



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 02:53 PM EDT

PDB ID : 9O3I / pdb\_00009o3i  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with ketolide telithromycin, mRNA, aminoacylated A-site Lys-tRNA<sup>Lys</sup>, P-site fMRC-peptidyl-tRNA<sup>Met</sup>, and deacylated E-site tRNA<sup>Lys</sup> at 2.80Å resolution  
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Kruglov, A.A.; Paranjpe, M.N.; Svetlov, M.S.; Polikanov, Y.S.  
Deposited on : 2025-04-07  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://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                      | : 9.0.015 (Gargrove)                                               |
| Density-Fitness           | : 1.0.12                                                           |
| Ideal geometry (proteins) | : Engh & Huber (2001)                                              |

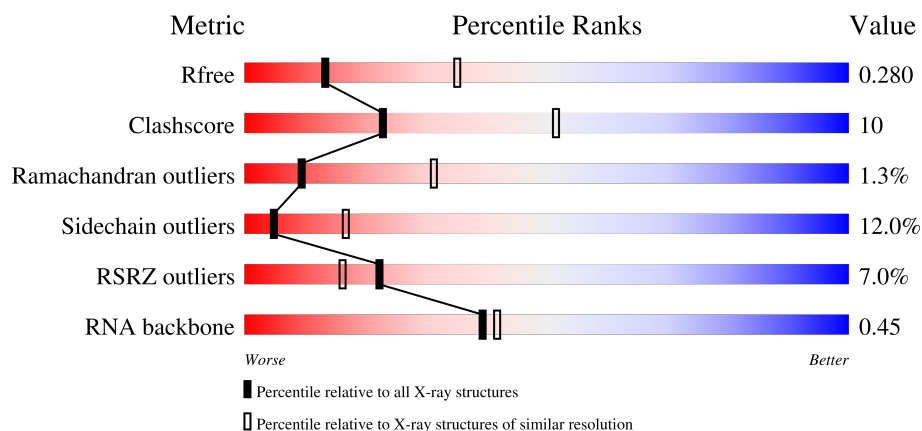
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



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

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

| Mol | Chain | Length | Quality of chain                                                                    |
|-----|-------|--------|-------------------------------------------------------------------------------------|
| 1   | 1A    | 2915   | <div> <div>4%</div> <div>59%</div> <div>32%</div> <div>8%</div> <div>.</div> </div> |
| 1   | 2A    | 2915   | <div> <div>3%</div> <div>53%</div> <div>35%</div> <div>8%</div> <div>.</div> </div> |

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

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| Mol | Chain | Length | Quality of chain      |
|-----|-------|--------|-----------------------|
| 2   | 1B    | 121    | %<br>59% 36% . .      |
| 2   | 2B    | 121    | 16%<br>40% 50% 10% .  |
| 3   | 1D    | 276    | %<br>74% 22% .        |
| 3   | 2D    | 276    | 3%<br>70% 28% .       |
| 4   | 1E    | 206    | 70% 26% . .           |
| 4   | 2E    | 206    | 3%<br>76% 21% . .     |
| 5   | 1F    | 210    | 65% 28% . .           |
| 5   | 2F    | 210    | %<br>53% 39% 5% .     |
| 6   | 1G    | 182    | 4%<br>59% 34% 6% .    |
| 6   | 2G    | 182    | 22%<br>49% 40% 9% . . |
| 7   | 1H    | 180    | %<br>66% 26% 5% .     |
| 7   | 2H    | 180    | 8%<br>63% 28% 6% .    |
| 8   | 1I    | 148    | 3%<br>61% 29% 8% .    |
| 8   | 2I    | 148    | 11%<br>56% 34% 9% .   |
| 9   | 1N    | 140    | %<br>70% 30%          |
| 9   | 2N    | 140    | 8%<br>74% 24% .       |
| 10  | 1O    | 122    | %<br>69% 27% .        |
| 10  | 2O    | 122    | 68% 30% .             |
| 11  | 1P    | 150    | %<br>67% 27% 5% .     |
| 11  | 2P    | 150    | 8%<br>67% 27% 5% . .  |
| 12  | 1Q    | 141    | %<br>69% 27% .        |
| 12  | 2Q    | 141    | 11%<br>55% 38% 7%     |
| 13  | 1R    | 118    | 70% 27% .             |
| 13  | 2R    | 118    | 70% 30%               |
| 14  | 1S    | 112    | %<br>63% 29% 5% .     |

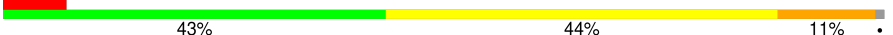
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14  | 2S    | 112    |                  |
| 15  | 1T    | 146    |                  |
| 15  | 2T    | 146    |                  |
| 16  | 1U    | 118    |                  |
| 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  | 2w    | 76     |                  |
| 55  | 1x    | 77     |                  |
| 55  | 2x    | 77     |                  |
| 56  | 1z    | 3      |                  |
| 56  | 2z    | 3      |                  |
| 57  | 1y    | 76     |                  |
| 57  | 2y    | 76     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58  | MG   | 2A    | 3715 | -         | -        | -       | X                |
| 62  | SF4  | 2d    | 303  | -         | -        | X       | -                |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 299377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | 1B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2577  | 1146 | 476 | 835 | 120 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2575  | 1146 | 476 | 833 | 120 |         |         |       |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 1G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1423  | 913 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 913 | 258 | 253 | 4 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1097  | 701 | 191 | 204 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 681 | 186 | 196 | 1 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | 1S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 873   | 550 | 174 | 149 |         |         |       |
| 14  | 2S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1240  | 795 | 222 | 220 | 3 |         |         |       |
| 21  | 2Z    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1271  | 814 | 228 | 227 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 10    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 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 MET-LYS-mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 53  | 1v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 283   | 128 | 59 | 83 | 13 |         |         |       |
| 53  | 2v    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 283   | 128 | 59 | 83 | 13 |         |         |       |

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Lys-tRNAlys.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 54  | 1w    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1599  | 718 | 282 | 524 | 74 | 1 |         |         |       |
| 54  | 2w    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1599  | 718 | 282 | 524 | 74 | 1 |         |         |       |

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMRC-tRNAcys RNA-part.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 55  | 1x    | 77       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1646  | 734 | 298 | 536 | 77 | 1 |         |         |       |
| 55  | 2x    | 77       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1646  | 734 | 298 | 536 | 77 | 1 |         |         |       |

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part.

| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---|---------|---------|-------|
| 56  | 1z    | 3        | Total | C  | N | O | S | 0       | 0       | 0     |
|     |       |          | 27    | 15 | 6 | 4 | 2 |         |         |       |
| 56  | 2z    | 3        | Total | C  | N | O | S | 0       | 0       | 0     |
|     |       |          | 27    | 15 | 6 | 4 | 2 |         |         |       |

- Molecule 57 is a RNA chain called E-site Deacylated tRNAlys.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 57  | 1y    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1577  | 705 | 277 | 520 | 74 | 1 |         |         |       |
| 57  | 2y    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1577  | 705 | 277 | 520 | 74 | 1 |         |         |       |

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 58  | 1A    | 1080     | Total | Mg   | 0       | 0       |
|     |       |          | 1080  | 1080 |         |         |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 58  | 1B    | 40       | Total<br>40 | Mg<br>40 | 0       | 0       |
| 58  | 1D    | 12       | Total<br>12 | Mg<br>12 | 0       | 0       |
| 58  | 1E    | 12       | Total<br>12 | Mg<br>12 | 0       | 0       |
| 58  | 1F    | 11       | Total<br>11 | Mg<br>11 | 0       | 0       |
| 58  | 1G    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 58  | 1N    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 58  | 1O    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 58  | 1P    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 58  | 1Q    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 58  | 1R    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 58  | 1S    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 58  | 1T    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 1U    | 10       | Total<br>10 | Mg<br>10 | 0       | 0       |
| 58  | 1V    | 8        | Total<br>8  | Mg<br>8  | 0       | 0       |
| 58  | 1W    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 58  | 1X    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 58  | 1Y    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 1Z    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 58  | 10    | 11       | Total<br>11 | Mg<br>11 | 0       | 0       |
| 58  | 11    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 58  | 12    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58  | 13    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 58  | 14    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 15    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 58  | 16    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | 17    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 58  | 18    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 58  | 19    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1a    | 209      | Total<br>209 | Mg<br>209 | 0       | 0       |
| 58  | 1b    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | 1l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | 1m    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1n    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | 1p    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 58  | 1t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1v    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | 1w    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 58  | 1x    | 12       | Total<br>12  | Mg<br>12  | 0       | 0       |
| 58  | 2A    | 824      | Total<br>824 | Mg<br>824 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 58  | 2B    | 19       | Total<br>19 | Mg<br>19 | 0       | 0       |
| 58  | 2D    | 8        | Total<br>8  | Mg<br>8  | 0       | 0       |
| 58  | 2E    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 58  | 2F    | 6        | Total<br>6  | Mg<br>6  | 0       | 0       |
| 58  | 2G    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 58  | 2N    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 58  | 2O    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 2P    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 2Q    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 2R    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 2T    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 58  | 2U    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 58  | 2V    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 2W    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 58  | 2X    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 2Y    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 58  | 2Z    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 58  | 20    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 58  | 21    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 58  | 23    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 58  | 25    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |

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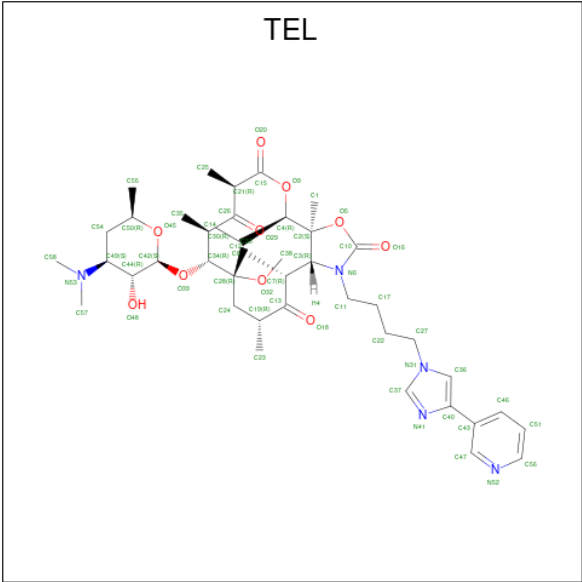
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| Mol | Chain | Residues | Atoms               | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 58  | 27    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 58  | 28    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 58  | 2a    | 211      | Total Mg<br>211 211 | 0       | 0       |
| 58  | 2d    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 58  | 2e    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2f    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2g    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2j    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2k    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2l    | 4        | Total Mg<br>4 4     | 0       | 0       |
| 58  | 2q    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 58  | 2r    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2t    | 1        | Total Mg<br>1 1     | 0       | 0       |
| 58  | 2v    | 3        | Total Mg<br>3 3     | 0       | 0       |
| 58  | 2w    | 2        | Total Mg<br>2 2     | 0       | 0       |
| 58  | 2x    | 5        | Total Mg<br>5 5     | 0       | 0       |

