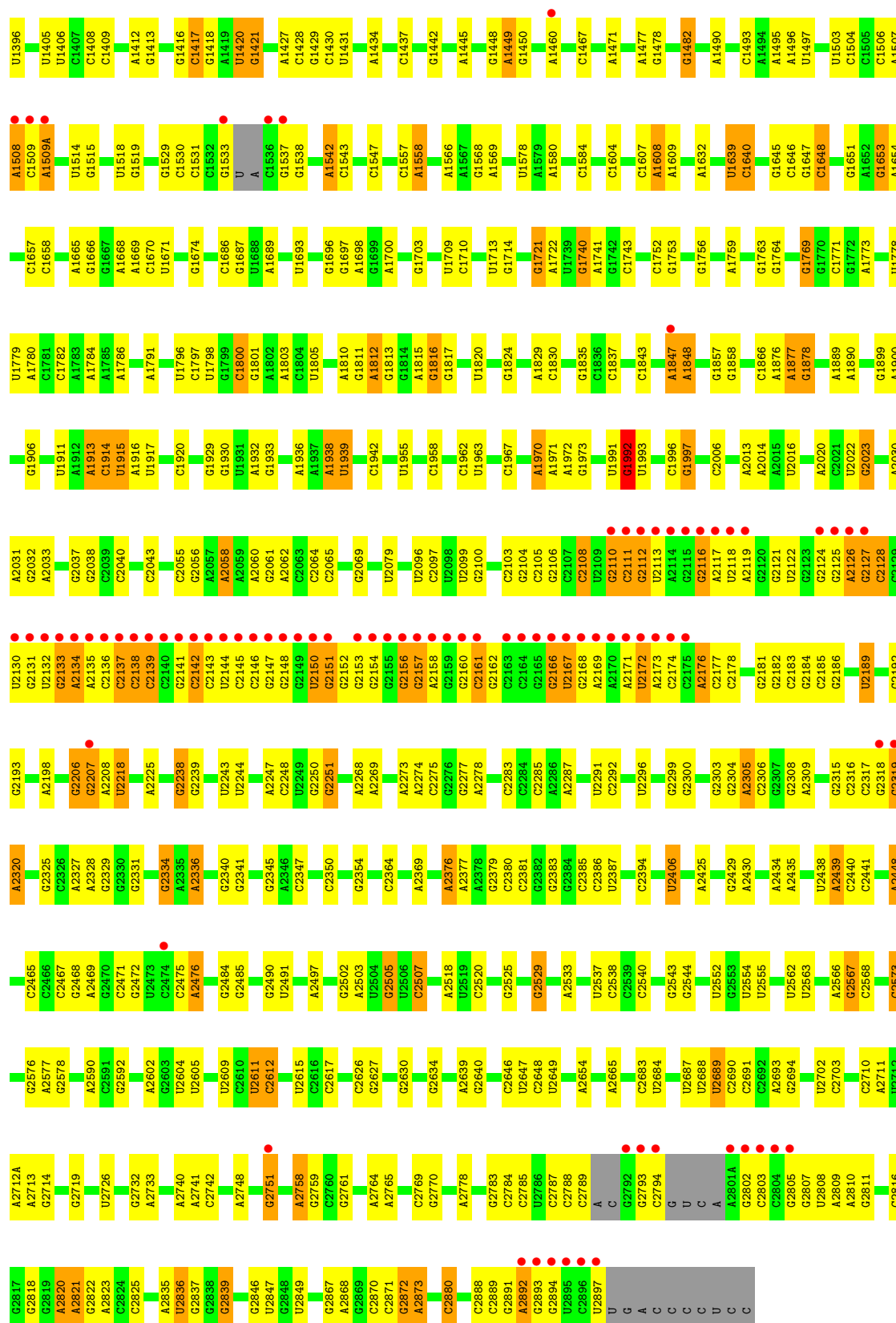




• Molecule 1: 23S Ribosomal RNA





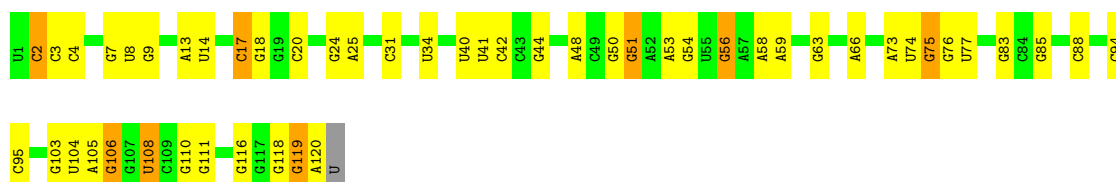


Chain 1B:  76% 20% ..



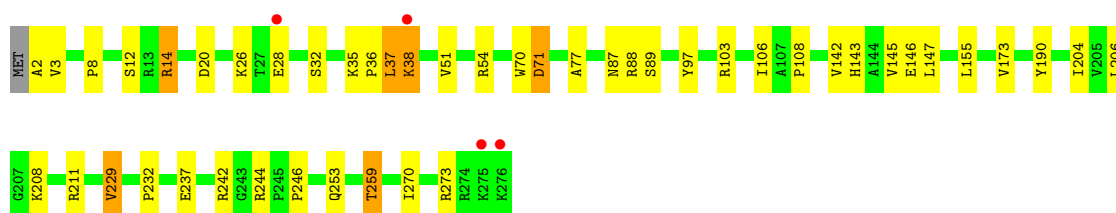
- Molecule 2: 5S Ribosomal RNA

Chain 2B:  58% 35% 7% .



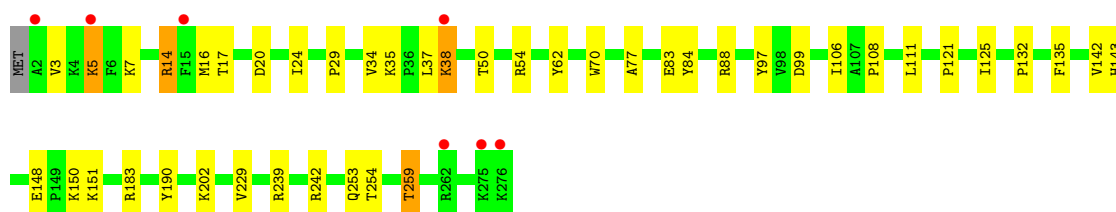
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  83% 15% .



- Molecule 3: 50S ribosomal protein L2

Chain 2D:  84% 14% 3% .



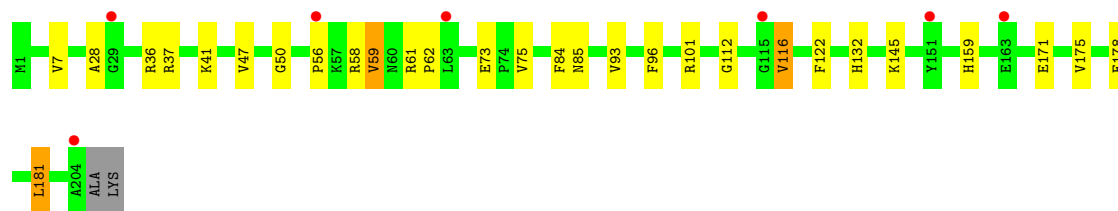
- Molecule 4: 50S ribosomal protein L3

Chain 1E:  86% 12% ..

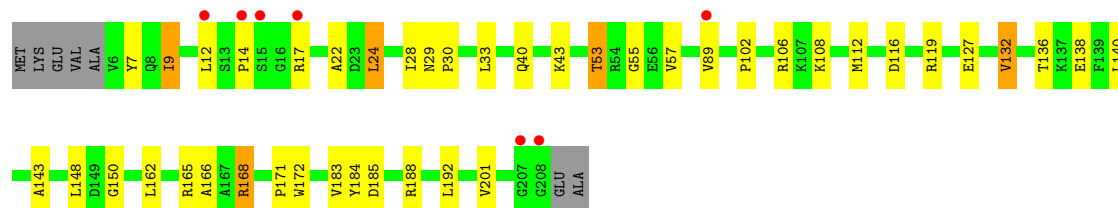
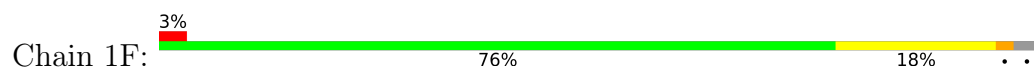


- Molecule 4: 50S ribosomal protein L3

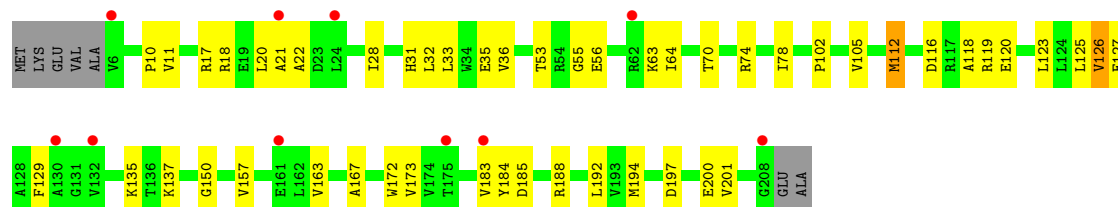
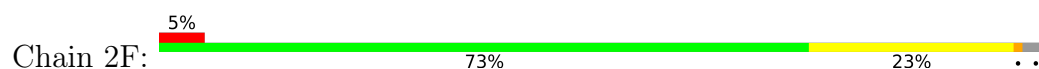
Chain 2E:  85% 13% ..



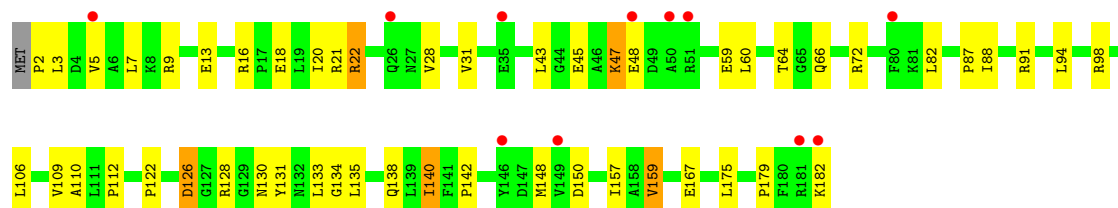
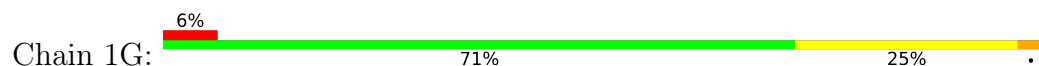
- Molecule 5: 50S ribosomal protein L4



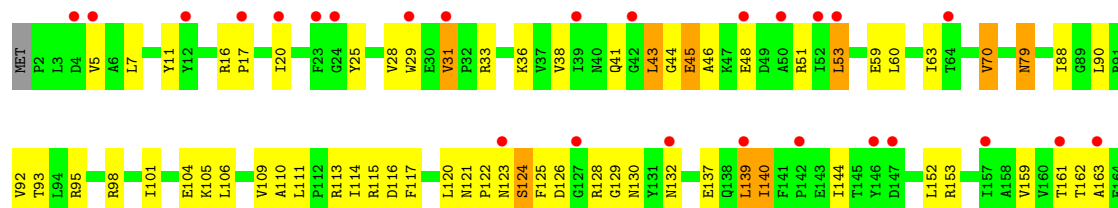
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

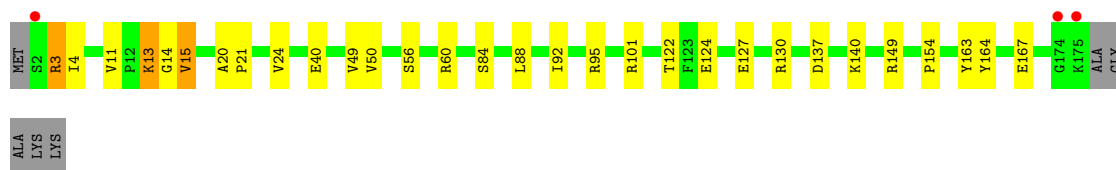
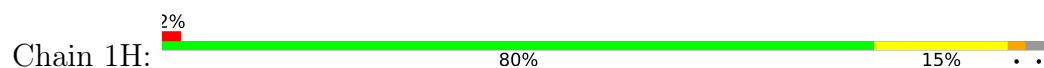


- Molecule 6: 50S ribosomal protein L5

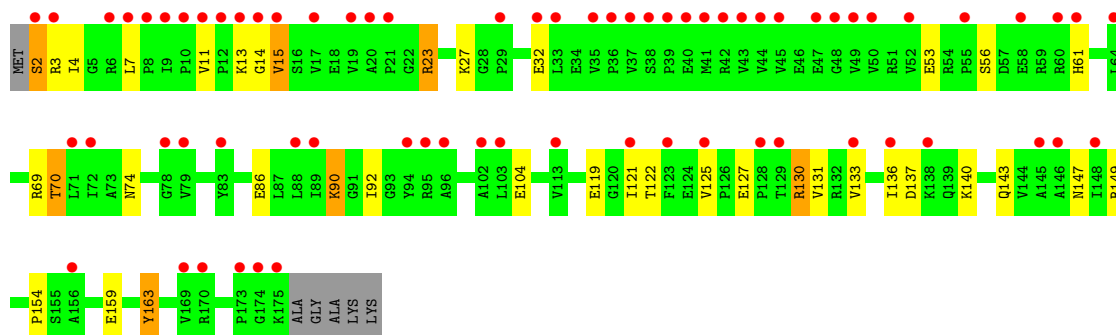
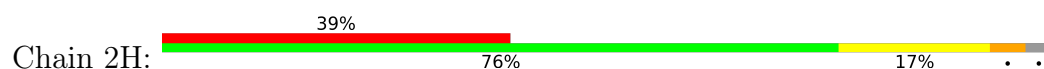




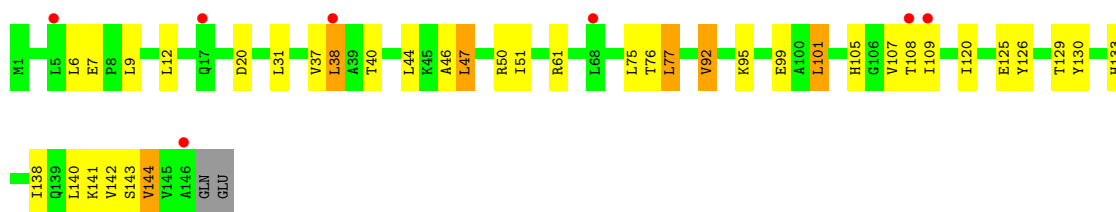
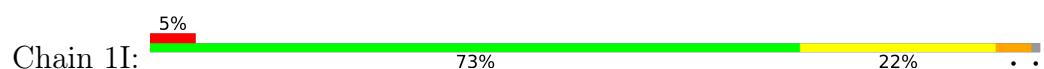
- Molecule 7: 50S ribosomal protein L6



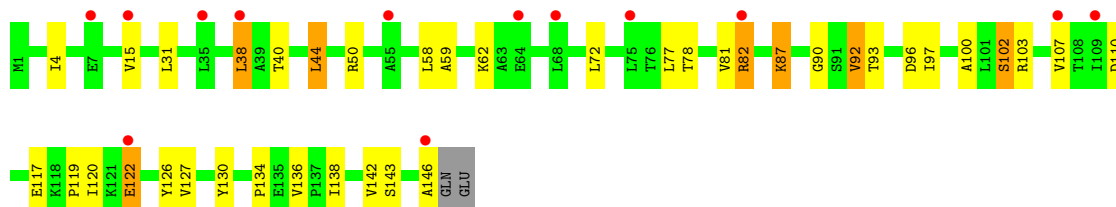
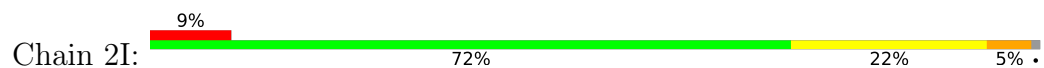
- Molecule 7: 50S ribosomal protein L6



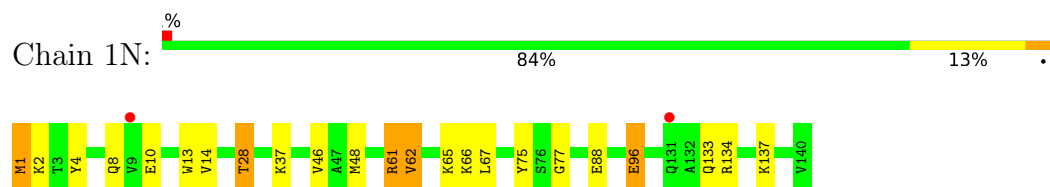
- Molecule 8: 50S ribosomal protein L9



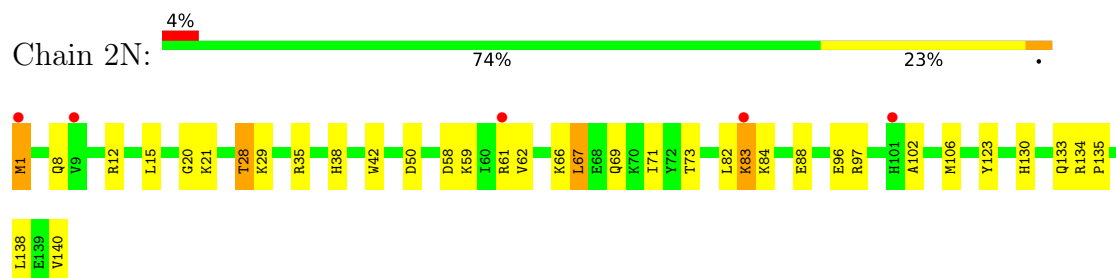
- Molecule 8: 50S ribosomal protein L9



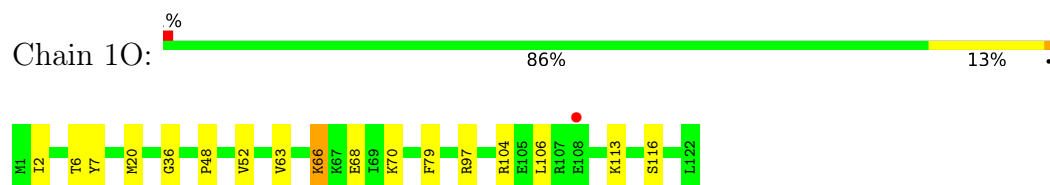
- Molecule 9: 50S ribosomal protein L13



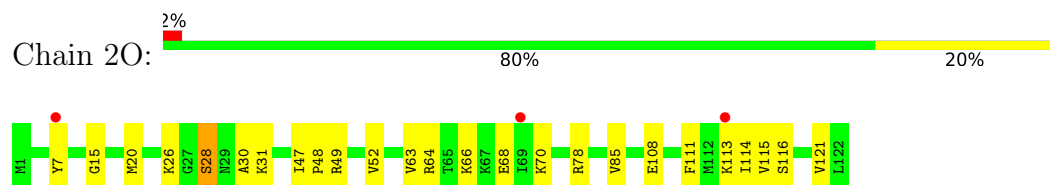
- Molecule 9: 50S ribosomal protein L13



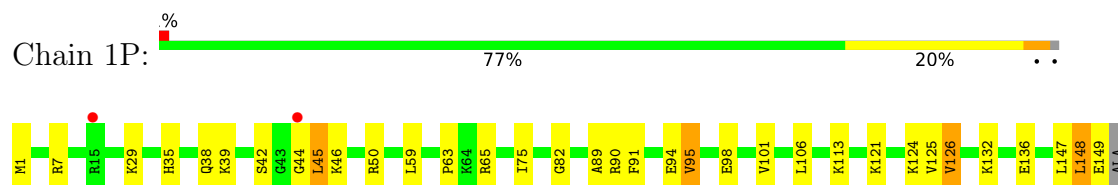
- Molecule 10: 50S ribosomal protein L14



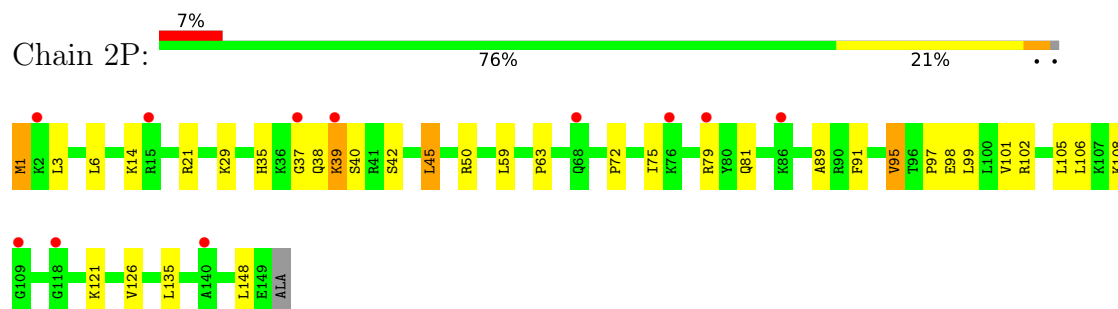
- Molecule 10: 50S ribosomal protein L14



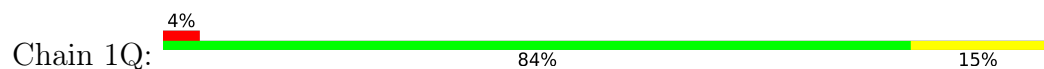
- Molecule 11: 50S ribosomal protein L15



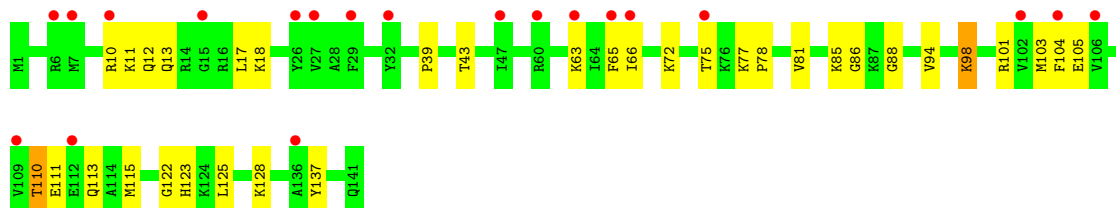
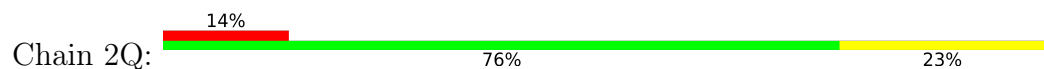
- Molecule 11: 50S ribosomal protein L15



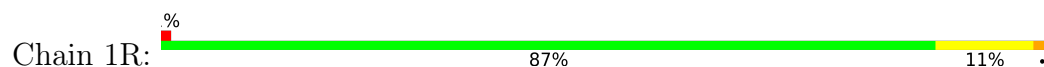
- Molecule 12: 50S ribosomal protein L16



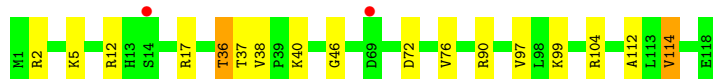
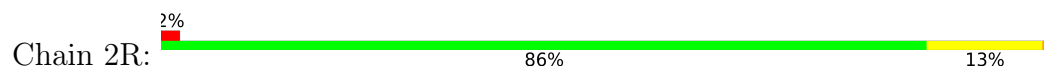
- Molecule 12: 50S ribosomal protein L16



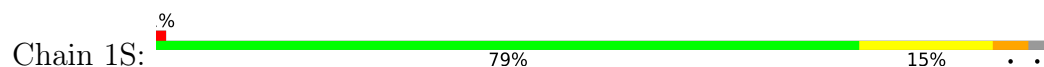
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

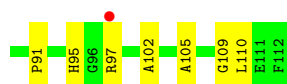


- Molecule 14: 50S ribosomal protein L18

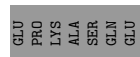
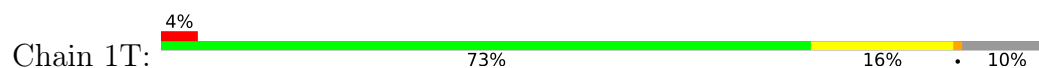


- Molecule 14: 50S ribosomal protein L18

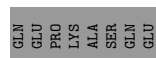
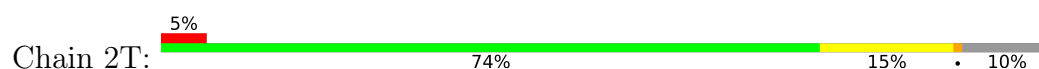




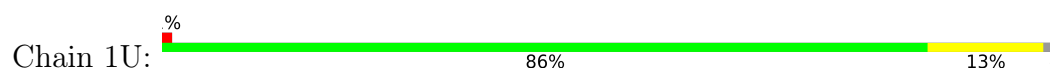
- Molecule 15: 50S ribosomal protein L19



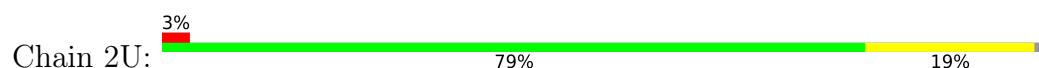
- Molecule 15: 50S ribosomal protein L19



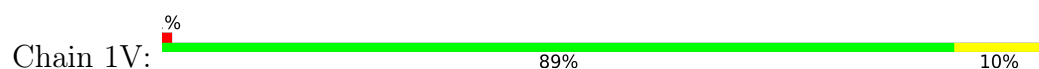
- Molecule 16: 50S ribosomal protein L20



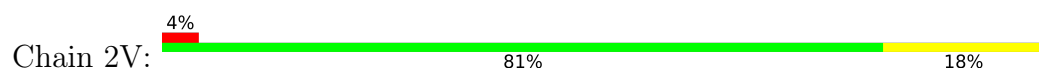
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

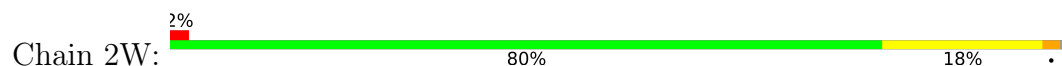




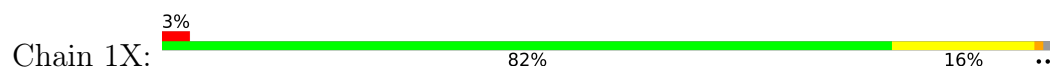
- Molecule 18: 50S ribosomal protein L22



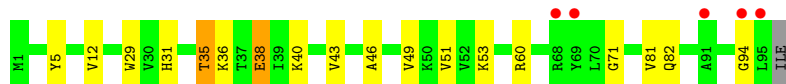
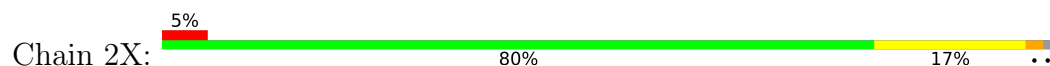
- Molecule 18: 50S ribosomal protein L22



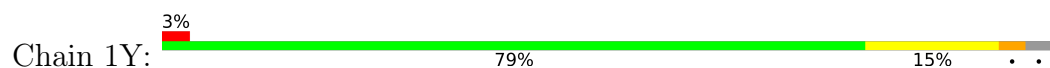
- Molecule 19: 50S ribosomal protein L23



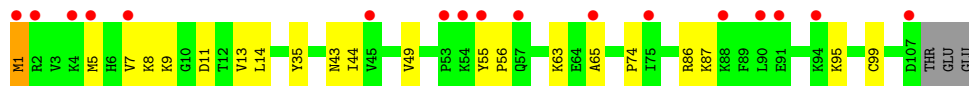
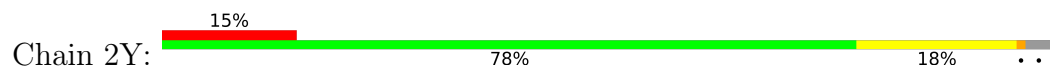
- Molecule 19: 50S ribosomal protein L23



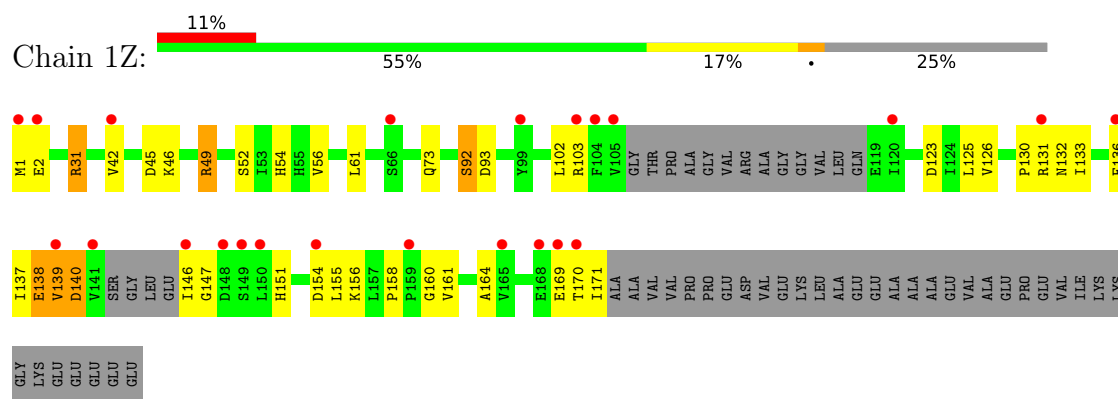
- Molecule 20: 50S ribosomal protein L24



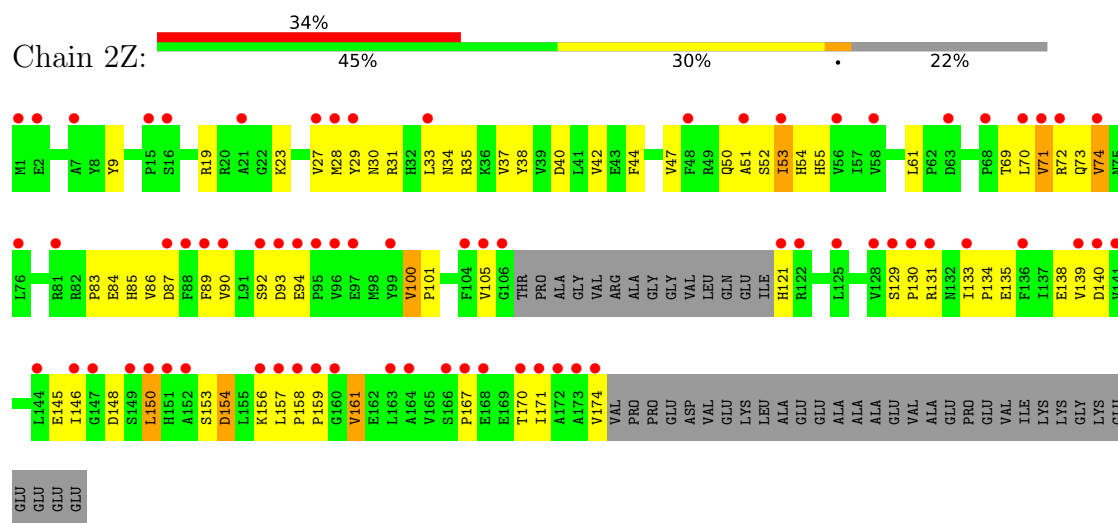
- Molecule 20: 50S ribosomal protein L24



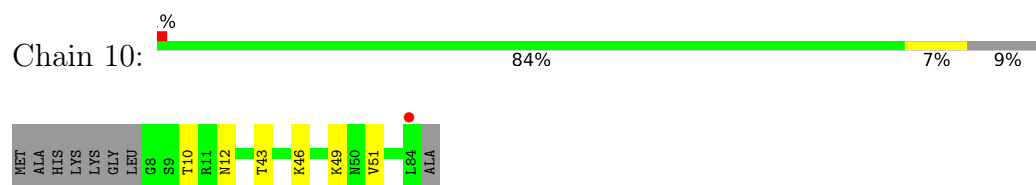
- Molecule 21: 50S ribosomal protein L25



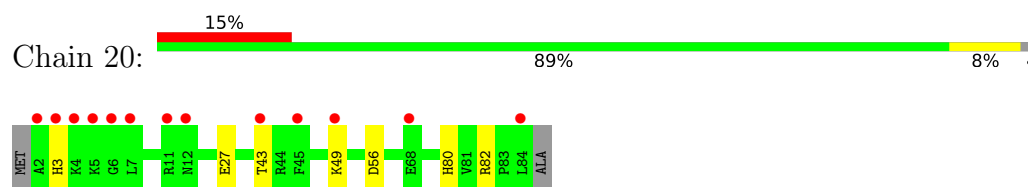
• Molecule 21: 50S ribosomal protein L25



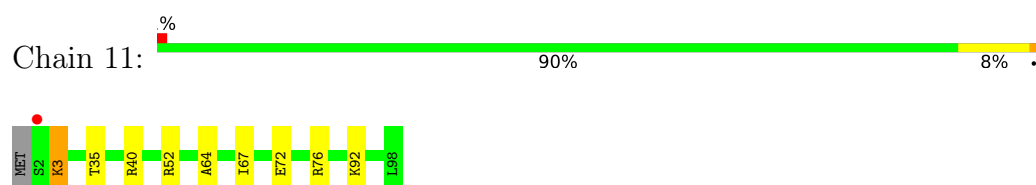
• Molecule 22: 50S ribosomal protein L27



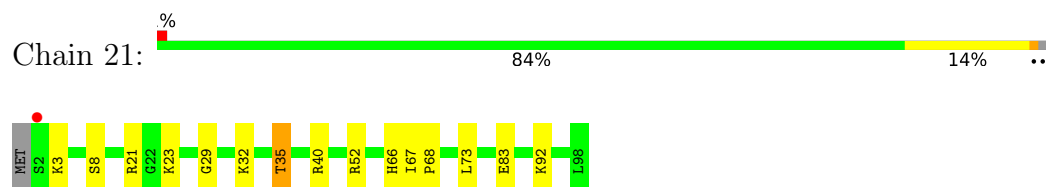
• Molecule 22: 50S ribosomal protein L27



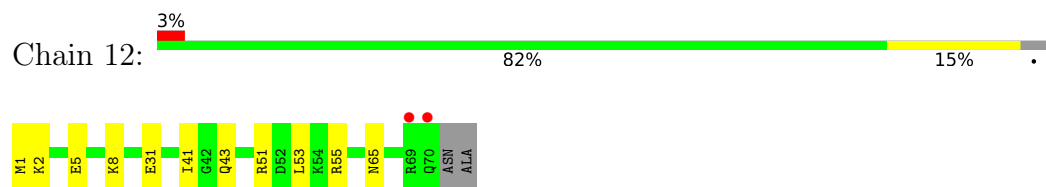
• Molecule 23: 50S ribosomal protein L28



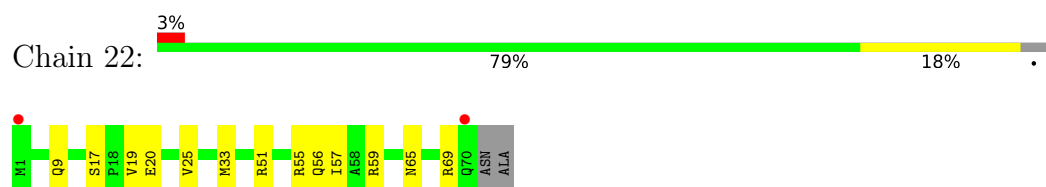
## • Molecule 23: 50S ribosomal protein L28



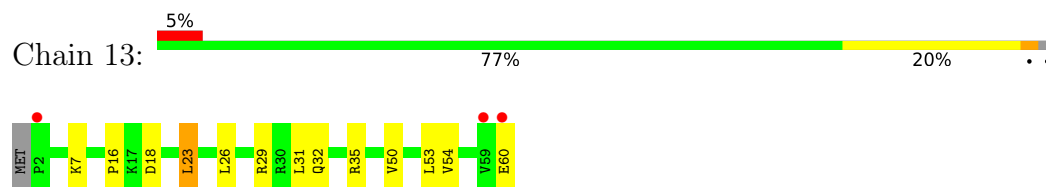
## • Molecule 24: 50S ribosomal protein L29



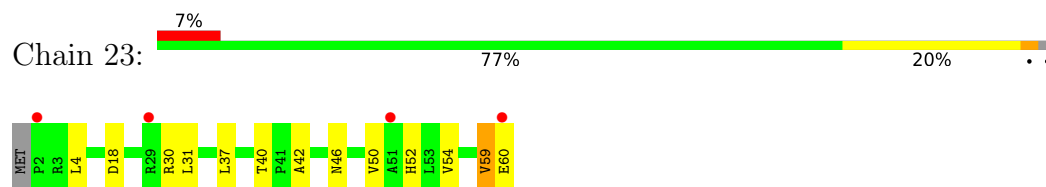
## • Molecule 24: 50S ribosomal protein L29



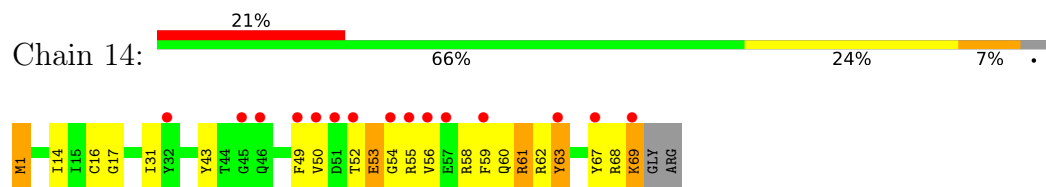
## • Molecule 25: 50S ribosomal protein L30



## • Molecule 25: 50S ribosomal protein L30

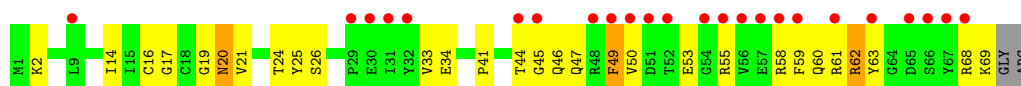


## • Molecule 26: 50S ribosomal protein L31

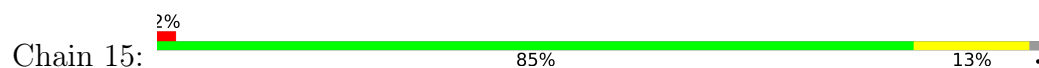


## • Molecule 26: 50S ribosomal protein L31

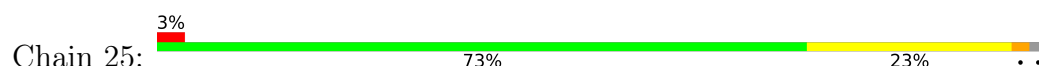




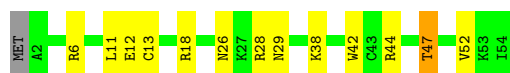
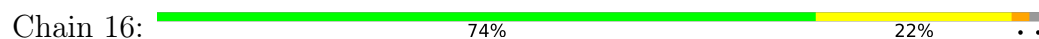
- Molecule 27: 50S ribosomal protein L32



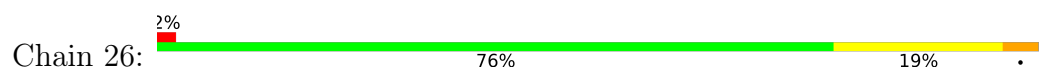
- Molecule 27: 50S ribosomal protein L32



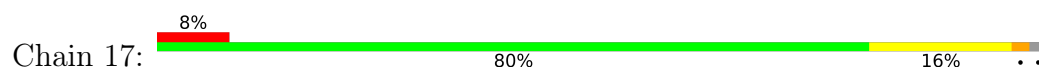
- Molecule 28: 50S ribosomal protein L33



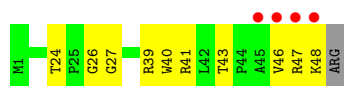
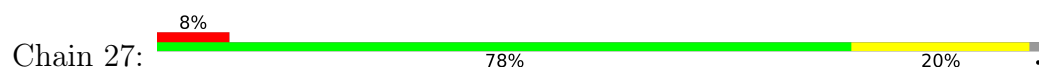
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

Chain 18:  85% 14%



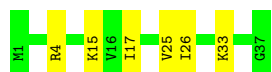
- Molecule 30: 50S ribosomal protein L35

Chain 28:  80% 18%



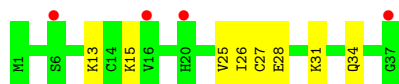
- Molecule 31: 50S ribosomal protein L36

Chain 19:  84% 16%



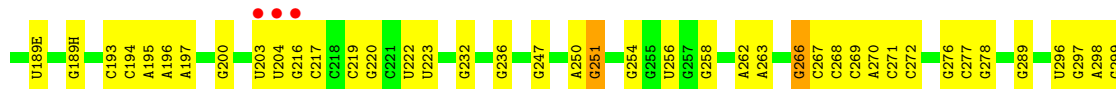
- Molecule 31: 50S ribosomal protein L36