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 59  | 1A    | 1        | Total K<br>1 1 | 0       | 0       |
| 59  | 2A    | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 60 is TELITHROMYCIN (CCD ID: TEL) (formula:  $C_{43}H_{65}N_5O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 60  | 1A    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 58    | 43 | 5 | 10 |         |         |
| 60  | 2A    | 1        | Total | C  | N | O  | 0       | 0       |
|     |       |          | 58    | 43 | 5 | 10 |         |         |

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

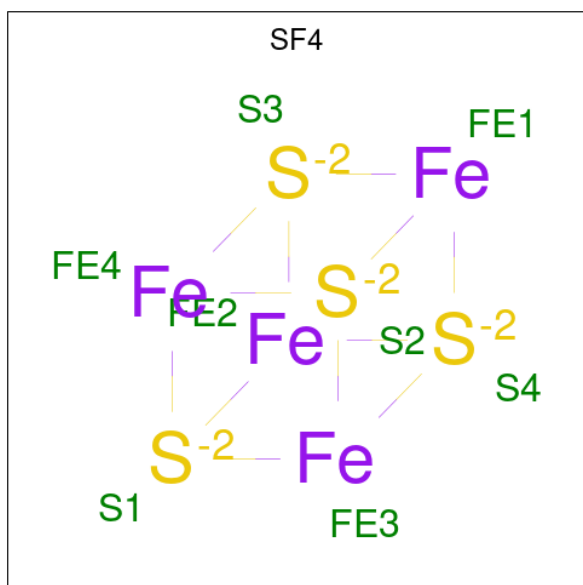
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 61  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 61  | 29    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | 2n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 62  | 1d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 62  | 2d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 63 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 63  | 1A    | 1780     | Total | O    | 0       | 0       |
|     |       |          | 1780  | 1780 |         |         |
| 63  | 1B    | 57       | Total | O    | 0       | 0       |
|     |       |          | 57    | 57   |         |         |
| 63  | 1D    | 24       | Total | O    | 0       | 0       |
|     |       |          | 24    | 24   |         |         |
| 63  | 1E    | 22       | Total | O    | 0       | 0       |
|     |       |          | 22    | 22   |         |         |
| 63  | 1F    | 14       | Total | O    | 0       | 0       |
|     |       |          | 14    | 14   |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 63  | 1G    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 63  | 1H    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 63  | 1I    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 1N    | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 63  | 1O    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | 1P    | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 63  | 1Q    | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 63  | 1R    | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 63  | 1S    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | 1T    | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 63  | 1U    | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 63  | 1V    | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 63  | 1W    | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 63  | 1X    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | 1Y    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 1Z    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 10    | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 63  | 11    | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 63  | 12    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | 13    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | 15    | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 63  | 16    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 17    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 18    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 63  | 1a    | 226      | Total<br>226 | O<br>226 | 0       | 0       |
| 63  | 1b    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 1e    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 1l    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 63  | 1m    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 1n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 1q    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 1v    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 1w    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 1x    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 63  | 1y    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2A    | 850      | Total<br>850 | O<br>850 | 0       | 0       |
| 63  | 2B    | 16       | Total<br>16  | O<br>16  | 0       | 0       |
| 63  | 2D    | 18       | Total<br>18  | O<br>18  | 0       | 0       |
| 63  | 2E    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 63  | 2F    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 63  | 2N    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2O    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 63  | 2P    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2Q    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2R    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 2T    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 63  | 2U    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 2W    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 2X    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 2Z    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 20    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 63  | 21    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 25    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 27    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 28    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 29    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2a    | 148      | Total<br>148 | O<br>148 | 0       | 0       |
| 63  | 2d    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2e    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2i    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2l    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 2p    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 2t    | 2        | Total<br>2   | O<br>2   | 0       | 0       |

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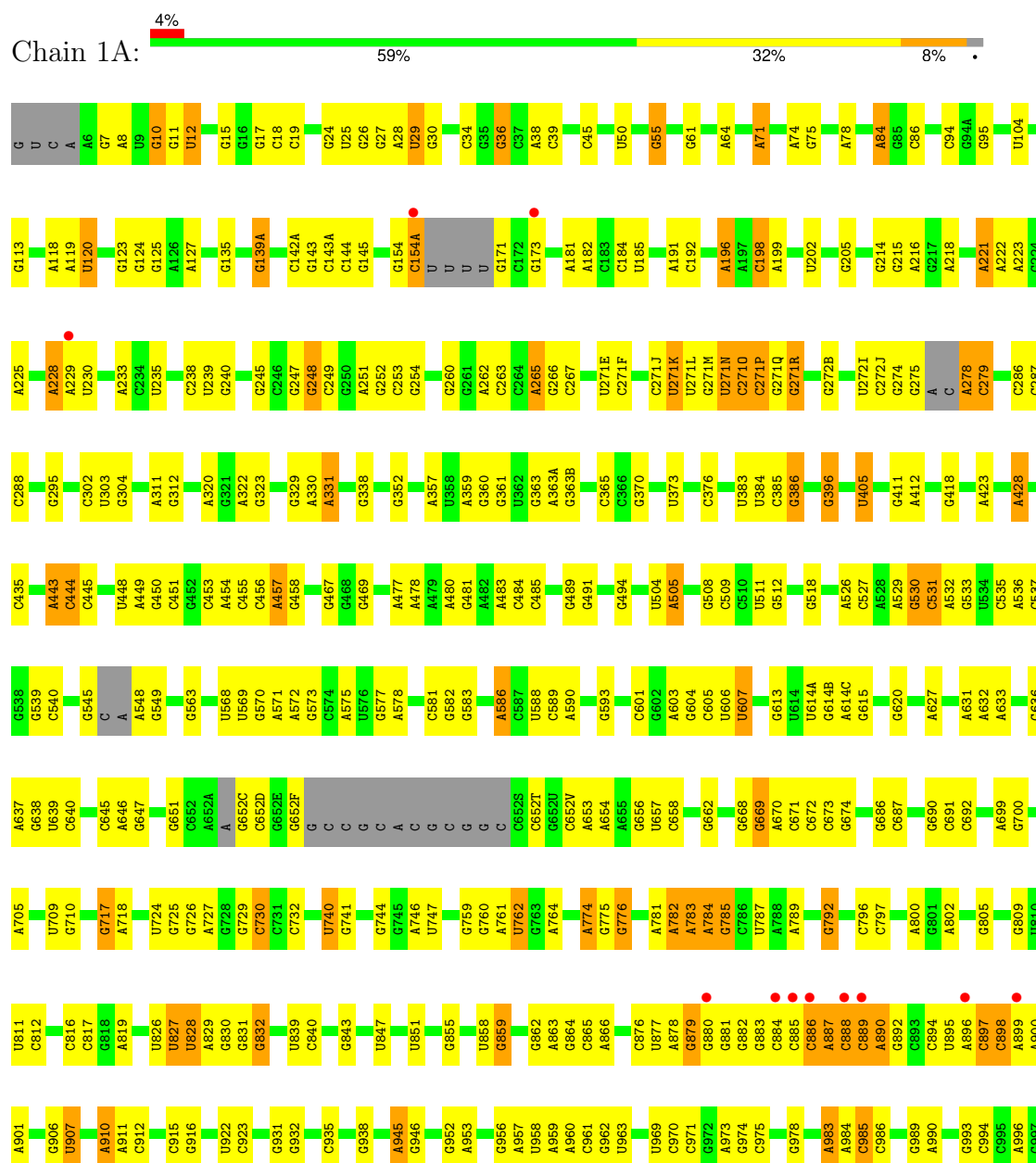
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 63  | 2v    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 63  | 2w    | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 63  | 2x    | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |

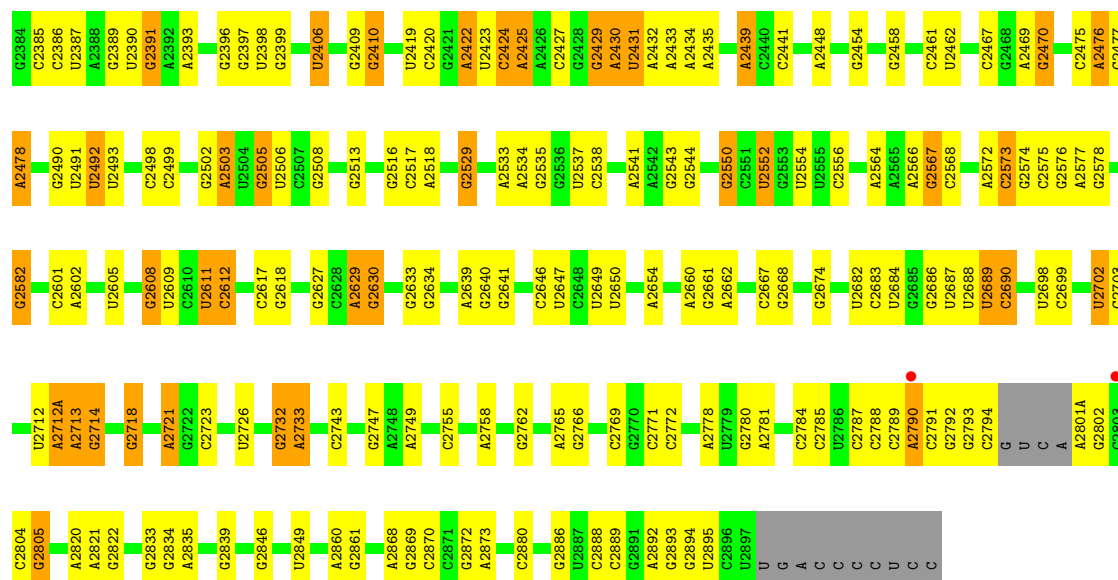
### 3 Residue-property plots

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.