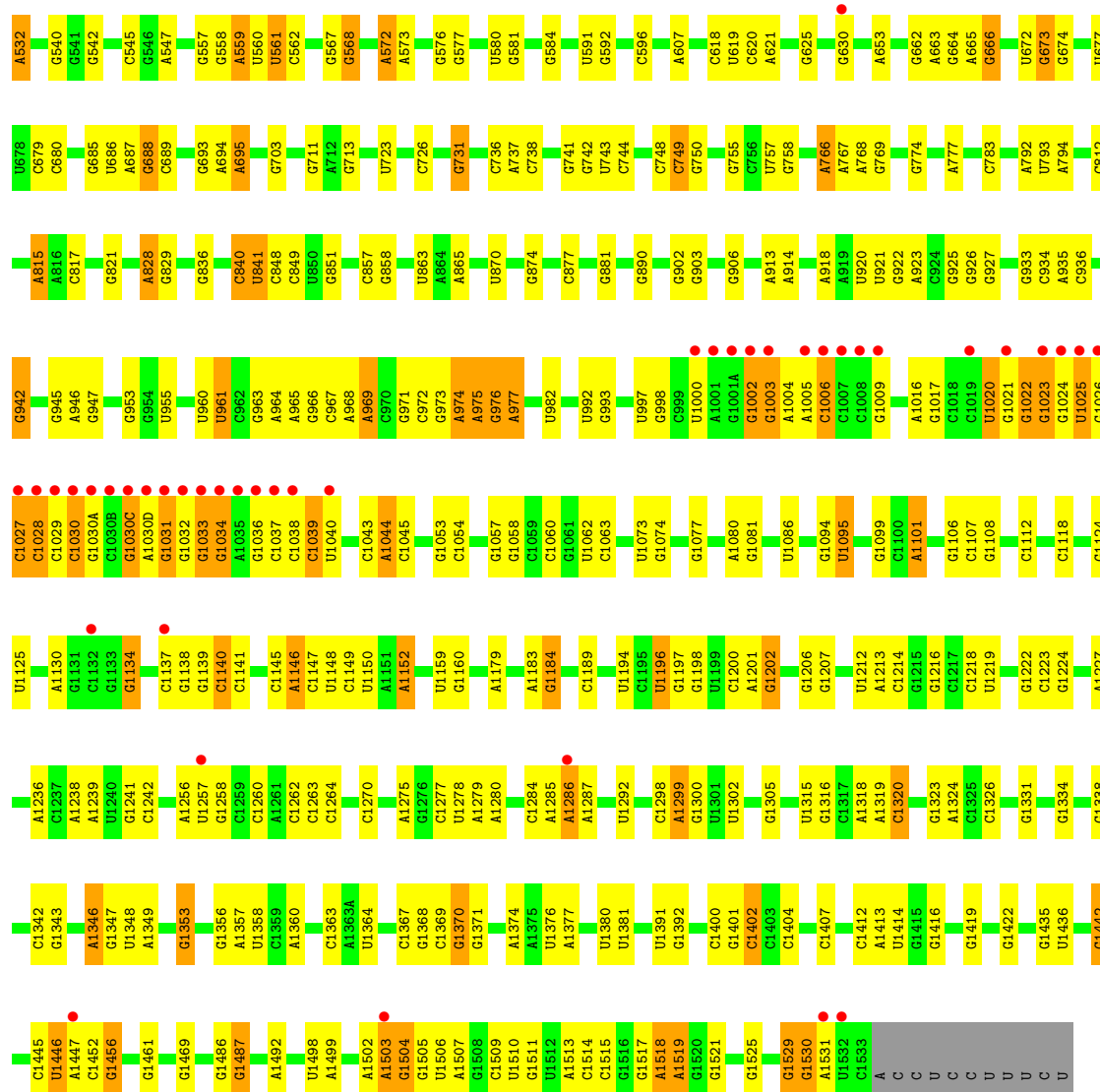
Chain 29:  11% 78% 22%



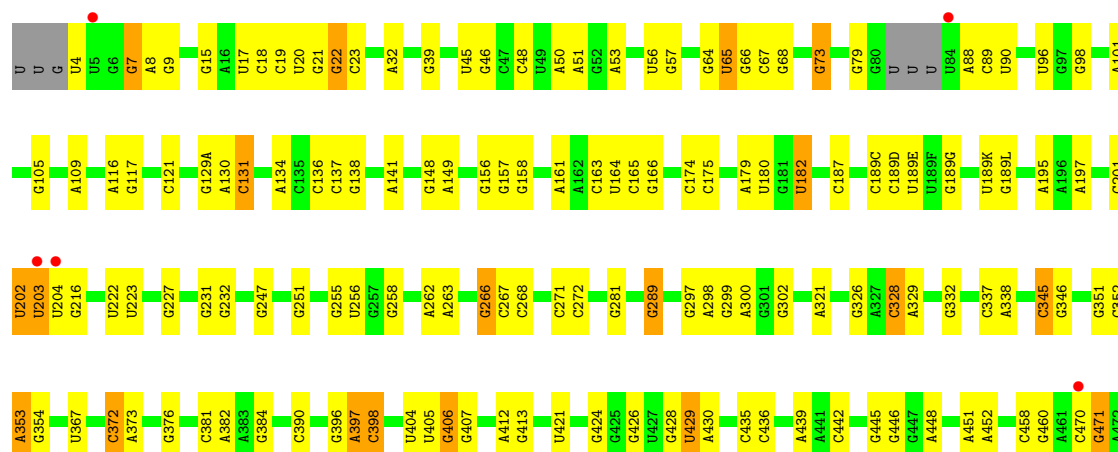
- Molecule 32: 16S Ribosomal RNA

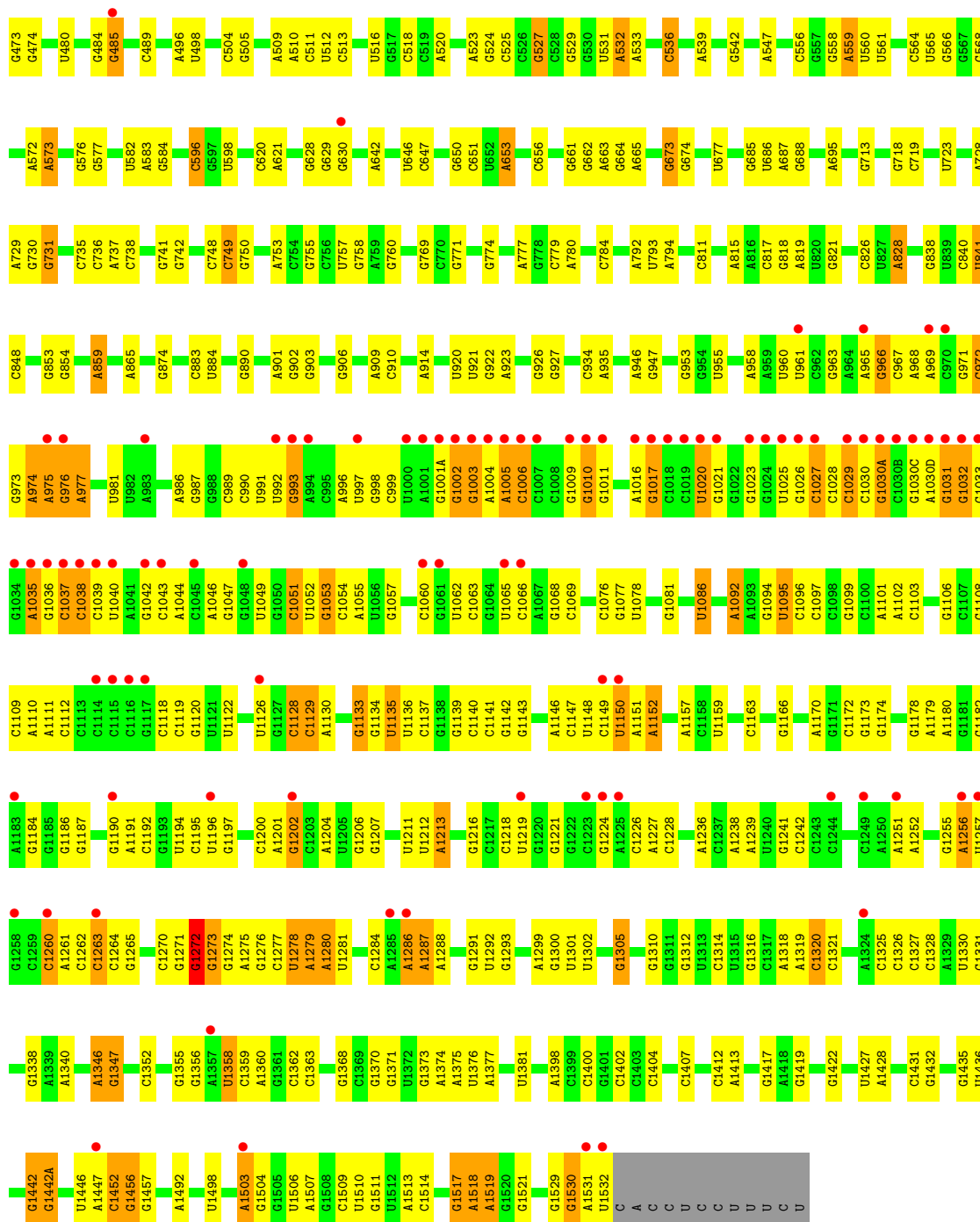
Chain 1a:  4% 63% 31% 5%

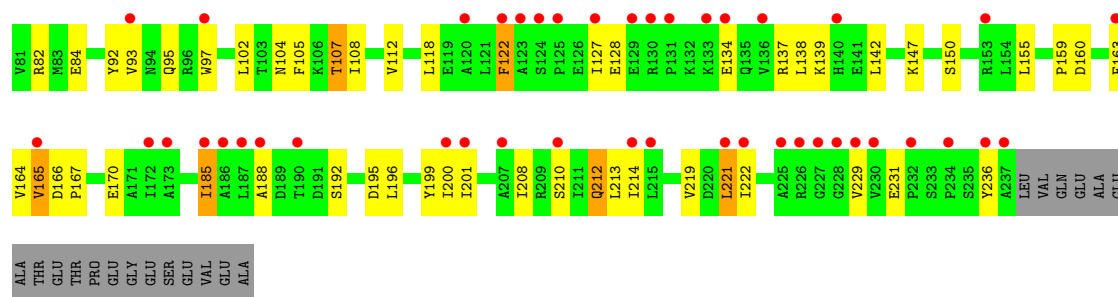




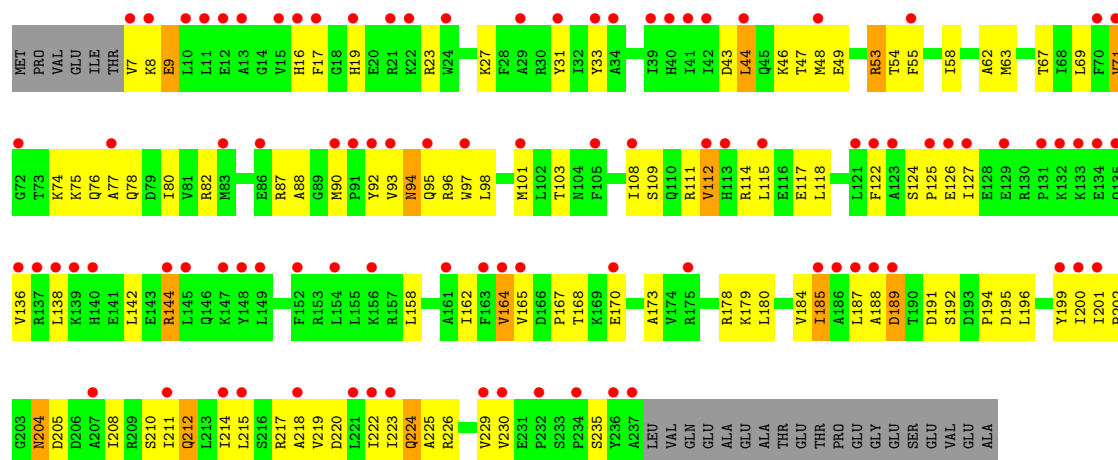
• Molecule 32: 16S Ribosomal RNA



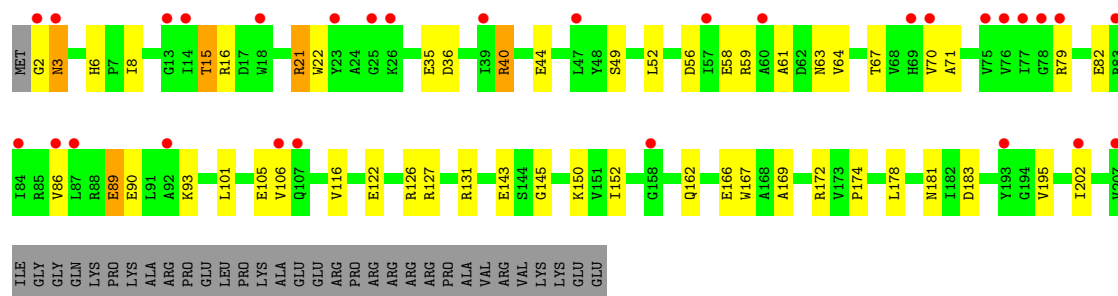




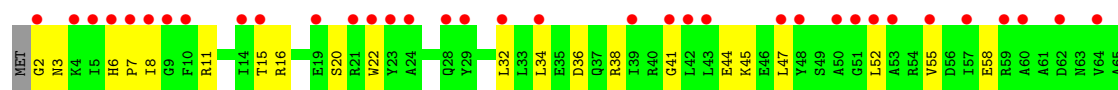
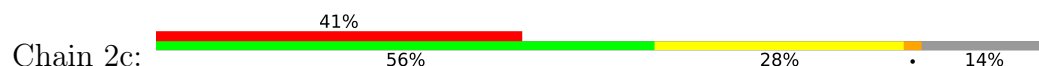
• Molecule 33: 30S ribosomal protein S2

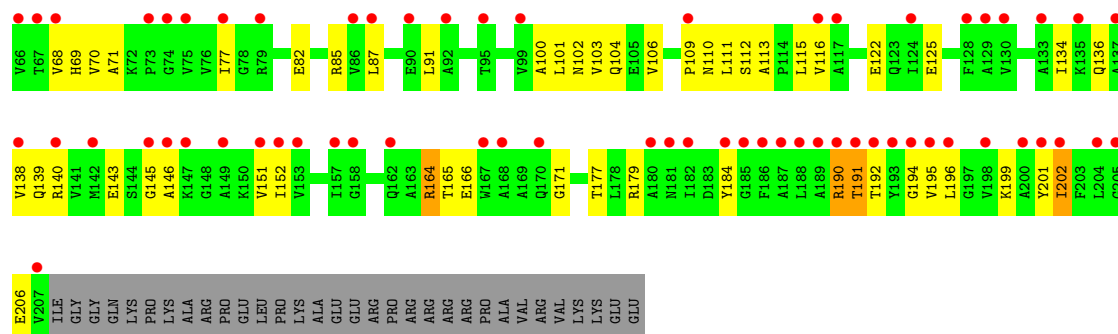


• Molecule 34: 30S ribosomal protein S3

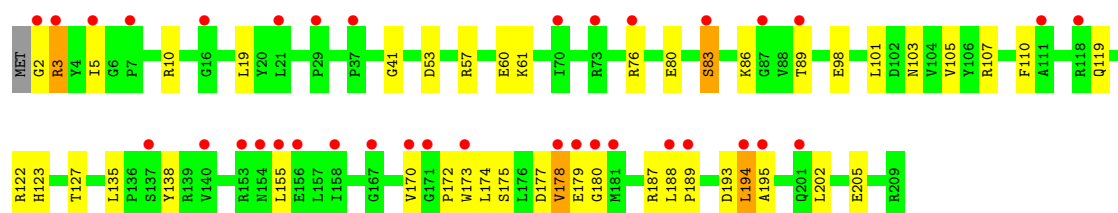
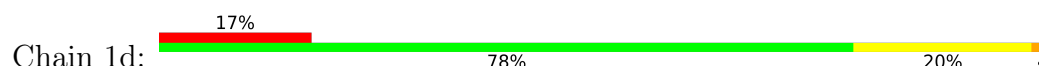


• Molecule 34: 30S ribosomal protein S3

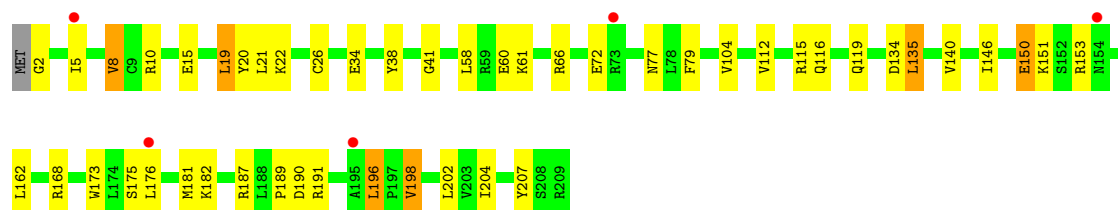
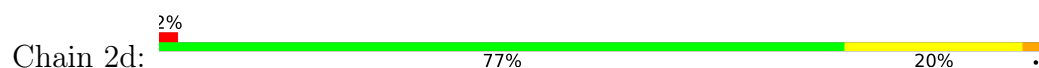




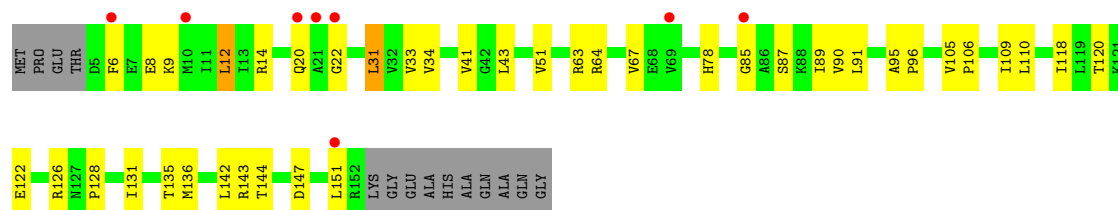
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

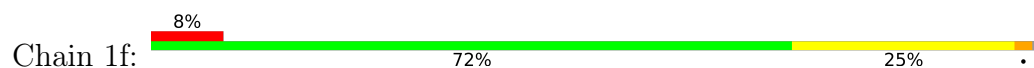


• Molecule 36: 30S ribosomal protein S5

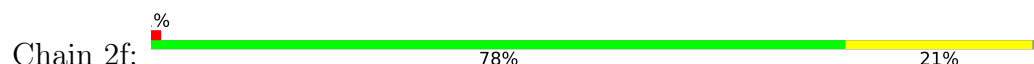




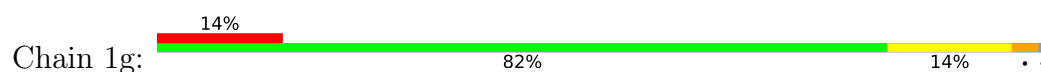
- Molecule 37: 30S ribosomal protein S6



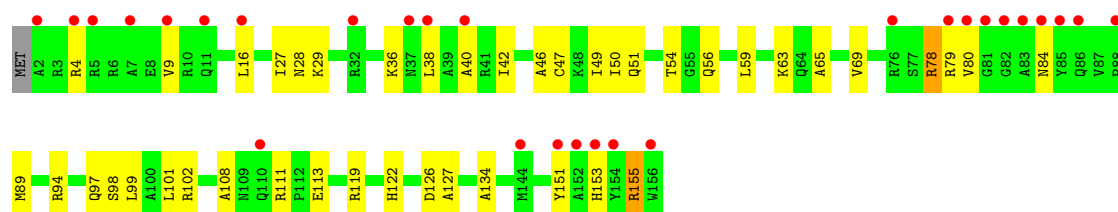
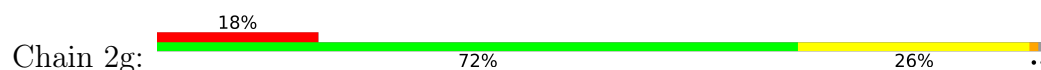
- Molecule 37: 30S ribosomal protein S6



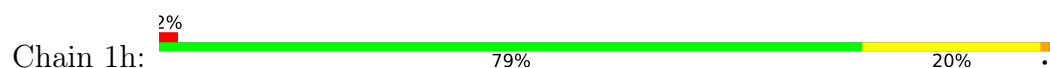
- Molecule 38: 30S ribosomal protein S7



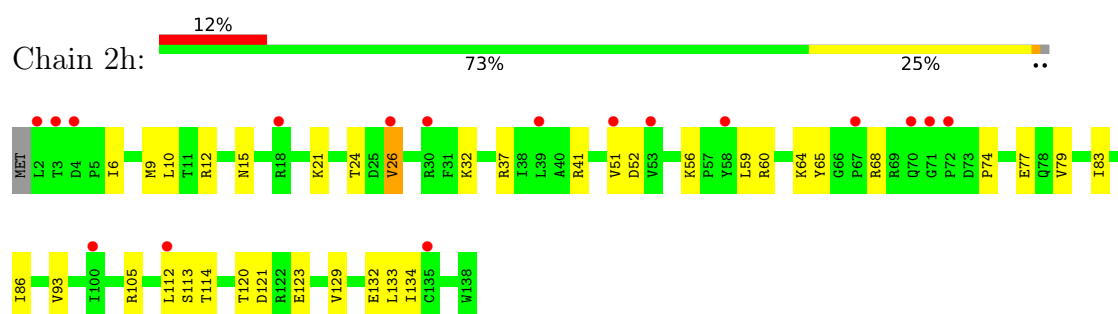
- Molecule 38: 30S ribosomal protein S7



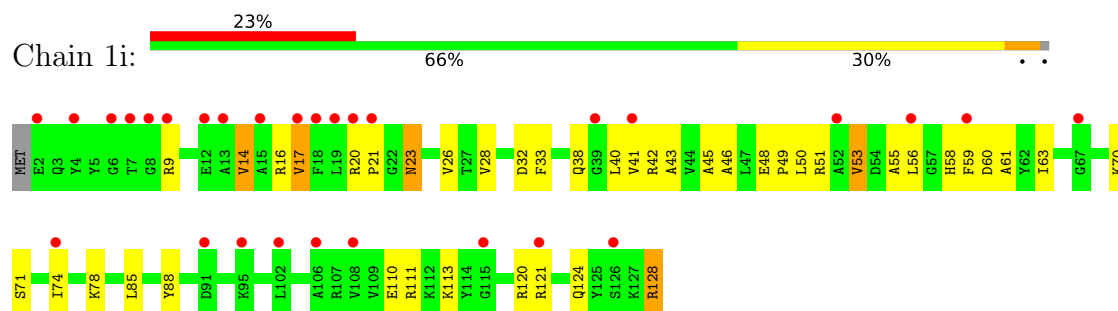
- Molecule 39: 30S ribosomal protein S8



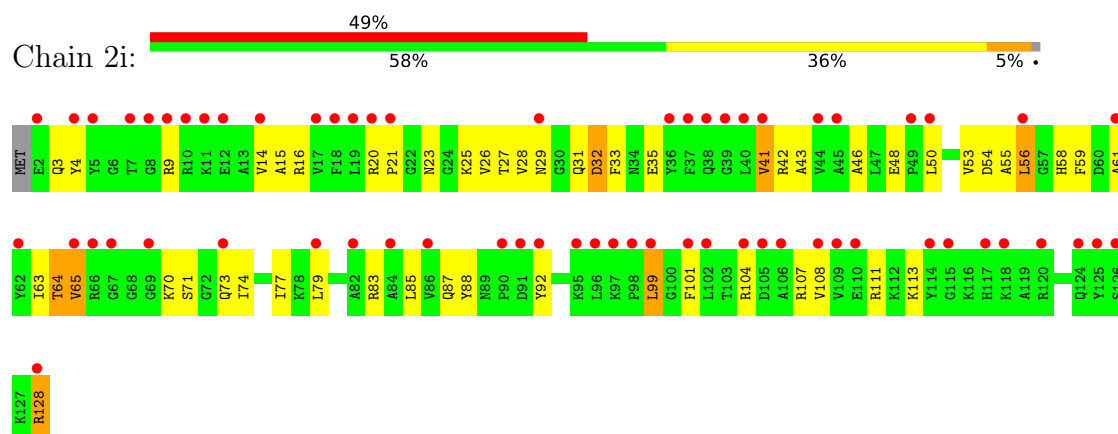
- Molecule 39: 30S ribosomal protein S8



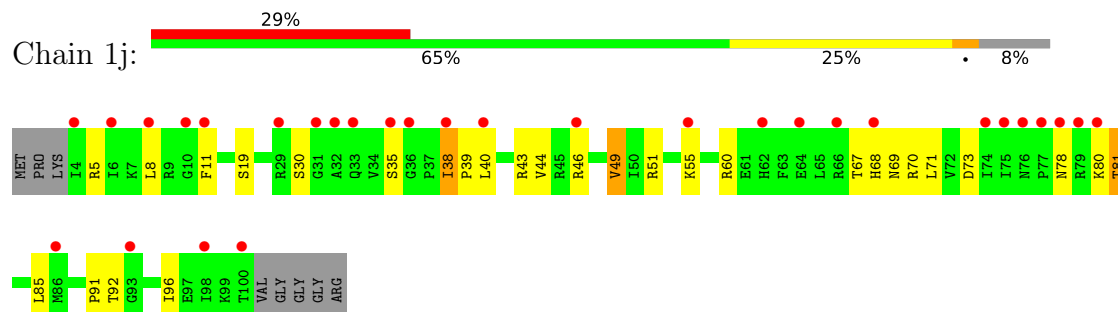
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

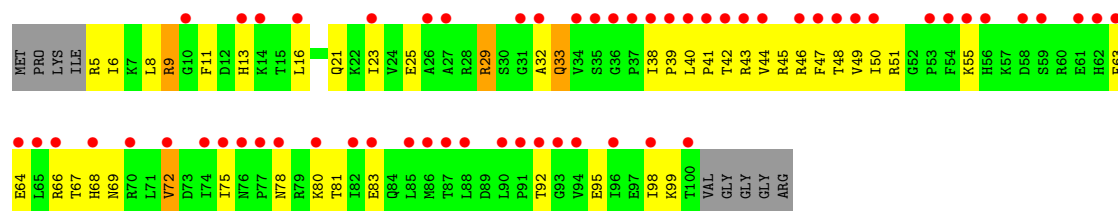


- Molecule 41: 30S ribosomal protein S10

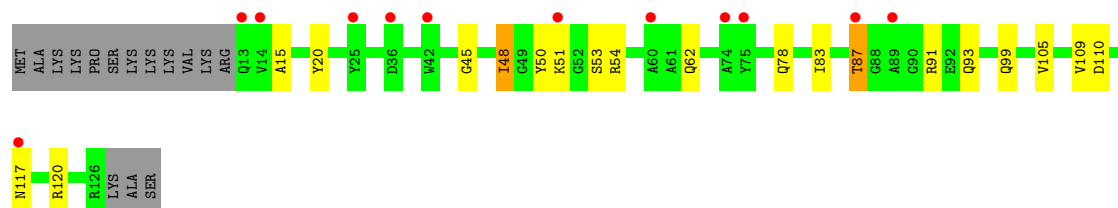
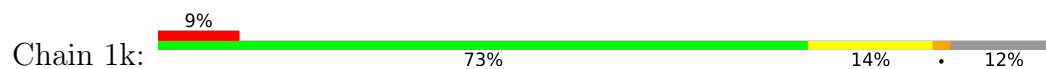


- Molecule 41: 30S ribosomal protein S10

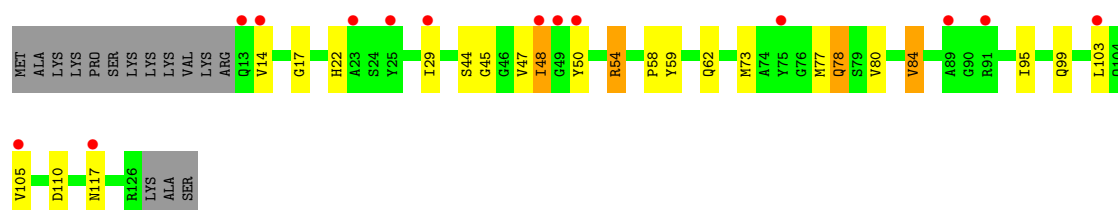
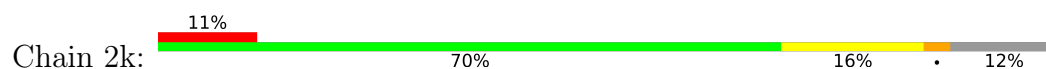




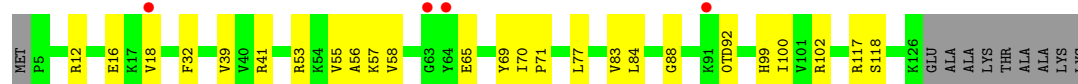
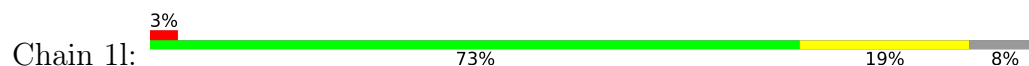
• Molecule 42: 30S ribosomal protein S11



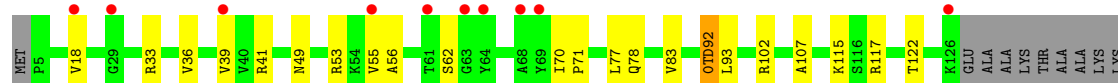
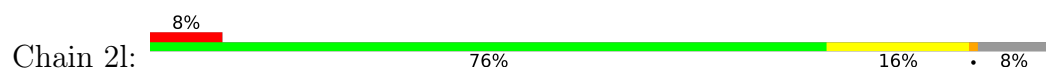
• Molecule 42: 30S ribosomal protein S11



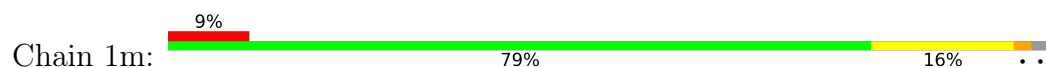
• Molecule 43: 30S ribosomal protein S12

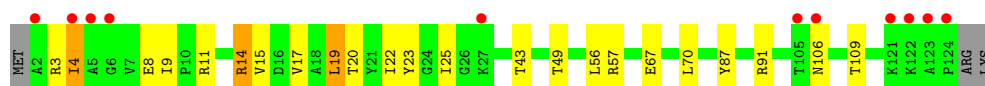


• Molecule 43: 30S ribosomal protein S12

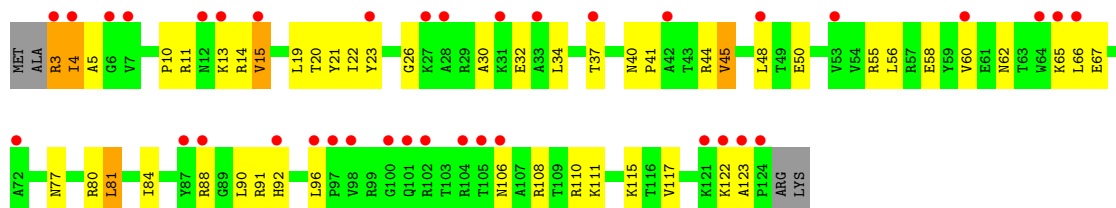


• Molecule 44: 30S ribosomal protein S13

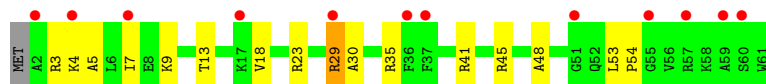
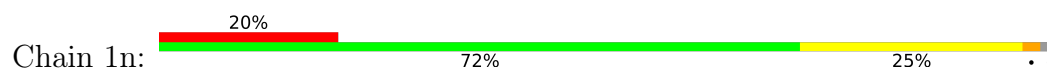




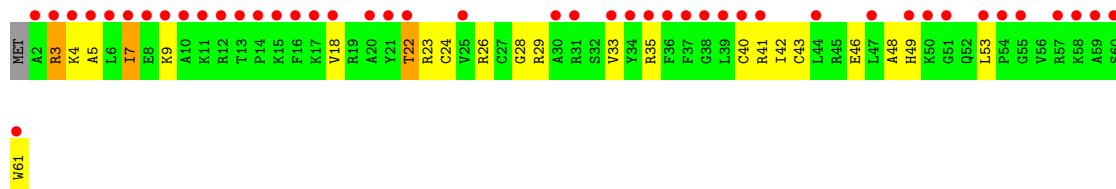
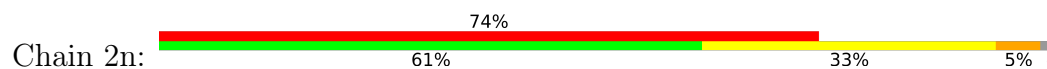
- Molecule 44: 30S ribosomal protein S13



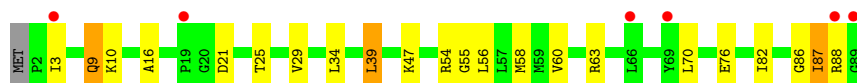
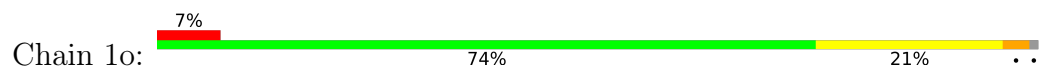
- Molecule 45: 30S ribosomal protein S14 type Z



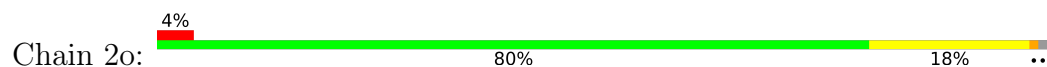
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

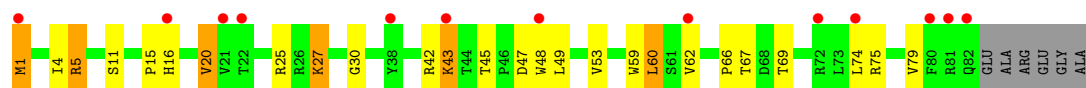


- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

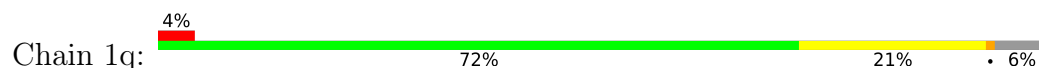




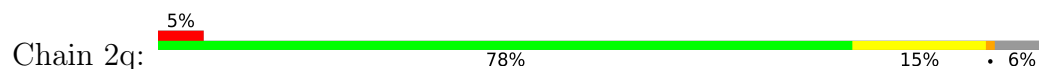
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



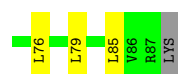
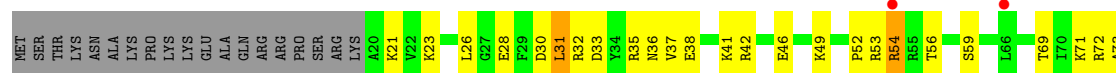
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

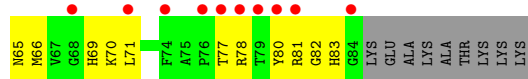
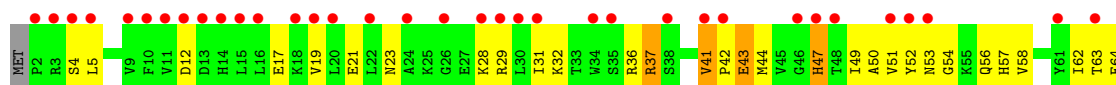
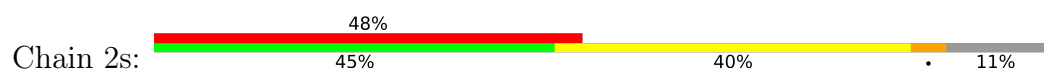


- Molecule 50: 30S ribosomal protein S19

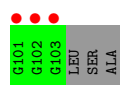
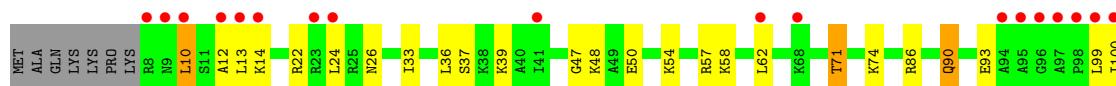




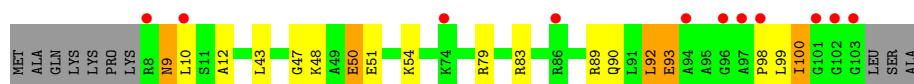
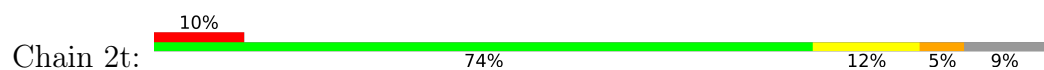
- Molecule 50: 30S ribosomal protein S19



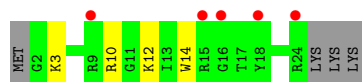
- Molecule 51: 30S ribosomal protein S20



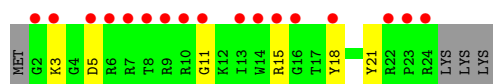
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

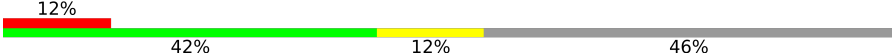


- Molecule 53: MF-mRNA

Chain 1v: 



• Molecule 53: MF-mRNA

Chain 2v: 



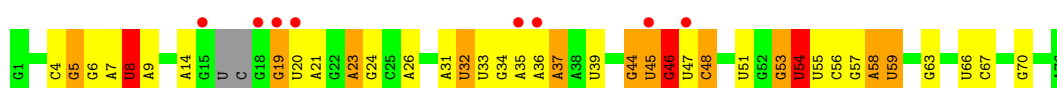
• Molecule 54: A- and E-site Deacylated tRNAp<sub>he</sub>

Chain 1w: 



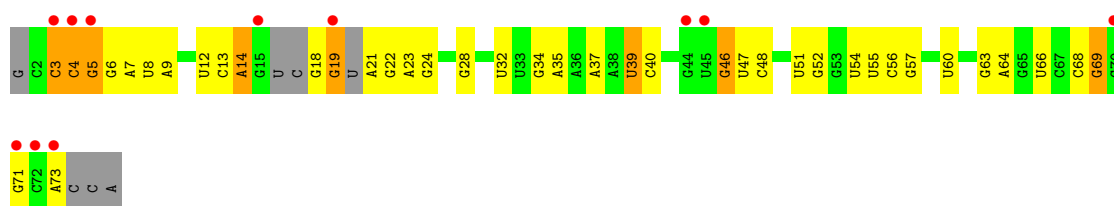
• Molecule 54: A- and E-site Deacylated tRNAp<sub>he</sub>

Chain 1y: 



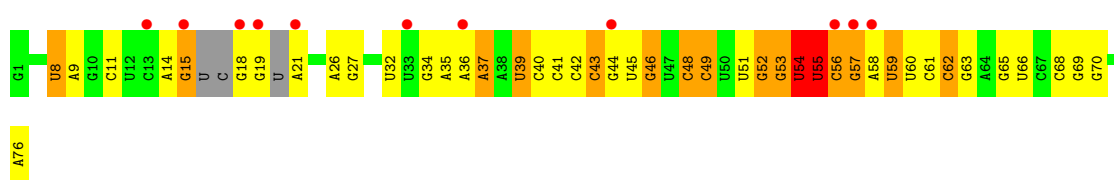
• Molecule 54: A- and E-site Deacylated tRNAp<sub>he</sub>

Chain 2w: 

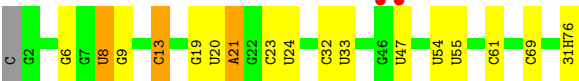
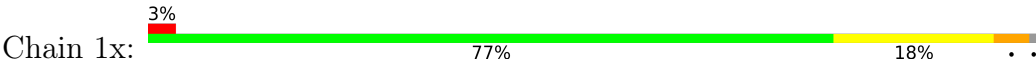


• Molecule 54: A- and E-site Deacylated tRNAp<sub>he</sub>

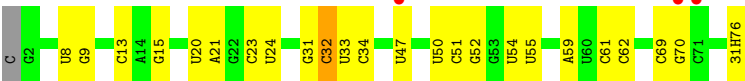
Chain 2y: 



• Molecule 55: P-site Aminoacyl-tRNA fMet-tRNA<sub>met</sub>



• Molecule 55: P-site Aminoacyl-tRNA fMet-tRNAmet



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.03Å 450.06Å 623.80Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 182.49 – 2.55<br>182.49 – 2.55                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (182.49-2.55)<br>100.0 (182.49-2.55)                  | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.17                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.30 (at 2.55Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.2                                                | Depositor        |
| R, $R_{free}$                                                           | 0.205 , 0.242<br>(Not available) , 0.228                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 95005 reflections (5.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 55.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.226                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 65.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 299373                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: 4SU, MG, 2MG, ZN, SF4, MIA, OMC, OMU, G7M, 5MC, UR3, 5MU, WC9, 2MA, 0TD, 4OC, OMG, M2G, K, 31H, PSU, MA6

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    | 0.28         | 1/68985 (0.0%) | 0.47        | 3/107677 (0.0%) |
| 1   | 2A    | 0.21         | 0/67269        | 0.40        | 1/104999 (0.0%) |
| 2   | 1B    | 0.21         | 0/2882         | 0.40        | 0/4494          |
| 2   | 2B    | 0.18         | 0/2879         | 0.36        | 0/4487          |
| 3   | 1D    | 0.27         | 0/2186         | 0.49        | 0/2944          |
| 3   | 2D    | 0.23         | 0/2186         | 0.45        | 0/2944          |
| 4   | 1E    | 0.26         | 0/1592         | 0.50        | 0/2149          |
| 4   | 2E    | 0.20         | 0/1592         | 0.42        | 0/2149          |
| 5   | 1F    | 0.25         | 0/1619         | 0.50        | 0/2193          |
| 5   | 2F    | 0.19         | 0/1615         | 0.45        | 0/2188          |
| 6   | 1G    | 0.22         | 0/1448         | 0.45        | 0/1957          |
| 6   | 2G    | 0.19         | 0/1453         | 0.40        | 0/1963          |
| 7   | 1H    | 0.21         | 0/1356         | 0.40        | 0/1834          |
| 7   | 2H    | 0.18         | 0/1356         | 0.35        | 0/1834          |
| 8   | 1I    | 0.19         | 0/1112         | 0.39        | 0/1514          |
| 8   | 2I    | 0.18         | 0/1079         | 0.40        | 0/1475          |
| 9   | 1N    | 0.24         | 0/1144         | 0.47        | 0/1543          |
| 9   | 2N    | 0.18         | 0/1144         | 0.40        | 0/1543          |
| 10  | 1O    | 0.25         | 0/943          | 0.45        | 0/1269          |
| 10  | 2O    | 0.19         | 0/943          | 0.42        | 0/1269          |
| 11  | 1P    | 0.25         | 0/1152         | 0.54        | 0/1533          |
| 11  | 2P    | 0.21         | 0/1152         | 0.51        | 0/1533          |
| 12  | 1Q    | 0.27         | 0/1143         | 0.49        | 0/1527          |
| 12  | 2Q    | 0.20         | 0/1143         | 0.42        | 0/1527          |
| 13  | 1R    | 0.27         | 0/982          | 0.50        | 0/1312          |
| 13  | 2R    | 0.20         | 0/982          | 0.44        | 0/1312          |
| 14  | 1S    | 0.21         | 0/883          | 0.46        | 0/1176          |
| 14  | 2S    | 0.20         | 0/880          | 0.43        | 0/1172          |
| 15  | 1T    | 0.23         | 0/1105         | 0.47        | 0/1477          |
| 15  | 2T    | 0.19         | 0/1097         | 0.42        | 0/1468          |
| 16  | 1U    | 0.28         | 0/977          | 0.46        | 0/1301          |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 16  | 2U    | 0.19         | 0/977   | 0.39        | 0/1301         |
| 17  | 1V    | 0.24         | 0/782   | 0.49        | 0/1049         |
| 17  | 2V    | 0.18         | 0/782   | 0.40        | 0/1049         |
| 18  | 1W    | 0.27         | 0/897   | 0.45        | 0/1205         |
| 18  | 2W    | 0.21         | 0/897   | 0.40        | 0/1205         |
| 19  | 1X    | 0.25         | 0/764   | 0.53        | 0/1025         |
| 19  | 2X    | 0.21         | 0/764   | 0.46        | 2/1025 (0.2%)  |
| 20  | 1Y    | 0.23         | 0/819   | 0.49        | 0/1095         |
| 20  | 2Y    | 0.19         | 0/819   | 0.45        | 0/1095         |
| 21  | 1Z    | 0.21         | 0/1267  | 0.47        | 0/1717         |
| 21  | 2Z    | 0.22         | 0/1299  | 0.46        | 0/1763         |
| 22  | 10    | 0.25         | 0/616   | 0.55        | 0/821          |
| 22  | 20    | 0.20         | 0/662   | 0.46        | 0/881          |
| 23  | 11    | 0.23         | 0/762   | 0.41        | 0/1014         |
| 23  | 21    | 0.21         | 0/762   | 0.40        | 0/1014         |
| 24  | 12    | 0.24         | 0/590   | 0.41        | 0/781          |
| 24  | 22    | 0.18         | 0/590   | 0.38        | 0/781          |
| 25  | 13    | 0.27         | 0/474   | 0.48        | 0/635          |
| 25  | 23    | 0.17         | 0/469   | 0.40        | 0/630          |
| 26  | 14    | 0.24         | 0/565   | 0.56        | 0/761          |
| 26  | 24    | 0.22         | 0/545   | 0.47        | 0/737          |
| 27  | 15    | 0.28         | 0/469   | 0.54        | 0/635          |
| 27  | 25    | 0.21         | 0/469   | 0.40        | 0/635          |
| 28  | 16    | 0.26         | 0/460   | 0.47        | 0/613          |
| 28  | 26    | 0.20         | 0/456   | 0.41        | 0/608          |
| 29  | 17    | 0.30         | 0/426   | 0.50        | 0/561          |
| 29  | 27    | 0.26         | 0/426   | 0.50        | 0/561          |
| 30  | 18    | 0.25         | 0/525   | 0.45        | 0/691          |
| 30  | 28    | 0.20         | 0/525   | 0.39        | 0/691          |
| 31  | 19    | 0.28         | 0/310   | 0.52        | 0/407          |
| 31  | 29    | 0.18         | 0/310   | 0.41        | 0/407          |
| 32  | 1a    | 0.20         | 0/35795 | 0.38        | 0/55864        |
| 32  | 2a    | 0.19         | 0/35886 | 0.37        | 3/56005 (0.0%) |
| 33  | 1b    | 0.21         | 0/1881  | 0.48        | 0/2542         |
| 33  | 2b    | 0.21         | 0/1860  | 0.48        | 0/2518         |
| 34  | 1c    | 0.19         | 0/1572  | 0.40        | 1/2126 (0.0%)  |
| 34  | 2c    | 0.21         | 0/1566  | 0.42        | 0/2119         |
| 35  | 1d    | 0.19         | 0/1685  | 0.40        | 0/2262         |
| 35  | 2d    | 0.19         | 0/1704  | 0.43        | 0/2284         |
| 36  | 1e    | 0.20         | 0/1145  | 0.44        | 0/1543         |
| 36  | 2e    | 0.20         | 0/1149  | 0.43        | 0/1548         |
| 37  | 1f    | 0.18         | 0/823   | 0.40        | 0/1115         |
| 37  | 2f    | 0.18         | 0/829   | 0.37        | 0/1123         |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 38  | 1g    | 0.18         | 0/1250          | 0.40        | 1/1679 (0.1%)    |
| 38  | 2g    | 0.18         | 0/1254          | 0.38        | 0/1683           |
| 39  | 1h    | 0.18         | 0/1108          | 0.41        | 0/1494           |
| 39  | 2h    | 0.18         | 0/1108          | 0.42        | 0/1494           |
| 40  | 1i    | 0.21         | 0/1002          | 0.46        | 0/1346           |
| 40  | 2i    | 0.22         | 0/997           | 0.47        | 0/1343           |
| 41  | 1j    | 0.21         | 0/722           | 0.47        | 0/982            |
| 41  | 2j    | 0.22         | 0/727           | 0.50        | 0/988            |
| 42  | 1k    | 0.18         | 0/844           | 0.39        | 0/1145           |
| 42  | 2k    | 0.18         | 0/848           | 0.37        | 0/1149           |
| 43  | 1l    | 0.21         | 0/937           | 0.41        | 0/1260           |
| 43  | 2l    | 0.18         | 0/937           | 0.40        | 0/1260           |
| 44  | 1m    | 0.19         | 0/969           | 0.50        | 0/1302           |
| 44  | 2m    | 0.21         | 0/961           | 0.45        | 0/1291           |
| 45  | 1n    | 0.19         | 0/501           | 0.43        | 0/664            |
| 45  | 2n    | 0.20         | 0/501           | 0.47        | 0/664            |
| 46  | 1o    | 0.19         | 0/739           | 0.36        | 0/985            |
| 46  | 2o    | 0.17         | 0/739           | 0.40        | 0/985            |
| 47  | 1p    | 0.21         | 0/697           | 0.47        | 0/939            |
| 47  | 2p    | 0.20         | 0/693           | 0.45        | 0/935            |
| 48  | 1q    | 0.18         | 0/836           | 0.42        | 0/1117           |
| 48  | 2q    | 0.17         | 0/836           | 0.42        | 0/1117           |
| 49  | 1r    | 0.20         | 0/560           | 0.42        | 0/746            |
| 49  | 2r    | 0.19         | 0/560           | 0.38        | 0/746            |
| 50  | 1s    | 0.20         | 0/667           | 0.46        | 0/900            |
| 50  | 2s    | 0.24         | 0/661           | 0.57        | 0/893            |
| 51  | 1t    | 0.19         | 0/730           | 0.49        | 0/965            |
| 51  | 2t    | 0.21         | 0/729           | 0.45        | 0/965            |
| 52  | 1u    | 0.18         | 0/203           | 0.44        | 0/266            |
| 52  | 2u    | 0.26         | 0/203           | 0.46        | 0/266            |
| 53  | 1v    | 0.19         | 0/310           | 0.33        | 0/480            |
| 53  | 2v    | 0.18         | 0/310           | 0.34        | 0/480            |
| 54  | 1w    | 0.27         | 1/1559 (0.1%)   | 0.38        | 0/2424           |
| 54  | 1y    | 0.28         | 2/1606 (0.1%)   | 0.39        | 0/2497           |
| 54  | 2w    | 0.31         | 1/1487 (0.1%)   | 0.40        | 0/2311           |
| 54  | 2y    | 0.27         | 0/1583          | 0.38        | 0/2459           |
| 55  | 1x    | 0.28         | 1/1700 (0.1%)   | 0.41        | 0/2650           |
| 55  | 2x    | 0.26         | 1/1700 (0.1%)   | 0.38        | 0/2650           |
| All | All   | 0.23         | 7/316426 (0.0%) | 0.42        | 11/473725 (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                   |
| All | All   | 0                   | 2                   |

The worst 5 of 7 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 54  | 1y    | 8    | 4SU  | O3'-P | 5.42 | 1.61        | 1.56     |
| 54  | 2w    | 46   | G7M  | O3'-P | 5.27 | 1.61        | 1.56     |
| 54  | 1y    | 46   | G7M  | O3'-P | 5.13 | 1.61        | 1.56     |
| 55  | 2x    | 8    | 4SU  | O3'-P | 5.07 | 1.61        | 1.56     |
| 1   | 1A    | 2552 | OMU  | O3'-P | 5.06 | 1.61        | 1.56     |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 1992 | G    | C2'-C3'-O3' | 7.65  | 120.98      | 109.50   |
| 1   | 2A    | 1992 | G    | C2'-C3'-O3' | 6.66  | 119.49      | 109.50   |
| 34  | 1c    | 86   | VAL  | N-CA-C      | -5.77 | 105.77      | 112.98   |
| 1   | 1A    | 1992 | G    | P-O3'-C3'   | 5.72  | 128.78      | 120.20   |
| 32  | 2a    | 1272 | G    | N1-C2-N2    | -5.56 | 99.53       | 116.20   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 11  | 1P    | 35  | HIS  | Peptide |
| 11  | 2P    | 35  | HIS  | Peptide |

## 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1A    | 61854 | 0        | 31201    | 432     | 0            |
| 1   | 2A    | 60324 | 0        | 30432    | 517     | 0            |
| 2   | 1B    | 2577  | 0        | 1305     | 17      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 2B    | 2575  | 0        | 1303     | 37      | 0            |
| 3   | 1D    | 2136  | 0        | 2218     | 29      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 33      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 16      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 20      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 23      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 35      | 0            |
| 6   | 1G    | 1423  | 0        | 1436     | 33      | 0            |
| 6   | 2G    | 1428  | 0        | 1438     | 49      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 14      | 0            |
| 7   | 2H    | 1330  | 0        | 1407     | 20      | 0            |
| 8   | 1I    | 1097  | 0        | 1140     | 23      | 0            |
| 8   | 2I    | 1064  | 0        | 1082     | 28      | 0            |
| 9   | 1N    | 1117  | 0        | 1184     | 13      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 26      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 10      | 0            |
| 10  | 2O    | 933   | 0        | 996      | 14      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 23      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 26      | 0            |
| 12  | 1Q    | 1122  | 0        | 1179     | 15      | 0            |
| 12  | 2Q    | 1122  | 0        | 1179     | 21      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 12      | 0            |
| 13  | 2R    | 968   | 0        | 1033     | 14      | 0            |
| 14  | 1S    | 873   | 0        | 927      | 18      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 34      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 12      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 10      | 0            |
| 16  | 1U    | 959   | 0        | 1019     | 11      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 15      | 0            |
| 17  | 1V    | 771   | 0        | 830      | 7       | 0            |
| 17  | 2V    | 771   | 0        | 830      | 14      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 6       | 0            |
| 18  | 2W    | 886   | 0        | 940      | 12      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 11      | 0            |
| 19  | 2X    | 750   | 0        | 813      | 12      | 0            |
| 20  | 1Y    | 806   | 0        | 881      | 13      | 0            |
| 20  | 2Y    | 806   | 0        | 881      | 12      | 0            |
| 21  | 1Z    | 1240  | 0        | 1240     | 25      | 0            |
| 21  | 2Z    | 1271  | 0        | 1273     | 55      | 0            |
| 22  | 10    | 608   | 0        | 622      | 7       | 0            |
| 22  | 20    | 653   | 0        | 674      | 6       | 0            |
| 23  | 11    | 755   | 0        | 826      | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | 21    | 755   | 0        | 826      | 12      | 0            |
| 24  | 12    | 588   | 0        | 643      | 6       | 0            |
| 24  | 22    | 588   | 0        | 643      | 7       | 0            |
| 25  | 13    | 469   | 0        | 518      | 7       | 0            |
| 25  | 23    | 464   | 0        | 514      | 7       | 0            |
| 26  | 14    | 552   | 0        | 533      | 19      | 0            |
| 26  | 24    | 532   | 0        | 503      | 20      | 0            |
| 27  | 15    | 455   | 0        | 465      | 4       | 0            |
| 27  | 25    | 455   | 0        | 465      | 8       | 0            |
| 28  | 16    | 453   | 0        | 473      | 7       | 0            |
| 28  | 26    | 449   | 0        | 469      | 6       | 0            |
| 29  | 17    | 418   | 0        | 467      | 5       | 0            |
| 29  | 27    | 418   | 0        | 467      | 6       | 0            |
| 30  | 18    | 517   | 0        | 582      | 6       | 0            |
| 30  | 28    | 517   | 0        | 582      | 9       | 0            |
| 31  | 19    | 307   | 0        | 335      | 3       | 0            |
| 31  | 29    | 307   | 0        | 335      | 6       | 0            |
| 32  | 1a    | 32246 | 0        | 16295    | 309     | 0            |
| 32  | 2a    | 32327 | 0        | 16338    | 357     | 0            |
| 33  | 1b    | 1846  | 0        | 1867     | 42      | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 69      | 0            |
| 34  | 1c    | 1548  | 0        | 1535     | 31      | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 45      | 0            |
| 35  | 1d    | 1655  | 0        | 1672     | 29      | 0            |
| 35  | 2d    | 1674  | 0        | 1714     | 34      | 0            |
| 36  | 1e    | 1129  | 0        | 1185     | 28      | 0            |
| 36  | 2e    | 1133  | 0        | 1191     | 35      | 0            |
| 37  | 1f    | 810   | 0        | 804      | 15      | 0            |
| 37  | 2f    | 816   | 0        | 808      | 17      | 0            |
| 38  | 1g    | 1231  | 0        | 1238     | 15      | 0            |
| 38  | 2g    | 1235  | 0        | 1249     | 30      | 0            |
| 39  | 1h    | 1088  | 0        | 1126     | 19      | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 25      | 0            |
| 40  | 1i    | 983   | 0        | 986      | 32      | 0            |
| 40  | 2i    | 978   | 0        | 966      | 41      | 0            |
| 41  | 1j    | 709   | 0        | 650      | 22      | 0            |
| 41  | 2j    | 714   | 0        | 672      | 33      | 0            |
| 42  | 1k    | 829   | 0        | 825      | 13      | 0            |
| 42  | 2k    | 833   | 0        | 836      | 16      | 0            |
| 43  | 1l    | 932   | 0        | 981      | 13      | 0            |
| 43  | 2l    | 932   | 0        | 980      | 10      | 0            |
| 44  | 1m    | 958   | 0        | 1002     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | 2m    | 950   | 0        | 988      | 34      | 0            |
| 45  | 1n    | 492   | 0        | 529      | 12      | 0            |
| 45  | 2n    | 492   | 0        | 529      | 20      | 0            |
| 46  | 1o    | 728   | 0        | 760      | 12      | 0            |
| 46  | 2o    | 728   | 0        | 760      | 13      | 0            |
| 47  | 1p    | 681   | 0        | 697      | 18      | 0            |
| 47  | 2p    | 677   | 0        | 686      | 16      | 0            |
| 48  | 1q    | 823   | 0        | 891      | 14      | 0            |
| 48  | 2q    | 823   | 0        | 891      | 9       | 0            |
| 49  | 1r    | 555   | 0        | 618      | 9       | 0            |
| 49  | 2r    | 555   | 0        | 618      | 19      | 0            |
| 50  | 1s    | 652   | 0        | 662      | 20      | 0            |
| 50  | 2s    | 646   | 0        | 644      | 36      | 0            |
| 51  | 1t    | 728   | 0        | 798      | 19      | 0            |
| 51  | 2t    | 727   | 0        | 796      | 11      | 0            |
| 52  | 1u    | 199   | 0        | 208      | 3       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 5       | 0            |
| 53  | 1v    | 277   | 0        | 140      | 4       | 0            |
| 53  | 2v    | 277   | 0        | 140      | 1       | 0            |
| 54  | 1w    | 1550  | 0        | 796      | 36      | 0            |
| 54  | 1y    | 1585  | 0        | 803      | 16      | 0            |
| 54  | 2w    | 1482  | 0        | 754      | 15      | 0            |
| 54  | 2y    | 1565  | 0        | 794      | 35      | 0            |
| 55  | 1x    | 1635  | 0        | 839      | 5       | 0            |
| 55  | 2x    | 1635  | 0        | 839      | 8       | 0            |
| 56  | 10    | 9     | 0        | 0        | 0       | 0            |
| 56  | 11    | 5     | 0        | 0        | 0       | 0            |
| 56  | 12    | 2     | 0        | 0        | 0       | 0            |
| 56  | 13    | 4     | 0        | 0        | 0       | 0            |
| 56  | 14    | 1     | 0        | 0        | 0       | 0            |
| 56  | 15    | 8     | 0        | 0        | 0       | 0            |
| 56  | 16    | 1     | 0        | 0        | 0       | 0            |
| 56  | 17    | 5     | 0        | 0        | 0       | 0            |
| 56  | 18    | 6     | 0        | 0        | 0       | 0            |
| 56  | 19    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1A    | 1097  | 0        | 0        | 0       | 0            |
| 56  | 1B    | 36    | 0        | 0        | 0       | 0            |
| 56  | 1D    | 11    | 0        | 0        | 0       | 0            |
| 56  | 1E    | 18    | 0        | 0        | 0       | 0            |
| 56  | 1F    | 13    | 0        | 0        | 0       | 0            |
| 56  | 1G    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1I    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | 1N    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1O    | 6     | 0        | 0        | 0       | 0            |
| 56  | 1P    | 5     | 0        | 0        | 0       | 0            |
| 56  | 1Q    | 7     | 0        | 0        | 0       | 0            |
| 56  | 1R    | 8     | 0        | 0        | 0       | 0            |
| 56  | 1S    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1T    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1U    | 10    | 0        | 0        | 0       | 0            |
| 56  | 1V    | 7     | 0        | 0        | 0       | 0            |
| 56  | 1W    | 4     | 0        | 0        | 0       | 0            |
| 56  | 1X    | 7     | 0        | 0        | 0       | 0            |
| 56  | 1Y    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1Z    | 3     | 0        | 0        | 0       | 0            |
| 56  | 1a    | 196   | 0        | 0        | 0       | 0            |
| 56  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1d    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1e    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1f    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1l    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1m    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1n    | 2     | 0        | 0        | 0       | 0            |
| 56  | 1r    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1t    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1w    | 5     | 0        | 0        | 0       | 0            |
| 56  | 1x    | 14    | 0        | 0        | 0       | 0            |
| 56  | 1y    | 1     | 0        | 0        | 0       | 0            |
| 56  | 20    | 4     | 0        | 0        | 0       | 0            |
| 56  | 21    | 1     | 0        | 0        | 0       | 0            |
| 56  | 23    | 1     | 0        | 0        | 0       | 0            |
| 56  | 25    | 4     | 0        | 0        | 0       | 0            |
| 56  | 27    | 3     | 0        | 0        | 0       | 0            |
| 56  | 28    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2A    | 808   | 0        | 0        | 0       | 0            |
| 56  | 2B    | 15    | 0        | 0        | 0       | 0            |
| 56  | 2D    | 6     | 0        | 0        | 0       | 0            |
| 56  | 2E    | 8     | 0        | 0        | 0       | 0            |
| 56  | 2F    | 7     | 0        | 0        | 0       | 0            |
| 56  | 2G    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2N    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2O    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2P    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2Q    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | 2R    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2T    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2U    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2V    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2W    | 5     | 0        | 0        | 0       | 0            |
| 56  | 2X    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2a    | 230   | 0        | 0        | 0       | 0            |
| 56  | 2d    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2e    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2f    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2j    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2l    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2q    | 2     | 0        | 0        | 0       | 0            |
| 56  | 2r    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 56  | 2v    | 3     | 0        | 0        | 0       | 0            |
| 56  | 2w    | 4     | 0        | 0        | 0       | 0            |
| 56  | 2x    | 5     | 0        | 0        | 0       | 0            |
| 56  | 2y    | 3     | 0        | 0        | 0       | 0            |
| 57  | 1A    | 34    | 0        | 0        | 1       | 0            |
| 57  | 2A    | 34    | 0        | 0        | 4       | 0            |
| 58  | 14    | 1     | 0        | 0        | 0       | 0            |
| 58  | 15    | 1     | 0        | 0        | 0       | 0            |
| 58  | 16    | 1     | 0        | 0        | 0       | 0            |
| 58  | 19    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 58  | 24    | 1     | 0        | 0        | 0       | 0            |
| 58  | 25    | 1     | 0        | 0        | 0       | 0            |
| 58  | 26    | 1     | 0        | 0        | 0       | 0            |
| 58  | 29    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 59  | 1d    | 8     | 0        | 0        | 0       | 0            |
| 59  | 2d    | 8     | 0        | 0        | 0       | 0            |
| 60  | 1x    | 1     | 0        | 0        | 0       | 0            |
| 60  | 2x    | 1     | 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            |
| 61  | 13    | 3     | 0        | 0        | 0       | 0            |
| 61  | 14    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61  | 15    | 4     | 0        | 0        | 0       | 0            |
| 61  | 16    | 2     | 0        | 0        | 0       | 0            |
| 61  | 17    | 12    | 0        | 0        | 2       | 0            |
| 61  | 18    | 9     | 0        | 0        | 0       | 0            |
| 61  | 1A    | 1899  | 0        | 0        | 55      | 0            |
| 61  | 1B    | 59    | 0        | 0        | 3       | 0            |
| 61  | 1D    | 27    | 0        | 0        | 1       | 0            |
| 61  | 1E    | 26    | 0        | 0        | 1       | 0            |
| 61  | 1F    | 16    | 0        | 0        | 1       | 0            |
| 61  | 1G    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1H    | 2     | 0        | 0        | 0       | 0            |
| 61  | 1N    | 6     | 0        | 0        | 0       | 0            |
| 61  | 1O    | 5     | 0        | 0        | 0       | 0            |
| 61  | 1P    | 22    | 0        | 0        | 1       | 0            |
| 61  | 1Q    | 8     | 0        | 0        | 0       | 0            |
| 61  | 1R    | 9     | 0        | 0        | 0       | 0            |
| 61  | 1S    | 3     | 0        | 0        | 1       | 0            |
| 61  | 1T    | 8     | 0        | 0        | 0       | 0            |
| 61  | 1U    | 14    | 0        | 0        | 0       | 0            |
| 61  | 1V    | 8     | 0        | 0        | 0       | 0            |
| 61  | 1W    | 8     | 0        | 0        | 2       | 0            |
| 61  | 1X    | 4     | 0        | 0        | 0       | 0            |
| 61  | 1Y    | 3     | 0        | 0        | 1       | 0            |
| 61  | 1Z    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1a    | 263   | 0        | 0        | 20      | 0            |
| 61  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1d    | 2     | 0        | 0        | 0       | 0            |
| 61  | 1f    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1g    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1l    | 3     | 0        | 0        | 0       | 0            |
| 61  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1q    | 2     | 0        | 0        | 0       | 0            |
| 61  | 1v    | 5     | 0        | 0        | 0       | 0            |
| 61  | 1w    | 7     | 0        | 0        | 0       | 0            |
| 61  | 1x    | 10    | 0        | 0        | 0       | 0            |
| 61  | 1y    | 1     | 0        | 0        | 0       | 0            |
| 61  | 20    | 4     | 0        | 0        | 0       | 0            |
| 61  | 21    | 7     | 0        | 0        | 1       | 0            |
| 61  | 23    | 2     | 0        | 0        | 0       | 0            |
| 61  | 27    | 4     | 0        | 0        | 0       | 0            |
| 61  | 28    | 3     | 0        | 0        | 0       | 0            |
| 61  | 29    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61  | 2A    | 974    | 0        | 0        | 49      | 0            |
| 61  | 2B    | 14     | 0        | 0        | 2       | 0            |
| 61  | 2D    | 19     | 0        | 0        | 0       | 0            |
| 61  | 2E    | 11     | 0        | 0        | 0       | 0            |
| 61  | 2F    | 10     | 0        | 0        | 0       | 0            |
| 61  | 2N    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2O    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2P    | 9      | 0        | 0        | 1       | 0            |
| 61  | 2Q    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2R    | 4      | 0        | 0        | 0       | 0            |
| 61  | 2T    | 4      | 0        | 0        | 0       | 0            |
| 61  | 2U    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2X    | 2      | 0        | 0        | 0       | 0            |
| 61  | 2a    | 184    | 0        | 0        | 16      | 0            |
| 61  | 2e    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2g    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2j    | 3      | 0        | 0        | 0       | 0            |
| 61  | 2l    | 3      | 0        | 0        | 0       | 0            |
| 61  | 2t    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2v    | 1      | 0        | 0        | 0       | 0            |
| 61  | 2x    | 4      | 0        | 0        | 0       | 0            |
| 61  | 2y    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 299373 | 0        | 196613   | 3107    | 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 6.

The worst 5 of 3107 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1A:1082:U:H3   | 1:1A:1086:A:N6    | 1.32                     | 1.24              |
| 1:1A:1054:A:H61  | 1:1A:1105:U:H3    | 1.15                     | 0.93              |
| 1:1A:2136:C:H42  | 1:1A:2155:G:H1    | 1.01                     | 0.93              |
| 33:2b:16:HIS:HB2 | 33:2b:204:ASN:HB3 | 1.49                     | 0.93              |
| 54:1w:2:C:H42    | 54:1w:71:G:H1     | 1.15                     | 0.93              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | 1D    | 215/218 (99%)  | 199 (93%) | 16 (7%)  | 13          | 17 |
| 3   | 2D    | 215/218 (99%)  | 205 (95%) | 10 (5%)  | 23          | 36 |
| 4   | 1E    | 164/166 (99%)  | 159 (97%) | 5 (3%)   | 36          | 53 |
| 4   | 2E    | 164/166 (99%)  | 159 (97%) | 5 (3%)   | 36          | 53 |
| 5   | 1F    | 160/166 (96%)  | 146 (91%) | 14 (9%)  | 9           | 12 |
| 5   | 2F    | 159/166 (96%)  | 151 (95%) | 8 (5%)   | 22          | 33 |
| 6   | 1G    | 143/156 (92%)  | 128 (90%) | 15 (10%) | 6           | 8  |
| 6   | 2G    | 143/156 (92%)  | 126 (88%) | 17 (12%) | 5           | 5  |
| 7   | 1H    | 144/148 (97%)  | 133 (92%) | 11 (8%)  | 12          | 17 |
| 7   | 2H    | 144/148 (97%)  | 128 (89%) | 16 (11%) | 6           | 6  |
| 8   | 1I    | 113/124 (91%)  | 99 (88%)  | 14 (12%) | 4           | 4  |
| 8   | 2I    | 105/124 (85%)  | 93 (89%)  | 12 (11%) | 5           | 6  |
| 9   | 1N    | 118/119 (99%)  | 107 (91%) | 11 (9%)  | 8           | 10 |
| 9   | 2N    | 118/119 (99%)  | 111 (94%) | 7 (6%)   | 18          | 27 |
| 10  | 1O    | 100/100 (100%) | 96 (96%)  | 4 (4%)   | 28          | 42 |
| 10  | 2O    | 100/100 (100%) | 93 (93%)  | 7 (7%)   | 14          | 19 |
| 11  | 1P    | 115/116 (99%)  | 106 (92%) | 9 (8%)   | 11          | 16 |
| 11  | 2P    | 115/116 (99%)  | 108 (94%) | 7 (6%)   | 17          | 25 |
| 12  | 1Q    | 111/111 (100%) | 106 (96%) | 5 (4%)   | 24          | 38 |
| 12  | 2Q    | 111/111 (100%) | 108 (97%) | 3 (3%)   | 39          | 58 |
| 13  | 1R    | 101/101 (100%) | 98 (97%)  | 3 (3%)   | 36          | 53 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 13  | 2R    | 101/101 (100%) | 99 (98%)  | 2 (2%)   | 48          | 67 |
| 14  | 1S    | 86/88 (98%)    | 77 (90%)  | 9 (10%)  | 6           | 8  |
| 14  | 2S    | 85/88 (97%)    | 77 (91%)  | 8 (9%)   | 8           | 10 |
| 15  | 1T    | 115/127 (91%)  | 108 (94%) | 7 (6%)   | 17          | 25 |
| 15  | 2T    | 113/127 (89%)  | 107 (95%) | 6 (5%)   | 20          | 31 |
| 16  | 1U    | 93/94 (99%)    | 91 (98%)  | 2 (2%)   | 45          | 64 |
| 16  | 2U    | 93/94 (99%)    | 88 (95%)  | 5 (5%)   | 20          | 30 |
| 17  | 1V    | 80/82 (98%)    | 78 (98%)  | 2 (2%)   | 42          | 60 |
| 17  | 2V    | 80/82 (98%)    | 75 (94%)  | 5 (6%)   | 16          | 23 |
| 18  | 1W    | 90/92 (98%)    | 88 (98%)  | 2 (2%)   | 45          | 64 |
| 18  | 2W    | 90/92 (98%)    | 86 (96%)  | 4 (4%)   | 25          | 38 |
| 19  | 1X    | 77/78 (99%)    | 76 (99%)  | 1 (1%)   | 61          | 76 |
| 19  | 2X    | 77/78 (99%)    | 74 (96%)  | 3 (4%)   | 28          | 43 |
| 20  | 1Y    | 85/91 (93%)    | 79 (93%)  | 6 (7%)   | 13          | 19 |
| 20  | 2Y    | 85/91 (93%)    | 79 (93%)  | 6 (7%)   | 13          | 19 |
| 21  | 1Z    | 135/179 (75%)  | 124 (92%) | 11 (8%)  | 11          | 15 |
| 21  | 2Z    | 137/179 (76%)  | 123 (90%) | 14 (10%) | 7           | 8  |
| 22  | 10    | 61/67 (91%)    | 60 (98%)  | 1 (2%)   | 55          | 73 |
| 22  | 20    | 65/67 (97%)    | 64 (98%)  | 1 (2%)   | 57          | 74 |
| 23  | 11    | 80/83 (96%)    | 78 (98%)  | 2 (2%)   | 42          | 60 |
| 23  | 21    | 80/83 (96%)    | 78 (98%)  | 2 (2%)   | 42          | 60 |
| 24  | 12    | 65/67 (97%)    | 63 (97%)  | 2 (3%)   | 35          | 53 |
| 24  | 22    | 65/67 (97%)    | 63 (97%)  | 2 (3%)   | 35          | 53 |
| 25  | 13    | 51/52 (98%)    | 47 (92%)  | 4 (8%)   | 11          | 16 |
| 25  | 23    | 50/52 (96%)    | 46 (92%)  | 4 (8%)   | 11          | 15 |
| 26  | 14    | 59/63 (94%)    | 50 (85%)  | 9 (15%)  | 3           | 2  |
| 26  | 24    | 53/63 (84%)    | 46 (87%)  | 7 (13%)  | 4           | 4  |
| 27  | 15    | 50/52 (96%)    | 48 (96%)  | 2 (4%)   | 28          | 42 |
| 27  | 25    | 50/52 (96%)    | 45 (90%)  | 5 (10%)  | 7           | 9  |
| 28  | 16    | 51/52 (98%)    | 49 (96%)  | 2 (4%)   | 28          | 43 |
| 28  | 26    | 50/52 (96%)    | 45 (90%)  | 5 (10%)  | 7           | 9  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 29  | 17    | 41/42 (98%)   | 37 (90%)  | 4 (10%)  | 7           | 9   |
| 29  | 27    | 41/42 (98%)   | 38 (93%)  | 3 (7%)   | 13          | 18  |
| 30  | 18    | 54/55 (98%)   | 52 (96%)  | 2 (4%)   | 30          | 45  |
| 30  | 28    | 54/55 (98%)   | 52 (96%)  | 2 (4%)   | 30          | 45  |
| 31  | 19    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 37          | 55  |
| 31  | 29    | 34/34 (100%)  | 34 (100%) | 0        | 100         | 100 |
| 33  | 1b    | 192/220 (87%) | 164 (85%) | 28 (15%) | 3           | 2   |
| 33  | 2b    | 187/220 (85%) | 153 (82%) | 34 (18%) | 2           | 1   |
| 34  | 1c    | 142/188 (76%) | 132 (93%) | 10 (7%)  | 14          | 19  |
| 34  | 2c    | 140/188 (74%) | 124 (89%) | 16 (11%) | 5           | 6   |
| 35  | 1d    | 169/181 (93%) | 157 (93%) | 12 (7%)  | 13          | 19  |
| 35  | 2d    | 173/181 (96%) | 161 (93%) | 12 (7%)  | 14          | 20  |
| 36  | 1e    | 113/123 (92%) | 106 (94%) | 7 (6%)   | 16          | 24  |
| 36  | 2e    | 114/123 (93%) | 106 (93%) | 8 (7%)   | 14          | 19  |
| 37  | 1f    | 84/90 (93%)   | 75 (89%)  | 9 (11%)  | 6           | 7   |
| 37  | 2f    | 85/90 (94%)   | 80 (94%)  | 5 (6%)   | 18          | 27  |
| 38  | 1g    | 119/127 (94%) | 107 (90%) | 12 (10%) | 7           | 8   |
| 38  | 2g    | 120/127 (94%) | 114 (95%) | 6 (5%)   | 22          | 33  |
| 39  | 1h    | 114/119 (96%) | 111 (97%) | 3 (3%)   | 40          | 59  |
| 39  | 2h    | 114/119 (96%) | 107 (94%) | 7 (6%)   | 17          | 25  |
| 40  | 1i    | 90/99 (91%)   | 83 (92%)  | 7 (8%)   | 11          | 16  |
| 40  | 2i    | 89/99 (90%)   | 77 (86%)  | 12 (14%) | 4           | 3   |
| 41  | 1j    | 66/92 (72%)   | 60 (91%)  | 6 (9%)   | 9           | 11  |
| 41  | 2j    | 69/92 (75%)   | 60 (87%)  | 9 (13%)  | 4           | 4   |
| 42  | 1k    | 82/99 (83%)   | 78 (95%)  | 4 (5%)   | 22          | 34  |
| 42  | 2k    | 83/99 (84%)   | 78 (94%)  | 5 (6%)   | 17          | 26  |
| 43  | 1l    | 96/108 (89%)  | 91 (95%)  | 5 (5%)   | 21          | 32  |
| 43  | 2l    | 96/108 (89%)  | 90 (94%)  | 6 (6%)   | 16          | 23  |
| 44  | 1m    | 93/101 (92%)  | 83 (89%)  | 10 (11%) | 6           | 7   |
| 44  | 2m    | 92/101 (91%)  | 81 (88%)  | 11 (12%) | 5           | 5   |
| 45  | 1n    | 49/50 (98%)   | 45 (92%)  | 4 (8%)   | 10          | 14  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 45  | 2n    | 49/50 (98%)      | 45 (92%)   | 4 (8%)   | 10          | 14  |
| 46  | 1o    | 78/80 (98%)      | 73 (94%)   | 5 (6%)   | 16          | 23  |
| 46  | 2o    | 78/80 (98%)      | 75 (96%)   | 3 (4%)   | 29          | 44  |
| 47  | 1p    | 69/74 (93%)      | 60 (87%)   | 9 (13%)  | 4           | 4   |
| 47  | 2p    | 68/74 (92%)      | 61 (90%)   | 7 (10%)  | 7           | 8   |
| 48  | 1q    | 94/97 (97%)      | 85 (90%)   | 9 (10%)  | 8           | 9   |
| 48  | 2q    | 94/97 (97%)      | 90 (96%)   | 4 (4%)   | 26          | 39  |
| 49  | 1r    | 59/77 (77%)      | 55 (93%)   | 4 (7%)   | 14          | 20  |
| 49  | 2r    | 59/77 (77%)      | 52 (88%)   | 7 (12%)  | 5           | 5   |
| 50  | 1s    | 69/80 (86%)      | 63 (91%)   | 6 (9%)   | 9           | 13  |
| 50  | 2s    | 67/80 (84%)      | 61 (91%)   | 6 (9%)   | 9           | 11  |
| 51  | 1t    | 70/82 (85%)      | 64 (91%)   | 6 (9%)   | 10          | 13  |
| 51  | 2t    | 70/82 (85%)      | 65 (93%)   | 5 (7%)   | 13          | 19  |
| 52  | 1u    | 18/22 (82%)      | 18 (100%)  | 0        | 100         | 100 |
| 52  | 2u    | 18/22 (82%)      | 18 (100%)  | 0        | 100         | 100 |
| All | All   | 9299/10064 (92%) | 8624 (93%) | 675 (7%) | 13          | 18  |

5 of 675 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 2Z    | 33  | LEU  |
| 36  | 2e    | 41  | VAL  |
| 21  | 2Z    | 170 | THR  |
| 20  | 2Y    | 99  | CYS  |
| 33  | 2b    | 112 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 2e    | 73  | ASN  |
| 50  | 2s    | 69  | HIS  |
| 38  | 2g    | 13  | GLN  |
| 42  | 2k    | 78  | GLN  |
| 37  | 1f    | 13  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2863/2915 (98%) | 404 (14%)         | 22 (0%)         |
| 1   | 2A    | 2791/2915 (95%) | 420 (15%)         | 27 (0%)         |
| 2   | 1B    | 119/121 (98%)   | 9 (7%)            | 0               |
| 2   | 2B    | 118/121 (97%)   | 23 (19%)          | 0               |
| 32  | 1a    | 1497/1521 (98%) | 216 (14%)         | 0               |
| 32  | 2a    | 1501/1521 (98%) | 244 (16%)         | 0               |
| 53  | 1v    | 12/24 (50%)     | 1 (8%)            | 0               |
| 53  | 2v    | 12/24 (50%)     | 2 (16%)           | 0               |
| 54  | 1w    | 70/76 (92%)     | 17 (24%)          | 0               |
| 54  | 1y    | 72/76 (94%)     | 23 (31%)          | 0               |
| 54  | 2w    | 66/76 (86%)     | 18 (27%)          | 0               |
| 54  | 2y    | 70/76 (92%)     | 19 (27%)          | 0               |
| 55  | 1x    | 74/77 (96%)     | 9 (12%)           | 0               |
| 55  | 2x    | 74/77 (96%)     | 8 (10%)           | 0               |
| All | All   | 9339/9620 (97%) | 1413 (15%)        | 49 (0%)         |

5 of 1413 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 34  | C    |
| 1   | 1A    | 45  | C    |
| 1   | 1A    | 71  | A    |
| 1   | 1A    | 74  | A    |

5 of 49 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 277  | C    |
| 1   | 2A    | 900  | A    |
| 1   | 2A    | 528  | A    |
| 1   | 2A    | 774  | A    |
| 1   | 2A    | 1210 | A    |