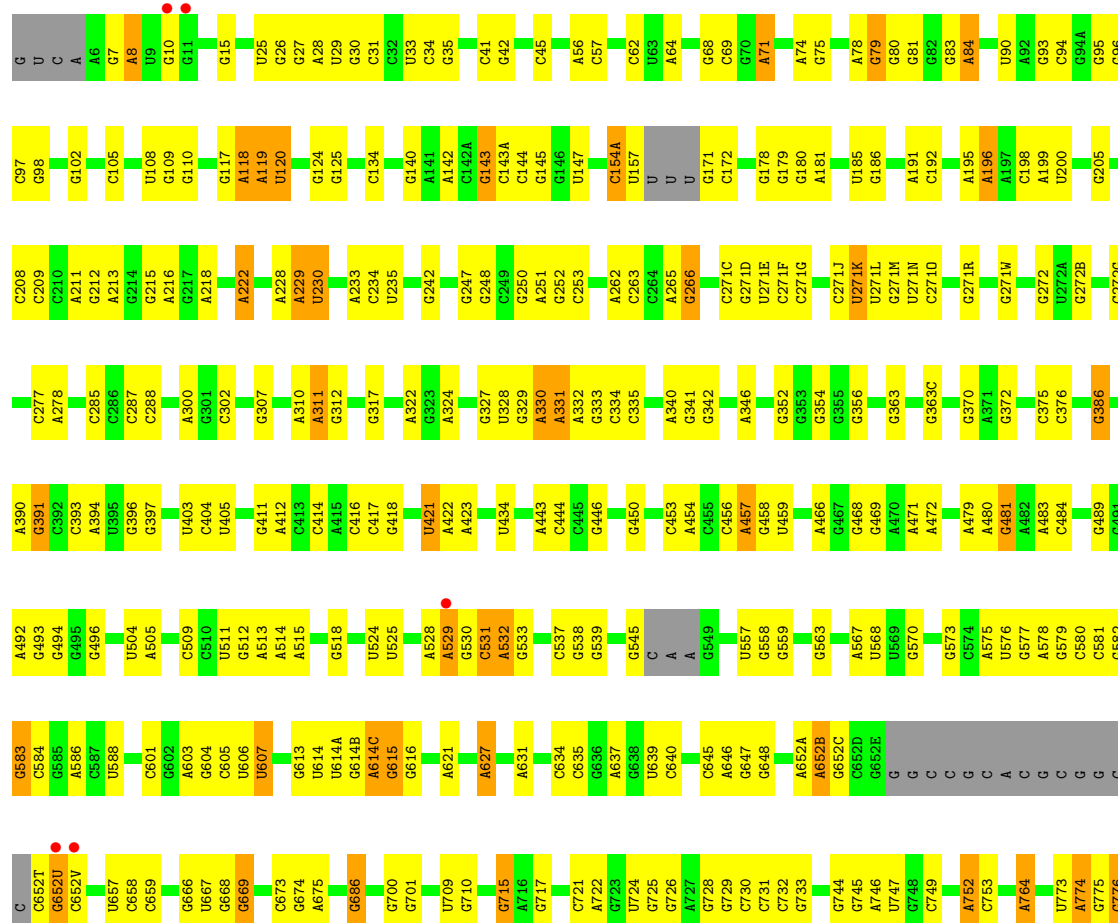
#### • Molecule 1: 23S Ribosomal RNA



|       |       |       |       |       |       |       |       |        |       |       |        |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|--------|-------|-------|
| G2308 | U2203 | C2137 | C2063 | C1967 | G1857 | U1757 | A1641 | A1508  | A1393 | G1266 | U1142  | C1071 | G999  |
| G2309 | C2205 | C2138 | C2065 | G1968 | G1858 | G1758 | G1642 | C1509  | U1394 | A1267 | U1142A | C1072 | G1003 |
| U2312 | G2206 | C2140 | C2066 | A1969 | G1859 | A1762 | G1647 | A1509A | U1395 | A1268 | A1142A | A1267 | G1003 |
| G2313 | G2207 | G2141 | G2067 | A1970 | G1865 | G1763 | C1648 | A1509B | U1396 | A1269 | A1143  | G1074 | G1007 |
| G2314 | U2208 | C2142 | U2268 | A1972 | A1877 | G1764 | G1649 | G1515  | C1399 | G1271 | G1149  | C1075 | G1008 |
| G2315 | U2218 | C2143 | G2069 |       | G1878 |       | G1650 | G1518  | U1405 | A1272 |        | A1009 |       |
| G2316 | G2219 | U2144 | U2074 | C1983 | G1878 | G1769 | G1651 | U1518  | U1406 | A1273 | C1152  | A1077 | A1010 |
| G2317 | U2075 | C2145 | U2075 | A1986 | G1882 | G1770 | G1651 | G1519  | U1407 | A1274 | C1153  | C1079 | G1011 |
| G2318 |       | C2146 |       |       | G1883 |       | C1663 | G1526  |       | U1292 | G1154  | C1080 | U1012 |
| G2319 |       | G2147 |       |       | G1883 | A1773 | A1664 | G1527  |       | C1293 | G1164  | U1081 | C1013 |
| A2320 |       | G2148 | U2079 | U1991 | G1889 | U1777 | A1665 | G1527  | G1416 | C1293 | U1165  | U1082 | U1014 |
| G2325 | G2234 | G2149 |       | G1992 | A1889 | U1777 | G1666 | C1532  | C1417 | C1297 | U1165  | U1083 |       |
| G2326 | G2235 | U2150 | U2086 | U1993 | G1899 | U1778 | G1667 | G      | G     |       | G1168  | A1084 | U1022 |
| A2327 | G2238 | G2152 | G2087 | C1996 | G1899 | U1779 | G1668 | U      | A     | U1300 | G1168  | A1085 | G1023 |
| G2328 | G2239 | G2153 | G2093 | G1997 | A1900 | A1780 | C1669 | A      | G     | A1301 | G1170  | A1086 | G1024 |
| G2329 | C2240 | G2154 | G2094 | G1997 | G1906 | A1783 | U1671 | C      | G     | A1301 | G1170  | A1087 | G1025 |
| G2330 | A2241 | G2155 | U2095 | G2012 | G1907 | A1784 | G1674 | G1537  | G1426 | G1310 | G1171  | A1088 | U1026 |
| G2331 | G2242 | G2156 | C2096 | A2013 | C1908 | A1785 | G1674 | G1538  | A1427 | U1090 | A1174  | A1027 |       |
| U2243 | U2243 | G2157 | C2097 | A2014 | C1908 | A1786 | G1678 | G1539  | C1428 | G1315 | U1175  | A1029 | A1028 |
| G2334 | U2244 | A2158 | U2098 |       | U1911 |       | G1678 | G1543  | G1429 | G1319 | A1177  | C1092 | G1030 |
| A2335 | U2245 | G2159 | U2099 |       | U1911 |       | G1678 | C1543  | C1430 | G1320 | C1178  |       |       |
| A2336 | G2246 | G2160 | G2100 | U2017 | C1914 | A1789 | G1682 | C1557  | U1431 |       |        |       | U1033 |
| G2337 | A2247 | C2161 | G2101 | A2020 | U1915 | C1790 | G1682 | C1557  | U1431 |       |        |       | G1034 |
|       | G2248 | G2162 | U2102 | A2020 | U1915 | A1791 | C1686 | A1558  | U1438 | G1325 | G1186  | A1096 | U1035 |
| G2340 | U2249 | C2163 | C2103 | U2022 | U1917 | U1794 | G1687 | A1558  | U1439 |       | G1187  | U1097 | U1036 |
| G2341 | G2250 | G2164 | G2104 | G2023 | A1918 | C1795 | U1688 | A1566  | G1440 | G1332 | U1188  | A1098 | G1037 |
| G2342 | G2251 | G2165 | C2105 | G2024 | A1919 | U1796 | U1688 | A1567  | G1441 | G1333 |        | A1099 | C1038 |
| C2343 | G2252 | G2166 | G2106 | C2025 | C1920 | C1797 | U1693 | G1568  | G1442 |       | C1201  | C1100 | G1039 |
| U2344 |       | U2167 | C2107 |       | G1921 | U1798 | C1694 | A1569  |       | G1338 |        | U1101 | C1040 |
| G2345 | G2255 | G2168 | C2108 | U2028 | G1929 | G1799 | C1695 | A1570  | A1445 | G1339 | A1213  | C1102 | C1041 |
| A2346 | G2256 | A2169 | U2109 | G2029 | G1930 | C1800 | G1696 | A1571  |       | U1340 | A1218  | A1103 | G1042 |
| G2347 | G2259 | A2170 | G2110 | A2030 | G1930 | G1801 | G1697 | A1572  | G1450 | U1341 | C1218  | C1104 | C1043 |
| U2348 |       | A2171 | C2111 | A2031 | G1939 | A1802 | A1698 |        |       | A1342 | U1105  | G1044 |       |
| G2349 | A2268 | U2172 | G2112 | G2032 | G1935 | A1803 | G1699 | U1578  | U1453 |       | A1226  | G1106 | A1045 |
| C2350 | A2269 | A2173 | G2113 | A2033 | A1936 | A1700 | G1699 | A1579  | U1455 | U1352 |        | G1107 | A1046 |
| G2354 | A2273 | C2174 | A2114 | G2034 | A1937 | A1812 | G1701 | A1580  | G1455 | A1353 | G1232  | U1108 | A1047 |
| G2359 |       | C2175 | G2115 | G2035 | A1938 | A1702 | G1702 | G1581  | G1461 | C1233 | G1233  | C1109 | A1048 |
| G2360 |       | A2176 | G2116 | C2036 | U1939 | A1815 | G1703 |        |       | U1357 | U1234  | G1110 |       |
| G2363 | G2277 | C2177 | A2117 | G2037 | U1940 | G1816 | G1703 | C1584  | C1467 | U1357 | G1235  | G1111 | G1051 |
| A2361 | U2278 | C2178 | U2113 | G2038 | C1941 | G1817 | U1709 | A1586  | C1468 | A1359 | G1236  | G1112 | C1052 |
| C2364 | G2279 | C2179 | A2119 | C2039 | C1942 | U1818 | C1710 | A1587  | C1468 | A1360 | G1237  | U1113 | C1053 |
| G2365 | G2280 | U2180 | G2120 |       |       | U1819 | C1711 | C1588  | A1477 | G1364 | G1238  | G1114 | G1054 |
| A2366 |       | G2181 | U2121 |       |       | A1819 | C1712 | C1589  | G1478 | G1365 | G1239  | G1115 | G1055 |
| G2367 | C2283 | G2182 | U2122 | C2043 | G1945 | G1823 | U1713 | G1584  | G1482 | A1365 | U1240  | C1116 | G1056 |
| G2375 | A2286 | C2183 | G2123 | G2049 | C1947 |       |       | G1594  | G1484 |       |        | G1117 | A1057 |
| G2376 | A2287 | G2184 | G2124 | C2050 | C1947 | G1826 | G1718 | G1595  | G1484 | G1371 | G1244  |       | A1058 |
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| G2378 | G2289 | G2186 | G2126 | G2052 | A1953 | G1828 | G1719 | C1607  | A1490 | G1377 | A1246  | U1060 |       |
| G2379 |       | G2187 | G2127 | G2053 | G1954 | A1829 | G1721 | A1608  | A1490 |       | A1247  | G1125 | U     |
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| G2379 |       | U2189 | C2129 | G2055 | C1988 | U1833 | U1739 | C1493  | C1494 |       | G1252  | U1130 | G1062 |
| A2377 | C2292 | G2190 | U2130 | G2056 | C1988 | U1833 | G1740 | A1614  | C1494 |       | A1253  | G1131 | G1063 |
| G2378 | U2296 | G2191 | G2131 | A2057 | C1988 | G1839 | A1741 | G1633  | G1500 |       | G1256  | C1135 | U1065 |
| G2379 |       | G2192 | U2132 | A2058 | C1962 | C1844 | G1742 | G1633  | G1500 |       |        | C1136 | U1066 |
| G2380 | C2301 | G2193 | G2133 | A2059 | U1963 | G1845 | C1743 | C1636  | C1504 |       |        | G1137 | A1067 |
| C2381 | G2302 |       | A2134 | A2060 | G1964 | G1845 | C1743 | A1637  | C1504 |       |        | A1139 | G1068 |
| G2382 |       | U2197 | C2135 | G2061 | C1965 | G1846 | G1746 | A1637  | C1505 |       |        | A1139 | A1069 |
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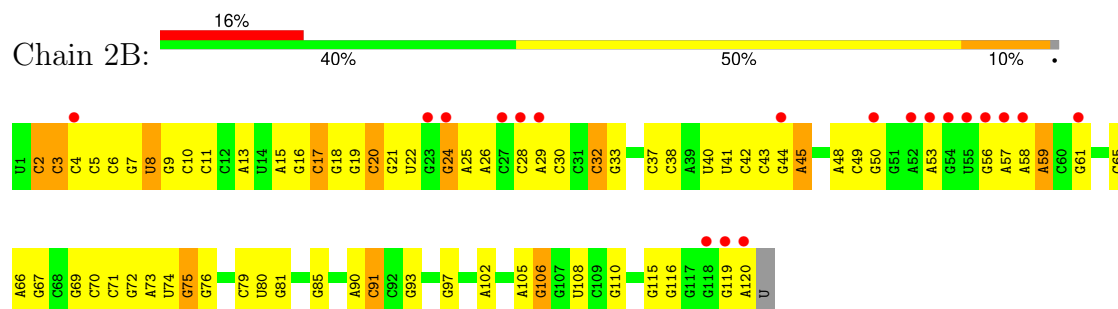
• Molecule 1: 23S Ribosomal RNA