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

88 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   | OMC  | 1A    | 1920 | 1       | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.87 | 0        |
| 1   | 5MU  | 2A    | 1915 | 1       | 19,22,23     | 1.46 | 5 (26%)  | 27,32,35    | 2.20 | 6 (22%)  |
| 54  | 5MU  | 2w    | 54   | 54      | 19,22,23     | 1.34 | 3 (15%)  | 27,32,35    | 1.87 | 7 (25%)  |
| 32  | 5MC  | 1a    | 967  | 32      | 19,22,23     | 1.73 | 2 (10%)  | 26,32,35    | 1.13 | 2 (7%)   |
| 32  | G7M  | 1a    | 527  | 32      | 23,26,27     | 1.53 | 3 (13%)  | 34,39,42    | 1.63 | 4 (11%)  |
| 1   | 2MA  | 1A    | 2503 | 56,1    | 22,25,26     | 1.45 | 5 (22%)  | 32,37,40    | 2.32 | 9 (28%)  |
| 32  | 5MC  | 2a    | 1400 | 32      | 19,22,23     | 1.67 | 3 (15%)  | 26,32,35    | 1.21 | 3 (11%)  |
| 54  | 5MU  | 1y    | 54   | 54      | 19,22,23     | 1.46 | 5 (26%)  | 27,32,35    | 1.72 | 6 (22%)  |
| 32  | 2MG  | 2a    | 1207 | 32      | 23,26,27     | 1.24 | 4 (17%)  | 33,38,41    | 2.23 | 8 (24%)  |
| 32  | MA6  | 1a    | 1518 | 32      | 23,26,27     | 0.42 | 0        | 33,38,41    | 1.99 | 9 (27%)  |
| 32  | M2G  | 1a    | 966  | 32      | 24,27,28     | 1.32 | 4 (16%)  | 33,40,43    | 1.84 | 6 (18%)  |
| 1   | OMG  | 1A    | 2251 | 55,56,1 | 23,26,27     | 1.24 | 3 (13%)  | 32,38,41    | 1.97 | 7 (21%)  |
| 32  | M2G  | 2a    | 966  | 32      | 24,27,28     | 1.28 | 3 (12%)  | 33,40,43    | 1.86 | 6 (18%)  |
| 54  | PSU  | 2w    | 55   | 54      | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.97 | 3 (14%)  |
| 54  | 5MU  | 1w    | 54   | 54      | 19,22,23     | 1.35 | 4 (21%)  | 27,32,35    | 2.07 | 6 (22%)  |
| 1   | 5MU  | 1A    | 1939 | 56,1    | 19,22,23     | 1.50 | 6 (31%)  | 27,32,35    | 2.01 | 5 (18%)  |
| 1   | PSU  | 1A    | 1911 | 1       | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 1.99 | 4 (19%)  |
| 1   | MA6  | 1A    | 2058 | 56,1    | 23,26,27     | 0.53 | 0        | 33,38,41    | 2.45 | 13 (39%) |
| 32  | 5MC  | 2a    | 967  | 32      | 19,22,23     | 1.66 | 3 (15%)  | 26,32,35    | 1.08 | 2 (7%)   |
| 32  | 5MC  | 2a    | 1404 | 32      | 19,22,23     | 1.81 | 3 (15%)  | 26,32,35    | 1.18 | 2 (7%)   |
| 32  | MA6  | 2a    | 1518 | 32      | 23,26,27     | 0.45 | 0        | 33,38,41    | 2.03 | 9 (27%)  |
| 32  | 5MC  | 1a    | 1404 | 32      | 19,22,23     | 1.73 | 3 (15%)  | 26,32,35    | 1.20 | 2 (7%)   |
| 1   | 2MA  | 2A    | 2503 | 56,1    | 22,25,26     | 1.49 | 5 (22%)  | 32,37,40    | 2.34 | 8 (25%)  |
| 54  | 4SU  | 2y    | 8    | 54      | 18,21,22     | 1.74 | 4 (22%)  | 25,30,33    | 2.21 | 4 (16%)  |
| 1   | MA6  | 2A    | 2058 | 1       | 23,26,27     | 0.49 | 0        | 33,38,41    | 2.20 | 12 (36%) |
| 32  | UR3  | 1a    | 1498 | 32      | 19,22,23     | 1.00 | 1 (5%)   | 26,32,35    | 1.79 | 4 (15%)  |
| 55  | 5MC  | 1x    | 32   | 55      | 19,22,23     | 1.65 | 3 (15%)  | 26,32,35    | 1.21 | 3 (11%)  |
| 54  | G7M  | 2w    | 46   | 54      | 23,26,27     | 1.47 | 5 (21%)  | 34,39,42    | 1.62 | 4 (11%)  |
| 43  | 0TD  | 1l    | 92   | 43      | 8,9,10       | 4.35 | 1 (12%)  | 6,11,13     | 7.57 | 2 (33%)  |
| 54  | PSU  | 1y    | 39   | 54      | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 1.82 | 3 (14%)  |
| 1   | OMU  | 2A    | 2552 | 56,1    | 19,22,23     | 1.16 | 2 (10%)  | 25,31,34    | 1.78 | 5 (20%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMU  | 1A    | 2552 | 56,1     | 19,22,23     | 1.26 | 3 (15%)  | 25,31,34    | 1.83 | 5 (20%)  |
| 32  | PSU  | 1a    | 516  | 56,32    | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 2.09 | 6 (28%)  |
| 32  | 5MC  | 1a    | 1407 | 32       | 19,22,23     | 1.60 | 2 (10%)  | 26,32,35    | 1.05 | 2 (7%)   |
| 54  | MIA  | 1w    | 37   | 54       | 28,31,32     | 2.36 | 6 (21%)  | 38,44,47    | 2.85 | 13 (34%) |
| 54  | G7M  | 2y    | 46   | 54       | 23,26,27     | 1.52 | 3 (13%)  | 34,39,42    | 1.75 | 4 (11%)  |
| 54  | G7M  | 1y    | 46   | 54       | 23,26,27     | 1.52 | 4 (17%)  | 34,39,42    | 1.70 | 4 (11%)  |
| 55  | 31H  | 1x    | 76   | 55,56,60 | 31,34,35     | 1.25 | 4 (12%)  | 35,47,50    | 2.05 | 13 (37%) |
| 32  | MA6  | 2a    | 1519 | 32       | 23,26,27     | 0.41 | 0        | 33,38,41    | 2.12 | 9 (27%)  |
| 32  | UR3  | 2a    | 1498 | 32       | 19,22,23     | 1.06 | 1 (5%)   | 26,32,35    | 1.74 | 3 (11%)  |
| 54  | PSU  | 1y    | 32   | 54       | 18,21,22     | 1.32 | 2 (11%)  | 21,30,33    | 1.97 | 3 (14%)  |
| 1   | OMC  | 2A    | 1920 | 1        | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.90 | 1 (4%)   |
| 1   | PSU  | 1A    | 1917 | 1        | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 2.02 | 3 (14%)  |
| 54  | PSU  | 2y    | 55   | 54       | 18,21,22     | 1.44 | 2 (11%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 1   | 5MC  | 1A    | 1962 | 56,1     | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.19 | 2 (7%)   |
| 54  | PSU  | 1w    | 32   | 56,54    | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.98 | 3 (14%)  |
| 55  | PSU  | 2x    | 55   | 55       | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 43  | 0TD  | 2l    | 92   | 43       | 8,9,10       | 4.46 | 1 (12%)  | 6,11,13     | 3.72 | 3 (50%)  |
| 1   | 5MU  | 2A    | 1939 | 56,1     | 19,22,23     | 1.45 | 6 (31%)  | 27,32,35    | 2.33 | 6 (22%)  |
| 55  | PSU  | 1x    | 55   | 55       | 18,21,22     | 1.33 | 2 (11%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 1   | 5MC  | 2A    | 1962 | 56,1     | 19,22,23     | 1.68 | 3 (15%)  | 26,32,35    | 1.16 | 3 (11%)  |
| 54  | G7M  | 1w    | 46   | 54       | 23,26,27     | 1.53 | 4 (17%)  | 34,39,42    | 1.61 | 4 (11%)  |
| 54  | PSU  | 1w    | 39   | 54       | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 1.94 | 3 (14%)  |
| 54  | PSU  | 2y    | 32   | 54       | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 1.98 | 3 (14%)  |
| 32  | 5MC  | 2a    | 1407 | 56,32    | 19,22,23     | 1.57 | 2 (10%)  | 26,32,35    | 1.16 | 2 (7%)   |
| 55  | 5MU  | 2x    | 54   | 55       | 19,22,23     | 1.37 | 5 (26%)  | 27,32,35    | 2.17 | 6 (22%)  |
| 54  | MIA  | 2y    | 37   | 54       | 21,24,32     | 1.63 | 3 (14%)  | 30,35,47    | 1.99 | 7 (23%)  |
| 1   | 5MC  | 1A    | 1942 | 1        | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.24 | 2 (7%)   |
| 54  | PSU  | 2y    | 39   | 54       | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 1.85 | 4 (19%)  |
| 55  | 4SU  | 2x    | 8    | 55       | 18,21,22     | 2.06 | 6 (33%)  | 25,30,33    | 1.38 | 5 (20%)  |
| 1   | PSU  | 1A    | 2605 | 56,1     | 18,21,22     | 1.43 | 3 (16%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 1   | 5MU  | 1A    | 1915 | 1        | 19,22,23     | 1.42 | 4 (21%)  | 27,32,35    | 2.21 | 6 (22%)  |
| 32  | MA6  | 1a    | 1519 | 32       | 23,26,27     | 0.45 | 0        | 33,38,41    | 2.10 | 9 (27%)  |
| 1   | PSU  | 2A    | 1917 | 1        | 18,21,22     | 1.32 | 2 (11%)  | 21,30,33    | 1.91 | 4 (19%)  |
| 54  | PSU  | 1y    | 55   | 54       | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 2.00 | 3 (14%)  |
| 54  | 5MU  | 2y    | 54   | 54       | 19,22,23     | 1.42 | 4 (21%)  | 27,32,35    | 2.09 | 7 (25%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | 2A    | 2251 | 55,1     | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 2.03 | 6 (18%)  |
| 55  | 5MC  | 2x    | 32   | 55       | 19,22,23     | 1.59 | 3 (15%)  | 26,32,35    | 1.27 | 3 (11%)  |
| 32  | 4OC  | 1a    | 1402 | 32       | 20,23,24     | 0.73 | 0        | 25,32,35    | 1.05 | 1 (4%)   |
| 1   | 5MC  | 2A    | 1942 | 1        | 19,22,23     | 1.60 | 3 (15%)  | 26,32,35    | 1.07 | 2 (7%)   |
| 32  | 2MG  | 1a    | 1207 | 32       | 23,26,27     | 1.23 | 2 (8%)   | 33,38,41    | 2.20 | 8 (24%)  |
| 54  | MIA  | 1y    | 37   | 54       | 21,24,32     | 1.67 | 4 (19%)  | 30,35,47    | 2.00 | 7 (23%)  |
| 54  | 4SU  | 1y    | 8    | 54       | 18,21,22     | 1.81 | 6 (33%)  | 25,30,33    | 1.80 | 4 (16%)  |
| 54  | PSU  | 2w    | 39   | 54       | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 1.94 | 3 (14%)  |
| 1   | PSU  | 2A    | 2605 | 1        | 18,21,22     | 1.37 | 3 (16%)  | 21,30,33    | 2.07 | 4 (19%)  |
| 54  | PSU  | 1w    | 55   | 54       | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 2.09 | 3 (14%)  |
| 32  | 5MC  | 1a    | 1400 | 32       | 19,22,23     | 1.66 | 3 (15%)  | 26,32,35    | 1.17 | 2 (7%)   |
| 54  | 4SU  | 1w    | 8    | 54       | 18,21,22     | 1.77 | 5 (27%)  | 25,30,33    | 1.80 | 5 (20%)  |
| 54  | PSU  | 2w    | 32   | 54       | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 1.93 | 4 (19%)  |
| 1   | PSU  | 2A    | 1911 | 1        | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 55  | 31H  | 2x    | 76   | 55,56,60 | 31,34,35     | 1.24 | 4 (12%)  | 35,47,50    | 1.97 | 11 (31%) |
| 54  | MIA  | 2w    | 37   | 54       | 24,27,32     | 2.11 | 6 (25%)  | 32,39,47    | 2.59 | 11 (34%) |
| 55  | 5MU  | 1x    | 54   | 55,56    | 19,22,23     | 1.44 | 5 (26%)  | 27,32,35    | 2.01 | 6 (22%)  |
| 32  | 4OC  | 2a    | 1402 | 32       | 20,23,24     | 0.78 | 0        | 25,32,35    | 0.96 | 1 (4%)   |
| 32  | PSU  | 2a    | 516  | 32       | 18,21,22     | 1.29 | 2 (11%)  | 21,30,33    | 2.10 | 4 (19%)  |
| 55  | 4SU  | 1x    | 8    | 55       | 18,21,22     | 2.35 | 6 (33%)  | 25,30,33    | 1.83 | 7 (28%)  |
| 54  | 4SU  | 2w    | 8    | 54       | 18,21,22     | 1.78 | 5 (27%)  | 25,30,33    | 2.02 | 5 (20%)  |
| 32  | G7M  | 2a    | 527  | 56,32    | 23,26,27     | 1.47 | 4 (17%)  | 34,39,42    | 1.71 | 5 (14%)  |

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   | OMC  | 1A    | 1920 | 1    | -       | 1/9/27/28 | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1915 | 1    | -       | 1/7/25/26 | 0/2/2/2 |
| 54  | 5MU  | 2w    | 54   | 54   | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 967  | 32   | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | G7M  | 1a    | 527  | 32   | -       | 3/7/25/26 | 0/3/3/3 |
| 1   | 2MA  | 1A    | 2503 | 56,1 | -       | 0/7/25/26 | 0/3/3/3 |
| 32  | 5MC  | 2a    | 1400 | 32   | -       | 1/7/25/26 | 0/2/2/2 |
| 54  | 5MU  | 1y    | 54   | 54   | -       | 2/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 32  | 2MG  | 2a    | 1207 | 32       | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | MA6  | 1a    | 1518 | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | M2G  | 1a    | 966  | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | OMG  | 1A    | 2251 | 55,56,1  | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | M2G  | 2a    | 966  | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 54  | PSU  | 2w    | 55   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 5MU  | 1w    | 54   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 56,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1911 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | 1A    | 2058 | 56,1     | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 5MC  | 2a    | 967  | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1404 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1518 | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1404 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 2A    | 2503 | 56,1     | -       | 2/7/25/26  | 0/3/3/3 |
| 54  | 4SU  | 2y    | 8    | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | MA6  | 2A    | 2058 | 1        | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | UR3  | 1a    | 1498 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MC  | 1x    | 32   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | G7M  | 2w    | 46   | 54       | -       | 1/7/25/26  | 0/3/3/3 |
| 43  | 0TD  | 1l    | 92   | 43       | -       | 2/7/12/14  | -       |
| 54  | PSU  | 1y    | 39   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2A    | 2552 | 56,1     | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMU  | 1A    | 2552 | 56,1     | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | PSU  | 1a    | 516  | 56,32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 1w    | 37   | 54       | -       | 1/15/33/34 | 0/3/3/3 |
| 54  | G7M  | 2y    | 46   | 54       | -       | 2/7/25/26  | 0/3/3/3 |
| 54  | G7M  | 1y    | 46   | 54       | -       | 1/7/25/26  | 0/3/3/3 |
| 55  | 31H  | 1x    | 76   | 55,56,60 | -       | 5/22/40/41 | 0/3/3/3 |
| 32  | MA6  | 2a    | 1519 | 32       | -       | 3/11/29/30 | 0/3/3/3 |
| 32  | UR3  | 2a    | 1498 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1y    | 32   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 2A    | 1920 | 1        | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2y    | 55   | 54       | -       | 3/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1962 | 56,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1w    | 32   | 56,54    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | PSU  | 2x    | 55   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43       | -       | 4/7/12/14  | -       |
| 1   | 5MU  | 2A    | 1939 | 56,1     | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|------|-------|------|----------|---------|------------|---------|
| 55  | PSU  | 1x    | 55   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 56,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | G7M  | 1w    | 46   | 54       | -       | 1/7/25/26  | 0/3/3/3 |
| 54  | PSU  | 1w    | 39   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2y    | 32   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 56,32    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU  | 2x    | 54   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 2y    | 37   | 54       | -       | 1/7/25/34  | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1942 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2y    | 39   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 2x    | 8    | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2605 | 56,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1519 | 32       | -       | 3/11/29/30 | 0/3/3/3 |
| 1   | PSU  | 2A    | 1917 | 1        | -       | 1/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1y    | 55   | 54       | -       | 1/7/25/26  | 0/2/2/2 |
| 54  | 5MU  | 2y    | 54   | 54       | -       | 3/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 55,1     | -       | 0/9/27/28  | 0/3/3/3 |
| 55  | 5MC  | 2x    | 32   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 4OC  | 1a    | 1402 | 32       | -       | 1/9/29/30  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32       | -       | 0/9/27/28  | 0/3/3/3 |
| 54  | MIA  | 1y    | 37   | 54       | -       | 0/7/25/34  | 0/3/3/3 |
| 54  | 4SU  | 1y    | 8    | 54       | -       | 3/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2w    | 39   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 2605 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1w    | 55   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1400 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 4SU  | 1w    | 8    | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2w    | 32   | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 31H  | 2x    | 76   | 55,56,60 | -       | 4/22/40/41 | 0/3/3/3 |
| 54  | MIA  | 2w    | 37   | 54       | -       | 2/11/29/34 | 0/3/3/3 |
| 55  | 5MU  | 1x    | 54   | 55,56    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 4OC  | 2a    | 1402 | 32       | -       | 1/9/29/30  | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 1x    | 8    | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 4SU  | 2w    | 8    | 54       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | G7M  | 2a    | 527  | 56,32    | -       | 3/7/25/26  | 0/3/3/3 |

The worst 5 of 252 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 43  | 2l    | 92  | 0TD  | CB-SB   | -12.18 | 1.70        | 1.82     |
| 43  | 1l    | 92  | 0TD  | CB-SB   | -11.84 | 1.70        | 1.82     |
| 54  | 1w    | 37  | MIA  | C2-S10  | -7.18  | 1.69        | 1.75     |
| 54  | 1w    | 37  | MIA  | C13-C14 | 6.81   | 1.52        | 1.32     |
| 54  | 2w    | 37  | MIA  | C2-S10  | -6.57  | 1.70        | 1.75     |

The worst 5 of 435 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB   | -18.12 | 69.79       | 102.36   |
| 54  | 1w    | 37   | MIA  | C12-C13-C14 | -9.42  | 110.10      | 127.01   |
| 54  | 2w    | 37   | MIA  | C5-C4-N3    | -9.08  | 117.61      | 127.18   |
| 54  | 1w    | 37   | MIA  | C5-C4-N3    | -8.21  | 118.53      | 127.18   |
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3    | -8.14  | 118.60      | 127.18   |

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 32  | 1a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 43  | 1l    | 92   | 0TD  | CA-CB-SB-CSB    |
| 43  | 1l    | 92   | 0TD  | CG-CB-SB-CSB    |
| 54  | 1w    | 37   | MIA  | C12-C13-C14-C16 |
| 55  | 1x    | 76   | 31H  | C-CA-CB-CG      |

There are no ring outliers.

31 monomers are involved in 43 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 2A    | 1915 | 5MU  | 1       | 0            |
| 1   | 1A    | 2503 | 2MA  | 1       | 0            |
| 54  | 1y    | 54   | 5MU  | 1       | 0            |
| 32  | 1a    | 1518 | MA6  | 1       | 0            |
| 32  | 2a    | 966  | M2G  | 1       | 0            |
| 1   | 1A    | 2058 | MA6  | 1       | 0            |
| 32  | 2a    | 1518 | MA6  | 4       | 0            |
| 54  | 2y    | 8    | 4SU  | 2       | 0            |
| 1   | 2A    | 2058 | MA6  | 3       | 0            |
| 1   | 1A    | 2552 | OMU  | 1       | 0            |
| 54  | 1w    | 37   | MIA  | 1       | 0            |
| 54  | 2y    | 46   | G7M  | 1       | 0            |
| 54  | 1y    | 46   | G7M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32  | 2a    | 1519 | MA6  | 2       | 0            |
| 54  | 1y    | 32   | PSU  | 1       | 0            |
| 54  | 2y    | 55   | PSU  | 7       | 0            |
| 43  | 2l    | 92   | 0TD  | 1       | 0            |
| 1   | 2A    | 1939 | 5MU  | 1       | 0            |
| 54  | 1w    | 46   | G7M  | 1       | 0            |
| 54  | 2y    | 37   | MIA  | 1       | 0            |
| 54  | 2y    | 39   | PSU  | 1       | 0            |
| 32  | 1a    | 1519 | MA6  | 1       | 0            |
| 54  | 2y    | 54   | 5MU  | 1       | 0            |
| 1   | 2A    | 2251 | OMG  | 1       | 0            |
| 55  | 2x    | 32   | 5MC  | 1       | 0            |
| 32  | 1a    | 1402 | 4OC  | 2       | 0            |
| 54  | 1y    | 37   | MIA  | 1       | 0            |
| 54  | 1y    | 8    | 4SU  | 1       | 0            |
| 54  | 2w    | 39   | PSU  | 1       | 0            |
| 54  | 1w    | 8    | 4SU  | 1       | 0            |
| 55  | 1x    | 8    | 4SU  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2682 ligands modelled in this entry, 2678 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 59  | SF4  | 2d    | 303  | 35   | 0,12,12      | -    | -           | -           |      |             |
| 57  | WC9  | 2A    | 3809 | -    | 34,37,37     | 1.36 | 5 (14%)     | 31,53,53    | 1.18 | 3 (9%)      |
| 59  | SF4  | 1d    | 302  | 35   | 0,12,12      | -    | -           | -           |      |             |
| 57  | WC9  | 1A    | 4098 | -    | 34,37,37     | 1.45 | 5 (14%)     | 31,53,53    | 1.36 | 6 (19%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 59  | SF4  | 2d    | 303  | 35   | -       | -          | 0/6/5/5 |
| 57  | WC9  | 2A    | 3809 | -    | -       | 2/28/71/71 | 0/3/4/4 |
| 59  | SF4  | 1d    | 302  | 35   | -       | -          | 0/6/5/5 |
| 57  | WC9  | 1A    | 4098 | -    | -       | 3/28/71/71 | 0/3/4/4 |

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

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 57  | 2A    | 3809 | WC9  | CAM-CBF | -4.74 | 1.40        | 1.51     |
| 57  | 1A    | 4098 | WC9  | CAM-CBF | -4.54 | 1.40        | 1.51     |
| 57  | 1A    | 4098 | WC9  | CD2-CAZ | -2.90 | 1.50        | 1.53     |
| 57  | 1A    | 4098 | WC9  | CAF-CAE | -2.85 | 1.48        | 1.53     |
| 57  | 2A    | 3809 | WC9  | OAW-CB  | 2.81  | 1.45        | 1.42     |

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

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | 2A    | 3809 | WC9  | CBC-CBB-CAZ | -3.14 | 110.58      | 116.68   |
| 57  | 1A    | 4098 | WC9  | CBC-CBB-CAZ | -3.05 | 110.77      | 116.68   |
| 57  | 1A    | 4098 | WC9  | CAF-OAA-CAB | -2.99 | 110.25      | 114.17   |
| 57  | 1A    | 4098 | WC9  | OAA-CAF-CAE | -2.79 | 106.47      | 110.32   |
| 57  | 2A    | 3809 | WC9  | CAF-OAA-CAB | -2.61 | 110.75      | 114.17   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

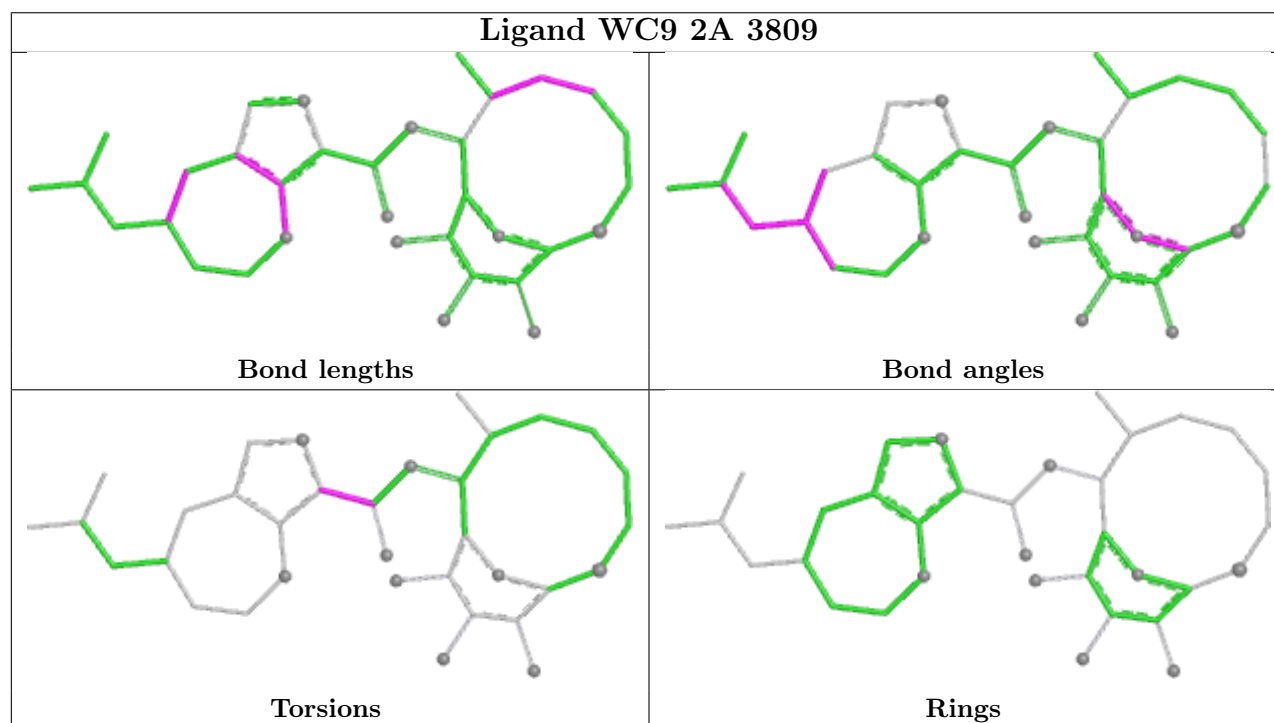
| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 57  | 1A    | 4098 | WC9  | O-C-CA-CB   |
| 57  | 2A    | 3809 | WC9  | O-C-CA-CB   |
| 57  | 1A    | 4098 | WC9  | NAL-C-CA-CB |
| 57  | 2A    | 3809 | WC9  | NAL-C-CA-CB |
| 57  | 1A    | 4098 | WC9  | O-C-CA-N    |

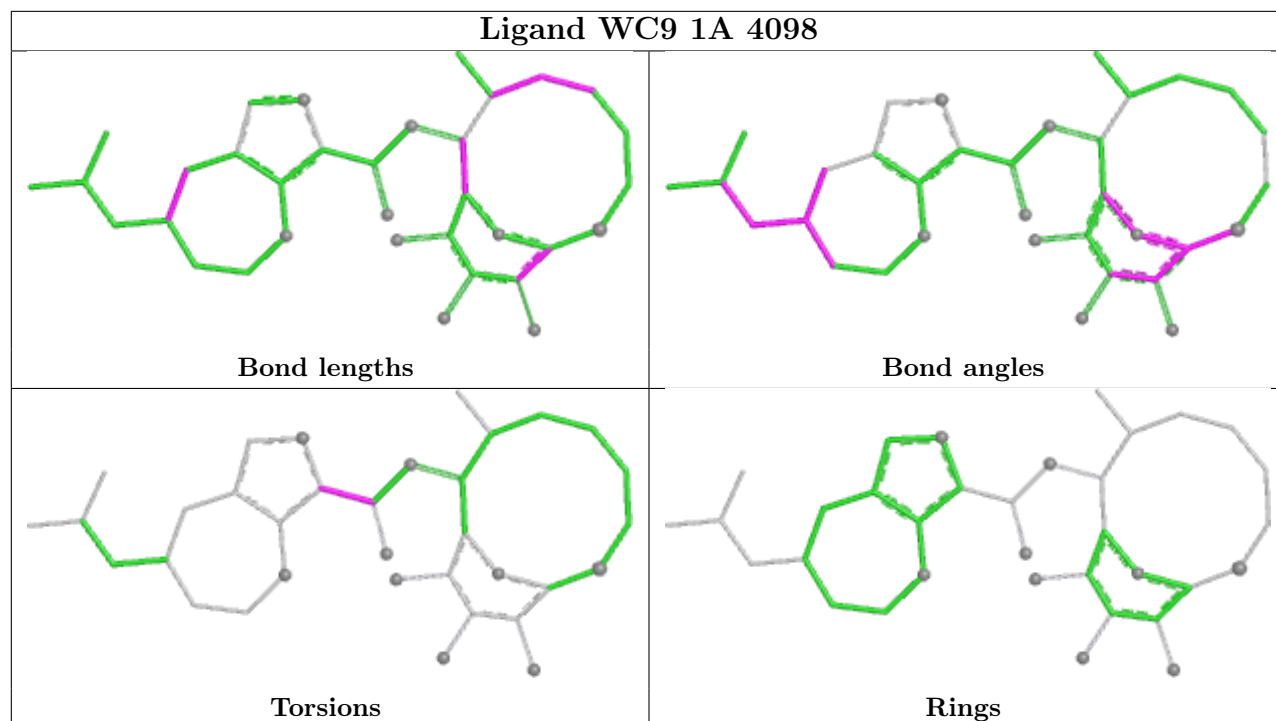
There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57  | 2A    | 3809 | WC9  | 4       | 0            |
| 57  | 1A    | 4098 | WC9  | 1       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |     |     | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-----|-----|-----------------------|---------|
| 1   | 1A    | 2859/2915 (98%) | -0.46  | 162 (5%)  | 29  | 29  | 24, 40, 98, 110       | 0       |
| 1   | 2A    | 2788/2915 (95%) | 0.01   | 139 (4%)  | 34  | 33  | 35, 58, 96, 108       | 0       |
| 2   | 1B    | 120/121 (99%)   | -0.28  | 0         | 100 | 100 | 35, 53, 67, 93        | 0       |
| 2   | 2B    | 120/121 (99%)   | 0.53   | 0         | 100 | 100 | 62, 75, 85, 97        | 0       |
| 3   | 1D    | 275/276 (99%)   | -0.09  | 4 (1%)    | 72  | 73  | 24, 40, 53, 82        | 0       |
| 3   | 2D    | 275/276 (99%)   | 0.25   | 7 (2%)    | 58  | 59  | 33, 50, 62, 82        | 0       |
| 4   | 1E    | 204/206 (99%)   | -0.13  | 2 (0%)    | 79  | 80  | 23, 42, 61, 74        | 0       |
| 4   | 2E    | 204/206 (99%)   | 0.58   | 7 (3%)    | 48  | 49  | 39, 60, 73, 83        | 0       |
| 5   | 1F    | 203/210 (96%)   | 0.14   | 7 (3%)    | 48  | 49  | 22, 46, 70, 89        | 0       |
| 5   | 2F    | 203/210 (96%)   | 0.63   | 10 (4%)   | 35  | 34  | 36, 68, 81, 87        | 0       |
| 6   | 1G    | 181/182 (99%)   | 0.67   | 11 (6%)   | 27  | 26  | 42, 62, 75, 89        | 0       |
| 6   | 2G    | 181/182 (99%)   | 1.35   | 29 (16%)  | 5   | 4   | 67, 77, 85, 92        | 0       |
| 7   | 1H    | 174/180 (96%)   | 0.30   | 3 (1%)    | 69  | 69  | 40, 55, 67, 77        | 0       |
| 7   | 2H    | 174/180 (96%)   | 1.91   | 70 (40%)  | 0   | 0   | 71, 85, 94, 96        | 0       |
| 8   | 1I    | 146/148 (98%)   | 0.99   | 7 (4%)    | 35  | 35  | 48, 75, 83, 86        | 0       |
| 8   | 2I    | 146/148 (98%)   | 1.07   | 13 (8%)   | 15  | 14  | 52, 74, 83, 88        | 0       |
| 9   | 1N    | 140/140 (100%)  | -0.04  | 2 (1%)    | 73  | 74  | 30, 41, 61, 76        | 0       |
| 9   | 2N    | 140/140 (100%)  | 0.87   | 5 (3%)    | 46  | 47  | 52, 67, 80, 88        | 0       |
| 10  | 1O    | 122/122 (100%)  | -0.04  | 1 (0%)    | 82  | 84  | 31, 43, 60, 66        | 0       |
| 10  | 2O    | 122/122 (100%)  | 0.63   | 3 (2%)    | 58  | 59  | 48, 61, 72, 76        | 0       |
| 11  | 1P    | 149/150 (99%)   | 0.21   | 2 (1%)    | 75  | 75  | 25, 50, 71, 78        | 0       |
| 11  | 2P    | 149/150 (99%)   | 0.83   | 11 (7%)   | 20  | 19  | 40, 68, 85, 91        | 0       |
| 12  | 1Q    | 141/141 (100%)  | 0.12   | 5 (3%)    | 47  | 48  | 30, 44, 62, 74        | 0       |
| 12  | 2Q    | 141/141 (100%)  | 1.11   | 20 (14%)  | 6   | 5   | 54, 68, 79, 88        | 0       |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | -0.22  | 1 (0%) 82 84   | 28, 38, 51, 61        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.36   | 2 (1%) 69 69   | 44, 54, 64, 74        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.34   | 1 (0%) 81 83   | 42, 53, 66, 69        | 0     |
| 14  | 2S    | 110/112 (98%)  | 1.13   | 12 (10%) 10 10 | 63, 73, 79, 85        | 0     |
| 15  | 1T    | 131/146 (89%)  | 0.29   | 6 (4%) 37 38   | 36, 49, 74, 83        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.79   | 8 (6%) 27 26   | 52, 65, 79, 85        | 0     |
| 16  | 1U    | 116/118 (98%)  | -0.33  | 1 (0%) 81 83   | 25, 33, 46, 68        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.67   | 3 (2%) 57 58   | 47, 63, 77, 83        | 0     |
| 17  | 1V    | 101/101 (100%) | -0.27  | 1 (0%) 79 80   | 25, 41, 58, 68        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.83   | 4 (3%) 42 43   | 44, 73, 81, 93        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.24  | 1 (0%) 81 83   | 27, 34, 54, 82        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.28   | 2 (1%) 67 68   | 43, 51, 67, 95        | 0     |
| 19  | 1X    | 95/96 (98%)    | 0.11   | 3 (3%) 50 51   | 31, 44, 69, 84        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.67   | 5 (5%) 32 31   | 46, 61, 75, 86        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.45   | 3 (2%) 55 56   | 37, 52, 69, 78        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 1.18   | 17 (15%) 5 4   | 57, 71, 83, 90        | 0     |
| 21  | 1Z    | 154/206 (74%)  | 1.05   | 23 (14%) 5 5   | 40, 67, 89, 93        | 0     |
| 21  | 2Z    | 160/206 (77%)  | 2.00   | 71 (44%) 0 0   | 70, 84, 93, 96        | 0     |
| 22  | 10    | 77/85 (90%)    | 0.02   | 1 (1%) 75 75   | 30, 41, 55, 72        | 0     |
| 22  | 20    | 83/85 (97%)    | 1.33   | 13 (15%) 5 4   | 46, 65, 78, 87        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.33   | 1 (1%) 79 80   | 31, 47, 75, 80        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.53   | 1 (1%) 79 80   | 39, 55, 75, 80        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.50   | 2 (2%) 53 55   | 41, 53, 65, 76        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.85   | 2 (2%) 53 55   | 58, 72, 80, 85        | 0     |
| 25  | 13    | 59/60 (98%)    | -0.02  | 3 (5%) 33 33   | 28, 38, 62, 81        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.90   | 4 (6%) 23 22   | 60, 68, 81, 89        | 0     |
| 26  | 14    | 69/71 (97%)    | 1.34   | 15 (21%) 2 2   | 57, 77, 90, 95        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.82   | 24 (34%) 1 0   | 76, 87, 95, 98        | 0     |
| 27  | 15    | 59/60 (98%)    | -0.28  | 1 (1%) 69 69   | 24, 35, 53, 60        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.32   | 2 (3%) 48 49   | 41, 53, 68, 82        | 0     |
| 28  | 16    | 53/54 (98%)    | -0.11  | 0 100 100      | 37, 45, 58, 63        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.59   | 1 (1%) 66 66   | 48, 61, 70, 75        | 0     |
| 29  | 17    | 48/49 (97%)     | 0.02   | 4 (8%) 17 17   | 24, 31, 64, 70        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.36   | 4 (8%) 17 17   | 36, 42, 70, 76        | 0     |
| 30  | 18    | 64/65 (98%)     | -0.21  | 0 100 100      | 29, 37, 44, 58        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.62   | 0 100 100      | 48, 56, 64, 70        | 0     |
| 31  | 19    | 37/37 (100%)    | -0.11  | 0 100 100      | 34, 42, 59, 62        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.21   | 4 (10%) 11 10  | 66, 72, 79, 83        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.30   | 60 (4%) 42 43  | 38, 69, 96, 108       | 0     |
| 32  | 2a    | 1491/1521 (98%) | 0.58   | 96 (6%) 25 24  | 48, 75, 96, 109       | 0     |
| 33  | 1b    | 231/256 (90%)   | 1.63   | 70 (30%) 1 0   | 67, 81, 90, 94        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.89   | 95 (41%) 0 0   | 73, 85, 91, 95        | 0     |
| 34  | 1c    | 206/239 (86%)   | 1.21   | 30 (14%) 6 5   | 64, 76, 86, 95        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.97   | 98 (47%) 0 0   | 75, 83, 90, 92        | 0     |
| 35  | 1d    | 208/209 (99%)   | 1.18   | 36 (17%) 4 3   | 55, 72, 81, 90        | 0     |
| 35  | 2d    | 208/209 (99%)   | 0.91   | 5 (2%) 59 61   | 60, 68, 76, 82        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.86   | 8 (5%) 31 31   | 53, 67, 77, 84        | 0     |
| 36  | 2e    | 148/162 (91%)   | 1.30   | 18 (12%) 8 7   | 60, 74, 82, 86        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.92   | 8 (8%) 18 18   | 59, 70, 78, 83        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.67   | 1 (1%) 79 80   | 60, 69, 77, 84        | 0     |
| 38  | 1g    | 155/156 (99%)   | 1.05   | 22 (14%) 6 5   | 64, 73, 85, 89        | 0     |
| 38  | 2g    | 155/156 (99%)   | 1.25   | 28 (18%) 3 3   | 68, 78, 88, 93        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.79   | 3 (2%) 62 63   | 55, 68, 74, 80        | 0     |
| 39  | 2h    | 137/138 (99%)   | 1.25   | 17 (12%) 8 7   | 67, 76, 81, 87        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.54   | 29 (22%) 2 2   | 59, 80, 87, 89        | 0     |
| 40  | 2i    | 127/128 (99%)   | 2.00   | 63 (49%) 0 0   | 72, 84, 90, 91        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.82   | 30 (30%) 1 0   | 59, 80, 89, 93        | 0     |
| 41  | 2j    | 96/105 (91%)    | 2.36   | 60 (62%) 0 0   | 75, 86, 92, 95        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.80   | 12 (10%) 11 11 | 45, 67, 78, 84        | 0     |
| 42  | 2k    | 114/129 (88%)   | 1.09   | 14 (12%) 8 7   | 55, 72, 82, 86        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.40   | 4 (3%) 49 50   | 46, 56, 70, 75        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.99   | 10 (8%) 17 17  | 54, 67, 78, 83        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 123/126 (97%)     | 1.08   | 11 (8%) 15 14   | 58, 73, 82, 90        | 0     |
| 44  | 2m    | 122/126 (96%)     | 1.78   | 37 (30%) 1 0    | 72, 83, 87, 93        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.39   | 12 (20%) 3 2    | 63, 72, 78, 80        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.62   | 45 (75%) 0 0    | 76, 83, 89, 93        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.83   | 6 (6%) 23 22    | 49, 67, 75, 82        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.90   | 4 (4%) 38 38    | 60, 72, 82, 85        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.46   | 13 (15%) 5 4    | 59, 72, 81, 86        | 0     |
| 47  | 2p    | 82/88 (93%)       | 1.09   | 7 (8%) 16 16    | 59, 69, 77, 82        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.91   | 4 (4%) 42 43    | 55, 68, 77, 80        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.88   | 5 (5%) 33 33    | 61, 72, 82, 84        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.79   | 4 (5%) 28 27    | 59, 67, 79, 82        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.82   | 2 (2%) 53 55    | 61, 70, 79, 83        | 0     |
| 50  | 1s    | 83/93 (89%)       | 1.13   | 8 (9%) 13 13    | 66, 76, 83, 89        | 0     |
| 50  | 2s    | 83/93 (89%)       | 2.19   | 45 (54%) 0 0    | 78, 86, 91, 96        | 0     |
| 51  | 1t    | 96/106 (90%)      | 1.34   | 21 (21%) 2 2    | 62, 73, 83, 85        | 0     |
| 51  | 2t    | 96/106 (90%)      | 1.12   | 11 (11%) 9 8    | 59, 71, 84, 85        | 0     |
| 52  | 1u    | 23/27 (85%)       | 1.32   | 5 (21%) 2 2     | 66, 70, 74, 79        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.50   | 17 (73%) 0 0    | 73, 79, 83, 85        | 0     |
| 53  | 1v    | 13/24 (54%)       | 0.37   | 0 100 100       | 50, 59, 81, 94        | 0     |
| 53  | 2v    | 13/24 (54%)       | 1.13   | 3 (23%) 2 1     | 64, 74, 92, 100       | 0     |
| 54  | 1w    | 65/76 (85%)       | 0.81   | 8 (12%) 8 7     | 58, 87, 98, 104       | 0     |
| 54  | 1y    | 67/76 (88%)       | 1.04   | 8 (11%) 9 8     | 39, 94, 101, 104      | 0     |
| 54  | 2w    | 62/76 (81%)       | 1.24   | 11 (17%) 4 3    | 74, 93, 102, 106      | 0     |
| 54  | 2y    | 66/76 (86%)       | 1.30   | 11 (16%) 4 3    | 52, 98, 103, 106      | 0     |
| 55  | 1x    | 71/77 (92%)       | 0.16   | 2 (2%) 55 56    | 32, 63, 81, 90        | 0     |
| 55  | 2x    | 71/77 (92%)       | 0.43   | 3 (4%) 40 41    | 49, 76, 88, 101       | 0     |
| All | All   | 20860/21748 (95%) | 0.49   | 1886 (9%) 15 14 | 22, 65, 90, 110       | 0     |

The worst 5 of 1886 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 44  | 2m    | 123 | ALA  | 10.0 |
| 1   | 1A    | 653 | A    | 8.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 45  | 2n    | 2      | ALA  | 8.0  |
| 1   | 2A    | 652(U) | G    | 7.7  |
| 1   | 2A    | 652(V) | C    | 7.6  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | PSU  | 2y    | 55   | 20/21 | 0.46 | 0.17 | 96,101,110,117             | 0     |
| 54  | G7M  | 2w    | 46   | 24/25 | 0.58 | 0.16 | 86,98,107,118              | 0     |
| 54  | 4SU  | 2y    | 8    | 20/21 | 0.61 | 0.15 | 94,99,103,117              | 0     |
| 54  | 5MU  | 1y    | 54   | 21/22 | 0.61 | 0.15 | 88,94,106,116              | 0     |
| 54  | G7M  | 2y    | 46   | 24/25 | 0.64 | 0.16 | 96,99,105,124              | 0     |
| 54  | G7M  | 1y    | 46   | 24/25 | 0.65 | 0.17 | 91,97,103,117              | 0     |
| 54  | G7M  | 1w    | 46   | 24/25 | 0.65 | 0.16 | 72,89,108,125              | 0     |
| 54  | 5MU  | 2y    | 54   | 21/22 | 0.67 | 0.15 | 93,98,108,122              | 0     |
| 54  | PSU  | 1y    | 55   | 20/21 | 0.68 | 0.13 | 91,98,108,119              | 0     |
| 54  | MIA  | 2y    | 37   | 22/30 | 0.69 | 0.16 | 83,93,104,117              | 0     |
| 54  | 4SU  | 1y    | 8    | 20/21 | 0.69 | 0.14 | 92,96,103,107              | 0     |
| 54  | PSU  | 2y    | 32   | 20/21 | 0.72 | 0.17 | 86,92,101,110              | 0     |
| 54  | PSU  | 2w    | 55   | 20/21 | 0.77 | 0.13 | 82,89,98,101               | 0     |
| 54  | 4SU  | 2w    | 8    | 20/21 | 0.78 | 0.14 | 92,97,102,108              | 0     |
| 54  | PSU  | 1y    | 39   | 20/21 | 0.79 | 0.14 | 84,87,98,100               | 0     |
| 54  | MIA  | 1y    | 37   | 22/30 | 0.80 | 0.15 | 81,88,95,103               | 0     |
| 54  | PSU  | 2y    | 39   | 20/21 | 0.84 | 0.13 | 84,89,97,104               | 0     |
| 54  | 5MU  | 2w    | 54   | 21/22 | 0.85 | 0.12 | 78,82,89,93                | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.86 | 0.13 | 76,86,89,90                | 0     |
| 54  | PSU  | 1w    | 55   | 20/21 | 0.86 | 0.11 | 68,79,86,88                | 0     |
| 54  | PSU  | 1y    | 32   | 20/21 | 0.87 | 0.13 | 80,88,92,96                | 0     |
| 54  | MIA  | 2w    | 37   | 25/30 | 0.87 | 0.15 | 61,76,87,107               | 0     |
| 54  | PSU  | 2w    | 32   | 20/21 | 0.88 | 0.13 | 76,85,97,99                | 0     |
| 55  | PSU  | 2x    | 55   | 20/21 | 0.89 | 0.11 | 69,75,83,89                | 0     |
| 55  | 5MU  | 2x    | 54   | 21/22 | 0.89 | 0.12 | 69,79,83,86                | 0     |
| 54  | MIA  | 1w    | 37   | 29/30 | 0.90 | 0.15 | 52,60,77,90                | 0     |
| 54  | 4SU  | 1w    | 8    | 20/21 | 0.90 | 0.11 | 80,85,90,92                | 0     |
| 32  | G7M  | 2a    | 527  | 24/25 | 0.91 | 0.14 | 57,66,70,74                | 0     |
| 55  | PSU  | 1x    | 55   | 20/21 | 0.91 | 0.10 | 56,62,72,77                | 0     |
| 55  | 4SU  | 2x    | 8    | 20/21 | 0.91 | 0.11 | 73,81,85,85                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.92 | 0.11 | 48,53,57,74                 | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.92 | 0.14 | 63,70,81,84                 | 0     |
| 55  | 5MU  | 1x    | 54   | 21/22 | 0.92 | 0.10 | 58,64,73,74                 | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.92 | 0.15 | 65,70,73,77                 | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.92 | 0.11 | 65,69,75,76                 | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.93 | 0.15 | 61,68,80,84                 | 0     |
| 54  | PSU  | 1w    | 32   | 20/21 | 0.93 | 0.11 | 63,71,81,82                 | 0     |
| 55  | 5MC  | 2x    | 32   | 21/22 | 0.93 | 0.12 | 68,71,77,79                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.93 | 0.10 | 57,62,73,75                 | 0     |
| 54  | 5MU  | 1w    | 54   | 21/22 | 0.93 | 0.10 | 57,70,73,78                 | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.93 | 0.11 | 48,54,59,63                 | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.94 | 0.09 | 59,62,67,71                 | 0     |
| 55  | 5MC  | 1x    | 32   | 21/22 | 0.94 | 0.13 | 54,59,63,71                 | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.94 | 0.10 | 54,61,67,68                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.94 | 0.12 | 45,53,63,69                 | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.94 | 0.10 | 54,62,64,65                 | 0     |
| 1   | MA6  | 2A    | 2058 | 24/25 | 0.94 | 0.11 | 38,49,57,59                 | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.94 | 0.10 | 64,72,76,82                 | 0     |
| 54  | PSU  | 2w    | 39   | 20/21 | 0.94 | 0.10 | 65,81,87,87                 | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.94 | 0.10 | 67,74,77,79                 | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.94 | 0.10 | 48,53,59,63                 | 0     |
| 55  | 4SU  | 1x    | 8    | 20/21 | 0.94 | 0.09 | 55,63,67,67                 | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.95 | 0.11 | 53,59,63,68                 | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.95 | 0.12 | 51,64,71,75                 | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.95 | 0.11 | 65,68,71,74                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.95 | 0.12 | 47,54,62,67                 | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.95 | 0.09 | 50,56,59,61                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.95 | 0.08 | 50,60,64,65                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.95 | 0.10 | 48,55,60,66                 | 0     |
| 55  | 31H  | 2x    | 76   | 32/33 | 0.96 | 0.09 | 41,47,60,65                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.96 | 0.09 | 39,50,58,68                 | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.96 | 0.13 | 54,61,69,72                 | 0     |
| 55  | 31H  | 1x    | 76   | 32/33 | 0.96 | 0.09 | 24,31,38,47                 | 10    |
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.96 | 0.08 | 46,52,57,58                 | 0     |
| 54  | PSU  | 1w    | 39   | 20/21 | 0.96 | 0.08 | 56,68,73,81                 | 0     |
| 1   | MA6  | 1A    | 2058 | 24/25 | 0.96 | 0.11 | 25,38,41,42                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.96 | 0.08 | 53,59,63,63                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.97 | 0.07 | 31,39,43,52                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.09 | 37,41,44,45                 | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.97 | 0.08 | 39,46,51,55                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.08 | 37,41,49,50                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.97 | 0.08 | 48,53,57,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.97 | 0.08 | 43,49,51,54                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.97 | 0.07 | 34,43,47,48                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.97 | 0.08 | 36,44,46,49                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.97 | 0.09 | 41,46,50,53                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.08 | 33,39,46,50                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.97 | 0.07 | 40,48,54,54                 | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.09 | 36,41,47,51                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.98 | 0.07 | 39,44,48,50                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.05 | 24,27,32,32                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.98 | 0.07 | 40,44,48,54                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.98 | 0.08 | 38,42,47,47                 | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.06 | 23,27,29,30                 | 0     |
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.98 | 0.07 | 27,32,34,38                 | 0     |
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.98 | 0.06 | 24,29,36,37                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.07 | 27,32,37,38                 | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.98 | 0.06 | 41,46,48,48                 | 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3643 | 1/1   | 0.44 | 0.30 | 85,85,85,85                 | 0     |
| 56  | MG   | 2a    | 1801 | 1/1   | 0.48 | 0.30 | 89,89,89,89                 | 0     |
| 56  | MG   | 1A    | 4061 | 1/1   | 0.49 | 0.25 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 4090 | 1/1   | 0.50 | 0.27 | 85,85,85,85                 | 0     |
| 56  | MG   | 1A    | 4073 | 1/1   | 0.52 | 0.28 | 86,86,86,86                 | 0     |
| 56  | MG   | 1a    | 1793 | 1/1   | 0.52 | 0.29 | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3703 | 1/1   | 0.53 | 0.28 | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1753 | 1/1   | 0.54 | 0.18 | 92,92,92,92                 | 0     |
| 56  | MG   | 1A    | 4007 | 1/1   | 0.56 | 0.16 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 4024 | 1/1   | 0.56 | 0.19 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3085 | 1/1   | 0.56 | 0.18 | 87,87,87,87                 | 0     |
| 56  | MG   | 1A    | 3966 | 1/1   | 0.57 | 0.24 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1Y    | 202  | 1/1   | 0.59 | 0.21 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 4072 | 1/1   | 0.59 | 0.27 | 78,78,78,78                 | 0     |
| 56  | MG   | 2a    | 1827 | 1/1   | 0.59 | 0.27 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1811 | 1/1   | 0.60 | 0.29 | 82,82,82,82                 | 0     |
| 56  | MG   | 2A    | 3532 | 1/1   | 0.60 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3714 | 1/1   | 0.61 | 0.23 | 82,82,82,82                 | 0     |
| 56  | MG   | 2d    | 302  | 1/1   | 0.61 | 0.29 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3295 | 1/1   | 0.62 | 0.23 | 79,79,79,79                 | 0     |
| 56  | MG   | 1B    | 229  | 1/1   | 0.62 | 0.20 | 87,87,87,87                 | 0     |
| 56  | MG   | 1A    | 4056 | 1/1   | 0.62 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3349 | 1/1   | 0.63 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1769 | 1/1   | 0.63 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | 2a    | 1622 | 1/1   | 0.63 | 0.17 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3620 | 1/1   | 0.64 | 0.21 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3244 | 1/1   | 0.64 | 0.35 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3808 | 1/1   | 0.64 | 0.24 | 73,73,73,73                 | 0     |
| 56  | MG   | 2a    | 1820 | 1/1   | 0.64 | 0.23 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3379 | 1/1   | 0.64 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 4012 | 1/1   | 0.64 | 0.16 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1734 | 1/1   | 0.65 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 1B    | 233  | 1/1   | 0.65 | 0.23 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3732 | 1/1   | 0.65 | 0.31 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3297 | 1/1   | 0.65 | 0.32 | 84,84,84,84                 | 0     |
| 56  | MG   | 1A    | 4076 | 1/1   | 0.66 | 0.17 | 76,76,76,76                 | 0     |
| 56  | MG   | 2j    | 201  | 1/1   | 0.66 | 0.18 | 85,85,85,85                 | 0     |
| 56  | MG   | 2a    | 1804 | 1/1   | 0.67 | 0.32 | 79,79,79,79                 | 0     |
| 56  | MG   | 2B    | 211  | 1/1   | 0.67 | 0.28 | 79,79,79,79                 | 0     |
| 56  | MG   | 1a    | 1721 | 1/1   | 0.67 | 0.34 | 88,88,88,88                 | 0     |
| 56  | MG   | 1A    | 3982 | 1/1   | 0.68 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3615 | 1/1   | 0.69 | 0.24 | 60,60,60,60                 | 0     |
| 56  | MG   | 2v    | 102  | 1/1   | 0.69 | 0.39 | 83,83,83,83                 | 0     |
| 56  | MG   | 2a    | 1624 | 1/1   | 0.70 | 0.26 | 84,84,84,84                 | 0     |
| 56  | MG   | 1A    | 3802 | 1/1   | 0.70 | 0.21 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3345 | 1/1   | 0.70 | 0.21 | 76,76,76,76                 | 0     |
| 56  | MG   | 2a    | 1755 | 1/1   | 0.70 | 0.20 | 84,84,84,84                 | 0     |
| 56  | MG   | 1A    | 3293 | 1/1   | 0.70 | 0.51 | 85,85,85,85                 | 0     |
| 56  | MG   | 2A    | 3058 | 1/1   | 0.70 | 0.30 | 85,85,85,85                 | 0     |
| 56  | MG   | 1A    | 3088 | 1/1   | 0.70 | 0.22 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3163 | 1/1   | 0.70 | 0.27 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3169 | 1/1   | 0.70 | 0.16 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3188 | 1/1   | 0.70 | 0.33 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3094 | 1/1   | 0.70 | 0.18 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3273 | 1/1   | 0.70 | 0.36 | 77,77,77,77                 | 0     |
| 56  | MG   | 1a    | 1635 | 1/1   | 0.70 | 0.31 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3195 | 1/1   | 0.71 | 0.17 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3336 | 1/1   | 0.71 | 0.43 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3205 | 1/1   | 0.71 | 0.33 | 78,78,78,78                 | 0     |
| 56  | MG   | 2a    | 1781 | 1/1   | 0.71 | 0.28 | 79,79,79,79                 | 0     |
| 56  | MG   | 2a    | 1797 | 1/1   | 0.71 | 0.23 | 83,83,83,83                 | 0     |
| 56  | MG   | 2A    | 3046 | 1/1   | 0.71 | 0.24 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3794 | 1/1   | 0.71 | 0.18 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3502 | 1/1   | 0.71 | 0.26 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3875 | 1/1   | 0.71 | 0.19 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1822 | 1/1   | 0.71 | 0.39 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3544 | 1/1   | 0.71 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1646 | 1/1   | 0.71 | 0.40 | 79,79,79,79                 | 0     |
| 56  | MG   | 2a    | 1722 | 1/1   | 0.71 | 0.47 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3765 | 1/1   | 0.71 | 0.14 | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3770 | 1/1   | 0.72 | 0.23 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3830 | 1/1   | 0.72 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 4041 | 1/1   | 0.72 | 0.26 | 75,75,75,75                 | 0     |
| 56  | MG   | 2a    | 1603 | 1/1   | 0.72 | 0.28 | 85,85,85,85                 | 0     |
| 56  | MG   | 2a    | 1616 | 1/1   | 0.72 | 0.29 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3530 | 1/1   | 0.72 | 0.21 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3794 | 1/1   | 0.72 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1662 | 1/1   | 0.72 | 0.31 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1670 | 1/1   | 0.73 | 0.31 | 76,76,76,76                 | 0     |
| 56  | MG   | 2a    | 1690 | 1/1   | 0.73 | 0.24 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1716 | 1/1   | 0.73 | 0.24 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 4040 | 1/1   | 0.73 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3057 | 1/1   | 0.73 | 0.27 | 66,66,66,66                 | 0     |
| 56  | MG   | 1O    | 206  | 1/1   | 0.73 | 0.24 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3671 | 1/1   | 0.73 | 0.20 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3993 | 1/1   | 0.73 | 0.14 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 4046 | 1/1   | 0.73 | 0.27 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 4087 | 1/1   | 0.73 | 0.25 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3771 | 1/1   | 0.73 | 0.14 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 4019 | 1/1   | 0.73 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3383 | 1/1   | 0.73 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3455 | 1/1   | 0.73 | 0.21 | 79,79,79,79                 | 0     |
| 56  | MG   | 1a    | 1761 | 1/1   | 0.73 | 0.23 | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3512 | 1/1   | 0.73 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3211 | 1/1   | 0.73 | 0.26 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3240 | 1/1   | 0.73 | 0.40 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1649 | 1/1   | 0.73 | 0.26 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3158 | 1/1   | 0.74 | 0.38 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 4018 | 1/1   | 0.74 | 0.26 | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1679 | 1/1   | 0.74 | 0.36 | 69,69,69,69                 | 0     |
| 56  | MG   | 2a    | 1621 | 1/1   | 0.74 | 0.23 | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3892 | 1/1   | 0.74 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1796 | 1/1   | 0.74 | 0.26 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3729 | 1/1   | 0.74 | 0.18 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3730 | 1/1   | 0.74 | 0.15 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1647 | 1/1   | 0.74 | 0.43 | 83,83,83,83                 | 0     |
| 56  | MG   | 1a    | 1760 | 1/1   | 0.74 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1654 | 1/1   | 0.74 | 0.28 | 84,84,84,84                 | 0     |
| 56  | MG   | 1A    | 3292 | 1/1   | 0.74 | 0.27 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1676 | 1/1   | 0.74 | 0.27 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3337 | 1/1   | 0.74 | 0.16 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3773 | 1/1   | 0.74 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3086 | 1/1   | 0.74 | 0.28 | 72,72,72,72                 | 0     |
| 56  | MG   | 2a    | 1749 | 1/1   | 0.75 | 0.14 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1752 | 1/1   | 0.75 | 0.23 | 90,90,90,90                 | 0     |
| 56  | MG   | 1A    | 3898 | 1/1   | 0.75 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3687 | 1/1   | 0.75 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | 1B    | 230  | 1/1   | 0.75 | 0.11 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1771 | 1/1   | 0.75 | 0.35 | 70,70,70,70                 | 0     |
| 56  | MG   | 2a    | 1634 | 1/1   | 0.75 | 0.42 | 79,79,79,79                 | 0     |
| 56  | MG   | 2a    | 1784 | 1/1   | 0.75 | 0.34 | 72,72,72,72                 | 0     |
| 56  | MG   | 2a    | 1792 | 1/1   | 0.75 | 0.34 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3171 | 1/1   | 0.75 | 0.18 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 4033 | 1/1   | 0.75 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | 1O    | 201  | 1/1   | 0.75 | 0.16 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3498 | 1/1   | 0.75 | 0.19 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3593 | 1/1   | 0.75 | 0.25 | 83,83,83,83                 | 0     |
| 56  | MG   | 2a    | 1814 | 1/1   | 0.75 | 0.41 | 81,81,81,81                 | 0     |
| 56  | MG   | 2A    | 3340 | 1/1   | 0.75 | 0.23 | 72,72,72,72                 | 0     |
| 56  | MG   | 1B    | 222  | 1/1   | 0.75 | 0.26 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1701 | 1/1   | 0.75 | 0.19 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3624 | 1/1   | 0.75 | 0.24 | 61,61,61,61                 | 0     |
| 56  | MG   | 1a    | 1774 | 1/1   | 0.75 | 0.25 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3666 | 1/1   | 0.75 | 0.25 | 72,72,72,72                 | 0     |
| 56  | MG   | 2y    | 103  | 1/1   | 0.75 | 0.16 | 85,85,85,85                 | 0     |
| 56  | MG   | 2A    | 3190 | 1/1   | 0.76 | 0.26 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3322 | 1/1   | 0.76 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1626 | 1/1   | 0.76 | 0.29 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 4074 | 1/1   | 0.76 | 0.24 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 4014 | 1/1   | 0.76 | 0.16 | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3933 | 1/1   | 0.76 | 0.15 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3600 | 1/1   | 0.76 | 0.23 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1653 | 1/1   | 0.76 | 0.34 | 77,77,77,77                 | 0     |
| 56  | MG   | 1a    | 1670 | 1/1   | 0.76 | 0.23 | 75,75,75,75                 | 0     |
| 56  | MG   | 2a    | 1798 | 1/1   | 0.76 | 0.34 | 71,71,71,71                 | 0     |
| 56  | MG   | 2a    | 1657 | 1/1   | 0.76 | 0.24 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3616 | 1/1   | 0.76 | 0.31 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1808 | 1/1   | 0.76 | 0.17 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3803 | 1/1   | 0.76 | 0.18 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1686 | 1/1   | 0.76 | 0.42 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3797 | 1/1   | 0.76 | 0.18 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1694 | 1/1   | 0.76 | 0.31 | 72,72,72,72                 | 0     |
| 56  | MG   | 2F    | 302  | 1/1   | 0.76 | 0.17 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3408 | 1/1   | 0.76 | 0.26 | 77,77,77,77                 | 0     |
| 56  | MG   | 2a    | 1612 | 1/1   | 0.76 | 0.24 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3418 | 1/1   | 0.76 | 0.21 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3687 | 1/1   | 0.76 | 0.14 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3589 | 1/1   | 0.77 | 0.17 | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1770 | 1/1   | 0.77 | 0.21 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3413 | 1/1   | 0.77 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3599 | 1/1   | 0.77 | 0.23 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3680 | 1/1   | 0.77 | 0.20 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3942 | 1/1   | 0.77 | 0.19 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3263 | 1/1   | 0.77 | 0.36 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3404 | 1/1   | 0.77 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1671 | 1/1   | 0.77 | 0.25 | 72,72,72,72                 | 0     |
| 56  | MG   | 1x    | 109  | 1/1   | 0.77 | 0.32 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3279 | 1/1   | 0.77 | 0.21 | 76,76,76,76                 | 0     |
| 56  | MG   | 2a    | 1611 | 1/1   | 0.77 | 0.29 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1698 | 1/1   | 0.77 | 0.29 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3432 | 1/1   | 0.77 | 0.26 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3026 | 1/1   | 0.77 | 0.22 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3680 | 1/1   | 0.77 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3835 | 1/1   | 0.77 | 0.15 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3466 | 1/1   | 0.77 | 0.24 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3232 | 1/1   | 0.77 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 1B    | 221  | 1/1   | 0.77 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1636 | 1/1   | 0.77 | 0.23 | 71,71,71,71                 | 0     |
| 56  | MG   | 2a    | 1745 | 1/1   | 0.78 | 0.29 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 4091 | 1/1   | 0.78 | 0.19 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3939 | 1/1   | 0.78 | 0.14 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3404 | 1/1   | 0.78 | 0.23 | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1754 | 1/1   | 0.78 | 0.14 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1677 | 1/1   | 0.78 | 0.32 | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1763 | 1/1   | 0.78 | 0.23 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3080 | 1/1   | 0.78 | 0.23 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3245 | 1/1   | 0.78 | 0.21 | 78,78,78,78                 | 0     |
| 56  | MG   | 2a    | 1630 | 1/1   | 0.78 | 0.36 | 82,82,82,82                 | 0     |
| 56  | MG   | 2A    | 3692 | 1/1   | 0.78 | 0.18 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3862 | 1/1   | 0.78 | 0.18 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1785 | 1/1   | 0.78 | 0.21 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3725 | 1/1   | 0.78 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3264 | 1/1   | 0.78 | 0.32 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3970 | 1/1   | 0.78 | 0.19 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3105 | 1/1   | 0.78 | 0.35 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3739 | 1/1   | 0.78 | 0.22 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3130 | 1/1   | 0.78 | 0.41 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3559 | 1/1   | 0.78 | 0.29 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3026 | 1/1   | 0.78 | 0.34 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3313 | 1/1   | 0.78 | 0.37 | 74,74,74,74                 | 0     |
| 56  | MG   | 2a    | 1816 | 1/1   | 0.78 | 0.29 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3807 | 1/1   | 0.78 | 0.24 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3523 | 1/1   | 0.78 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 2D    | 303  | 1/1   | 0.78 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3350 | 1/1   | 0.78 | 0.30 | 71,71,71,71                 | 0     |
| 56  | MG   | 14    | 101  | 1/1   | 0.78 | 0.20 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1607 | 1/1   | 0.78 | 0.26 | 79,79,79,79                 | 0     |
| 56  | MG   | 1a    | 1632 | 1/1   | 0.78 | 0.31 | 83,83,83,83                 | 0     |
| 56  | MG   | 1A    | 3358 | 1/1   | 0.79 | 0.20 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3945 | 1/1   | 0.79 | 0.19 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1736 | 1/1   | 0.79 | 0.35 | 81,81,81,81                 | 0     |
| 56  | MG   | 2A    | 3097 | 1/1   | 0.79 | 0.33 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1749 | 1/1   | 0.79 | 0.20 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3810 | 1/1   | 0.79 | 0.22 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3475 | 1/1   | 0.79 | 0.18 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3705 | 1/1   | 0.79 | 0.18 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3516 | 1/1   | 0.79 | 0.19 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3980 | 1/1   | 0.79 | 0.11 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3731 | 1/1   | 0.79 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1786 | 1/1   | 0.79 | 0.35 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1786 | 1/1   | 0.79 | 0.21 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3299 | 1/1   | 0.79 | 0.21 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1656 | 1/1   | 0.79 | 0.13 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3568 | 1/1   | 0.79 | 0.25 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3923 | 1/1   | 0.79 | 0.14 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3553 | 1/1   | 0.79 | 0.45 | 78,78,78,78                 | 0     |
| 56  | MG   | 2a    | 1803 | 1/1   | 0.79 | 0.36 | 66,66,66,66                 | 0     |
| 56  | MG   | 1D    | 310  | 1/1   | 0.79 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1805 | 1/1   | 0.79 | 0.27 | 84,84,84,84                 | 0     |
| 56  | MG   | 2A    | 3798 | 1/1   | 0.79 | 0.23 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3784 | 1/1   | 0.79 | 0.29 | 85,85,85,85                 | 0     |
| 56  | MG   | 2A    | 3206 | 1/1   | 0.79 | 0.26 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1694 | 1/1   | 0.79 | 0.29 | 73,73,73,73                 | 0     |
| 56  | MG   | 2E    | 302  | 1/1   | 0.79 | 0.17 | 76,76,76,76                 | 0     |
| 56  | MG   | 2E    | 307  | 1/1   | 0.79 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3352 | 1/1   | 0.79 | 0.30 | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1602 | 1/1   | 0.79 | 0.17 | 86,86,86,86                 | 0     |
| 56  | MG   | 2a    | 1723 | 1/1   | 0.79 | 0.31 | 70,70,70,70                 | 0     |
| 56  | MG   | 2l    | 204  | 1/1   | 0.79 | 0.18 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3356 | 1/1   | 0.79 | 0.25 | 62,62,62,62                 | 0     |
| 56  | MG   | 2y    | 101  | 1/1   | 0.79 | 0.13 | 85,85,85,85                 | 0     |
| 56  | MG   | 2y    | 102  | 1/1   | 0.79 | 0.39 | 79,79,79,79                 | 0     |
| 56  | MG   | 1a    | 1686 | 1/1   | 0.79 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3496 | 1/1   | 0.80 | 0.16 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 4079 | 1/1   | 0.80 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1737 | 1/1   | 0.80 | 0.36 | 83,83,83,83                 | 0     |
| 56  | MG   | 1E    | 317  | 1/1   | 0.80 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3063 | 1/1   | 0.80 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3248 | 1/1   | 0.80 | 0.19 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3258 | 1/1   | 0.80 | 0.19 | 82,82,82,82                 | 0     |
| 56  | MG   | 2A    | 3068 | 1/1   | 0.80 | 0.15 | 63,63,63,63                 | 0     |
| 56  | MG   | 1F    | 312  | 1/1   | 0.80 | 0.21 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 4085 | 1/1   | 0.80 | 0.25 | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1727 | 1/1   | 0.80 | 0.23 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3595 | 1/1   | 0.80 | 0.13 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3598 | 1/1   | 0.80 | 0.26 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3584 | 1/1   | 0.80 | 0.22 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3100 | 1/1   | 0.80 | 0.23 | 81,81,81,81                 | 0     |
| 56  | MG   | 1a    | 1742 | 1/1   | 0.80 | 0.21 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3109 | 1/1   | 0.80 | 0.26 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3617 | 1/1   | 0.80 | 0.18 | 82,82,82,82                 | 0     |
| 56  | MG   | 1A    | 3721 | 1/1   | 0.80 | 0.23 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3146 | 1/1   | 0.80 | 0.18 | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1758 | 1/1   | 0.80 | 0.15 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3665 | 1/1   | 0.80 | 0.17 | 76,76,76,76                 | 0     |
| 56  | MG   | 2a    | 1641 | 1/1   | 0.80 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 4057 | 1/1   | 0.80 | 0.14 | 25,25,25,25                 | 0     |
| 56  | MG   | 1a    | 1603 | 1/1   | 0.80 | 0.21 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3349 | 1/1   | 0.80 | 0.29 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3445 | 1/1   | 0.80 | 0.19 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3354 | 1/1   | 0.80 | 0.30 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3987 | 1/1   | 0.80 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | 1B    | 228  | 1/1   | 0.80 | 0.15 | 74,74,74,74                 | 0     |
| 56  | MG   | 1x    | 103  | 1/1   | 0.80 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3323 | 1/1   | 0.80 | 0.23 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3268 | 1/1   | 0.80 | 0.17 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3820 | 1/1   | 0.80 | 0.23 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3222 | 1/1   | 0.80 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | 2q    | 202  | 1/1   | 0.80 | 0.21 | 83,83,83,83                 | 0     |
| 56  | MG   | 2A    | 3236 | 1/1   | 0.80 | 0.33 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3468 | 1/1   | 0.80 | 0.21 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3237 | 1/1   | 0.80 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3792 | 1/1   | 0.80 | 0.19 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3400 | 1/1   | 0.81 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3164 | 1/1   | 0.81 | 0.20 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3728 | 1/1   | 0.81 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3734 | 1/1   | 0.81 | 0.15 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3270 | 1/1   | 0.81 | 0.19 | 72,72,72,72                 | 0     |
| 56  | MG   | 1b    | 301  | 1/1   | 0.81 | 0.19 | 81,81,81,81                 | 0     |
| 56  | MG   | 1A    | 3838 | 1/1   | 0.81 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3164 | 1/1   | 0.81 | 0.33 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3187 | 1/1   | 0.81 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3793 | 1/1   | 0.81 | 0.24 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3536 | 1/1   | 0.81 | 0.19 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3795 | 1/1   | 0.81 | 0.19 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3540 | 1/1   | 0.81 | 0.26 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3298 | 1/1   | 0.81 | 0.23 | 85,85,85,85                 | 0     |
| 56  | MG   | 2B    | 205  | 1/1   | 0.81 | 0.32 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 4062 | 1/1   | 0.81 | 0.20 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3035 | 1/1   | 0.81 | 0.23 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3419 | 1/1   | 0.81 | 0.17 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1766 | 1/1   | 0.81 | 0.27 | 83,83,83,83                 | 0     |
| 56  | MG   | 2a    | 1768 | 1/1   | 0.81 | 0.22 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3425 | 1/1   | 0.81 | 0.21 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3198 | 1/1   | 0.81 | 0.48 | 77,77,77,77                 | 0     |
| 56  | MG   | 2l    | 101  | 1/1   | 0.81 | 0.17 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3338 | 1/1   | 0.81 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1703 | 1/1   | 0.81 | 0.30 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1604 | 1/1   | 0.81 | 0.22 | 82,82,82,82                 | 0     |
| 56  | MG   | 2a    | 1605 | 1/1   | 0.81 | 0.28 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3342 | 1/1   | 0.81 | 0.14 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3644 | 1/1   | 0.81 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3907 | 1/1   | 0.81 | 0.15 | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1615 | 1/1   | 0.81 | 0.45 | 78,78,78,78                 | 0     |
| 56  | MG   | 2a    | 1800 | 1/1   | 0.81 | 0.31 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3217 | 1/1   | 0.81 | 0.24 | 86,86,86,86                 | 0     |
| 56  | MG   | 2a    | 1802 | 1/1   | 0.81 | 0.17 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3219 | 1/1   | 0.81 | 0.24 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3077 | 1/1   | 0.81 | 0.26 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3635 | 1/1   | 0.81 | 0.28 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3377 | 1/1   | 0.81 | 0.34 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1809 | 1/1   | 0.81 | 0.29 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3656 | 1/1   | 0.81 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3369 | 1/1   | 0.81 | 0.39 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3804 | 1/1   | 0.81 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1637 | 1/1   | 0.81 | 0.33 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3390 | 1/1   | 0.81 | 0.37 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3391 | 1/1   | 0.81 | 0.30 | 76,76,76,76                 | 0     |
| 56  | MG   | 1l    | 102  | 1/1   | 0.81 | 0.22 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3385 | 1/1   | 0.81 | 0.29 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3701 | 1/1   | 0.81 | 0.22 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3707 | 1/1   | 0.81 | 0.22 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3709 | 1/1   | 0.81 | 0.32 | 76,76,76,76                 | 0     |
| 56  | MG   | 2w    | 104  | 1/1   | 0.81 | 0.34 | 81,81,81,81                 | 0     |
| 56  | MG   | 2a    | 1668 | 1/1   | 0.81 | 0.31 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3413 | 1/1   | 0.81 | 0.14 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3467 | 1/1   | 0.81 | 0.17 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3425 | 1/1   | 0.82 | 0.21 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3839 | 1/1   | 0.82 | 0.14 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3254 | 1/1   | 0.82 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1707 | 1/1   | 0.82 | 0.24 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3856 | 1/1   | 0.82 | 0.15 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3860 | 1/1   | 0.82 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3478 | 1/1   | 0.82 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1733 | 1/1   | 0.82 | 0.26 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3484 | 1/1   | 0.82 | 0.13 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3971 | 1/1   | 0.82 | 0.21 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3112 | 1/1   | 0.82 | 0.27 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3426 | 1/1   | 0.82 | 0.17 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1782 | 1/1   | 0.82 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3287 | 1/1   | 0.82 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3874 | 1/1   | 0.82 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3800 | 1/1   | 0.82 | 0.28 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3676 | 1/1   | 0.82 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3742 | 1/1   | 0.82 | 0.25 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3547 | 1/1   | 0.82 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3552 | 1/1   | 0.82 | 0.14 | 39,39,39,39                 | 0     |
| 56  | MG   | 1w    | 104  | 1/1   | 0.82 | 0.24 | 75,75,75,75                 | 0     |
| 56  | MG   | 1x    | 102  | 1/1   | 0.82 | 0.22 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1774 | 1/1   | 0.82 | 0.21 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3320 | 1/1   | 0.82 | 0.29 | 77,77,77,77                 | 0     |
| 56  | MG   | 2a    | 1783 | 1/1   | 0.82 | 0.16 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3526 | 1/1   | 0.82 | 0.28 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3325 | 1/1   | 0.82 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3326 | 1/1   | 0.82 | 0.27 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1789 | 1/1   | 0.82 | 0.29 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3327 | 1/1   | 0.82 | 0.34 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3306 | 1/1   | 0.82 | 0.35 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3604 | 1/1   | 0.82 | 0.17 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3612 | 1/1   | 0.82 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3193 | 1/1   | 0.82 | 0.28 | 72,72,72,72                 | 0     |
| 56  | MG   | 1x    | 113  | 1/1   | 0.82 | 0.19 | 85,85,85,85                 | 0     |
| 56  | MG   | 2A    | 3197 | 1/1   | 0.82 | 0.12 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3583 | 1/1   | 0.82 | 0.25 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3203 | 1/1   | 0.82 | 0.17 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3625 | 1/1   | 0.82 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3833 | 1/1   | 0.82 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3327 | 1/1   | 0.82 | 0.31 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3644 | 1/1   | 0.82 | 0.32 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3049 | 1/1   | 0.82 | 0.25 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3213 | 1/1   | 0.82 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3215 | 1/1   | 0.82 | 0.45 | 59,59,59,59                 | 0     |
| 56  | MG   | 1a    | 1705 | 1/1   | 0.82 | 0.11 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1718 | 1/1   | 0.82 | 0.15 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3682 | 1/1   | 0.82 | 0.18 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3389 | 1/1   | 0.82 | 0.29 | 78,78,78,78                 | 0     |
| 56  | MG   | 1O    | 205  | 1/1   | 0.82 | 0.18 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3606 | 1/1   | 0.82 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | 2r    | 101  | 1/1   | 0.82 | 0.23 | 82,82,82,82                 | 0     |
| 56  | MG   | 1a    | 1735 | 1/1   | 0.82 | 0.11 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1T    | 201  | 1/1   | 0.82 | 0.19 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 4086 | 1/1   | 0.82 | 0.20 | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1748 | 1/1   | 0.82 | 0.17 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3420 | 1/1   | 0.82 | 0.28 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3083 | 1/1   | 0.83 | 0.16 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3958 | 1/1   | 0.83 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3846 | 1/1   | 0.83 | 0.13 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3096 | 1/1   | 0.83 | 0.30 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3429 | 1/1   | 0.83 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1689 | 1/1   | 0.83 | 0.29 | 71,71,71,71                 | 0     |
| 56  | MG   | 1a    | 1725 | 1/1   | 0.83 | 0.21 | 82,82,82,82                 | 0     |
| 56  | MG   | 2A    | 3433 | 1/1   | 0.83 | 0.24 | 82,82,82,82                 | 0     |
| 56  | MG   | 1B    | 234  | 1/1   | 0.83 | 0.18 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3715 | 1/1   | 0.83 | 0.18 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 4050 | 1/1   | 0.83 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3274 | 1/1   | 0.83 | 0.26 | 69,69,69,69                 | 0     |
| 56  | MG   | 1E    | 314  | 1/1   | 0.83 | 0.17 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3101 | 1/1   | 0.83 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1728 | 1/1   | 0.83 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3530 | 1/1   | 0.83 | 0.36 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3296 | 1/1   | 0.83 | 0.41 | 84,84,84,84                 | 0     |
| 56  | MG   | 2A    | 3742 | 1/1   | 0.83 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3757 | 1/1   | 0.83 | 0.25 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3758 | 1/1   | 0.83 | 0.21 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3698 | 1/1   | 0.83 | 0.18 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3521 | 1/1   | 0.83 | 0.13 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3294 | 1/1   | 0.83 | 0.17 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3782 | 1/1   | 0.83 | 0.14 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3256 | 1/1   | 0.83 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3305 | 1/1   | 0.83 | 0.18 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3539 | 1/1   | 0.83 | 0.21 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3307 | 1/1   | 0.83 | 0.24 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3889 | 1/1   | 0.83 | 0.26 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3995 | 1/1   | 0.83 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3708 | 1/1   | 0.83 | 0.24 | 60,60,60,60                 | 0     |
| 56  | MG   | 2B    | 203  | 1/1   | 0.83 | 0.28 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 4008 | 1/1   | 0.83 | 0.11 | 69,69,69,69                 | 0     |
| 56  | MG   | 2B    | 206  | 1/1   | 0.83 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 4080 | 1/1   | 0.83 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1622 | 1/1   | 0.83 | 0.27 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 4011 | 1/1   | 0.83 | 0.17 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3497 | 1/1   | 0.83 | 0.13 | 80,80,80,80                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1642 | 1/1   | 0.83 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | 1a    | 1649 | 1/1   | 0.83 | 0.23 | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1652 | 1/1   | 0.83 | 0.35 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3602 | 1/1   | 0.83 | 0.18 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 4013 | 1/1   | 0.83 | 0.12 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3609 | 1/1   | 0.83 | 0.16 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 4088 | 1/1   | 0.83 | 0.16 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3043 | 1/1   | 0.83 | 0.30 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3586 | 1/1   | 0.83 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3024 | 1/1   | 0.83 | 0.29 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3374 | 1/1   | 0.83 | 0.36 | 66,66,66,66                 | 0     |
| 56  | MG   | 1B    | 212  | 1/1   | 0.83 | 0.30 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1680 | 1/1   | 0.83 | 0.32 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3628 | 1/1   | 0.83 | 0.25 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3638 | 1/1   | 0.83 | 0.21 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3638 | 1/1   | 0.83 | 0.22 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3065 | 1/1   | 0.83 | 0.19 | 60,60,60,60                 | 0     |
| 56  | MG   | 2a    | 1828 | 1/1   | 0.83 | 0.29 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3238 | 1/1   | 0.83 | 0.22 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3651 | 1/1   | 0.83 | 0.22 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3371 | 1/1   | 0.83 | 0.28 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1645 | 1/1   | 0.83 | 0.34 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3396 | 1/1   | 0.83 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3099 | 1/1   | 0.83 | 0.17 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3786 | 1/1   | 0.83 | 0.21 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3673 | 1/1   | 0.83 | 0.10 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3677 | 1/1   | 0.83 | 0.22 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3679 | 1/1   | 0.83 | 0.19 | 82,82,82,82                 | 0     |
| 56  | MG   | 1A    | 3412 | 1/1   | 0.84 | 0.15 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3180 | 1/1   | 0.84 | 0.24 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3959 | 1/1   | 0.84 | 0.20 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3965 | 1/1   | 0.84 | 0.14 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3089 | 1/1   | 0.84 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3695 | 1/1   | 0.84 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3095 | 1/1   | 0.84 | 0.14 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3329 | 1/1   | 0.84 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3483 | 1/1   | 0.84 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3370 | 1/1   | 0.84 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3334 | 1/1   | 0.84 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3104 | 1/1   | 0.84 | 0.24 | 75,75,75,75                 | 0     |
| 56  | MG   | 2a    | 1693 | 1/1   | 0.84 | 0.27 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3513 | 1/1   | 0.84 | 0.22 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1697 | 1/1   | 0.84 | 0.30 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3720 | 1/1   | 0.84 | 0.21 | 73,73,73,73                 | 0     |
| 56  | MG   | 10    | 108  | 1/1   | 0.84 | 0.24 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3528 | 1/1   | 0.84 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1708 | 1/1   | 0.84 | 0.23 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3573 | 1/1   | 0.84 | 0.23 | 46,46,46,46                 | 0     |
| 56  | MG   | 11    | 104  | 1/1   | 0.84 | 0.17 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3145 | 1/1   | 0.84 | 0.34 | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1726 | 1/1   | 0.84 | 0.30 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3984 | 1/1   | 0.84 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3147 | 1/1   | 0.84 | 0.21 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3153 | 1/1   | 0.84 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3546 | 1/1   | 0.84 | 0.29 | 74,74,74,74                 | 0     |
| 56  | MG   | 2a    | 1739 | 1/1   | 0.84 | 0.43 | 79,79,79,79                 | 0     |
| 56  | MG   | 2a    | 1743 | 1/1   | 0.84 | 0.21 | 78,78,78,78                 | 0     |
| 56  | MG   | 1a    | 1777 | 1/1   | 0.84 | 0.22 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1602 | 1/1   | 0.84 | 0.28 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3553 | 1/1   | 0.84 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3438 | 1/1   | 0.84 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1788 | 1/1   | 0.84 | 0.19 | 84,84,84,84                 | 0     |
| 56  | MG   | 1a    | 1791 | 1/1   | 0.84 | 0.13 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3376 | 1/1   | 0.84 | 0.24 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3994 | 1/1   | 0.84 | 0.15 | 75,75,75,75                 | 0     |
| 56  | MG   | 2B    | 201  | 1/1   | 0.84 | 0.34 | 78,78,78,78                 | 0     |
| 56  | MG   | 11    | 202  | 1/1   | 0.84 | 0.17 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3465 | 1/1   | 0.84 | 0.32 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3594 | 1/1   | 0.84 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | 2B    | 208  | 1/1   | 0.84 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3598 | 1/1   | 0.84 | 0.28 | 59,59,59,59                 | 0     |
| 56  | MG   | 2B    | 212  | 1/1   | 0.84 | 0.35 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3347 | 1/1   | 0.84 | 0.17 | 57,57,57,57                 | 0     |
| 56  | MG   | 2D    | 306  | 1/1   | 0.84 | 0.29 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3199 | 1/1   | 0.84 | 0.32 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3350 | 1/1   | 0.84 | 0.31 | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1791 | 1/1   | 0.84 | 0.23 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3348 | 1/1   | 0.84 | 0.21 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1795 | 1/1   | 0.84 | 0.22 | 74,74,74,74                 | 0     |
| 56  | MG   | 2G    | 201  | 1/1   | 0.84 | 0.17 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3634 | 1/1   | 0.84 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | 25    | 101  | 1/1   | 0.84 | 0.28 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3015 | 1/1   | 0.84 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3362 | 1/1   | 0.84 | 0.38 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 4093 | 1/1   | 0.84 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3212 | 1/1   | 0.84 | 0.17 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1606 | 1/1   | 0.84 | 0.31 | 81,81,81,81                 | 0     |
| 56  | MG   | 1a    | 1665 | 1/1   | 0.84 | 0.26 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3633 | 1/1   | 0.84 | 0.22 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3634 | 1/1   | 0.84 | 0.19 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1613 | 1/1   | 0.84 | 0.41 | 81,81,81,81                 | 0     |
| 56  | MG   | 1A    | 3895 | 1/1   | 0.84 | 0.22 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3637 | 1/1   | 0.84 | 0.18 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3245 | 1/1   | 0.84 | 0.19 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3641 | 1/1   | 0.84 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1623 | 1/1   | 0.84 | 0.38 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3047 | 1/1   | 0.84 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3496 | 1/1   | 0.84 | 0.16 | 81,81,81,81                 | 0     |
| 56  | MG   | 2A    | 3234 | 1/1   | 0.84 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3651 | 1/1   | 0.84 | 0.16 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1635 | 1/1   | 0.84 | 0.23 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3401 | 1/1   | 0.84 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3934 | 1/1   | 0.84 | 0.14 | 65,65,65,65                 | 0     |
| 56  | MG   | 2w    | 101  | 1/1   | 0.84 | 0.14 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1639 | 1/1   | 0.84 | 0.34 | 76,76,76,76                 | 0     |
| 56  | MG   | 2x    | 105  | 1/1   | 0.84 | 0.16 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3678 | 1/1   | 0.84 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3195 | 1/1   | 0.84 | 0.36 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 4043 | 1/1   | 0.84 | 0.17 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3431 | 1/1   | 0.85 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3382 | 1/1   | 0.85 | 0.31 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3252 | 1/1   | 0.85 | 0.20 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3088 | 1/1   | 0.85 | 0.34 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1659 | 1/1   | 0.85 | 0.22 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3699 | 1/1   | 0.85 | 0.19 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3733 | 1/1   | 0.85 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3260 | 1/1   | 0.85 | 0.19 | 80,80,80,80                 | 0     |
| 56  | MG   | 2A    | 3092 | 1/1   | 0.85 | 0.17 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1677 | 1/1   | 0.85 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1682 | 1/1   | 0.85 | 0.19 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1737 | 1/1   | 0.85 | 0.12 | 80,80,80,80                 | 0     |
| 56  | MG   | 2a    | 1688 | 1/1   | 0.85 | 0.36 | 72,72,72,72                 | 0     |
| 56  | MG   | 1a    | 1741 | 1/1   | 0.85 | 0.26 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3722 | 1/1   | 0.85 | 0.17 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 4051 | 1/1   | 0.85 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3499 | 1/1   | 0.85 | 0.20 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1696 | 1/1   | 0.85 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3968 | 1/1   | 0.85 | 0.11 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3503 | 1/1   | 0.85 | 0.16 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1699 | 1/1   | 0.85 | 0.18 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3845 | 1/1   | 0.85 | 0.16 | 75,75,75,75                 | 0     |
| 56  | MG   | 1a    | 1750 | 1/1   | 0.85 | 0.14 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3740 | 1/1   | 0.85 | 0.22 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3520 | 1/1   | 0.85 | 0.17 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1718 | 1/1   | 0.85 | 0.17 | 80,80,80,80                 | 0     |
| 56  | MG   | 2A    | 3752 | 1/1   | 0.85 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3423 | 1/1   | 0.85 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3976 | 1/1   | 0.85 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3120 | 1/1   | 0.85 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 4064 | 1/1   | 0.85 | 0.15 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3850 | 1/1   | 0.85 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3006 | 1/1   | 0.85 | 0.35 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3744 | 1/1   | 0.85 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3542 | 1/1   | 0.85 | 0.35 | 84,84,84,84                 | 0     |