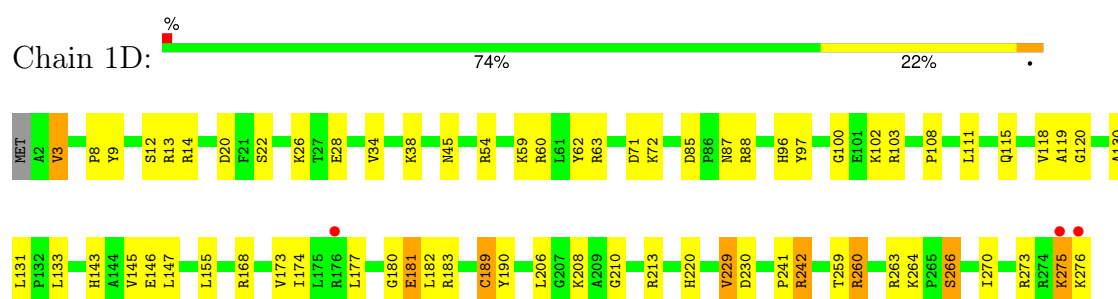
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| U1963 | A1847 | G1756 | A1610 | C1513  | G1429  | C1333 | G1235 | G1149 | G1017 | G942  | G869 | A783 |
| U1964 | A1848 | G1757 | A1614 | U1514  | C1430  | C1336 | G1236 | G1150 | U1019 | U943  | G873 | A784 |
| C1962 | A1853 | G1758 | C1617 | G1519  | A1434  | A1336 | U1239 | C1152 | A1020 | A945  | G874 | G785 |
| U1963 | A1861 | G1763 | G1627 | G1525  | C1437  | G1337 | A1241 | C1153 | A1021 | G946  | A878 | G786 |
| C1965 | A1866 | G1764 | G1628 | A1528  | G1441  | A1349 | A1246 | A1155 | G1022 | G947  | A879 | U787 |
| A1966 | G1865 | G1773 | G1633 | A1528A | G1442  | U1352 | A1247 | U1159 | G1025 | C951  | G880 | A788 |
| C1967 | C1866 | U1777 | G1636 | C1530  | G1444  | A1359 | G1252 | C1161 | A1028 | A957  | G881 | G792 |
| G1968 | A1876 | U1778 | A1637 | C1531  | G1445  | A1360 | A1253 | G1162 | G1029 | U958  | G882 | G793 |
| A1970 | A1877 | U1779 | G1638 | U1533  | G1448  | C1363 | A1254 | U1166 | A1032 | A959  | G883 | G801 |
| A1971 | G1878 | A1780 | C1640 | A      | G1449  | C1364 | G1256 | U1167 | U1027 | A887  | G884 | A802 |
| A1972 | C1781 | G1782 | C1645 | C1536  | G1450  | A1365 | G1260 | G1168 | G1030 | C886  | G885 | G805 |
| G1975 | C1882 | A1783 | G1645 | G1541  | A1452  | G1368 | G1265 | G1169 | U1033 | G961  | C888 | C806 |
| G1984 | G1883 | A1784 | C1646 | G1546  | A1460  | G1369 | U1263 | G1170 | G1034 | G962  | C889 | U807 |
| A1889 | A1785 | G1647 | C1648 | C1547  | G1461  | C1370 | G1266 | G1171 | U1035 | U963  | G890 | G808 |
| A1890 | A1786 | C1648 | C1648 | C1548  | C1462  | G1371 | U1267 | G     | G1036 | C964  | G892 | G809 |
| U1993 | G1899 | G1653 | A1654 | C1548  | C1463  | U1372 | U1268 | U     | U1038 | G966  | C894 | U811 |
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| A1901 | G1792 | G1667 | G1667 | A1558  | C1467  | C1377 | A1268 | C1178 | G1042 | C971  | C897 | C815 |
| C1902 | C1793 | U1671 | U1671 | A1559  | C1468  | A1378 | A1271 | C1179 | C1043 | G972  | C898 | C816 |
| G1906 | C1795 | G1674 | G1674 | G1560  | A1469  | A1379 | A1272 | C1180 | A     | A973  | A999 | C817 |
| C1908 | U1796 | G1674 | G1674 | A1562  | G1470  | C1380 | U1273 | G1183 | A     | C975  | A901 | G818 |
| C1909 | U1798 | C1686 | C1686 | A1566  | A1471  | A1384 | A1274 | U     | G     | A980  | C902 | A820 |
| U2011 | G1799 | G1687 | G1687 | A1567  | G1472  | G1385 | A1275 | G1186 | G     | A983  | C903 | A821 |
| G2012 | C1801 | U1688 | U1688 | A1567  | G1474  | C1386 | A1278 | G1187 | C     | A988  | C904 | C815 |
| A2014 | A1912 | A1689 | A1689 | A1569  | G1476  | G1388 | G1280 | G1192 | A     | G987  | U907 | C816 |
| G2018 | C1914 | U1693 | U1693 | C1577  | A1477  | G1389 | U1288 | G1193 | C     | G989  | C908 | C817 |
| A2019 | A1915 | G1696 | G1696 | U1578  | G1478  | U1394 | C1291 | C1201 | C     | A910  | C909 | U827 |
| U2022 | U1917 | G1697 | G1697 | A1579  | G1482  | A1395 | C1291 | G1202 | G     | A911  | U828 | U828 |
| C2023 | C1920 | A1698 | A1698 | G1581  | A1486  | C1399 | C1295 | A1204 | A     | C914  | G832 | G832 |
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| A2031 | G1929 | C1711 | C1711 | G1594  | U1497  | C1407 | G1303 | A1213 | A     | C995  | G916 | G916 |
| G2032 | U1930 | G1714 | G1714 | G1595  | C1498  | G1416 | G1309 | A1214 | U     | A996  | G917 | G917 |
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| G2037 | A1936 | G1721 | G1721 | C1600  | U1503  | G1418 | C1314 | C1221 | G     | C1005 | G919 | G919 |
| G2038 | A1937 | A1722 | A1722 | G1601  | C1504  | A1419 | C1315 | G1223 | G     | C1006 | G920 | G920 |
| C2039 | U1938 | G1739 | G1739 | U1602  | C1505  | U1420 | A1316 | U1224 | A     | A1010 | U921 | U921 |
| U2041 | G1939 | G1740 | G1740 | A1603  | C1506  | G1421 | A1317 | A1226 | G     | A933  | U922 | G854 |
| G2042 | C1942 | A1741 | A1741 | C1604  | A1507  | G1422 | G1324 | G1230 | C     | U1011 | C923 | G855 |
| C2043 | U1945 | C1745 | C1745 | C1607  | A1508  | G1423 | G1325 | G1231 | A     | U1012 | C924 | C856 |
| A2051 | U1946 | U1834 | U1834 | A1608  | A1509A | G1424 | C1327 | C1233 | G     | U1013 | C925 | C857 |
|       |       |       |       |        |        | A1427 |       |       | C     | G1064 | A926 | U888 |
|       |       |       |       |        |        |       |       |       | A     | C1006 | A926 | G889 |
|       |       |       |       |        |        |       |       |       | A     | A1010 | G932 | U860 |
|       |       |       |       |        |        |       |       |       | G     | A933  | G932 | A861 |
|       |       |       |       |        |        |       |       |       | A     | U1011 | G936 | G862 |
|       |       |       |       |        |        |       |       |       | A     | U1012 | U937 | A863 |
|       |       |       |       |        |        |       |       |       | G     | U1013 | G938 | G864 |
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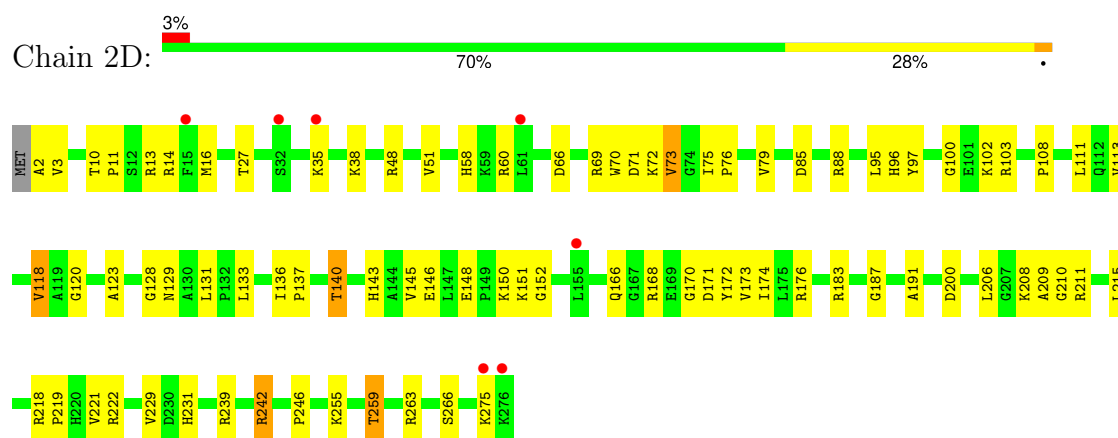
- Molecule 2: 5S Ribosomal RNA



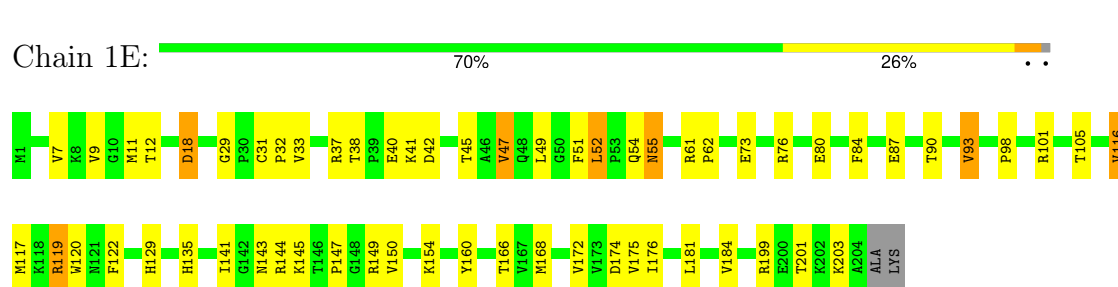
- Molecule 3: 50S ribosomal protein L2



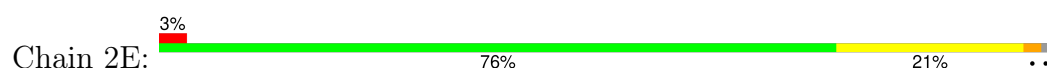
- Molecule 3: 50S ribosomal protein L2

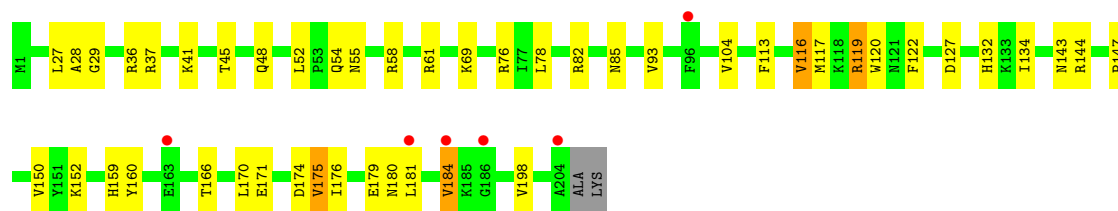


- Molecule 4: 50S ribosomal protein L3



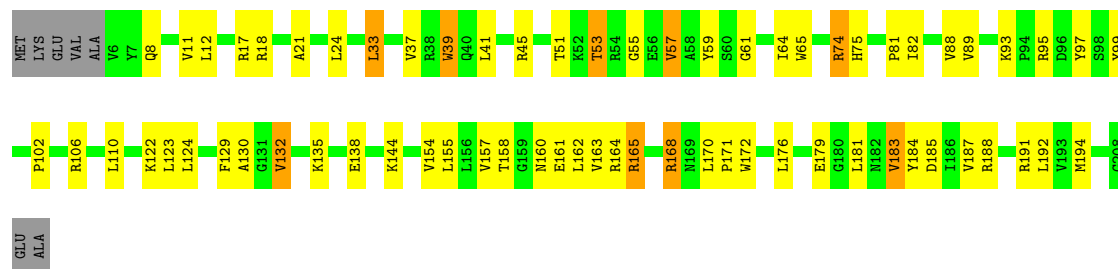
- Molecule 4: 50S ribosomal protein L3





• Molecule 5: 50S ribosomal protein L4

Chain 1F: 65% 28%



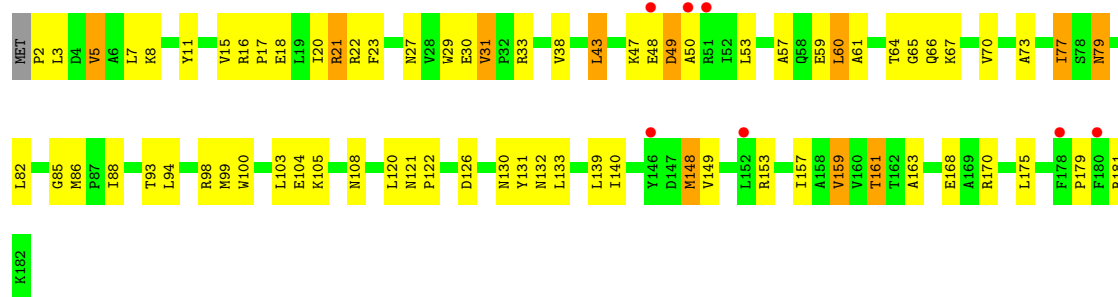
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 53% 39% 5%



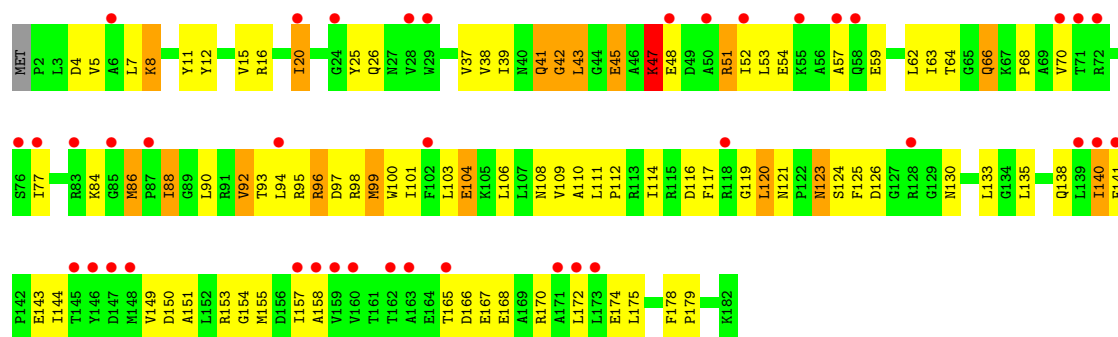
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 59% 34% 6%

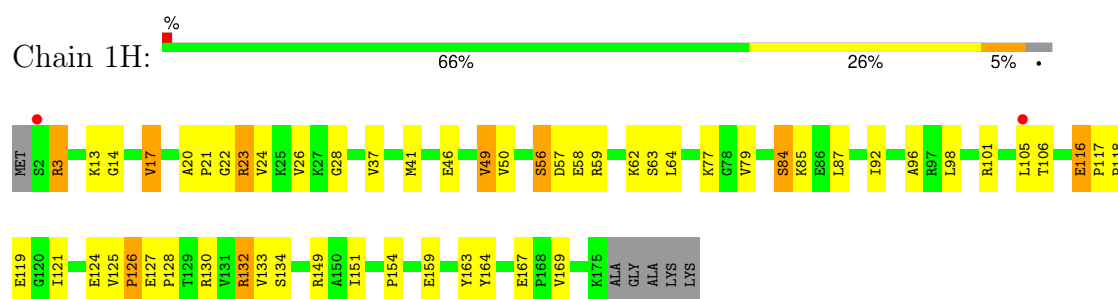


• Molecule 6: 50S ribosomal protein L5

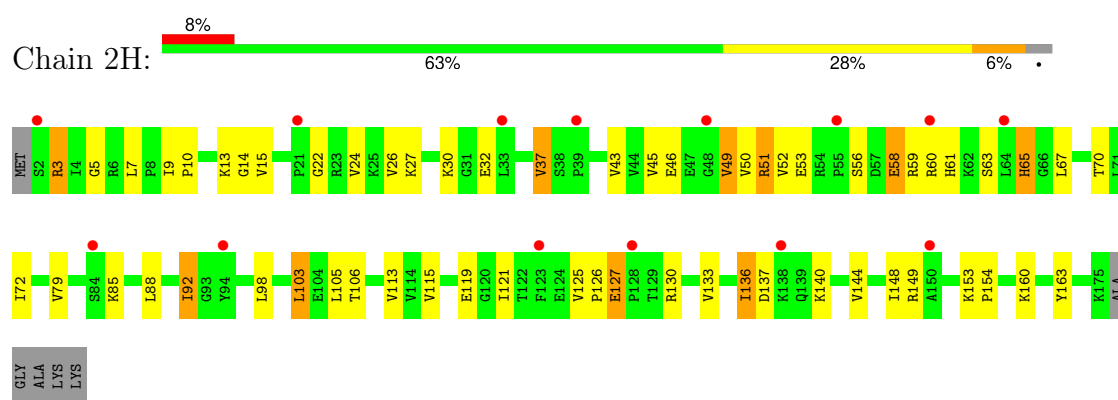
Chain 2G: 49% 40% 9%



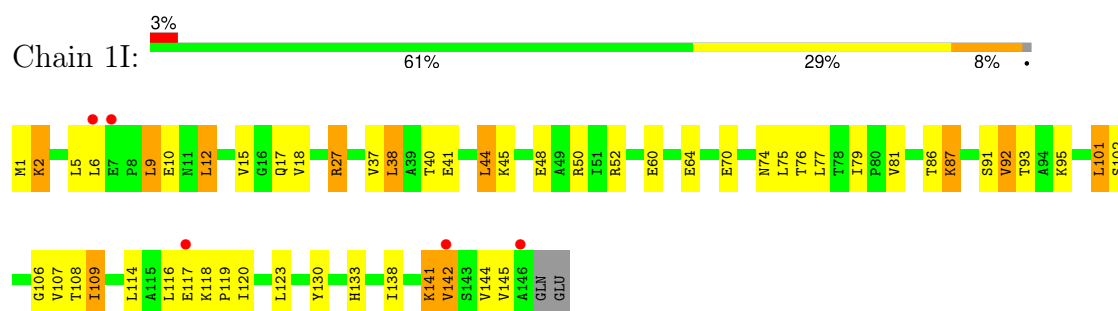
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