| 56  | MG   | 2A    | 3309 | 1/1   | 0.85 | 0.33 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 4075 | 1/1   | 0.85 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3315 | 1/1   | 0.85 | 0.11 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3387 | 1/1   | 0.85 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3989 | 1/1   | 0.85 | 0.33 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3555 | 1/1   | 0.85 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1756 | 1/1   | 0.85 | 0.29 | 74,74,74,74                 | 0     |
| 56  | MG   | 2a    | 1762 | 1/1   | 0.85 | 0.19 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3556 | 1/1   | 0.85 | 0.24 | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1620 | 1/1   | 0.85 | 0.33 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3359 | 1/1   | 0.85 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3065 | 1/1   | 0.85 | 0.22 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3184 | 1/1   | 0.85 | 0.27 | 80,80,80,80                 | 0     |
| 56  | MG   | 1A    | 3181 | 1/1   | 0.85 | 0.24 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3596 | 1/1   | 0.85 | 0.20 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3797 | 1/1   | 0.85 | 0.09 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3410 | 1/1   | 0.85 | 0.34 | 75,75,75,75                 | 0     |
| 56  | MG   | 1x    | 106  | 1/1   | 0.85 | 0.25 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3578 | 1/1   | 0.85 | 0.33 | 63,63,63,63                 | 0     |
| 56  | MG   | 2F    | 303  | 1/1   | 0.85 | 0.33 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3580 | 1/1   | 0.85 | 0.34 | 62,62,62,62                 | 0     |
| 56  | MG   | 2W    | 201  | 1/1   | 0.85 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3005 | 1/1   | 0.85 | 0.15 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3200 | 1/1   | 0.85 | 0.20 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1660 | 1/1   | 0.85 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3353 | 1/1   | 0.85 | 0.29 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3291 | 1/1   | 0.85 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | 1B    | 211  | 1/1   | 0.85 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3360 | 1/1   | 0.85 | 0.14 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3470 | 1/1   | 0.85 | 0.38 | 69,69,69,69                 | 0     |
| 56  | MG   | 2a    | 1610 | 1/1   | 0.85 | 0.21 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3707 | 1/1   | 0.85 | 0.09 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1678 | 1/1   | 0.85 | 0.33 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3378 | 1/1   | 0.85 | 0.21 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3476 | 1/1   | 0.85 | 0.38 | 58,58,58,58                 | 0     |
| 56  | MG   | 1B    | 223  | 1/1   | 0.85 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1812 | 1/1   | 0.85 | 0.20 | 73,73,73,73                 | 0     |
| 56  | MG   | 2a    | 1619 | 1/1   | 0.85 | 0.18 | 79,79,79,79                 | 0     |
| 56  | MG   | 1A    | 3717 | 1/1   | 0.85 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3062 | 1/1   | 0.85 | 0.38 | 74,74,74,74                 | 0     |
| 56  | MG   | 2a    | 1821 | 1/1   | 0.85 | 0.32 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3230 | 1/1   | 0.85 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3831 | 1/1   | 0.85 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3398 | 1/1   | 0.85 | 0.12 | 71,71,71,71                 | 0     |
| 56  | MG   | 2a    | 1829 | 1/1   | 0.85 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3652 | 1/1   | 0.85 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1633 | 1/1   | 0.85 | 0.40 | 70,70,70,70                 | 0     |
| 56  | MG   | 2l    | 202  | 1/1   | 0.85 | 0.10 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3654 | 1/1   | 0.85 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3950 | 1/1   | 0.85 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3488 | 1/1   | 0.85 | 0.15 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 4042 | 1/1   | 0.85 | 0.07 | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 3233 | 1/1   | 0.85 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | 2w    | 102  | 1/1   | 0.85 | 0.21 | 83,83,83,83                 | 0     |
| 56  | MG   | 1D    | 311  | 1/1   | 0.85 | 0.25 | 42,42,42,42                 | 0     |
| 56  | MG   | 1E    | 309  | 1/1   | 0.85 | 0.22 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3426 | 1/1   | 0.85 | 0.23 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3247 | 1/1   | 0.85 | 0.30 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1648 | 1/1   | 0.85 | 0.26 | 80,80,80,80                 | 0     |
| 56  | MG   | 1A    | 3983 | 1/1   | 0.86 | 0.15 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3183 | 1/1   | 0.86 | 0.11 | 81,81,81,81                 | 0     |
| 56  | MG   | 1E    | 310  | 1/1   | 0.86 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3778 | 1/1   | 0.86 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 4063 | 1/1   | 0.86 | 0.12 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3505 | 1/1   | 0.86 | 0.17 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1700 | 1/1   | 0.86 | 0.10 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3208 | 1/1   | 0.86 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3582 | 1/1   | 0.86 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3584 | 1/1   | 0.86 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 4065 | 1/1   | 0.86 | 0.25 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3590 | 1/1   | 0.86 | 0.30 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3591 | 1/1   | 0.86 | 0.34 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 4068 | 1/1   | 0.86 | 0.29 | 65,65,65,65                 | 0     |
| 56  | MG   | 2B    | 202  | 1/1   | 0.86 | 0.17 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3906 | 1/1   | 0.86 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | 2a    | 1731 | 1/1   | 0.86 | 0.33 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3357 | 1/1   | 0.86 | 0.39 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3506 | 1/1   | 0.86 | 0.19 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3908 | 1/1   | 0.86 | 0.16 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3369 | 1/1   | 0.86 | 0.40 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3373 | 1/1   | 0.86 | 0.34 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3074 | 1/1   | 0.86 | 0.26 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3376 | 1/1   | 0.86 | 0.30 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3916 | 1/1   | 0.86 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | 1Z    | 302  | 1/1   | 0.86 | 0.08 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3231 | 1/1   | 0.86 | 0.20 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3999 | 1/1   | 0.86 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3385 | 1/1   | 0.86 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 4006 | 1/1   | 0.86 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1747 | 1/1   | 0.86 | 0.21 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3605 | 1/1   | 0.86 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1601 | 1/1   | 0.86 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3393 | 1/1   | 0.86 | 0.15 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3267 | 1/1   | 0.86 | 0.32 | 72,72,72,72                 | 0     |
| 56  | MG   | 1a    | 1601 | 1/1   | 0.86 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1757 | 1/1   | 0.86 | 0.16 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3246 | 1/1   | 0.86 | 0.16 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3516 | 1/1   | 0.86 | 0.20 | 82,82,82,82                 | 0     |
| 56  | MG   | 2a    | 1608 | 1/1   | 0.86 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3837 | 1/1   | 0.86 | 0.15 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3517 | 1/1   | 0.86 | 0.19 | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1621 | 1/1   | 0.86 | 0.30 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3944 | 1/1   | 0.86 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3428 | 1/1   | 0.86 | 0.23 | 76,76,76,76                 | 0     |
| 56  | MG   | 2a    | 1794 | 1/1   | 0.86 | 0.15 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3108 | 1/1   | 0.86 | 0.43 | 74,74,74,74                 | 0     |
| 56  | MG   | 2a    | 1617 | 1/1   | 0.86 | 0.23 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3403 | 1/1   | 0.86 | 0.16 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3947 | 1/1   | 0.86 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3668 | 1/1   | 0.86 | 0.15 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3115 | 1/1   | 0.86 | 0.25 | 88,88,88,88                 | 0     |
| 56  | MG   | 2A    | 3442 | 1/1   | 0.86 | 0.35 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1625 | 1/1   | 0.86 | 0.29 | 74,74,74,74                 | 0     |
| 56  | MG   | 1a    | 1636 | 1/1   | 0.86 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1789 | 1/1   | 0.86 | 0.35 | 82,82,82,82                 | 0     |
| 56  | MG   | 2a    | 1806 | 1/1   | 0.86 | 0.29 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3133 | 1/1   | 0.86 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3139 | 1/1   | 0.86 | 0.36 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3291 | 1/1   | 0.86 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3140 | 1/1   | 0.86 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1813 | 1/1   | 0.86 | 0.24 | 84,84,84,84                 | 0     |
| 56  | MG   | 1a    | 1638 | 1/1   | 0.86 | 0.27 | 70,70,70,70                 | 0     |
| 56  | MG   | 2a    | 1815 | 1/1   | 0.86 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3525 | 1/1   | 0.86 | 0.24 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1644 | 1/1   | 0.86 | 0.21 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3704 | 1/1   | 0.86 | 0.19 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3706 | 1/1   | 0.86 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | 1l    | 201  | 1/1   | 0.86 | 0.10 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3144 | 1/1   | 0.86 | 0.25 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3158 | 1/1   | 0.86 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3540 | 1/1   | 0.86 | 0.13 | 69,69,69,69                 | 0     |
| 56  | MG   | 2e    | 201  | 1/1   | 0.86 | 0.10 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3168 | 1/1   | 0.86 | 0.28 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3522 | 1/1   | 0.86 | 0.21 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3046 | 1/1   | 0.86 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1661 | 1/1   | 0.86 | 0.27 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3029 | 1/1   | 0.86 | 0.13 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3185 | 1/1   | 0.86 | 0.33 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3418 | 1/1   | 0.86 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3040 | 1/1   | 0.86 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3881 | 1/1   | 0.86 | 0.11 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3248 | 1/1   | 0.86 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3389 | 1/1   | 0.86 | 0.29 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3039 | 1/1   | 0.86 | 0.33 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3766 | 1/1   | 0.86 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | 1a    | 1755 | 1/1   | 0.87 | 0.26 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3311 | 1/1   | 0.87 | 0.34 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3312 | 1/1   | 0.87 | 0.26 | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1759 | 1/1   | 0.87 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | 13    | 104  | 1/1   | 0.87 | 0.23 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3605 | 1/1   | 0.87 | 0.26 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3606 | 1/1   | 0.87 | 0.16 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3341 | 1/1   | 0.87 | 0.16 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3610 | 1/1   | 0.87 | 0.14 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3611 | 1/1   | 0.87 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3997 | 1/1   | 0.87 | 0.09 | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3613 | 1/1   | 0.87 | 0.10 | 71,71,71,71                 | 0     |
| 56  | MG   | 1a    | 1762 | 1/1   | 0.87 | 0.14 | 67,67,67,67                 | 0     |
| 56  | MG   | 1a    | 1765 | 1/1   | 0.87 | 0.21 | 73,73,73,73                 | 0     |
| 56  | MG   | 15    | 108  | 1/1   | 0.87 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3450 | 1/1   | 0.87 | 0.23 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 4005 | 1/1   | 0.87 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3460 | 1/1   | 0.87 | 0.22 | 73,73,73,73                 | 0     |
| 56  | MG   | 1a    | 1604 | 1/1   | 0.87 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1617 | 1/1   | 0.87 | 0.20 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3657 | 1/1   | 0.87 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3363 | 1/1   | 0.87 | 0.19 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3189 | 1/1   | 0.87 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3365 | 1/1   | 0.87 | 0.19 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3366 | 1/1   | 0.87 | 0.26 | 72,72,72,72                 | 0     |
| 56  | MG   | 1a    | 1794 | 1/1   | 0.87 | 0.28 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1662 | 1/1   | 0.87 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3192 | 1/1   | 0.87 | 0.36 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3927 | 1/1   | 0.87 | 0.18 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3375 | 1/1   | 0.87 | 0.31 | 62,62,62,62                 | 0     |
| 56  | MG   | 1e    | 3100 | 1/1   | 0.87 | 0.12 | 76,76,76,76                 | 0     |
| 56  | MG   | 1a    | 1624 | 1/1   | 0.87 | 0.25 | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1678 | 1/1   | 0.87 | 0.20 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3661 | 1/1   | 0.87 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3315 | 1/1   | 0.87 | 0.37 | 75,75,75,75                 | 0     |
| 56  | MG   | 1n    | 101  | 1/1   | 0.87 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | 1n    | 102  | 1/1   | 0.87 | 0.23 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3406 | 1/1   | 0.87 | 0.29 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3387 | 1/1   | 0.87 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 4097 | 1/1   | 0.87 | 0.28 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3469 | 1/1   | 0.87 | 0.21 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3020 | 1/1   | 0.87 | 0.19 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3555 | 1/1   | 0.87 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 4022 | 1/1   | 0.87 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3397 | 1/1   | 0.87 | 0.18 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3572 | 1/1   | 0.87 | 0.17 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3706 | 1/1   | 0.87 | 0.25 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3405 | 1/1   | 0.87 | 0.18 | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1711 | 1/1   | 0.87 | 0.40 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3406 | 1/1   | 0.87 | 0.32 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3020 | 1/1   | 0.87 | 0.34 | 69,69,69,69                 | 0     |
| 56  | MG   | 2a    | 1721 | 1/1   | 0.87 | 0.30 | 84,84,84,84                 | 0     |
| 56  | MG   | 1A    | 3948 | 1/1   | 0.87 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3415 | 1/1   | 0.87 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3221 | 1/1   | 0.87 | 0.18 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3027 | 1/1   | 0.87 | 0.19 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3224 | 1/1   | 0.87 | 0.18 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3225 | 1/1   | 0.87 | 0.16 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3028 | 1/1   | 0.87 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3172 | 1/1   | 0.87 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3233 | 1/1   | 0.87 | 0.21 | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1742 | 1/1   | 0.87 | 0.35 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3036 | 1/1   | 0.87 | 0.16 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3733 | 1/1   | 0.87 | 0.11 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3735 | 1/1   | 0.87 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3956 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3434 | 1/1   | 0.87 | 0.16 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3437 | 1/1   | 0.87 | 0.19 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3574 | 1/1   | 0.87 | 0.15 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3447 | 1/1   | 0.87 | 0.29 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3575 | 1/1   | 0.87 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3764 | 1/1   | 0.87 | 0.35 | 86,86,86,86                 | 0     |
| 56  | MG   | 2A    | 3239 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3576 | 1/1   | 0.87 | 0.16 | 57,57,57,57                 | 0     |
| 56  | MG   | 1E    | 307  | 1/1   | 0.87 | 0.22 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3772 | 1/1   | 0.87 | 0.22 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3481 | 1/1   | 0.87 | 0.16 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3052 | 1/1   | 0.87 | 0.25 | 72,72,72,72                 | 0     |
| 56  | MG   | 2a    | 1775 | 1/1   | 0.87 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1778 | 1/1   | 0.87 | 0.34 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1780 | 1/1   | 0.87 | 0.18 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3004 | 1/1   | 0.87 | 0.09 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3786 | 1/1   | 0.87 | 0.18 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3495 | 1/1   | 0.87 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1684 | 1/1   | 0.87 | 0.24 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3104 | 1/1   | 0.87 | 0.33 | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1691 | 1/1   | 0.87 | 0.25 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3058 | 1/1   | 0.87 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1695 | 1/1   | 0.87 | 0.19 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3261 | 1/1   | 0.87 | 0.29 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3803 | 1/1   | 0.87 | 0.17 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3804 | 1/1   | 0.87 | 0.20 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3262 | 1/1   | 0.87 | 0.29 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1698 | 1/1   | 0.87 | 0.33 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3524 | 1/1   | 0.87 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3861 | 1/1   | 0.87 | 0.23 | 49,49,49,49                 | 0     |
| 56  | MG   | 1G    | 204  | 1/1   | 0.87 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1710 | 1/1   | 0.87 | 0.23 | 68,68,68,68                 | 0     |
| 56  | MG   | 2B    | 209  | 1/1   | 0.87 | 0.32 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3533 | 1/1   | 0.87 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3740 | 1/1   | 0.87 | 0.25 | 63,63,63,63                 | 0     |
| 56  | MG   | 2B    | 215  | 1/1   | 0.87 | 0.31 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3538 | 1/1   | 0.87 | 0.17 | 68,68,68,68                 | 0     |
| 56  | MG   | 1O    | 204  | 1/1   | 0.87 | 0.18 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3098 | 1/1   | 0.87 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3091 | 1/1   | 0.87 | 0.24 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3500 | 1/1   | 0.87 | 0.25 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1730 | 1/1   | 0.87 | 0.18 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1734 | 1/1   | 0.87 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1817 | 1/1   | 0.87 | 0.25 | 78,78,78,78                 | 0     |
| 56  | MG   | 2N    | 201  | 1/1   | 0.87 | 0.15 | 83,83,83,83                 | 0     |
| 56  | MG   | 2P    | 201  | 1/1   | 0.87 | 0.18 | 61,61,61,61                 | 0     |
| 56  | MG   | 2T    | 201  | 1/1   | 0.87 | 0.18 | 71,71,71,71                 | 0     |
| 56  | MG   | 1P    | 205  | 1/1   | 0.87 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | 2O    | 101  | 1/1   | 0.87 | 0.25 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3099 | 1/1   | 0.87 | 0.19 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1830 | 1/1   | 0.87 | 0.21 | 77,77,77,77                 | 0     |
| 56  | MG   | 1Q    | 204  | 1/1   | 0.87 | 0.15 | 72,72,72,72                 | 0     |
| 56  | MG   | 27    | 102  | 1/1   | 0.87 | 0.28 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3306 | 1/1   | 0.87 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | 1S    | 202  | 1/1   | 0.87 | 0.18 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3752 | 1/1   | 0.87 | 0.16 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3580 | 1/1   | 0.87 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | 1V    | 206  | 1/1   | 0.87 | 0.25 | 68,68,68,68                 | 0     |
| 56  | MG   | 2v    | 101  | 1/1   | 0.87 | 0.31 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3503 | 1/1   | 0.87 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3316 | 1/1   | 0.87 | 0.21 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3264 | 1/1   | 0.87 | 0.17 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3321 | 1/1   | 0.87 | 0.34 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3592 | 1/1   | 0.87 | 0.16 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3397 | 1/1   | 0.87 | 0.12 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 10    | 109  | 1/1   | 0.87 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1751 | 1/1   | 0.87 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | 1N    | 201  | 1/1   | 0.88 | 0.18 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3136 | 1/1   | 0.88 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1618 | 1/1   | 0.88 | 0.20 | 71,71,71,71                 | 0     |
| 56  | MG   | 1a    | 1743 | 1/1   | 0.88 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3471 | 1/1   | 0.88 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3144 | 1/1   | 0.88 | 0.21 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3614 | 1/1   | 0.88 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3407 | 1/1   | 0.88 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3479 | 1/1   | 0.88 | 0.25 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3205 | 1/1   | 0.88 | 0.14 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1627 | 1/1   | 0.88 | 0.29 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 4031 | 1/1   | 0.88 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3582 | 1/1   | 0.88 | 0.23 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3160 | 1/1   | 0.88 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3162 | 1/1   | 0.88 | 0.15 | 68,68,68,68                 | 0     |
| 56  | MG   | 1R    | 208  | 1/1   | 0.88 | 0.29 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3411 | 1/1   | 0.88 | 0.21 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3166 | 1/1   | 0.88 | 0.23 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3636 | 1/1   | 0.88 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3751 | 1/1   | 0.88 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3909 | 1/1   | 0.88 | 0.32 | 66,66,66,66                 | 0     |
| 56  | MG   | 1Y    | 201  | 1/1   | 0.88 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3642 | 1/1   | 0.88 | 0.15 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3372 | 1/1   | 0.88 | 0.24 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3911 | 1/1   | 0.88 | 0.13 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3914 | 1/1   | 0.88 | 0.10 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3143 | 1/1   | 0.88 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3920 | 1/1   | 0.88 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1661 | 1/1   | 0.88 | 0.44 | 74,74,74,74                 | 0     |
| 56  | MG   | 1a    | 1780 | 1/1   | 0.88 | 0.23 | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1663 | 1/1   | 0.88 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3657 | 1/1   | 0.88 | 0.09 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 4053 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3753 | 1/1   | 0.88 | 0.10 | 22,22,22,22                 | 0     |
| 56  | MG   | 2a    | 1674 | 1/1   | 0.88 | 0.25 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3001 | 1/1   | 0.88 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3782 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3669 | 1/1   | 0.88 | 0.15 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3286 | 1/1   | 0.88 | 0.16 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1685 | 1/1   | 0.88 | 0.14 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3935 | 1/1   | 0.88 | 0.15 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3675 | 1/1   | 0.88 | 0.15 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3054 | 1/1   | 0.88 | 0.13 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3202 | 1/1   | 0.88 | 0.25 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1691 | 1/1   | 0.88 | 0.41 | 73,73,73,73                 | 0     |
| 56  | MG   | 2a    | 1692 | 1/1   | 0.88 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1795 | 1/1   | 0.88 | 0.35 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3501 | 1/1   | 0.88 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3246 | 1/1   | 0.88 | 0.29 | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1611 | 1/1   | 0.88 | 0.29 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3401 | 1/1   | 0.88 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3210 | 1/1   | 0.88 | 0.18 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3622 | 1/1   | 0.88 | 0.16 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3103 | 1/1   | 0.88 | 0.33 | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1706 | 1/1   | 0.88 | 0.32 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3637 | 1/1   | 0.88 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3806 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3708 | 1/1   | 0.88 | 0.12 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1714 | 1/1   | 0.88 | 0.33 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1623 | 1/1   | 0.88 | 0.28 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3951 | 1/1   | 0.88 | 0.09 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3419 | 1/1   | 0.88 | 0.38 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3716 | 1/1   | 0.88 | 0.30 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3717 | 1/1   | 0.88 | 0.14 | 80,80,80,80                 | 0     |
| 56  | MG   | 1a    | 1626 | 1/1   | 0.88 | 0.32 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 4078 | 1/1   | 0.88 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1730 | 1/1   | 0.88 | 0.28 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3068 | 1/1   | 0.88 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | 1x    | 115  | 1/1   | 0.88 | 0.29 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3642 | 1/1   | 0.88 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3809 | 1/1   | 0.88 | 0.15 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3390 | 1/1   | 0.88 | 0.14 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3811 | 1/1   | 0.88 | 0.22 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3816 | 1/1   | 0.88 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1651 | 1/1   | 0.88 | 0.21 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1747 | 1/1   | 0.88 | 0.12 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3301 | 1/1   | 0.88 | 0.27 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3445 | 1/1   | 0.88 | 0.22 | 59,59,59,59                 | 0     |
| 56  | MG   | 1a    | 1654 | 1/1   | 0.88 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3453 | 1/1   | 0.88 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3762 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3454 | 1/1   | 0.88 | 0.25 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3398 | 1/1   | 0.88 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3458 | 1/1   | 0.88 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3241 | 1/1   | 0.88 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3243 | 1/1   | 0.88 | 0.16 | 80,80,80,80                 | 0     |
| 56  | MG   | 1a    | 1659 | 1/1   | 0.88 | 0.22 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3044 | 1/1   | 0.88 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3974 | 1/1   | 0.88 | 0.23 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 4095 | 1/1   | 0.88 | 0.24 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3788 | 1/1   | 0.88 | 0.13 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3489 | 1/1   | 0.88 | 0.22 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3673 | 1/1   | 0.88 | 0.19 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1663 | 1/1   | 0.88 | 0.30 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3053 | 1/1   | 0.88 | 0.16 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3256 | 1/1   | 0.88 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3519 | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3457 | 1/1   | 0.88 | 0.14 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3801 | 1/1   | 0.88 | 0.25 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3059 | 1/1   | 0.88 | 0.15 | 81,81,81,81                 | 0     |
| 56  | MG   | 1a    | 1674 | 1/1   | 0.88 | 0.31 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3808 | 1/1   | 0.88 | 0.12 | 74,74,74,74                 | 0     |
| 56  | MG   | 1B    | 215  | 1/1   | 0.88 | 0.23 | 64,64,64,64                 | 0     |
| 56  | MG   | 1B    | 218  | 1/1   | 0.88 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3458 | 1/1   | 0.88 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3459 | 1/1   | 0.88 | 0.27 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3690 | 1/1   | 0.88 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3277 | 1/1   | 0.88 | 0.24 | 74,74,74,74                 | 0     |
| 56  | MG   | 1a    | 1685 | 1/1   | 0.88 | 0.37 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3282 | 1/1   | 0.88 | 0.15 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3286 | 1/1   | 0.88 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | 2B    | 213  | 1/1   | 0.88 | 0.26 | 67,67,67,67                 | 0     |
| 56  | MG   | 1B    | 226  | 1/1   | 0.88 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3289 | 1/1   | 0.88 | 0.40 | 72,72,72,72                 | 0     |
| 56  | MG   | 1a    | 1689 | 1/1   | 0.88 | 0.33 | 63,63,63,63                 | 0     |
| 56  | MG   | 2E    | 301  | 1/1   | 0.88 | 0.29 | 73,73,73,73                 | 0     |
| 56  | MG   | 1B    | 227  | 1/1   | 0.88 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3528 | 1/1   | 0.88 | 0.30 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3551 | 1/1   | 0.88 | 0.20 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3529 | 1/1   | 0.88 | 0.33 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3399 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3853 | 1/1   | 0.88 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | 2O    | 201  | 1/1   | 0.88 | 0.25 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3304 | 1/1   | 0.88 | 0.41 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3855 | 1/1   | 0.88 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | 2V    | 201  | 1/1   | 0.88 | 0.34 | 54,54,54,54                 | 0     |
| 56  | MG   | 1D    | 308  | 1/1   | 0.88 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | 2X    | 101  | 1/1   | 0.88 | 0.12 | 77,77,77,77                 | 0     |
| 56  | MG   | 1a    | 1712 | 1/1   | 0.88 | 0.16 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3463 | 1/1   | 0.88 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3355 | 1/1   | 0.88 | 0.18 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3314 | 1/1   | 0.88 | 0.32 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3303 | 1/1   | 0.88 | 0.28 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3715 | 1/1   | 0.88 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3317 | 1/1   | 0.88 | 0.19 | 79,79,79,79                 | 0     |
| 56  | MG   | 2A    | 3318 | 1/1   | 0.88 | 0.18 | 85,85,85,85                 | 0     |
| 56  | MG   | 2t    | 201  | 1/1   | 0.88 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3869 | 1/1   | 0.88 | 0.16 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3872 | 1/1   | 0.88 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3257 | 1/1   | 0.88 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3324 | 1/1   | 0.88 | 0.27 | 70,70,70,70                 | 0     |
| 56  | MG   | 2w    | 103  | 1/1   | 0.88 | 0.14 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3114 | 1/1   | 0.88 | 0.16 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3362 | 1/1   | 0.88 | 0.24 | 64,64,64,64                 | 0     |
| 56  | MG   | 1F    | 313  | 1/1   | 0.88 | 0.23 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3125 | 1/1   | 0.88 | 0.16 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3263 | 1/1   | 0.88 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3021 | 1/1   | 0.89 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3025 | 1/1   | 0.89 | 0.31 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3726 | 1/1   | 0.89 | 0.19 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3179 | 1/1   | 0.89 | 0.20 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3525 | 1/1   | 0.89 | 0.28 | 67,67,67,67                 | 0     |
| 56  | MG   | 1U    | 203  | 1/1   | 0.89 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3207 | 1/1   | 0.89 | 0.10 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3531 | 1/1   | 0.89 | 0.20 | 73,73,73,73                 | 0     |
| 56  | MG   | 2a    | 1680 | 1/1   | 0.89 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | 1V    | 207  | 1/1   | 0.89 | 0.15 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1684 | 1/1   | 0.89 | 0.37 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3328 | 1/1   | 0.89 | 0.37 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3335 | 1/1   | 0.89 | 0.22 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3910 | 1/1   | 0.89 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3748 | 1/1   | 0.89 | 0.26 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3038 | 1/1   | 0.89 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 4083 | 1/1   | 0.89 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3308 | 1/1   | 0.89 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3761 | 1/1   | 0.89 | 0.13 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 10    | 106  | 1/1   | 0.89 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3545 | 1/1   | 0.89 | 0.18 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3204 | 1/1   | 0.89 | 0.16 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3344 | 1/1   | 0.89 | 0.13 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3550 | 1/1   | 0.89 | 0.16 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1717 | 1/1   | 0.89 | 0.16 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3595 | 1/1   | 0.89 | 0.28 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1705 | 1/1   | 0.89 | 0.16 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3048 | 1/1   | 0.89 | 0.22 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3915 | 1/1   | 0.89 | 0.11 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3475 | 1/1   | 0.89 | 0.25 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3558 | 1/1   | 0.89 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1712 | 1/1   | 0.89 | 0.28 | 74,74,74,74                 | 0     |
| 56  | MG   | 11    | 103  | 1/1   | 0.89 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3055 | 1/1   | 0.89 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3574 | 1/1   | 0.89 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1720 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3355 | 1/1   | 0.89 | 0.23 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3821 | 1/1   | 0.89 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3922 | 1/1   | 0.89 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1725 | 1/1   | 0.89 | 0.23 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3585 | 1/1   | 0.89 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1727 | 1/1   | 0.89 | 0.29 | 85,85,85,85                 | 0     |
| 56  | MG   | 1A    | 4092 | 1/1   | 0.89 | 0.20 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1729 | 1/1   | 0.89 | 0.44 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3060 | 1/1   | 0.89 | 0.25 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3285 | 1/1   | 0.89 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | 18    | 101  | 1/1   | 0.89 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 18    | 104  | 1/1   | 0.89 | 0.21 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3594 | 1/1   | 0.89 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 19    | 101  | 1/1   | 0.89 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | 2a    | 1740 | 1/1   | 0.89 | 0.31 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3069 | 1/1   | 0.89 | 0.18 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 4094 | 1/1   | 0.89 | 0.10 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3527 | 1/1   | 0.89 | 0.22 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3832 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | 1B    | 207  | 1/1   | 0.89 | 0.20 | 73,73,73,73                 | 0     |
| 56  | MG   | 2A    | 3084 | 1/1   | 0.89 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3609 | 1/1   | 0.89 | 0.22 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3382 | 1/1   | 0.89 | 0.35 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3608 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1612 | 1/1   | 0.89 | 0.14 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 4015 | 1/1   | 0.89 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3242 | 1/1   | 0.89 | 0.26 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3732 | 1/1   | 0.89 | 0.09 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3936 | 1/1   | 0.89 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3210 | 1/1   | 0.89 | 0.15 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3313 | 1/1   | 0.89 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 4026 | 1/1   | 0.89 | 0.16 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 4029 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3249 | 1/1   | 0.89 | 0.12 | 67,67,67,67                 | 0     |
| 56  | MG   | 2Q    | 203  | 1/1   | 0.89 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3400 | 1/1   | 0.89 | 0.30 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3250 | 1/1   | 0.89 | 0.17 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 4030 | 1/1   | 0.89 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 2W    | 203  | 1/1   | 0.89 | 0.28 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3631 | 1/1   | 0.89 | 0.11 | 68,68,68,68                 | 0     |
| 56  | MG   | 1a    | 1769 | 1/1   | 0.89 | 0.16 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1788 | 1/1   | 0.89 | 0.41 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3738 | 1/1   | 0.89 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3407 | 1/1   | 0.89 | 0.17 | 61,61,61,61                 | 0     |
| 56  | MG   | 25    | 103  | 1/1   | 0.89 | 0.22 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1793 | 1/1   | 0.89 | 0.21 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3494 | 1/1   | 0.89 | 0.09 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3410 | 1/1   | 0.89 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3259 | 1/1   | 0.89 | 0.11 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3640 | 1/1   | 0.89 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3106 | 1/1   | 0.89 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1779 | 1/1   | 0.89 | 0.13 | 81,81,81,81                 | 0     |
| 56  | MG   | 1A    | 3531 | 1/1   | 0.89 | 0.37 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1781 | 1/1   | 0.89 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3421 | 1/1   | 0.89 | 0.18 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3641 | 1/1   | 0.89 | 0.11 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3533 | 1/1   | 0.89 | 0.20 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3655 | 1/1   | 0.89 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | 1B    | 235  | 1/1   | 0.89 | 0.19 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3287 | 1/1   | 0.89 | 0.30 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3456 | 1/1   | 0.89 | 0.25 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3662 | 1/1   | 0.89 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3761 | 1/1   | 0.89 | 0.16 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3135 | 1/1   | 0.89 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3762 | 1/1   | 0.89 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3960 | 1/1   | 0.89 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3654 | 1/1   | 0.89 | 0.09 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3864 | 1/1   | 0.89 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3674 | 1/1   | 0.89 | 0.17 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3293 | 1/1   | 0.89 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1826 | 1/1   | 0.89 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 4058 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1629 | 1/1   | 0.89 | 0.11 | 93,93,93,93                 | 0     |
| 56  | MG   | 1A    | 3655 | 1/1   | 0.89 | 0.11 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3223 | 1/1   | 0.89 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1666 | 1/1   | 0.89 | 0.31 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3684 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3155 | 1/1   | 0.89 | 0.39 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3691 | 1/1   | 0.89 | 0.11 | 63,63,63,63                 | 0     |
| 56  | MG   | 2l    | 203  | 1/1   | 0.89 | 0.14 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3302 | 1/1   | 0.89 | 0.15 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3224 | 1/1   | 0.89 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1643 | 1/1   | 0.89 | 0.18 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3260 | 1/1   | 0.89 | 0.27 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3133 | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3337 | 1/1   | 0.89 | 0.21 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3340 | 1/1   | 0.89 | 0.30 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3344 | 1/1   | 0.89 | 0.26 | 55,55,55,55                 | 0     |
| 56  | MG   | 1x    | 114  | 1/1   | 0.89 | 0.18 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3508 | 1/1   | 0.89 | 0.27 | 41,41,41,41                 | 0     |
| 56  | MG   | 2x    | 104  | 1/1   | 0.89 | 0.34 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3062 | 1/1   | 0.89 | 0.34 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3013 | 1/1   | 0.89 | 0.34 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3468 | 1/1   | 0.89 | 0.19 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 4077 | 1/1   | 0.89 | 0.10 | 62,62,62,62                 | 0     |
| 58  | ZN   | 24    | 501  | 1/1   | 0.89 | 0.15 | 132,132,132,132             | 0     |
| 60  | K    | 2x    | 101  | 1/1   | 0.89 | 0.28 | 81,81,81,81                 | 0     |
| 56  | MG   | 2A    | 3174 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3182 | 1/1   | 0.90 | 0.22 | 67,67,67,67                 | 0     |
| 56  | MG   | 1S    | 201  | 1/1   | 0.90 | 0.34 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3004 | 1/1   | 0.90 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1675 | 1/1   | 0.90 | 0.34 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3187 | 1/1   | 0.90 | 0.19 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3541 | 1/1   | 0.90 | 0.10 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1688 | 1/1   | 0.90 | 0.35 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3332 | 1/1   | 0.90 | 0.18 | 71,71,71,71                 | 0     |
| 56  | MG   | 1S    | 203  | 1/1   | 0.90 | 0.08 | 73,73,73,73                 | 0     |
| 56  | MG   | 1a    | 1690 | 1/1   | 0.90 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3551 | 1/1   | 0.90 | 0.18 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3194 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3428 | 1/1   | 0.90 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3792 | 1/1   | 0.90 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3656 | 1/1   | 0.90 | 0.08 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3343 | 1/1   | 0.90 | 0.09 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3182 | 1/1   | 0.90 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3032 | 1/1   | 0.90 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1704 | 1/1   | 0.90 | 0.20 | 71,71,71,71                 | 0     |
| 56  | MG   | 2a    | 1695 | 1/1   | 0.90 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3554 | 1/1   | 0.90 | 0.18 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3660 | 1/1   | 0.90 | 0.09 | 27,27,27,27                 | 0     |
| 56  | MG   | 1a    | 1708 | 1/1   | 0.90 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3567 | 1/1   | 0.90 | 0.24 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3444 | 1/1   | 0.90 | 0.18 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3560 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3780 | 1/1   | 0.90 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3351 | 1/1   | 0.90 | 0.20 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3446 | 1/1   | 0.90 | 0.17 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3787 | 1/1   | 0.90 | 0.27 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1710 | 1/1   | 0.90 | 0.26 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3353 | 1/1   | 0.90 | 0.19 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3791 | 1/1   | 0.90 | 0.14 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3208 | 1/1   | 0.90 | 0.10 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3359 | 1/1   | 0.90 | 0.20 | 38,38,38,38                 | 0     |
| 56  | MG   | 1B    | 203  | 1/1   | 0.90 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3588 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3249 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3363 | 1/1   | 0.90 | 0.45 | 74,74,74,74                 | 0     |
| 56  | MG   | 1a    | 1731 | 1/1   | 0.90 | 0.24 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3314 | 1/1   | 0.90 | 0.18 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3802 | 1/1   | 0.90 | 0.17 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3367 | 1/1   | 0.90 | 0.30 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3254 | 1/1   | 0.90 | 0.18 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3805 | 1/1   | 0.90 | 0.29 | 74,74,74,74                 | 0     |
| 56  | MG   | 1B    | 213  | 1/1   | 0.90 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3819 | 1/1   | 0.90 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1740 | 1/1   | 0.90 | 0.14 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3227 | 1/1   | 0.90 | 0.21 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3053 | 1/1   | 0.90 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3462 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3232 | 1/1   | 0.90 | 0.12 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3829 | 1/1   | 0.90 | 0.09 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1746 | 1/1   | 0.90 | 0.14 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3607 | 1/1   | 0.90 | 0.31 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3515 | 1/1   | 0.90 | 0.11 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3710 | 1/1   | 0.90 | 0.14 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3386 | 1/1   | 0.90 | 0.45 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3076 | 1/1   | 0.90 | 0.21 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3587 | 1/1   | 0.90 | 0.14 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3078 | 1/1   | 0.90 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | 2E    | 305  | 1/1   | 0.90 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1760 | 1/1   | 0.90 | 0.15 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3035 | 1/1   | 0.90 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | 2F    | 301  | 1/1   | 0.90 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3082 | 1/1   | 0.90 | 0.16 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3194 | 1/1   | 0.90 | 0.34 | 42,42,42,42                 | 0     |
| 56  | MG   | 2F    | 304  | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3596 | 1/1   | 0.90 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3618 | 1/1   | 0.90 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3619 | 1/1   | 0.90 | 0.23 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 4044 | 1/1   | 0.90 | 0.12 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3727 | 1/1   | 0.90 | 0.12 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3333 | 1/1   | 0.90 | 0.11 | 63,63,63,63                 | 0     |
| 56  | MG   | 2T    | 203  | 1/1   | 0.90 | 0.26 | 65,65,65,65                 | 0     |
| 56  | MG   | 2U    | 201  | 1/1   | 0.90 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3626 | 1/1   | 0.90 | 0.16 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3627 | 1/1   | 0.90 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3844 | 1/1   | 0.90 | 0.27 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3295 | 1/1   | 0.90 | 0.11 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3226 | 1/1   | 0.90 | 0.18 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1763 | 1/1   | 0.90 | 0.21 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3416 | 1/1   | 0.90 | 0.19 | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1767 | 1/1   | 0.90 | 0.10 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3411 | 1/1   | 0.90 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1768 | 1/1   | 0.90 | 0.09 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3851 | 1/1   | 0.90 | 0.36 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3621 | 1/1   | 0.90 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1639 | 1/1   | 0.90 | 0.18 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1799 | 1/1   | 0.90 | 0.19 | 71,71,71,71                 | 0     |
| 56  | MG   | 1E    | 311  | 1/1   | 0.90 | 0.11 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3739 | 1/1   | 0.90 | 0.08 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3650 | 1/1   | 0.90 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3049 | 1/1   | 0.90 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | 2a    | 1609 | 1/1   | 0.90 | 0.41 | 77,77,77,77                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3110 | 1/1   | 0.90 | 0.49 | 77,77,77,77                 | 0     |
| 56  | MG   | 1E    | 318  | 1/1   | 0.90 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | 1F    | 311  | 1/1   | 0.90 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3275 | 1/1   | 0.90 | 0.36 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1810 | 1/1   | 0.90 | 0.13 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1653 | 1/1   | 0.90 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3198 | 1/1   | 0.90 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3635 | 1/1   | 0.90 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3435 | 1/1   | 0.90 | 0.31 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3422 | 1/1   | 0.90 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 1I    | 201  | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3307 | 1/1   | 0.90 | 0.22 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3865 | 1/1   | 0.90 | 0.19 | 39,39,39,39                 | 0     |
| 56  | MG   | 1d    | 301  | 1/1   | 0.90 | 0.15 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3168 | 1/1   | 0.90 | 0.25 | 39,39,39,39                 | 0     |
| 56  | MG   | 2a    | 1825 | 1/1   | 0.90 | 0.30 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3486 | 1/1   | 0.90 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3392 | 1/1   | 0.90 | 0.34 | 74,74,74,74                 | 0     |
| 56  | MG   | 2A    | 3678 | 1/1   | 0.90 | 0.20 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3459 | 1/1   | 0.90 | 0.31 | 65,65,65,65                 | 0     |
| 56  | MG   | 1m    | 3002 | 1/1   | 0.90 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3650 | 1/1   | 0.90 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3301 | 1/1   | 0.90 | 0.29 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3686 | 1/1   | 0.90 | 0.33 | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1672 | 1/1   | 0.90 | 0.26 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1638 | 1/1   | 0.90 | 0.40 | 78,78,78,78                 | 0     |
| 56  | MG   | 1r    | 101  | 1/1   | 0.90 | 0.30 | 69,69,69,69                 | 0     |
| 56  | MG   | 1Q    | 201  | 1/1   | 0.90 | 0.27 | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1642 | 1/1   | 0.90 | 0.33 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3159 | 1/1   | 0.90 | 0.23 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3778 | 1/1   | 0.90 | 0.08 | 69,69,69,69                 | 0     |
| 56  | MG   | 1R    | 202  | 1/1   | 0.90 | 0.33 | 64,64,64,64                 | 0     |
| 56  | MG   | 2v    | 103  | 1/1   | 0.90 | 0.26 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3310 | 1/1   | 0.90 | 0.20 | 72,72,72,72                 | 0     |
| 56  | MG   | 1R    | 205  | 1/1   | 0.90 | 0.26 | 58,58,58,58                 | 0     |