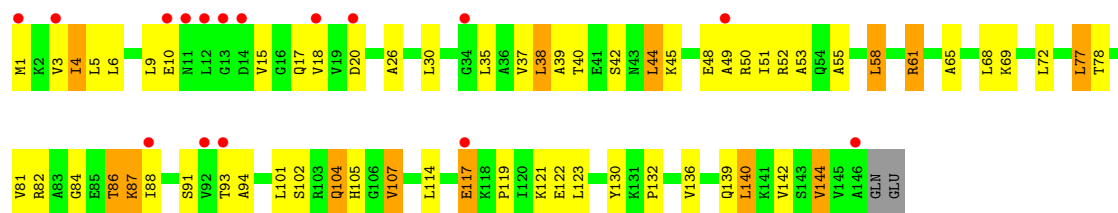


• Molecule 8: 50S ribosomal protein L9

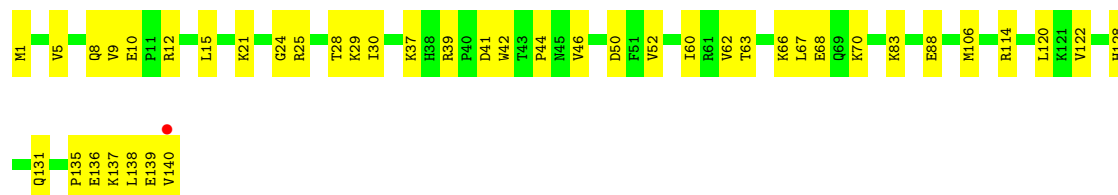


• Molecule 8: 50S ribosomal protein L9

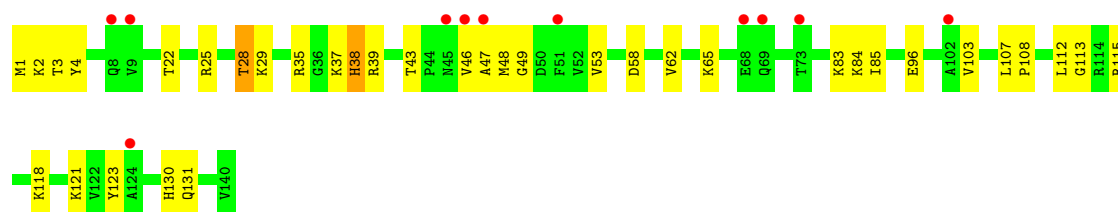
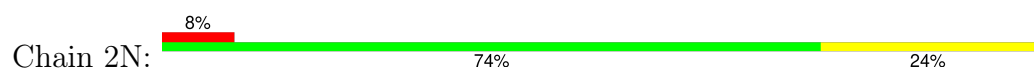




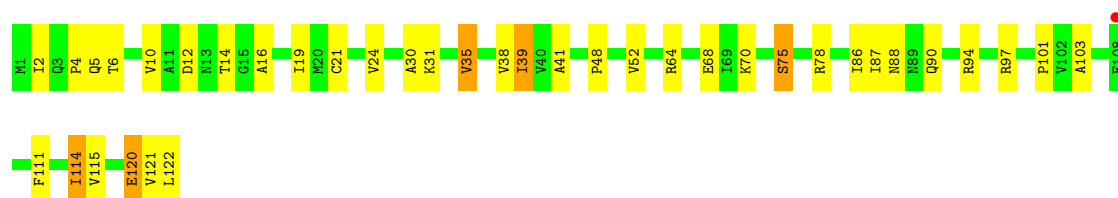
● Molecule 9: 50S ribosomal protein L13



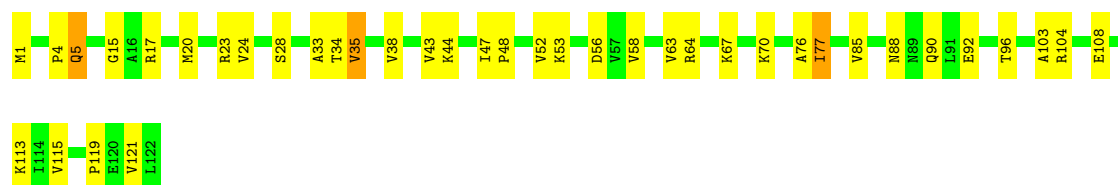
● Molecule 9: 50S ribosomal protein L13



● Molecule 10: 50S ribosomal protein L14

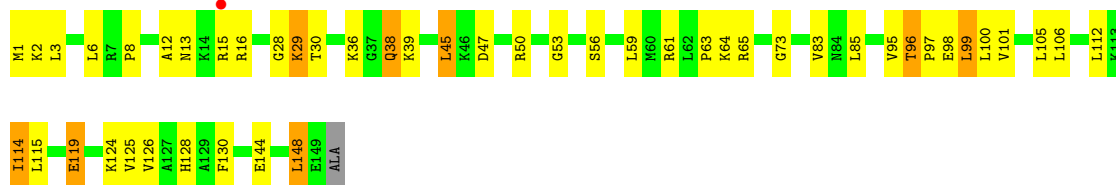


● Molecule 10: 50S ribosomal protein L14



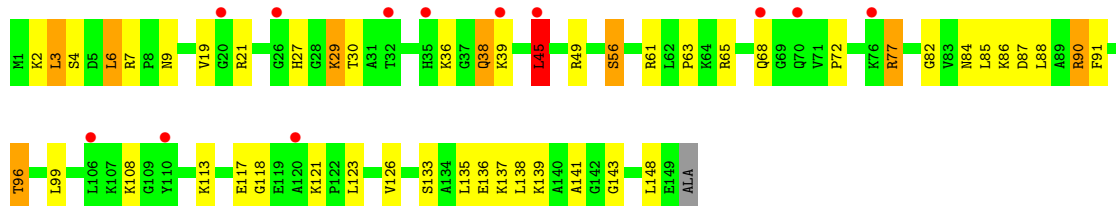
● Molecule 11: 50S ribosomal protein L15

Chain 1P: 



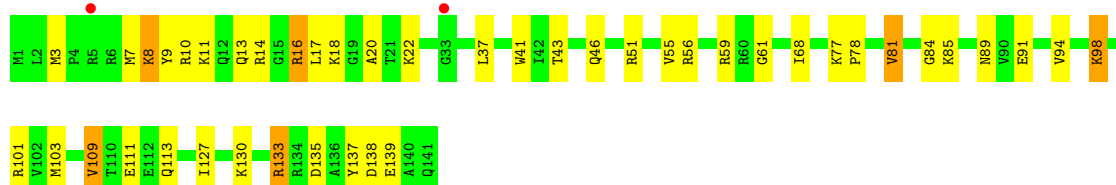
- Molecule 11: 50S ribosomal protein L15

Chain 2P: 



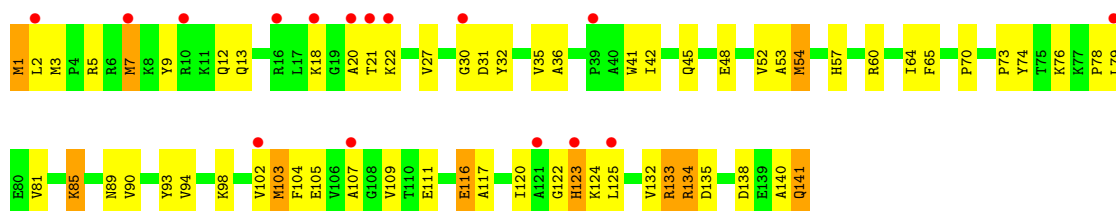
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 



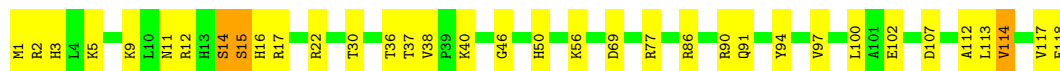
- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 



- Molecule 13: 50S ribosomal protein L17

Chain 1R: 



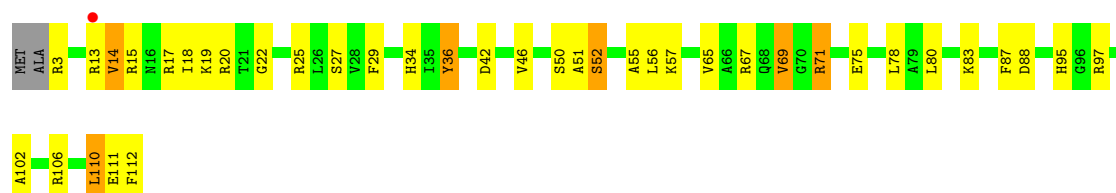
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  70% 30%



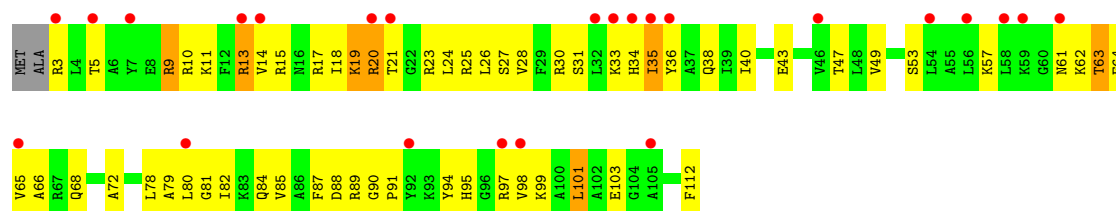
• Molecule 14: 50S ribosomal protein L18

Chain 1S:  63% 29% 5%



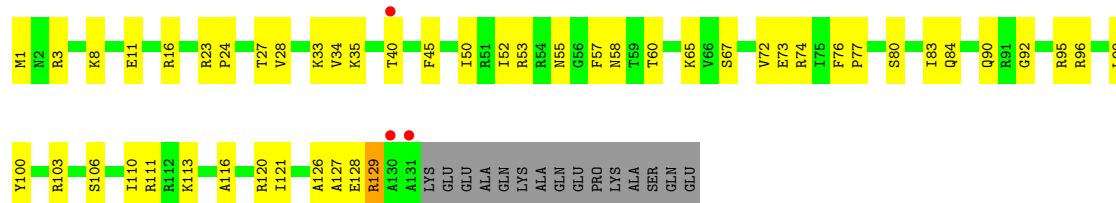
• Molecule 14: 50S ribosomal protein L18

Chain 2S:  21% 45% 47% 6%



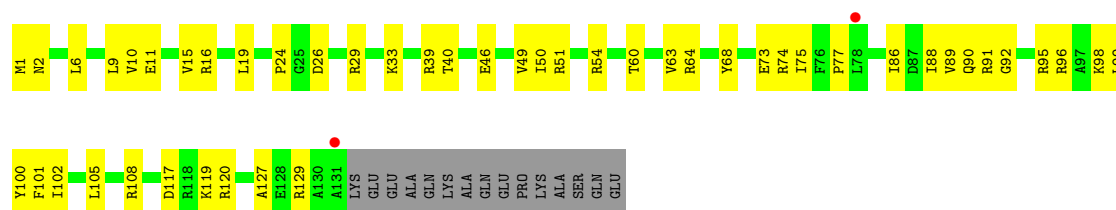
• Molecule 15: 50S ribosomal protein L19

Chain 1T:  2% 56% 33% 10%

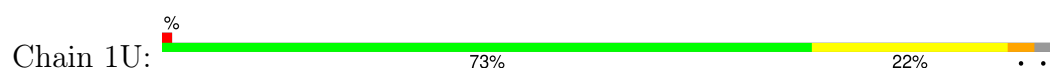


• Molecule 15: 50S ribosomal protein L19

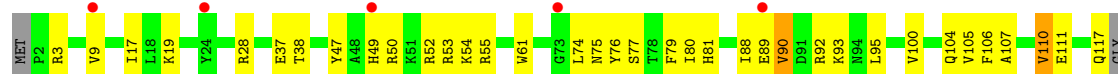
Chain 2T:  57% 33% 10%



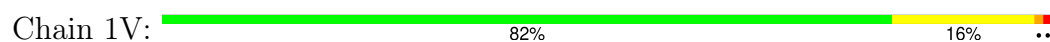
• Molecule 16: 50S ribosomal protein L20



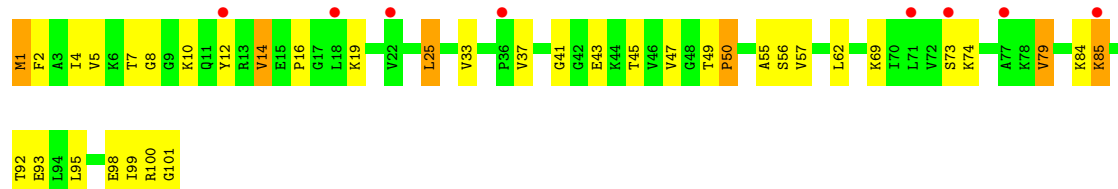
- Molecule 16: 50S ribosomal protein L20



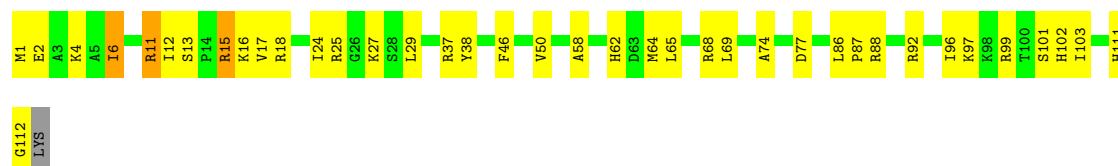
- Molecule 17: 50S ribosomal protein L21



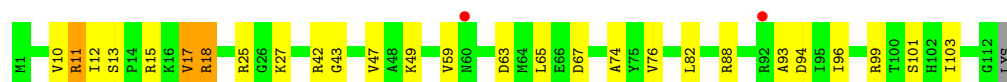
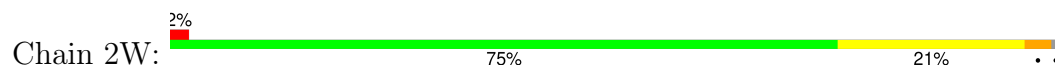
- Molecule 17: 50S ribosomal protein L21



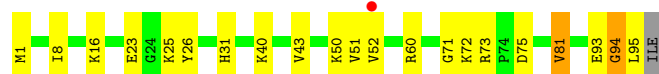
- Molecule 18: 50S ribosomal protein L22



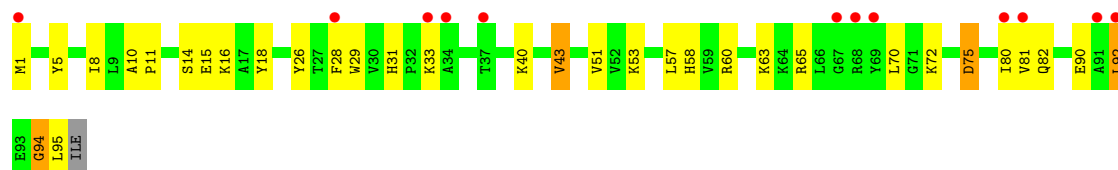
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



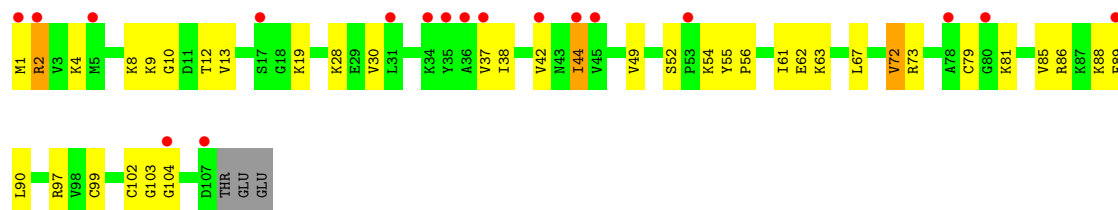
Chain 2X: 



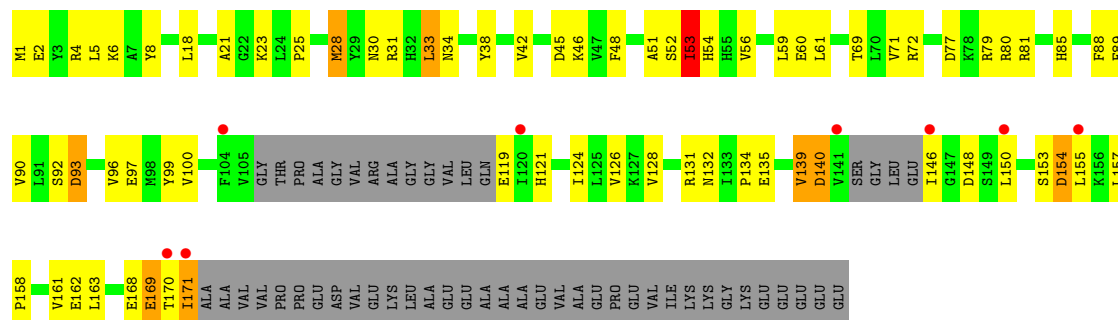
Chain 1Y: 

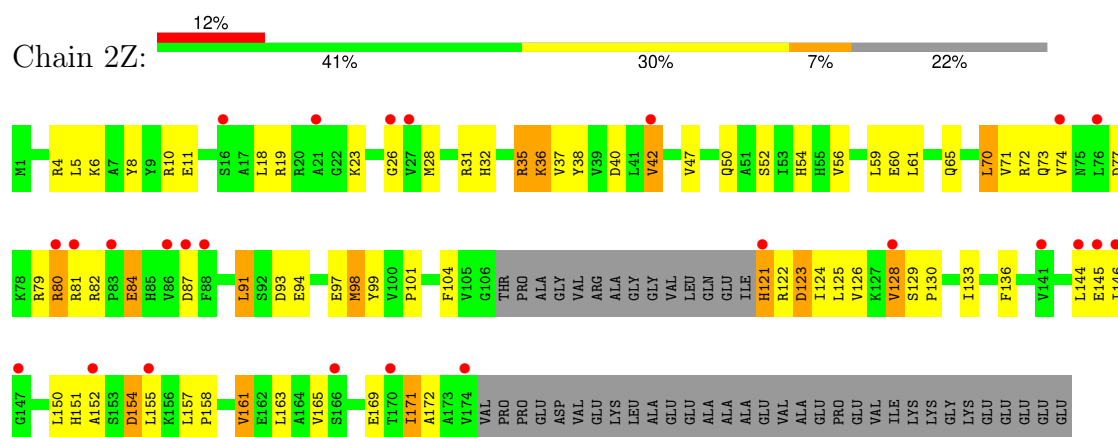


Chain 2Y: 

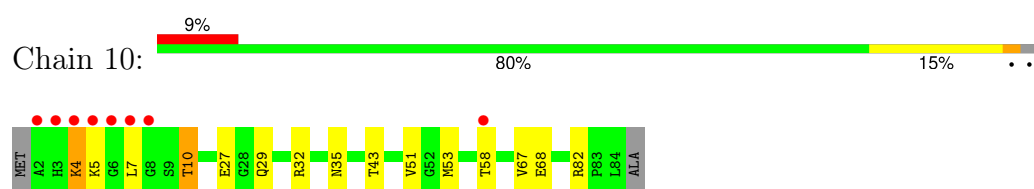


Chain 1Z: 