| 56  | MG   | 1x    | 107  | 1/1   | 0.90 | 0.22 | 71,71,71,71                 | 0     |
| 56  | MG   | 2a    | 1651 | 1/1   | 0.90 | 0.15 | 74,74,74,74                 | 0     |
| 56  | MG   | 2x    | 103  | 1/1   | 0.90 | 0.11 | 72,72,72,72                 | 0     |
| 56  | MG   | 1R    | 206  | 1/1   | 0.90 | 0.18 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3517 | 1/1   | 0.90 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3167 | 1/1   | 0.90 | 0.22 | 62,62,62,62                 | 0     |
| 56  | MG   | 1x    | 112  | 1/1   | 0.90 | 0.21 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1682 | 1/1   | 0.90 | 0.31 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3887 | 1/1   | 0.90 | 0.13 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3719 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1631 | 1/1   | 0.91 | 0.28 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1632 | 1/1   | 0.91 | 0.29 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3482 | 1/1   | 0.91 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | 1W    | 201  | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 4070 | 1/1   | 0.91 | 0.26 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3554 | 1/1   | 0.91 | 0.30 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3940 | 1/1   | 0.91 | 0.11 | 58,58,58,58                 | 0     |
| 56  | MG   | 10    | 102  | 1/1   | 0.91 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3676 | 1/1   | 0.91 | 0.21 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3266 | 1/1   | 0.91 | 0.31 | 74,74,74,74                 | 0     |
| 56  | MG   | 10    | 105  | 1/1   | 0.91 | 0.24 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3272 | 1/1   | 0.91 | 0.18 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3483 | 1/1   | 0.91 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3443 | 1/1   | 0.91 | 0.29 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3564 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3169 | 1/1   | 0.91 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3448 | 1/1   | 0.91 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3690 | 1/1   | 0.91 | 0.24 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3570 | 1/1   | 0.91 | 0.27 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3694 | 1/1   | 0.91 | 0.22 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1655 | 1/1   | 0.91 | 0.34 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3693 | 1/1   | 0.91 | 0.12 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3280 | 1/1   | 0.91 | 0.18 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3696 | 1/1   | 0.91 | 0.18 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3456 | 1/1   | 0.91 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3107 | 1/1   | 0.91 | 0.21 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3283 | 1/1   | 0.91 | 0.19 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3284 | 1/1   | 0.91 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3427 | 1/1   | 0.91 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3090 | 1/1   | 0.91 | 0.27 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3479 | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3710 | 1/1   | 0.91 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3713 | 1/1   | 0.91 | 0.14 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3480 | 1/1   | 0.91 | 0.26 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3952 | 1/1   | 0.91 | 0.09 | 69,69,69,69                 | 0     |
| 56  | MG   | 2a    | 1681 | 1/1   | 0.91 | 0.32 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3825 | 1/1   | 0.91 | 0.12 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3292 | 1/1   | 0.91 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3828 | 1/1   | 0.91 | 0.10 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3432 | 1/1   | 0.91 | 0.18 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3724 | 1/1   | 0.91 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3119 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3434 | 1/1   | 0.91 | 0.12 | 76,76,76,76                 | 0     |
| 56  | MG   | 2A    | 3727 | 1/1   | 0.91 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3234 | 1/1   | 0.91 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3512 | 1/1   | 0.91 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3126 | 1/1   | 0.91 | 0.19 | 78,78,78,78                 | 0     |
| 56  | MG   | 1a    | 1772 | 1/1   | 0.91 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3261 | 1/1   | 0.91 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3734 | 1/1   | 0.91 | 0.18 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3321 | 1/1   | 0.91 | 0.18 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3713 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3244 | 1/1   | 0.91 | 0.26 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3741 | 1/1   | 0.91 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | 2a    | 1703 | 1/1   | 0.91 | 0.31 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3356 | 1/1   | 0.91 | 0.16 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3744 | 1/1   | 0.91 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3747 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3141 | 1/1   | 0.91 | 0.18 | 63,63,63,63                 | 0     |
| 56  | MG   | 2a    | 1709 | 1/1   | 0.91 | 0.19 | 77,77,77,77                 | 0     |
| 56  | MG   | 1A    | 3975 | 1/1   | 0.91 | 0.10 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3311 | 1/1   | 0.91 | 0.09 | 63,63,63,63                 | 0     |
| 56  | MG   | 1B    | 202  | 1/1   | 0.91 | 0.31 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3719 | 1/1   | 0.91 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | 2a    | 1715 | 1/1   | 0.91 | 0.14 | 69,69,69,69                 | 0     |
| 56  | MG   | 1B    | 204  | 1/1   | 0.91 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3455 | 1/1   | 0.91 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3357 | 1/1   | 0.91 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3326 | 1/1   | 0.91 | 0.16 | 60,60,60,60                 | 0     |
| 56  | MG   | 1a    | 1627 | 1/1   | 0.91 | 0.30 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3849 | 1/1   | 0.91 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3543 | 1/1   | 0.91 | 0.20 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3593 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3779 | 1/1   | 0.91 | 0.12 | 69,69,69,69                 | 0     |
| 56  | MG   | 1B    | 216  | 1/1   | 0.91 | 0.09 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3731 | 1/1   | 0.91 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3785 | 1/1   | 0.91 | 0.18 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3992 | 1/1   | 0.91 | 0.13 | 66,66,66,66                 | 0     |
| 56  | MG   | 2a    | 1732 | 1/1   | 0.91 | 0.45 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3511 | 1/1   | 0.91 | 0.28 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1643 | 1/1   | 0.91 | 0.17 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3790 | 1/1   | 0.91 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3330 | 1/1   | 0.91 | 0.11 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3297 | 1/1   | 0.91 | 0.31 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1741 | 1/1   | 0.91 | 0.11 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3513 | 1/1   | 0.91 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3172 | 1/1   | 0.91 | 0.25 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3736 | 1/1   | 0.91 | 0.11 | 24,24,24,24                 | 0     |
| 56  | MG   | 2a    | 1746 | 1/1   | 0.91 | 0.15 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3176 | 1/1   | 0.91 | 0.18 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3339 | 1/1   | 0.91 | 0.26 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3737 | 1/1   | 0.91 | 0.11 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3360 | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3571 | 1/1   | 0.91 | 0.11 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3572 | 1/1   | 0.91 | 0.25 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3863 | 1/1   | 0.91 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | 2a    | 1759 | 1/1   | 0.91 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3579 | 1/1   | 0.91 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3806 | 1/1   | 0.91 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | 1B    | 231  | 1/1   | 0.91 | 0.09 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3581 | 1/1   | 0.91 | 0.11 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1767 | 1/1   | 0.91 | 0.11 | 72,72,72,72                 | 0     |
| 56  | MG   | 1x    | 108  | 1/1   | 0.91 | 0.34 | 76,76,76,76                 | 0     |
| 56  | MG   | 1a    | 1657 | 1/1   | 0.91 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3346 | 1/1   | 0.91 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3586 | 1/1   | 0.91 | 0.24 | 69,69,69,69                 | 0     |
| 56  | MG   | 2B    | 207  | 1/1   | 0.91 | 0.12 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3361 | 1/1   | 0.91 | 0.24 | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1777 | 1/1   | 0.91 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3093 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 56  | MG   | 2B    | 210  | 1/1   | 0.91 | 0.33 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 4010 | 1/1   | 0.91 | 0.10 | 64,64,64,64                 | 0     |
| 56  | MG   | 1D    | 302  | 1/1   | 0.91 | 0.22 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3003 | 1/1   | 0.91 | 0.24 | 57,57,57,57                 | 0     |
| 56  | MG   | 2B    | 214  | 1/1   | 0.91 | 0.29 | 67,67,67,67                 | 0     |
| 56  | MG   | 1D    | 304  | 1/1   | 0.91 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3330 | 1/1   | 0.91 | 0.26 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3870 | 1/1   | 0.91 | 0.20 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1668 | 1/1   | 0.91 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3019 | 1/1   | 0.91 | 0.19 | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1669 | 1/1   | 0.91 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3743 | 1/1   | 0.91 | 0.13 | 42,42,42,42                 | 0     |
| 56  | MG   | 2E    | 308  | 1/1   | 0.91 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3610 | 1/1   | 0.91 | 0.22 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3747 | 1/1   | 0.91 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3878 | 1/1   | 0.91 | 0.14 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3749 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3368 | 1/1   | 0.91 | 0.35 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3368 | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3120 | 1/1   | 0.91 | 0.16 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3131 | 1/1   | 0.91 | 0.10 | 65,65,65,65                 | 0     |
| 56  | MG   | 1F    | 310  | 1/1   | 0.91 | 0.17 | 55,55,55,55                 | 0     |
| 56  | MG   | 2R    | 201  | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 4027 | 1/1   | 0.91 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | 2T    | 202  | 1/1   | 0.91 | 0.12 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3042 | 1/1   | 0.91 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | 2T    | 204  | 1/1   | 0.91 | 0.22 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3756 | 1/1   | 0.91 | 0.13 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3897 | 1/1   | 0.91 | 0.17 | 70,70,70,70                 | 0     |
| 56  | MG   | 2V    | 202  | 1/1   | 0.91 | 0.18 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3414 | 1/1   | 0.91 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3335 | 1/1   | 0.91 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3372 | 1/1   | 0.91 | 0.25 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3384 | 1/1   | 0.91 | 0.24 | 57,57,57,57                 | 0     |
| 56  | MG   | 20    | 102  | 1/1   | 0.91 | 0.18 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3229 | 1/1   | 0.91 | 0.10 | 78,78,78,78                 | 0     |
| 56  | MG   | 2A    | 3621 | 1/1   | 0.91 | 0.22 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1823 | 1/1   | 0.91 | 0.32 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3770 | 1/1   | 0.91 | 0.11 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3051 | 1/1   | 0.91 | 0.18 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3388 | 1/1   | 0.91 | 0.31 | 63,63,63,63                 | 0     |
| 56  | MG   | 1O    | 203  | 1/1   | 0.91 | 0.20 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3774 | 1/1   | 0.91 | 0.13 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3777 | 1/1   | 0.91 | 0.12 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3375 | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 4045 | 1/1   | 0.91 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3912 | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | 2I    | 201  | 1/1   | 0.91 | 0.18 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3474 | 1/1   | 0.91 | 0.23 | 50,50,50,50                 | 0     |
| 56  | MG   | 1Q    | 205  | 1/1   | 0.91 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3027 | 1/1   | 0.91 | 0.23 | 82,82,82,82                 | 0     |
| 56  | MG   | 2A    | 3402 | 1/1   | 0.91 | 0.15 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3649 | 1/1   | 0.91 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3919 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3534 | 1/1   | 0.91 | 0.24 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3538 | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1729 | 1/1   | 0.91 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3250 | 1/1   | 0.91 | 0.15 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3230 | 1/1   | 0.91 | 0.10 | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1620 | 1/1   | 0.91 | 0.10 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3542 | 1/1   | 0.91 | 0.26 | 64,64,64,64                 | 0     |
| 56  | MG   | 1T    | 202  | 1/1   | 0.91 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3251 | 1/1   | 0.91 | 0.28 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3549 | 1/1   | 0.91 | 0.39 | 61,61,61,61                 | 0     |
| 56  | MG   | 1U    | 204  | 1/1   | 0.91 | 0.27 | 40,40,40,40                 | 0     |
| 56  | MG   | 1V    | 202  | 1/1   | 0.91 | 0.23 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3664 | 1/1   | 0.91 | 0.13 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3422 | 1/1   | 0.91 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3480 | 1/1   | 0.91 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3082 | 1/1   | 0.92 | 0.28 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3967 | 1/1   | 0.92 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1637 | 1/1   | 0.92 | 0.28 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3824 | 1/1   | 0.92 | 0.19 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3558 | 1/1   | 0.92 | 0.27 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3207 | 1/1   | 0.92 | 0.16 | 64,64,64,64                 | 0     |
| 56  | MG   | 1a    | 1640 | 1/1   | 0.92 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3392 | 1/1   | 0.92 | 0.13 | 62,62,62,62                 | 0     |
| 56  | MG   | 1x    | 111  | 1/1   | 0.92 | 0.17 | 37,37,37,37                 | 0     |
| 56  | MG   | 1B    | 219  | 1/1   | 0.92 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3691 | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3481 | 1/1   | 0.92 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3667 | 1/1   | 0.92 | 0.12 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3415 | 1/1   | 0.92 | 0.35 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3700 | 1/1   | 0.92 | 0.10 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3978 | 1/1   | 0.92 | 0.08 | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 3702 | 1/1   | 0.92 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3011 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1644 | 1/1   | 0.92 | 0.12 | 83,83,83,83                 | 0     |
| 56  | MG   | 2A    | 3223 | 1/1   | 0.92 | 0.17 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3568 | 1/1   | 0.92 | 0.13 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3704 | 1/1   | 0.92 | 0.07 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3226 | 1/1   | 0.92 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3056 | 1/1   | 0.92 | 0.27 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3485 | 1/1   | 0.92 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3274 | 1/1   | 0.92 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3683 | 1/1   | 0.92 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3364 | 1/1   | 0.92 | 0.23 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1656 | 1/1   | 0.92 | 0.18 | 82,82,82,82                 | 0     |
| 56  | MG   | 1A    | 3492 | 1/1   | 0.92 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3365 | 1/1   | 0.92 | 0.15 | 62,62,62,62                 | 0     |
| 56  | MG   | 2a    | 1660 | 1/1   | 0.92 | 0.09 | 59,59,59,59                 | 0     |
| 56  | MG   | 1a    | 1664 | 1/1   | 0.92 | 0.28 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3235 | 1/1   | 0.92 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3848 | 1/1   | 0.92 | 0.12 | 25,25,25,25                 | 0     |
| 56  | MG   | 2a    | 1666 | 1/1   | 0.92 | 0.34 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3714 | 1/1   | 0.92 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3366 | 1/1   | 0.92 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3037 | 1/1   | 0.92 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1672 | 1/1   | 0.92 | 0.19 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3697 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 4001 | 1/1   | 0.92 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3324 | 1/1   | 0.92 | 0.22 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3040 | 1/1   | 0.92 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3705 | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3041 | 1/1   | 0.92 | 0.23 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3149 | 1/1   | 0.92 | 0.19 | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1673 | 1/1   | 0.92 | 0.33 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3089 | 1/1   | 0.92 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1675 | 1/1   | 0.92 | 0.30 | 63,63,63,63                 | 0     |
| 56  | MG   | 1E    | 312  | 1/1   | 0.92 | 0.13 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3202 | 1/1   | 0.92 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3857 | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3451 | 1/1   | 0.92 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3452 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3289 | 1/1   | 0.92 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | 1a    | 1681 | 1/1   | 0.92 | 0.31 | 55,55,55,55                 | 0     |
| 56  | MG   | 1F    | 309  | 1/1   | 0.92 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3374 | 1/1   | 0.92 | 0.19 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3247 | 1/1   | 0.92 | 0.25 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3439 | 1/1   | 0.92 | 0.28 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3460 | 1/1   | 0.92 | 0.18 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3463 | 1/1   | 0.92 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1687 | 1/1   | 0.92 | 0.22 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3443 | 1/1   | 0.92 | 0.12 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3477 | 1/1   | 0.92 | 0.10 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3061 | 1/1   | 0.92 | 0.37 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3018 | 1/1   | 0.92 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3379 | 1/1   | 0.92 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3265 | 1/1   | 0.92 | 0.19 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3601 | 1/1   | 0.92 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3267 | 1/1   | 0.92 | 0.33 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3487 | 1/1   | 0.92 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3746 | 1/1   | 0.92 | 0.18 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3488 | 1/1   | 0.92 | 0.07 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3269 | 1/1   | 0.92 | 0.35 | 60,60,60,60                 | 0     |
| 56  | MG   | 1N    | 203  | 1/1   | 0.92 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3755 | 1/1   | 0.92 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3108 | 1/1   | 0.92 | 0.30 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3071 | 1/1   | 0.92 | 0.23 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3759 | 1/1   | 0.92 | 0.12 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 4025 | 1/1   | 0.92 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3505 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3506 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3765 | 1/1   | 0.92 | 0.16 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3509 | 1/1   | 0.92 | 0.11 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3002 | 1/1   | 0.92 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3608 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3451 | 1/1   | 0.92 | 0.21 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3079 | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3879 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3339 | 1/1   | 0.92 | 0.15 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3882 | 1/1   | 0.92 | 0.14 | 30,30,30,30                 | 0     |
| 56  | MG   | 1a    | 1713 | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3886 | 1/1   | 0.92 | 0.08 | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3288 | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 1R    | 201  | 1/1   | 0.92 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3290 | 1/1   | 0.92 | 0.11 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3789 | 1/1   | 0.92 | 0.17 | 69,69,69,69                 | 0     |
| 56  | MG   | 1a    | 1719 | 1/1   | 0.92 | 0.16 | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1720 | 1/1   | 0.92 | 0.20 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3616 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3294 | 1/1   | 0.92 | 0.19 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3888 | 1/1   | 0.92 | 0.08 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3620 | 1/1   | 0.92 | 0.16 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3541 | 1/1   | 0.92 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3252 | 1/1   | 0.92 | 0.14 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3341 | 1/1   | 0.92 | 0.23 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3896 | 1/1   | 0.92 | 0.26 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3253 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3393 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3347 | 1/1   | 0.92 | 0.29 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3760 | 1/1   | 0.92 | 0.08 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3123 | 1/1   | 0.92 | 0.19 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3807 | 1/1   | 0.92 | 0.13 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3124 | 1/1   | 0.92 | 0.24 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3764 | 1/1   | 0.92 | 0.08 | 34,34,34,34                 | 0     |
| 56  | MG   | 2a    | 1773 | 1/1   | 0.92 | 0.10 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3305 | 1/1   | 0.92 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3126 | 1/1   | 0.92 | 0.29 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3312 | 1/1   | 0.92 | 0.16 | 68,68,68,68                 | 0     |
| 56  | MG   | 1X    | 104  | 1/1   | 0.92 | 0.41 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1779 | 1/1   | 0.92 | 0.24 | 78,78,78,78                 | 0     |
| 56  | MG   | 1A    | 3771 | 1/1   | 0.92 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3117 | 1/1   | 0.92 | 0.28 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3564 | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3565 | 1/1   | 0.92 | 0.16 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3258 | 1/1   | 0.92 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3354 | 1/1   | 0.92 | 0.17 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3122 | 1/1   | 0.92 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | 1Z    | 303  | 1/1   | 0.92 | 0.23 | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1790 | 1/1   | 0.92 | 0.14 | 67,67,67,67                 | 0     |
| 56  | MG   | 1a    | 1752 | 1/1   | 0.92 | 0.14 | 77,77,77,77                 | 0     |
| 56  | MG   | 1a    | 1753 | 1/1   | 0.92 | 0.19 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3535 | 1/1   | 0.92 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3134 | 1/1   | 0.92 | 0.21 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3652 | 1/1   | 0.92 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | 2E    | 303  | 1/1   | 0.92 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3653 | 1/1   | 0.92 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | 2E    | 306  | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3259 | 1/1   | 0.92 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3329 | 1/1   | 0.92 | 0.35 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3790 | 1/1   | 0.92 | 0.13 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3932 | 1/1   | 0.92 | 0.11 | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3334 | 1/1   | 0.92 | 0.11 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3791 | 1/1   | 0.92 | 0.10 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3539 | 1/1   | 0.92 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | 13    | 103  | 1/1   | 0.92 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3309 | 1/1   | 0.92 | 0.28 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3149 | 1/1   | 0.92 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3795 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | 15    | 103  | 1/1   | 0.92 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1771 | 1/1   | 0.92 | 0.15 | 81,81,81,81                 | 0     |
| 56  | MG   | 1A    | 3409 | 1/1   | 0.92 | 0.19 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3658 | 1/1   | 0.92 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1776 | 1/1   | 0.92 | 0.14 | 78,78,78,78                 | 0     |
| 56  | MG   | 18    | 102  | 1/1   | 0.92 | 0.24 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3011 | 1/1   | 0.92 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | 2a    | 1818 | 1/1   | 0.92 | 0.21 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1819 | 1/1   | 0.92 | 0.25 | 65,65,65,65                 | 0     |
| 56  | MG   | 18    | 105  | 1/1   | 0.92 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3943 | 1/1   | 0.92 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | 2W    | 202  | 1/1   | 0.92 | 0.43 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3351 | 1/1   | 0.92 | 0.27 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3664 | 1/1   | 0.92 | 0.08 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3668 | 1/1   | 0.92 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3228 | 1/1   | 0.92 | 0.15 | 40,40,40,40                 | 0     |
| 56  | MG   | 20    | 104  | 1/1   | 0.92 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3017 | 1/1   | 0.92 | 0.20 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3949 | 1/1   | 0.92 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3175 | 1/1   | 0.92 | 0.21 | 68,68,68,68                 | 0     |
| 56  | MG   | 25    | 104  | 1/1   | 0.92 | 0.14 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3477 | 1/1   | 0.92 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3178 | 1/1   | 0.92 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3179 | 1/1   | 0.92 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | 1a    | 1614 | 1/1   | 0.92 | 0.18 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3364 | 1/1   | 0.92 | 0.28 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3623 | 1/1   | 0.92 | 0.28 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3140 | 1/1   | 0.92 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1796 | 1/1   | 0.92 | 0.15 | 72,72,72,72                 | 0     |
| 56  | MG   | 1a    | 1619 | 1/1   | 0.92 | 0.35 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3683 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | 1B    | 201  | 1/1   | 0.92 | 0.21 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3371 | 1/1   | 0.92 | 0.35 | 62,62,62,62                 | 0     |
| 56  | MG   | 1f    | 3101 | 1/1   | 0.92 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3191 | 1/1   | 0.92 | 0.11 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3812 | 1/1   | 0.92 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3813 | 1/1   | 0.92 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3684 | 1/1   | 0.92 | 0.17 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3685 | 1/1   | 0.92 | 0.09 | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3196 | 1/1   | 0.92 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3962 | 1/1   | 0.92 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1631 | 1/1   | 0.92 | 0.23 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3686 | 1/1   | 0.92 | 0.10 | 29,29,29,29                 | 0     |
| 56  | MG   | 1w    | 105  | 1/1   | 0.92 | 0.29 | 67,67,67,67                 | 0     |
| 56  | MG   | 2a    | 1652 | 1/1   | 0.93 | 0.13 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3519 | 1/1   | 0.93 | 0.20 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3643 | 1/1   | 0.93 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | 1U    | 202  | 1/1   | 0.93 | 0.23 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3440 | 1/1   | 0.93 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3442 | 1/1   | 0.93 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 4084 | 1/1   | 0.93 | 0.09 | 32,32,32,32                 | 0     |
| 56  | MG   | 1V    | 203  | 1/1   | 0.93 | 0.38 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3552 | 1/1   | 0.93 | 0.28 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3491 | 1/1   | 0.93 | 0.18 | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1696 | 1/1   | 0.93 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | 1a    | 1697 | 1/1   | 0.93 | 0.37 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3737 | 1/1   | 0.93 | 0.06 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3745 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1702 | 1/1   | 0.93 | 0.39 | 66,66,66,66                 | 0     |
| 56  | MG   | 1W    | 203  | 1/1   | 0.93 | 0.25 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3237 | 1/1   | 0.93 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 4089 | 1/1   | 0.93 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3969 | 1/1   | 0.93 | 0.17 | 66,66,66,66                 | 0     |
| 56  | MG   | 1Y    | 203  | 1/1   | 0.93 | 0.35 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3269 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1679 | 1/1   | 0.93 | 0.28 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3749 | 1/1   | 0.93 | 0.09 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3316 | 1/1   | 0.93 | 0.22 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3130 | 1/1   | 0.93 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | 2a    | 1683 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 56  | MG   | 10    | 104  | 1/1   | 0.93 | 0.18 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3858 | 1/1   | 0.93 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3447 | 1/1   | 0.93 | 0.08 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3209 | 1/1   | 0.93 | 0.37 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3449 | 1/1   | 0.93 | 0.17 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3402 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3162 | 1/1   | 0.93 | 0.35 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3054 | 1/1   | 0.93 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3557 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3452 | 1/1   | 0.93 | 0.09 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3050 | 1/1   | 0.93 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3986 | 1/1   | 0.93 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3775 | 1/1   | 0.93 | 0.07 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3777 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3561 | 1/1   | 0.93 | 0.11 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3361 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 56  | MG   | 1B    | 208  | 1/1   | 0.93 | 0.24 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3567 | 1/1   | 0.93 | 0.10 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3783 | 1/1   | 0.93 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | 1B    | 209  | 1/1   | 0.93 | 0.11 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3866 | 1/1   | 0.93 | 0.14 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3867 | 1/1   | 0.93 | 0.26 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3200 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3576 | 1/1   | 0.93 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3766 | 1/1   | 0.93 | 0.07 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3066 | 1/1   | 0.93 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1713 | 1/1   | 0.93 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3288 | 1/1   | 0.93 | 0.12 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3873 | 1/1   | 0.93 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1744 | 1/1   | 0.93 | 0.12 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3165 | 1/1   | 0.93 | 0.17 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3579 | 1/1   | 0.93 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3016 | 1/1   | 0.93 | 0.25 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3581 | 1/1   | 0.93 | 0.31 | 72,72,72,72                 | 0     |
| 56  | MG   | 1B    | 225  | 1/1   | 0.93 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | 2a    | 1724 | 1/1   | 0.93 | 0.36 | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1605 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3081 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3380 | 1/1   | 0.93 | 0.20 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3381 | 1/1   | 0.93 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3331 | 1/1   | 0.93 | 0.33 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3134 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1754 | 1/1   | 0.93 | 0.13 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3251 | 1/1   | 0.93 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3787 | 1/1   | 0.93 | 0.10 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3464 | 1/1   | 0.93 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | 2B    | 204  | 1/1   | 0.93 | 0.14 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3170 | 1/1   | 0.93 | 0.16 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3890 | 1/1   | 0.93 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3588 | 1/1   | 0.93 | 0.15 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3093 | 1/1   | 0.93 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3520 | 1/1   | 0.93 | 0.21 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3171 | 1/1   | 0.93 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3394 | 1/1   | 0.93 | 0.10 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3395 | 1/1   | 0.93 | 0.25 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3524 | 1/1   | 0.93 | 0.26 | 50,50,50,50                 | 0     |
| 56  | MG   | 2a    | 1750 | 1/1   | 0.93 | 0.12 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3338 | 1/1   | 0.93 | 0.20 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3253 | 1/1   | 0.93 | 0.18 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1628 | 1/1   | 0.93 | 0.21 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3219 | 1/1   | 0.93 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3298 | 1/1   | 0.93 | 0.22 | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1634 | 1/1   | 0.93 | 0.15 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3221 | 1/1   | 0.93 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1761 | 1/1   | 0.93 | 0.13 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3136 | 1/1   | 0.93 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 4028 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3622 | 1/1   | 0.93 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3607 | 1/1   | 0.93 | 0.08 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3079 | 1/1   | 0.93 | 0.10 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3711 | 1/1   | 0.93 | 0.15 | 37,37,37,37                 | 0     |
| 56  | MG   | 1E    | 315  | 1/1   | 0.93 | 0.20 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3063 | 1/1   | 0.93 | 0.36 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1772 | 1/1   | 0.93 | 0.22 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3416 | 1/1   | 0.93 | 0.31 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3629 | 1/1   | 0.93 | 0.12 | 77,77,77,77                 | 0     |
| 56  | MG   | 2A    | 3268 | 1/1   | 0.93 | 0.17 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1776 | 1/1   | 0.93 | 0.16 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3632 | 1/1   | 0.93 | 0.08 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 4036 | 1/1   | 0.93 | 0.07 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1645 | 1/1   | 0.93 | 0.21 | 70,70,70,70                 | 0     |
| 56  | MG   | 2R    | 202  | 1/1   | 0.93 | 0.24 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3271 | 1/1   | 0.93 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 2a    | 1782 | 1/1   | 0.93 | 0.23 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3087 | 1/1   | 0.93 | 0.13 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3424 | 1/1   | 0.93 | 0.19 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3123 | 1/1   | 0.93 | 0.23 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1650 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3615 | 1/1   | 0.93 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3276 | 1/1   | 0.93 | 0.23 | 58,58,58,58                 | 0     |
| 56  | MG   | 2A    | 3430 | 1/1   | 0.93 | 0.24 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3814 | 1/1   | 0.93 | 0.10 | 28,28,28,28                 | 0     |
| 56  | MG   | 2A    | 3648 | 1/1   | 0.93 | 0.13 | 35,35,35,35                 | 0     |
| 56  | MG   | 2W    | 205  | 1/1   | 0.93 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3649 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3278 | 1/1   | 0.93 | 0.23 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3148 | 1/1   | 0.93 | 0.22 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3817 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3281 | 1/1   | 0.93 | 0.29 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3718 | 1/1   | 0.93 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | 25    | 102  | 1/1   | 0.93 | 0.19 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3441 | 1/1   | 0.93 | 0.18 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3430 | 1/1   | 0.93 | 0.18 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3137 | 1/1   | 0.93 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | 28    | 101  | 1/1   | 0.93 | 0.33 | 61,61,61,61                 | 0     |
| 56  | MG   | 28    | 102  | 1/1   | 0.93 | 0.16 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3285 | 1/1   | 0.93 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1807 | 1/1   | 0.93 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3928 | 1/1   | 0.93 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3537 | 1/1   | 0.93 | 0.29 | 61,61,61,61                 | 0     |
| 56  | MG   | 1N    | 205  | 1/1   | 0.93 | 0.23 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3142 | 1/1   | 0.93 | 0.21 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3822 | 1/1   | 0.93 | 0.22 | 52,52,52,52                 | 0     |
| 56  | MG   | 1O    | 202  | 1/1   | 0.93 | 0.17 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3431 | 1/1   | 0.93 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3722 | 1/1   | 0.93 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3457 | 1/1   | 0.93 | 0.19 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3723 | 1/1   | 0.93 | 0.13 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3151 | 1/1   | 0.93 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3152 | 1/1   | 0.93 | 0.16 | 68,68,68,68                 | 0     |
| 56  | MG   | 2a    | 1614 | 1/1   | 0.93 | 0.22 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3462 | 1/1   | 0.93 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3724 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3464 | 1/1   | 0.93 | 0.14 | 75,75,75,75                 | 0     |
| 56  | MG   | 2A    | 3467 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3154 | 1/1   | 0.93 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3470 | 1/1   | 0.93 | 0.13 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3685 | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3474 | 1/1   | 0.93 | 0.16 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3626 | 1/1   | 0.93 | 0.06 | 42,42,42,42                 | 0     |
| 56  | MG   | 2d    | 301  | 1/1   | 0.93 | 0.41 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3629 | 1/1   | 0.93 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | 1x    | 104  | 1/1   | 0.93 | 0.25 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1671 | 1/1   | 0.93 | 0.15 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3161 | 1/1   | 0.93 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3633 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3262 | 1/1   | 0.93 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 1Q    | 207  | 1/1   | 0.93 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3165 | 1/1   | 0.93 | 0.17 | 71,71,71,71                 | 0     |
| 56  | MG   | 2A    | 3700 | 1/1   | 0.93 | 0.10 | 68,68,68,68                 | 0     |
| 56  | MG   | 1x    | 110  | 1/1   | 0.93 | 0.09 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3128 | 1/1   | 0.93 | 0.24 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3836 | 1/1   | 0.93 | 0.07 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3498 | 1/1   | 0.93 | 0.15 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3184 | 1/1   | 0.93 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3151 | 1/1   | 0.93 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3543 | 1/1   | 0.93 | 0.22 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3504 | 1/1   | 0.93 | 0.21 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3002 | 1/1   | 0.93 | 0.28 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3840 | 1/1   | 0.93 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3841 | 1/1   | 0.93 | 0.12 | 66,66,66,66                 | 0     |
| 56  | MG   | 1a    | 1683 | 1/1   | 0.93 | 0.32 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3843 | 1/1   | 0.93 | 0.11 | 24,24,24,24                 | 0     |
| 56  | MG   | 2A    | 3180 | 1/1   | 0.93 | 0.24 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3720 | 1/1   | 0.93 | 0.11 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3545 | 1/1   | 0.93 | 0.16 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 4002 | 1/1   | 0.94 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3745 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3532 | 1/1   | 0.94 | 0.08 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3328 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3105 | 1/1   | 0.94 | 0.15 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3107 | 1/1   | 0.94 | 0.31 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3611 | 1/1   | 0.94 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3370 | 1/1   | 0.94 | 0.37 | 68,68,68,68                 | 0     |
| 56  | MG   | 2A    | 3756 | 1/1   | 0.94 | 0.20 | 73,73,73,73                 | 0     |
| 56  | MG   | 1A    | 3893 | 1/1   | 0.94 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3612 | 1/1   | 0.94 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1607 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3760 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 1a    | 1610 | 1/1   | 0.94 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3613 | 1/1   | 0.94 | 0.14 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3239 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3241 | 1/1   | 0.94 | 0.35 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3900 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3768 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3901 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3569 | 1/1   | 0.94 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | 1B    | 236  | 1/1   | 0.94 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3902 | 1/1   | 0.94 | 0.11 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3774 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3031 | 1/1   | 0.94 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3112 | 1/1   | 0.94 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3381 | 1/1   | 0.94 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3625 | 1/1   | 0.94 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | 1E    | 303  | 1/1   | 0.94 | 0.15 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3437 | 1/1   | 0.94 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3336 | 1/1   | 0.94 | 0.11 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3101 | 1/1   | 0.94 | 0.16 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3818 | 1/1   | 0.94 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3587 | 1/1   | 0.94 | 0.16 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3150 | 1/1   | 0.94 | 0.19 | 37,37,37,37                 | 0     |
| 56  | MG   | 2a    | 1704 | 1/1   | 0.94 | 0.27 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3490 | 1/1   | 0.94 | 0.14 | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1775 | 1/1   | 0.94 | 0.08 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3255 | 1/1   | 0.94 | 0.21 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 4034 | 1/1   | 0.94 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3257 | 1/1   | 0.94 | 0.10 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3117 | 1/1   | 0.94 | 0.25 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 4038 | 1/1   | 0.94 | 0.18 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3091 | 1/1   | 0.94 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 1F    | 305  | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3122 | 1/1   | 0.94 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1783 | 1/1   | 0.94 | 0.09 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3601 | 1/1   | 0.94 | 0.20 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3729 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | 1a    | 1787 | 1/1   | 0.94 | 0.26 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3121 | 1/1   | 0.94 | 0.27 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3827 | 1/1   | 0.94 | 0.17 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3639 | 1/1   | 0.94 | 0.14 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3092 | 1/1   | 0.94 | 0.14 | 28,28,28,28                 | 0     |
| 56  | MG   | 1G    | 202  | 1/1   | 0.94 | 0.27 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3414 | 1/1   | 0.94 | 0.13 | 41,41,41,41                 | 0     |
| 56  | MG   | 2A    | 3129 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | 1G    | 203  | 1/1   | 0.94 | 0.08 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3343 | 1/1   | 0.94 | 0.22 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 4048 | 1/1   | 0.94 | 0.06 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 4049 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3396 | 1/1   | 0.94 | 0.30 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3735 | 1/1   | 0.94 | 0.08 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3423 | 1/1   | 0.94 | 0.20 | 63,63,63,63                 | 0     |
| 56  | MG   | 1N    | 206  | 1/1   | 0.94 | 0.21 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1738 | 1/1   | 0.94 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3563 | 1/1   | 0.94 | 0.11 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3647 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3427 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3047 | 1/1   | 0.94 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3499 | 1/1   | 0.94 | 0.16 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2a    | 1744 | 1/1   | 0.94 | 0.15 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 4060 | 1/1   | 0.94 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3941 | 1/1   | 0.94 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3448 | 1/1   | 0.94 | 0.22 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1667 | 1/1   | 0.94 | 0.20 | 63,63,63,63                 | 0     |
| 56  | MG   | 2E    | 304  | 1/1   | 0.94 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3150 | 1/1   | 0.94 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3299 | 1/1   | 0.94 | 0.15 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3436 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3166 | 1/1   | 0.94 | 0.21 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3438 | 1/1   | 0.94 | 0.32 | 65,65,65,65                 | 0     |
| 56  | MG   | 2a    | 1758 | 1/1   | 0.94 | 0.21 | 60,60,60,60                 | 0     |
| 56  | MG   | 2A    | 3440 | 1/1   | 0.94 | 0.33 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3167 | 1/1   | 0.94 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | 1x    | 105  | 1/1   | 0.94 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | 2F    | 307  | 1/1   | 0.94 | 0.24 | 49,49,49,49                 | 0     |
| 56  | MG   | 1Q    | 206  | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3156 | 1/1   | 0.94 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3157 | 1/1   | 0.94 | 0.13 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 4067 | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | 2Q    | 202  | 1/1   | 0.94 | 0.23 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3213 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3454 | 1/1   | 0.94 | 0.27 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3645 | 1/1   | 0.94 | 0.14 | 69,69,69,69                 | 0     |
| 56  | MG   | 2A    | 3646 | 1/1   | 0.94 | 0.18 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3509 | 1/1   | 0.94 | 0.50 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3750 | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 56  | MG   | 1R    | 207  | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3214 | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3303 | 1/1   | 0.94 | 0.34 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3653 | 1/1   | 0.94 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3216 | 1/1   | 0.94 | 0.21 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3955 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3001 | 1/1   | 0.94 | 0.25 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3034 | 1/1   | 0.94 | 0.22 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3659 | 1/1   | 0.94 | 0.10 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3308 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3220 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3669 | 1/1   | 0.94 | 0.12 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3095 | 1/1   | 0.94 | 0.21 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3173 | 1/1   | 0.94 | 0.23 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3471 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3472 | 1/1   | 0.94 | 0.11 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3473 | 1/1   | 0.94 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3129 | 1/1   | 0.94 | 0.21 | 57,57,57,57                 | 0     |
| 56  | MG   | 27    | 103  | 1/1   | 0.94 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3672 | 1/1   | 0.94 | 0.11 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3964 | 1/1   | 0.94 | 0.15 | 66,66,66,66                 | 0     |
| 56  | MG   | 28    | 103  | 1/1   | 0.94 | 0.32 | 56,56,56,56                 | 0     |
| 56  | MG   | 1U    | 209  | 1/1   | 0.94 | 0.19 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3177 | 1/1   | 0.94 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3016 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3060 | 1/1   | 0.94 | 0.15 | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3319 | 1/1   | 0.94 | 0.37 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3083 | 1/1   | 0.94 | 0.20 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3522 | 1/1   | 0.94 | 0.31 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3486 | 1/1   | 0.94 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3022 | 1/1   | 0.94 | 0.17 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3061 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3102 | 1/1   | 0.94 | 0.05 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3492 | 1/1   | 0.94 | 0.25 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3495 | 1/1   | 0.94 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3689 | 1/1   | 0.94 | 0.20 | 71,71,71,71                 | 0     |
| 56  | MG   | 1A    | 3320 | 1/1   | 0.94 | 0.08 | 51,51,51,51                 | 0     |
| 56  | MG   | 1W    | 204  | 1/1   | 0.94 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 1X    | 102  | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3500 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3776 | 1/1   | 0.94 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 1X    | 105  | 1/1   | 0.94 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3231 | 1/1   | 0.94 | 0.20 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3698 | 1/1   | 0.94 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3333 | 1/1   | 0.94 | 0.18 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3322 | 1/1   | 0.94 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | 1a    | 1707 | 1/1   | 0.94 | 0.30 | 70,70,70,70                 | 0     |
| 56  | MG   | 1A    | 3780 | 1/1   | 0.94 | 0.06 | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1709 | 1/1   | 0.94 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3515 | 1/1   | 0.94 | 0.12 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3868 | 1/1   | 0.94 | 0.22 | 35,35,35,35                 | 0     |
| 56  | MG   | 1a    | 1711 | 1/1   | 0.94 | 0.17 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3025 | 1/1   | 0.94 | 0.20 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3692 | 1/1   | 0.94 | 0.10 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3871 | 1/1   | 0.94 | 0.16 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3785 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | 2f    | 202  | 1/1   | 0.94 | 0.10 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3523 | 1/1   | 0.94 | 0.09 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3693 | 1/1   | 0.94 | 0.10 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 3600 | 1/1   | 0.94 | 0.10 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3718 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3526 | 1/1   | 0.94 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | 2q    | 201  | 1/1   | 0.94 | 0.36 | 74,74,74,74                 | 0     |
| 56  | MG   | 1A    | 3988 | 1/1   | 0.94 | 0.08 | 18,18,18,18                 | 0     |
| 56  | MG   | 1A    | 3696 | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 56  | MG   | 1B    | 210  | 1/1   | 0.94 | 0.11 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3272 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | 1l    | 105  | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3604 | 1/1   | 0.94 | 0.08 | 29,29,29,29                 | 0     |
| 56  | MG   | 2A    | 3537 | 1/1   | 0.94 | 0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1732 | 1/1   | 0.94 | 0.20 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3214 | 1/1   | 0.94 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1733 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | 2x    | 102  | 1/1   | 0.94 | 0.28 | 72,72,72,72                 | 0     |
| 56  | MG   | 2A    | 3216 | 1/1   | 0.94 | 0.21 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3793 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | 1B    | 214  | 1/1   | 0.94 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3022 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3883 | 1/1   | 0.94 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3885 | 1/1   | 0.94 | 0.08 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3279 | 1/1   | 0.94 | 0.13 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3548 | 1/1   | 0.94 | 0.10 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3823 | 1/1   | 0.95 | 0.28 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 3996 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3769 | 1/1   | 0.95 | 0.06 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3421 | 1/1   | 0.95 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1673 | 1/1   | 0.95 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3188 | 1/1   | 0.95 | 0.28 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3386 | 1/1   | 0.95 | 0.10 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3597 | 1/1   | 0.95 | 0.09 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3325 | 1/1   | 0.95 | 0.18 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 4003 | 1/1   | 0.95 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3776 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3903 | 1/1   | 0.95 | 0.20 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3681 | 1/1   | 0.95 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | 1y    | 101  | 1/1   | 0.95 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3544 | 1/1   | 0.95 | 0.16 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1693 | 1/1   | 0.95 | 0.19 | 44,44,44,44                 | 0     |
| 56  | MG   | 1Z    | 301  | 1/1   | 0.95 | 0.20 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3784 | 1/1   | 0.95 | 0.12 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3191 | 1/1   | 0.95 | 0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | 1B    | 217  | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3007 | 1/1   | 0.95 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | 1A    | 4009 | 1/1   | 0.95 | 0.09 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3504 | 1/1   | 0.95 | 0.24 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3005 | 1/1   | 0.95 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3300 | 1/1   | 0.95 | 0.09 | 76,76,76,76                 | 0     |
| 56  | MG   | 1A    | 3754 | 1/1   | 0.95 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3152 | 1/1   | 0.95 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3913 | 1/1   | 0.95 | 0.06 | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1706 | 1/1   | 0.95 | 0.34 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3796 | 1/1   | 0.95 | 0.07 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3300 | 1/1   | 0.95 | 0.13 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3023 | 1/1   | 0.95 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3799 | 1/1   | 0.95 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3449 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3197 | 1/1   | 0.95 | 0.29 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3510 | 1/1   | 0.95 | 0.26 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3917 | 1/1   | 0.95 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3302 | 1/1   | 0.95 | 0.41 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3030 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | 2A    | 3031 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3618 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 56  | MG   | 1B    | 232  | 1/1   | 0.95 | 0.10 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3842 | 1/1   | 0.95 | 0.19 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3183 | 1/1   | 0.95 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 3100 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 56  | MG   | 17    | 105  | 1/1   | 0.95 | 0.11 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1717 | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3925 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3465 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3466 | 1/1   | 0.95 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3767 | 1/1   | 0.95 | 0.10 | 23,23,23,23                 | 0     |
| 56  | MG   | 1a    | 1722 | 1/1   | 0.95 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3639 | 1/1   | 0.95 | 0.06 | 61,61,61,61                 | 0     |
| 56  | MG   | 1D    | 301  | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3323 | 1/1   | 0.95 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3768 | 1/1   | 0.95 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | 18    | 106  | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3045 | 1/1   | 0.95 | 0.15 | 37,37,37,37                 | 0     |
| 56  | MG   | 2D    | 301  | 1/1   | 0.95 | 0.18 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2D    | 302  | 1/1   | 0.95 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3930 | 1/1   | 0.95 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | 2D    | 305  | 1/1   | 0.95 | 0.32 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3476 | 1/1   | 0.95 | 0.11 | 33,33,33,33                 | 0     |
| 56  | MG   | 2a    | 1736 | 1/1   | 0.95 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3435 | 1/1   | 0.95 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | 1D    | 309  | 1/1   | 0.95 | 0.13 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3565 | 1/1   | 0.95 | 0.30 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3331 | 1/1   | 0.95 | 0.12 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3050 | 1/1   | 0.95 | 0.08 | 65,65,65,65                 | 0     |
| 56  | MG   | 2A    | 3482 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3566 | 1/1   | 0.95 | 0.17 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 4037 | 1/1   | 0.95 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | 1a    | 1606 | 1/1   | 0.95 | 0.32 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3775 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3658 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | 2a    | 1748 | 1/1   | 0.95 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | 1A    | 4039 | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 56  | MG   | 2F    | 305  | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 2a    | 1751 | 1/1   | 0.95 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | 2F    | 306  | 1/1   | 0.95 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3056 | 1/1   | 0.95 | 0.06 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3490 | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3436 | 1/1   | 0.95 | 0.23 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3938 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3852 | 1/1   | 0.95 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 2Q    | 201  | 1/1   | 0.95 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 2A    | 3497 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 1a    | 1616 | 1/1   | 0.95 | 0.05 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3627 | 1/1   | 0.95 | 0.07 | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3670 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | 2a    | 1764 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1765 | 1/1   | 0.95 | 0.12 | 80,80,80,80                 | 0     |
| 56  | MG   | 1A    | 3628 | 1/1   | 0.95 | 0.08 | 23,23,23,23                 | 0     |
| 56  | MG   | 1E    | 316  | 1/1   | 0.95 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3225 | 1/1   | 0.95 | 0.20 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3632 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3348 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3273 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3859 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3511 | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1625 | 1/1   | 0.95 | 0.10 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3218 | 1/1   | 0.95 | 0.16 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3514 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3709 | 1/1   | 0.95 | 0.05 | 16,16,16,16                 | 0     |
| 56  | MG   | 2A    | 3220 | 1/1   | 0.95 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3160 | 1/1   | 0.95 | 0.22 | 36,36,36,36                 | 0     |
| 56  | MG   | 20    | 103  | 1/1   | 0.95 | 0.23 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3201 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1629 | 1/1   | 0.95 | 0.23 | 74,74,74,74                 | 0     |
| 56  | MG   | 23    | 101  | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3358 | 1/1   | 0.95 | 0.34 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3521 | 1/1   | 0.95 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3478 | 1/1   | 0.95 | 0.10 | 61,61,61,61                 | 0     |
| 56  | MG   | 2a    | 1787 | 1/1   | 0.95 | 0.31 | 65,65,65,65                 | 0     |
| 56  | MG   | 1a    | 1633 | 1/1   | 0.95 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | 27    | 101  | 1/1   | 0.95 | 0.29 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3281 | 1/1   | 0.95 | 0.29 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3953 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3954 | 1/1   | 0.95 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3640 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 56  | MG   | 1N    | 202  | 1/1   | 0.95 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3087 | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3367 | 1/1   | 0.95 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3405 | 1/1   | 0.95 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | 2A    | 3703 | 1/1   | 0.95 | 0.10 | 69,69,69,69                 | 0     |
| 56  | MG   | 1A    | 3142 | 1/1   | 0.95 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3801 | 1/1   | 0.95 | 0.33 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3163 | 1/1   | 0.95 | 0.23 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3015 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1647 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1648 | 1/1   | 0.95 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3648 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3711 | 1/1   | 0.95 | 0.07 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3712 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3805 | 1/1   | 0.95 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3069 | 1/1   | 0.95 | 0.16 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3102 | 1/1   | 0.95 | 0.17 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3103 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3876 | 1/1   | 0.95 | 0.08 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3549 | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1784 | 1/1   | 0.95 | 0.08 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3877 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3721 | 1/1   | 0.95 | 0.25 | 80,80,80,80                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3725 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3132 | 1/1   | 0.95 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3972 | 1/1   | 0.95 | 0.07 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3973 | 1/1   | 0.95 | 0.10 | 61,61,61,61                 | 0     |
| 56  | MG   | 1a    | 1792 | 1/1   | 0.95 | 0.13 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3113 | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 4082 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | 2a    | 1824 | 1/1   | 0.95 | 0.16 | 72,72,72,72                 | 0     |
| 56  | MG   | 1A    | 3489 | 1/1   | 0.95 | 0.34 | 55,55,55,55                 | 0     |
| 56  | MG   | 1R    | 203  | 1/1   | 0.95 | 0.25 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3118 | 1/1   | 0.95 | 0.08 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3562 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3373 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 56  | MG   | 2A    | 3736 | 1/1   | 0.95 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3346 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3738 | 1/1   | 0.95 | 0.08 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3884 | 1/1   | 0.95 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | 2f    | 201  | 1/1   | 0.95 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | 2a    | 1640 | 1/1   | 0.95 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | 1A    | 3589 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3981 | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3591 | 1/1   | 0.95 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3290 | 1/1   | 0.95 | 0.23 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3573 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3235 | 1/1   | 0.95 | 0.23 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3575 | 1/1   | 0.95 | 0.16 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3536 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3041 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | 2a    | 1650 | 1/1   | 0.95 | 0.31 | 62,62,62,62                 | 0     |
| 56  | MG   | 2A    | 3750 | 1/1   | 0.95 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3891 | 1/1   | 0.95 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3753 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | 1w    | 101  | 1/1   | 0.95 | 0.07 | 48,48,48,48                 | 0     |
| 56  | MG   | 1w    | 102  | 1/1   | 0.95 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3597 | 1/1   | 0.95 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | 2A    | 3138 | 1/1   | 0.95 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | 1U    | 206  | 1/1   | 0.95 | 0.20 | 43,43,43,43                 | 0     |
| 56  | MG   | 1U    | 207  | 1/1   | 0.95 | 0.32 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3990 | 1/1   | 0.95 | 0.08 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3666 | 1/1   | 0.95 | 0.06 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3238 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 56  | MG   | 2a    | 1664 | 1/1   | 0.95 | 0.21 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | ZN   | 14    | 102  | 1/1   | 0.95 | 0.10 | 111,111,111,111             | 0     |
| 56  | MG   | 2a    | 1665 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 60  | K    | 1x    | 101  | 1/1   | 0.95 | 0.29 | 75,75,75,75                 | 0     |
| 56  | MG   | 1A    | 3113 | 1/1   | 0.95 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3124 | 1/1   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3675 | 1/1   | 0.96 | 0.07 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3439 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3076 | 1/1   | 0.96 | 0.19 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3128 | 1/1   | 0.96 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3119 | 1/1   | 0.96 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | 1a    | 1646 | 1/1   | 0.96 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3317 | 1/1   | 0.96 | 0.24 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3446 | 1/1   | 0.96 | 0.16 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3318 | 1/1   | 0.96 | 0.08 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 4066 | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3957 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 56  | MG   | 2a    | 1702 | 1/1   | 0.96 | 0.10 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3450 | 1/1   | 0.96 | 0.10 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3772 | 1/1   | 0.96 | 0.05 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3077 | 1/1   | 0.96 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3473 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | 1Q    | 203  | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 56  | MG   | 1a    | 1655 | 1/1   | 0.96 | 0.20 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3961 | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3599 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 56  | MG   | 1a    | 1658 | 1/1   | 0.96 | 0.11 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3963 | 1/1   | 0.96 | 0.19 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3420 | 1/1   | 0.96 | 0.20 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3148 | 1/1   | 0.96 | 0.06 | 55,55,55,55                 | 0     |
| 56  | MG   | 1w    | 103  | 1/1   | 0.96 | 0.13 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3121 | 1/1   | 0.96 | 0.32 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3602 | 1/1   | 0.96 | 0.12 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3781 | 1/1   | 0.96 | 0.04 | 47,47,47,47                 | 0     |
| 56  | MG   | 2a    | 1719 | 1/1   | 0.96 | 0.19 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3603 | 1/1   | 0.96 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3078 | 1/1   | 0.96 | 0.11 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3271 | 1/1   | 0.96 | 0.17 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3227 | 1/1   | 0.96 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3695 | 1/1   | 0.96 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3032 | 1/1   | 0.96 | 0.21 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3185 | 1/1   | 0.96 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3277 | 1/1   | 0.96 | 0.11 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3701 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3880 | 1/1   | 0.96 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3153 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3154 | 1/1   | 0.96 | 0.23 | 41,41,41,41                 | 0     |
| 56  | MG   | 1U    | 205  | 1/1   | 0.96 | 0.16 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3796 | 1/1   | 0.96 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3189 | 1/1   | 0.96 | 0.19 | 36,36,36,36                 | 0     |
| 56  | MG   | 2a    | 1735 | 1/1   | 0.96 | 0.38 | 57,57,57,57                 | 0     |
| 56  | MG   | 1U    | 208  | 1/1   | 0.96 | 0.23 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3433 | 1/1   | 0.96 | 0.09 | 64,64,64,64                 | 0     |
| 56  | MG   | 1U    | 210  | 1/1   | 0.96 | 0.40 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 4096 | 1/1   | 0.96 | 0.08 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3487 | 1/1   | 0.96 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | 2A    | 3008 | 1/1   | 0.96 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3377 | 1/1   | 0.96 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3491 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3617 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3157 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3380 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | 2R    | 203  | 1/1   | 0.96 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3017 | 1/1   | 0.96 | 0.07 | 58,58,58,58                 | 0     |
| 56  | MG   | 1B    | 205  | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3181 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3547 | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3501 | 1/1   | 0.96 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3712 | 1/1   | 0.96 | 0.10 | 53,53,53,53                 | 0     |
| 56  | MG   | 1a    | 1692 | 1/1   | 0.96 | 0.23 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3548 | 1/1   | 0.96 | 0.16 | 34,34,34,34                 | 0     |
| 56  | MG   | 1X    | 107  | 1/1   | 0.96 | 0.10 | 59,59,59,59                 | 0     |
| 56  | MG   | 2a    | 1757 | 1/1   | 0.96 | 0.06 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3193 | 1/1   | 0.96 | 0.43 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3550 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3510 | 1/1   | 0.96 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3236 | 1/1   | 0.96 | 0.19 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3029 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3493 | 1/1   | 0.96 | 0.30 | 45,45,45,45                 | 0     |
| 56  | MG   | 1a    | 1700 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3694 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 4000 | 1/1   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3033 | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3080 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | 10    | 101  | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3630 | 1/1   | 0.96 | 0.11 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3159 | 1/1   | 0.96 | 0.15 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3196 | 1/1   | 0.96 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3201 | 1/1   | 0.96 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3556 | 1/1   | 0.96 | 0.16 | 35,35,35,35                 | 0     |
| 56  | MG   | 1B    | 220  | 1/1   | 0.96 | 0.08 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3388 | 1/1   | 0.96 | 0.38 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3527 | 1/1   | 0.96 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3636 | 1/1   | 0.96 | 0.09 | 17,17,17,17                 | 0     |
| 56  | MG   | 1A    | 3561 | 1/1   | 0.96 | 0.28 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3081 | 1/1   | 0.96 | 0.20 | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1715 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3019 | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | 12    | 101  | 1/1   | 0.96 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | 12    | 102  | 1/1   | 0.96 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | 13    | 102  | 1/1   | 0.96 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3043 | 1/1   | 0.96 | 0.13 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3826 | 1/1   | 0.96 | 0.06 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3086 | 1/1   | 0.96 | 0.23 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1726 | 1/1   | 0.96 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3044 | 1/1   | 0.96 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | 15    | 104  | 1/1   | 0.96 | 0.21 | 44,44,44,44                 | 0     |
| 56  | MG   | 15    | 106  | 1/1   | 0.96 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3203 | 1/1   | 0.96 | 0.07 | 25,25,25,25                 | 0     |
| 56  | MG   | 16    | 101  | 1/1   | 0.96 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | 17    | 103  | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | 17    | 104  | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3204 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3918 | 1/1   | 0.96 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3064 | 1/1   | 0.96 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 4023 | 1/1   | 0.96 | 0.08 | 51,51,51,51                 | 0     |
| 56  | MG   | 2A    | 3228 | 1/1   | 0.96 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | 1a    | 1739 | 1/1   | 0.96 | 0.05 | 52,52,52,52                 | 0     |
| 56  | MG   | 2A    | 3067 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 56  | MG   | 2a    | 1628 | 1/1   | 0.96 | 0.38 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3646 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3023 | 1/1   | 0.96 | 0.08 | 16,16,16,16                 | 0     |
| 56  | MG   | 1A    | 3507 | 1/1   | 0.96 | 0.30 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3073 | 1/1   | 0.96 | 0.17 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3067 | 1/1   | 0.96 | 0.05 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3075 | 1/1   | 0.96 | 0.29 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3453 | 1/1   | 0.96 | 0.22 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1a    | 1745 | 1/1   | 0.96 | 0.09 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 3926 | 1/1   | 0.96 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3036 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3059 | 1/1   | 0.96 | 0.39 | 66,66,66,66                 | 0     |
| 56  | MG   | 2A    | 3570 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3929 | 1/1   | 0.96 | 0.06 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3212 | 1/1   | 0.96 | 0.05 | 44,44,44,44                 | 0     |
| 56  | MG   | 1E    | 306  | 1/1   | 0.96 | 0.17 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1608 | 1/1   | 0.96 | 0.26 | 55,55,55,55                 | 0     |
| 56  | MG   | 1a    | 1609 | 1/1   | 0.96 | 0.09 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 4035 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3578 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3255 | 1/1   | 0.96 | 0.16 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1756 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3514 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3403 | 1/1   | 0.96 | 0.31 | 50,50,50,50                 | 0     |
| 56  | MG   | 2A    | 3090 | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | 1a    | 1613 | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3075 | 1/1   | 0.96 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3115 | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | 1E    | 313  | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3409 | 1/1   | 0.96 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3215 | 1/1   | 0.96 | 0.22 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3937 | 1/1   | 0.96 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3412 | 1/1   | 0.96 | 0.19 | 70,70,70,70                 | 0     |
| 56  | MG   | 1a    | 1764 | 1/1   | 0.96 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3310 | 1/1   | 0.96 | 0.34 | 61,61,61,61                 | 0     |
| 56  | MG   | 1A    | 3661 | 1/1   | 0.96 | 0.05 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3847 | 1/1   | 0.96 | 0.08 | 22,22,22,22                 | 0     |
| 56  | MG   | 2A    | 3417 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 56  | MG   | 1F    | 303  | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 56  | MG   | 2a    | 1669 | 1/1   | 0.96 | 0.29 | 84,84,84,84                 | 0     |
| 56  | MG   | 1A    | 3662 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 56  | MG   | 1F    | 306  | 1/1   | 0.96 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | 1F    | 307  | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3116 | 1/1   | 0.96 | 0.19 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3603 | 1/1   | 0.96 | 0.11 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3758 | 1/1   | 0.96 | 0.07 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3217 | 1/1   | 0.96 | 0.08 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3174 | 1/1   | 0.96 | 0.36 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3946 | 1/1   | 0.96 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | 1G    | 201  | 1/1   | 0.96 | 0.11 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3590 | 1/1   | 0.96 | 0.17 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 4054 | 1/1   | 0.96 | 0.13 | 17,17,17,17                 | 0     |
| 56  | MG   | 2x    | 106  | 1/1   | 0.96 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3854 | 1/1   | 0.96 | 0.11 | 58,58,58,58                 | 0     |
| 56  | MG   | 1a    | 1785 | 1/1   | 0.96 | 0.06 | 57,57,57,57                 | 0     |
| 56  | MG   | 1A    | 3763 | 1/1   | 0.96 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3671 | 1/1   | 0.96 | 0.05 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 4059 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 58  | ZN   | 2n    | 501  | 1/1   | 0.96 | 0.06 | 97,97,97,97                 | 0     |
| 56  | MG   | 1A    | 3178 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | 1a    | 1790 | 1/1   | 0.96 | 0.15 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3147 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3098 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 56  | MG   | 15    | 102  | 1/1   | 0.97 | 0.25 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3074 | 1/1   | 0.97 | 0.09 | 32,32,32,32                 | 0     |
| 56  | MG   | 1F    | 302  | 1/1   | 0.97 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3894 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3469 | 1/1   | 0.97 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 15    | 107  | 1/1   | 0.97 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3977 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 4069 | 1/1   | 0.97 | 0.21 | 57,57,57,57                 | 0     |
| 56  | MG   | 17    | 102  | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3345 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | 1F    | 308  | 1/1   | 0.97 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3042 | 1/1   | 0.97 | 0.23 | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1699 | 1/1   | 0.97 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3111 | 1/1   | 0.97 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3051 | 1/1   | 0.97 | 0.15 | 31,31,31,31                 | 0     |
| 56  | MG   | 2A    | 3754 | 1/1   | 0.97 | 0.06 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3125 | 1/1   | 0.97 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | 18    | 103  | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3218 | 1/1   | 0.97 | 0.19 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3116 | 1/1   | 0.97 | 0.28 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3052 | 1/1   | 0.97 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3485 | 1/1   | 0.97 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3985 | 1/1   | 0.97 | 0.04 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3461 | 1/1   | 0.97 | 0.21 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3028 | 1/1   | 0.97 | 0.16 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3741 | 1/1   | 0.97 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 3352 | 1/1   | 0.97 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3592 | 1/1   | 0.97 | 0.23 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3663 | 1/1   | 0.97 | 0.10 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3109 | 1/1   | 0.97 | 0.31 | 37,37,37,37                 | 0     |
| 56  | MG   | 1N    | 204  | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3630 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | 2A    | 3127 | 1/1   | 0.97 | 0.08 | 52,52,52,52                 | 0     |
| 56  | MG   | 1a    | 1716 | 1/1   | 0.97 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3746 | 1/1   | 0.97 | 0.05 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3222 | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3408 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3009 | 1/1   | 0.97 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3155 | 1/1   | 0.97 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3998 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3111 | 1/1   | 0.97 | 0.20 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3064 | 1/1   | 0.97 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | 1a    | 1615 | 1/1   | 0.97 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3674 | 1/1   | 0.97 | 0.05 | 56,56,56,56                 | 0     |
| 56  | MG   | 1a    | 1728 | 1/1   | 0.97 | 0.07 | 53,53,53,53                 | 0     |
| 56  | MG   | 1P    | 202  | 1/1   | 0.97 | 0.27 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3143 | 1/1   | 0.97 | 0.16 | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1618 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 56  | MG   | 1P    | 204  | 1/1   | 0.97 | 0.30 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3190 | 1/1   | 0.97 | 0.21 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3265 | 1/1   | 0.97 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | 2A    | 3518 | 1/1   | 0.97 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3472 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3921 | 1/1   | 0.97 | 0.06 | 15,15,15,15                 | 0     |
| 56  | MG   | 1A    | 3759 | 1/1   | 0.97 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3266 | 1/1   | 0.97 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3007 | 1/1   | 0.97 | 0.05 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3192 | 1/1   | 0.97 | 0.24 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3066 | 1/1   | 0.97 | 0.15 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3034 | 1/1   | 0.97 | 0.11 | 27,27,27,27                 | 0     |
| 56  | MG   | 1B    | 206  | 1/1   | 0.97 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 1R    | 204  | 1/1   | 0.97 | 0.33 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3270 | 1/1   | 0.97 | 0.28 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3039 | 1/1   | 0.97 | 0.30 | 38,38,38,38                 | 0     |
| 56  | MG   | 2a    | 1658 | 1/1   | 0.97 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3319 | 1/1   | 0.97 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3688 | 1/1   | 0.97 | 0.10 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 4016 | 1/1   | 0.97 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3135 | 1/1   | 0.97 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3033 | 1/1   | 0.97 | 0.24 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3424 | 1/1   | 0.97 | 0.08 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3137 | 1/1   | 0.97 | 0.24 | 31,31,31,31                 | 0     |
| 56  | MG   | 1a    | 1641 | 1/1   | 0.97 | 0.06 | 51,51,51,51                 | 0     |
| 56  | MG   | 1A    | 3484 | 1/1   | 0.97 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3275 | 1/1   | 0.97 | 0.23 | 42,42,42,42                 | 0     |
| 56  | MG   | 2A    | 3170 | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3139 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3118 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3699 | 1/1   | 0.97 | 0.09 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3141 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 56  | MG   | 2A    | 3681 | 1/1   | 0.97 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3282 | 1/1   | 0.97 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3283 | 1/1   | 0.97 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | 1B    | 224  | 1/1   | 0.97 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | 1A    | 4032 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3783 | 1/1   | 0.97 | 0.09 | 23,23,23,23                 | 0     |
| 56  | MG   | 2D    | 304  | 1/1   | 0.97 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3284 | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3085 | 1/1   | 0.97 | 0.23 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3030 | 1/1   | 0.97 | 0.23 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3332 | 1/1   | 0.97 | 0.29 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3240 | 1/1   | 0.97 | 0.28 | 32,32,32,32                 | 0     |
| 56  | MG   | 2a    | 1687 | 1/1   | 0.97 | 0.18 | 40,40,40,40                 | 0     |
| 56  | MG   | 1X    | 101  | 1/1   | 0.97 | 0.28 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3072 | 1/1   | 0.97 | 0.14 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3560 | 1/1   | 0.97 | 0.16 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3383 | 1/1   | 0.97 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3563 | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3384 | 1/1   | 0.97 | 0.28 | 33,33,33,33                 | 0     |
| 56  | MG   | 1a    | 1778 | 1/1   | 0.97 | 0.09 | 67,67,67,67                 | 0     |
| 56  | MG   | 2A    | 3566 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3441 | 1/1   | 0.97 | 0.16 | 39,39,39,39                 | 0     |
| 56  | MG   | 2A    | 3702 | 1/1   | 0.97 | 0.07 | 70,70,70,70                 | 0     |
| 56  | MG   | 2A    | 3070 | 1/1   | 0.97 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3145 | 1/1   | 0.97 | 0.18 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3072 | 1/1   | 0.97 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | 1A    | 3206 | 1/1   | 0.97 | 0.08 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3798 | 1/1   | 0.97 | 0.07 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3502 | 1/1   | 0.97 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3146 | 1/1   | 0.97 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3569 | 1/1   | 0.97 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3175 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3577 | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 10    | 103  | 1/1   | 0.97 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | 2A    | 3444 | 1/1   | 0.97 | 0.08 | 70,70,70,70                 | 0     |
| 56  | MG   | 1E    | 302  | 1/1   | 0.97 | 0.19 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3571 | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 56  | MG   | 1E    | 304  | 1/1   | 0.97 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3583 | 1/1   | 0.97 | 0.11 | 36,36,36,36                 | 0     |
| 56  | MG   | 1E    | 305  | 1/1   | 0.97 | 0.19 | 34,34,34,34                 | 0     |
| 56  | MG   | 1a    | 1676 | 1/1   | 0.97 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3209 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3176 | 1/1   | 0.97 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3391 | 1/1   | 0.97 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3645 | 1/1   | 0.97 | 0.10 | 53,53,53,53                 | 0     |
| 56  | MG   | 1A    | 3177 | 1/1   | 0.97 | 0.09 | 21,21,21,21                 | 0     |
| 56  | MG   | 1A    | 3342 | 1/1   | 0.97 | 0.31 | 40,40,40,40                 | 0     |
| 56  | MG   | 2A    | 3728 | 1/1   | 0.97 | 0.10 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3394 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 57  | WC9  | 2A    | 3809 | 34/34 | 0.97 | 0.09 | 35,43,48,51                 | 0     |
| 56  | MG   | 1A    | 3395 | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 58  | ZN   | 2Y    | 501  | 1/1   | 0.97 | 0.05 | 88,88,88,88                 | 0     |
| 56  | MG   | 1A    | 3730 | 1/1   | 0.97 | 0.05 | 55,55,55,55                 | 0     |
| 56  | MG   | 2A    | 3094 | 1/1   | 0.97 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | 1A    | 3815 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | 1m    | 3001 | 1/1   | 0.97 | 0.10 | 56,56,56,56                 | 0     |
| 56  | MG   | 1A    | 3296 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3243 | 1/1   | 0.98 | 0.07 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3757 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3084 | 1/1   | 0.98 | 0.14 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3577 | 1/1   | 0.98 | 0.14 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3073 | 1/1   | 0.98 | 0.07 | 14,14,14,14                 | 0     |
| 56  | MG   | 1a    | 1723 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1724 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3417 | 1/1   | 0.98 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | 1A    | 3659 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | 2a    | 1667 | 1/1   | 0.98 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3008 | 1/1   | 0.98 | 0.12 | 27,27,27,27                 | 0     |
| 56  | MG   | 2A    | 3743 | 1/1   | 0.98 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 4052 | 1/1   | 0.98 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3619 | 1/1   | 0.98 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3038 | 1/1   | 0.98 | 0.21 | 33,33,33,33                 | 0     |
| 56  | MG   | 11    | 101  | 1/1   | 0.98 | 0.30 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3199 | 1/1   | 0.98 | 0.13 | 19,19,19,19                 | 0     |
| 56  | MG   | 1A    | 3045 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3665 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3624 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3304 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3585 | 1/1   | 0.98 | 0.10 | 12,12,12,12                 | 0     |
| 56  | MG   | 13    | 101  | 1/1   | 0.98 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3773 | 1/1   | 0.98 | 0.06 | 22,22,22,22                 | 0     |
| 56  | MG   | 1A    | 3670 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3138 | 1/1   | 0.98 | 0.30 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3672 | 1/1   | 0.98 | 0.05 | 27,27,27,27                 | 0     |
| 56  | MG   | 1P    | 201  | 1/1   | 0.98 | 0.43 | 39,39,39,39                 | 0     |
| 56  | MG   | 2W    | 204  | 1/1   | 0.98 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 4004 | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3660 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 56  | MG   | 2X    | 102  | 1/1   | 0.98 | 0.08 | 54,54,54,54                 | 0     |
| 56  | MG   | 2A    | 3186 | 1/1   | 0.98 | 0.05 | 65,65,65,65                 | 0     |
| 56  | MG   | 1P    | 203  | 1/1   | 0.98 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3663 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3006 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | 15    | 105  | 1/1   | 0.98 | 0.22 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3009 | 1/1   | 0.98 | 0.04 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3518 | 1/1   | 0.98 | 0.07 | 56,56,56,56                 | 0     |
| 56  | MG   | 2A    | 3010 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | 1A    | 3779 | 1/1   | 0.98 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3012 | 1/1   | 0.98 | 0.07 | 46,46,46,46                 | 0     |
| 56  | MG   | 1Q    | 202  | 1/1   | 0.98 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3014 | 1/1   | 0.98 | 0.26 | 49,49,49,49                 | 0     |
| 56  | MG   | 17    | 101  | 1/1   | 0.98 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3278 | 1/1   | 0.98 | 0.27 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 4071 | 1/1   | 0.98 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | 1A    | 3726 | 1/1   | 0.98 | 0.07 | 25,25,25,25                 | 0     |
| 56  | MG   | 2A    | 3781 | 1/1   | 0.98 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | 1A    | 3631 | 1/1   | 0.98 | 0.06 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3677 | 1/1   | 0.98 | 0.08 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3055 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | 1D    | 303  | 1/1   | 0.98 | 0.09 | 18,18,18,18                 | 0     |
| 56  | MG   | 2A    | 3024 | 1/1   | 0.98 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3280 | 1/1   | 0.98 | 0.34 | 39,39,39,39                 | 0     |
| 56  | MG   | 1D    | 305  | 1/1   | 0.98 | 0.20 | 35,35,35,35                 | 0     |
| 56  | MG   | 1D    | 306  | 1/1   | 0.98 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | 1D    | 307  | 1/1   | 0.98 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | 1A    | 3161 | 1/1   | 0.98 | 0.24 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3682 | 1/1   | 0.98 | 0.06 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 2A    | 3688 | 1/1   | 0.98 | 0.06 | 58,58,58,58                 | 0     |
| 56  | MG   | 1A    | 3429 | 1/1   | 0.98 | 0.22 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 4017 | 1/1   | 0.98 | 0.04 | 48,48,48,48                 | 0     |
| 56  | MG   | 1E    | 301  | 1/1   | 0.98 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | 2A    | 3493 | 1/1   | 0.98 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3494 | 1/1   | 0.98 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | 1a    | 1770 | 1/1   | 0.98 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3557 | 1/1   | 0.98 | 0.07 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3010 | 1/1   | 0.98 | 0.04 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3559 | 1/1   | 0.98 | 0.15 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3106 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3057 | 1/1   | 0.98 | 0.06 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3689 | 1/1   | 0.98 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | 1E    | 308  | 1/1   | 0.98 | 0.12 | 30,30,30,30                 | 0     |
| 56  | MG   | 2A    | 3131 | 1/1   | 0.98 | 0.18 | 46,46,46,46                 | 0     |
| 56  | MG   | 2A    | 3132 | 1/1   | 0.98 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | 1A    | 3562 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3186 | 1/1   | 0.98 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3507 | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3799 | 1/1   | 0.98 | 0.05 | 47,47,47,47                 | 0     |
| 56  | MG   | 1A    | 3800 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 56  | MG   | 1V    | 201  | 1/1   | 0.98 | 0.16 | 33,33,33,33                 | 0     |
| 56  | MG   | 1A    | 3048 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3003 | 1/1   | 0.98 | 0.06 | 22,22,22,22                 | 0     |
| 56  | MG   | 1V    | 205  | 1/1   | 0.98 | 0.24 | 54,54,54,54                 | 0     |
| 56  | MG   | 1A    | 3211 | 1/1   | 0.98 | 0.14 | 36,36,36,36                 | 0     |
| 56  | MG   | 1a    | 1701 | 1/1   | 0.98 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3127 | 1/1   | 0.98 | 0.35 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3110 | 1/1   | 0.98 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3697 | 1/1   | 0.98 | 0.06 | 15,15,15,15                 | 0     |
| 56  | MG   | 1F    | 301  | 1/1   | 0.98 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3012 | 1/1   | 0.98 | 0.03 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3096 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 56  | MG   | 1X    | 103  | 1/1   | 0.98 | 0.05 | 48,48,48,48                 | 0     |
| 56  | MG   | 1F    | 304  | 1/1   | 0.98 | 0.08 | 36,36,36,36                 | 0     |
| 56  | MG   | 2A    | 3723 | 1/1   | 0.98 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | 1a    | 1630 | 1/1   | 0.98 | 0.16 | 33,33,33,33                 | 0     |
| 57  | WC9  | 1A    | 4098 | 34/34 | 0.98 | 0.07 | 22,27,32,33                 | 0     |
| 56  | MG   | 1A    | 3097 | 1/1   | 0.98 | 0.17 | 22,22,22,22                 | 0     |
| 56  | MG   | 1X    | 106  | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 3114 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 56  | MG   | 2A    | 3529 | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | ZN   | 29    | 501  | 1/1   | 0.98 | 0.04 | 76,76,76,76                 | 0     |
| 56  | MG   | 1a    | 1714 | 1/1   | 0.98 | 0.04 | 35,35,35,35                 | 0     |
| 59  | SF4  | 1d    | 302  | 8/8   | 0.98 | 0.05 | 64,70,73,76                 | 0     |
| 56  | MG   | 1A    | 3242 | 1/1   | 0.98 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | 1A    | 3924 | 1/1   | 0.98 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | 2A    | 3508 | 1/1   | 0.99 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | 1U    | 201  | 1/1   | 0.99 | 0.20 | 34,34,34,34                 | 0     |
| 56  | MG   | 1A    | 3834 | 1/1   | 0.99 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3229 | 1/1   | 0.99 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3899 | 1/1   | 0.99 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | 2A    | 3751 | 1/1   | 0.99 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | 1A    | 3679 | 1/1   | 0.99 | 0.05 | 30,30,30,30                 | 0     |
| 56  | MG   | 10    | 107  | 1/1   | 0.99 | 0.03 | 41,41,41,41                 | 0     |
| 56  | MG   | 1A    | 3173 | 1/1   | 0.99 | 0.11 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3276 | 1/1   | 0.99 | 0.11 | 28,28,28,28                 | 0     |
| 56  | MG   | 1A    | 3667 | 1/1   | 0.99 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3904 | 1/1   | 0.99 | 0.05 | 31,31,31,31                 | 0     |
| 56  | MG   | 1A    | 3979 | 1/1   | 0.99 | 0.10 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3905 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 56  | MG   | 1A    | 3021 | 1/1   | 0.99 | 0.02 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3931 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 56  | MG   | 1V    | 204  | 1/1   | 0.99 | 0.12 | 32,32,32,32                 | 0     |
| 56  | MG   | 2A    | 3763 | 1/1   | 0.99 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 3378 | 1/1   | 0.99 | 0.22 | 24,24,24,24                 | 0     |
| 56  | MG   | 1A    | 3037 | 1/1   | 0.99 | 0.14 | 25,25,25,25                 | 0     |
| 56  | MG   | 1A    | 3070 | 1/1   | 0.99 | 0.08 | 14,14,14,14                 | 0     |
| 56  | MG   | 2A    | 3767 | 1/1   | 0.99 | 0.04 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 3748 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 56  | MG   | 2A    | 3018 | 1/1   | 0.99 | 0.11 | 29,29,29,29                 | 0     |
| 56  | MG   | 1W    | 202  | 1/1   | 0.99 | 0.18 | 37,37,37,37                 | 0     |
| 56  | MG   | 1a    | 1766 | 1/1   | 0.99 | 0.05 | 57,57,57,57                 | 0     |
| 56  | MG   | 2A    | 3399 | 1/1   | 0.99 | 0.11 | 25,25,25,25                 | 0     |
| 56  | MG   | 15    | 101  | 1/1   | 0.99 | 0.17 | 34,34,34,34                 | 0     |
| 56  | MG   | 1t    | 201  | 1/1   | 0.99 | 0.04 | 64,64,64,64                 | 0     |
| 56  | MG   | 2A    | 3534 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3535 | 1/1   | 0.99 | 0.02 | 42,42,42,42                 | 0     |
| 56  | MG   | 1A    | 3546 | 1/1   | 0.99 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | 1A    | 3071 | 1/1   | 0.99 | 0.12 | 29,29,29,29                 | 0     |
| 56  | MG   | 1A    | 3156 | 1/1   | 0.99 | 0.23 | 39,39,39,39                 | 0     |
| 56  | MG   | 1A    | 3769 | 1/1   | 0.99 | 0.03 | 35,35,35,35                 | 0     |
| 56  | MG   | 1A    | 4047 | 1/1   | 0.99 | 0.03 | 39,39,39,39                 | 0     |
| 56  | MG   | 1a    | 1773 | 1/1   | 0.99 | 0.04 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | 1A    | 3991 | 1/1   | 0.99 | 0.05 | 36,36,36,36                 | 0     |
| 56  | MG   | 1A    | 3788 | 1/1   | 0.99 | 0.06 | 23,23,23,23                 | 0     |
| 56  | MG   | 1A    | 4081 | 1/1   | 0.99 | 0.04 | 37,37,37,37                 | 0     |
| 56  | MG   | 1A    | 4020 | 1/1   | 0.99 | 0.02 | 26,26,26,26                 | 0     |
| 56  | MG   | 1a    | 1738 | 1/1   | 0.99 | 0.06 | 62,62,62,62                 | 0     |
| 56  | MG   | 1A    | 4021 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 58  | ZN   | 1Y    | 204  | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 56  | MG   | 1A    | 3789 | 1/1   | 0.99 | 0.04 | 27,27,27,27                 | 0     |
| 58  | ZN   | 15    | 109  | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 58  | ZN   | 1n    | 103  | 1/1   | 0.99 | 0.04 | 68,68,68,68                 | 0     |
| 56  | MG   | 1A    | 3013 | 1/1   | 0.99 | 0.13 | 30,30,30,30                 | 0     |
| 56  | MG   | 1A    | 3623 | 1/1   | 0.99 | 0.06 | 25,25,25,25                 | 0     |
| 58  | ZN   | 25    | 105  | 1/1   | 0.99 | 0.04 | 60,60,60,60                 | 0     |
| 58  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 56  | MG   | 1A    | 4055 | 1/1   | 0.99 | 0.09 | 33,33,33,33                 | 0     |
| 56  | MG   | 2A    | 3461 | 1/1   | 0.99 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | 2A    | 3647 | 1/1   | 0.99 | 0.04 | 37,37,37,37                 | 0     |
| 59  | SF4  | 2d    | 303  | 8/8   | 0.99 | 0.05 | 64,66,74,76                 | 0     |
| 56  | MG   | 1A    | 3014 | 1/1   | 0.99 | 0.05 | 27,27,27,27                 | 0     |
| 56  | MG   | 1A    | 3755 | 1/1   | 0.99 | 0.06 | 47,47,47,47                 | 0     |
| 58  | ZN   | 19    | 102  | 1/1   | 1.00 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | 1A    | 3716 | 1/1   | 1.00 | 0.06 | 26,26,26,26                 | 0     |
| 56  | MG   | 1A    | 3614 | 1/1   | 1.00 | 0.07 | 36,36,36,36                 | 0     |
| 58  | ZN   | 16    | 102  | 1/1   | 1.00 | 0.02 | 43,43,43,43                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.