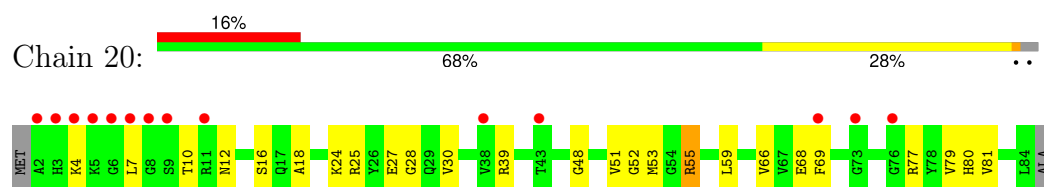




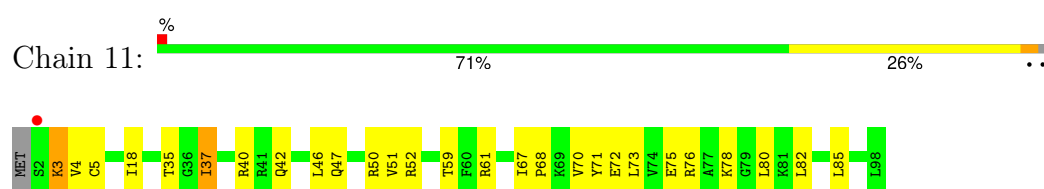
- Molecule 22: 50S ribosomal protein L27



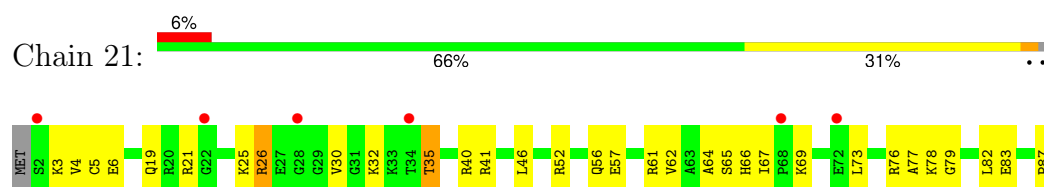
- Molecule 22: 50S ribosomal protein L27



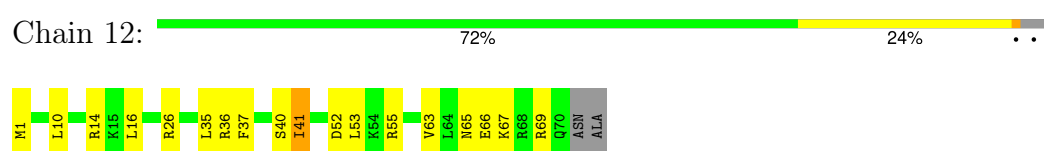
- Molecule 23: 50S ribosomal protein L28



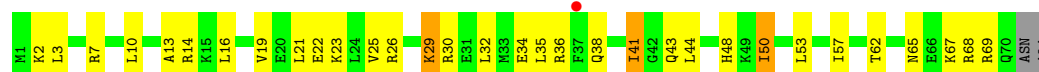
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



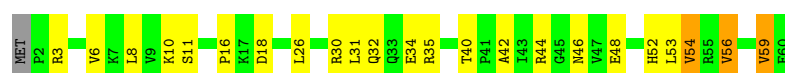
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



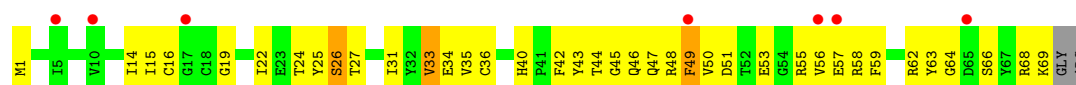
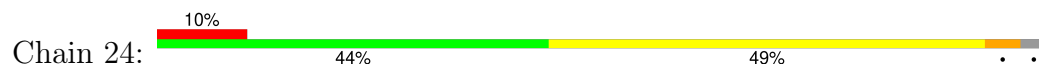
- Molecule 25: 50S ribosomal protein L30



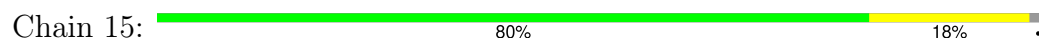
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



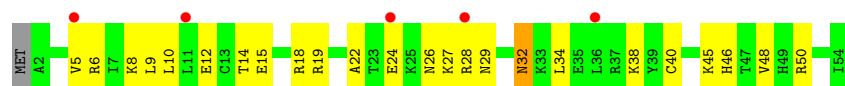
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



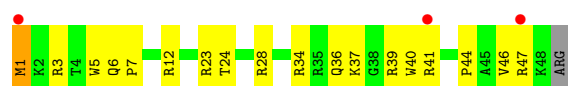
- Molecule 28: 50S ribosomal protein L33



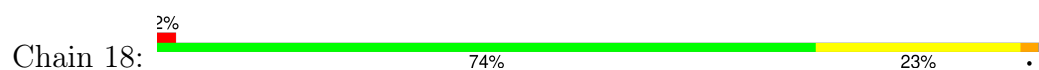
- Molecule 29: 50S ribosomal protein L34



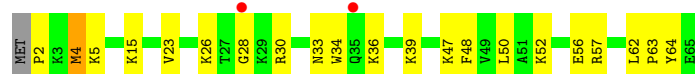
- Molecule 29: 50S ribosomal protein L34



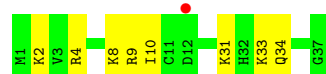
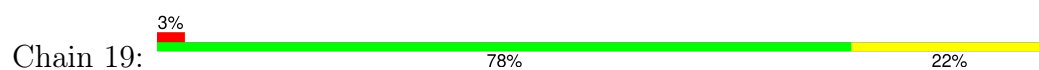
- Molecule 30: 50S ribosomal protein L35



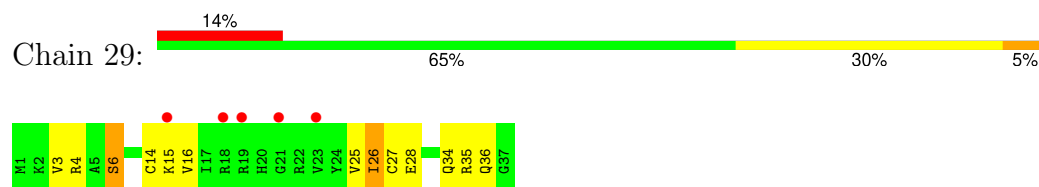
- Molecule 30: 50S ribosomal protein L35



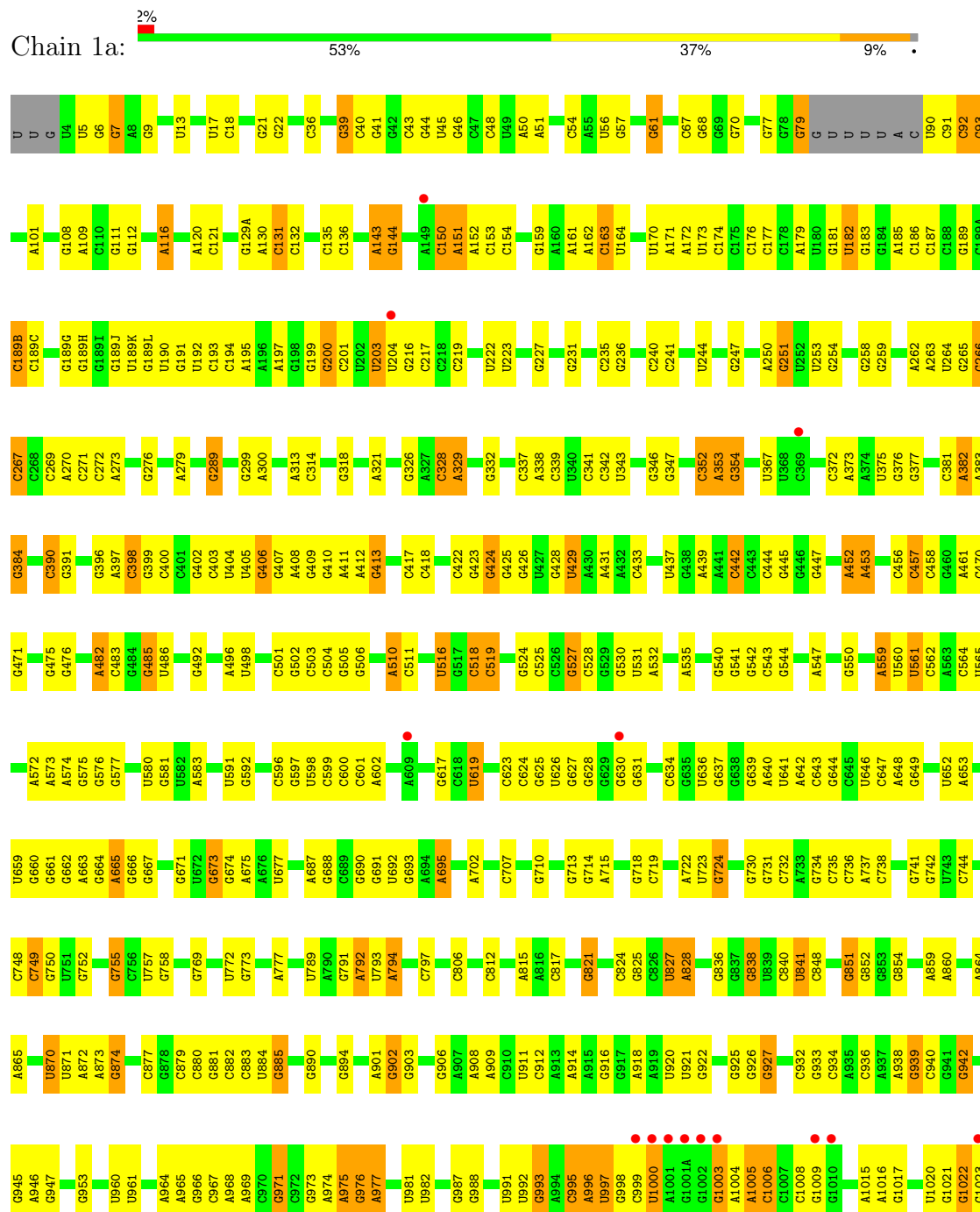
- Molecule 31: 50S ribosomal protein L36

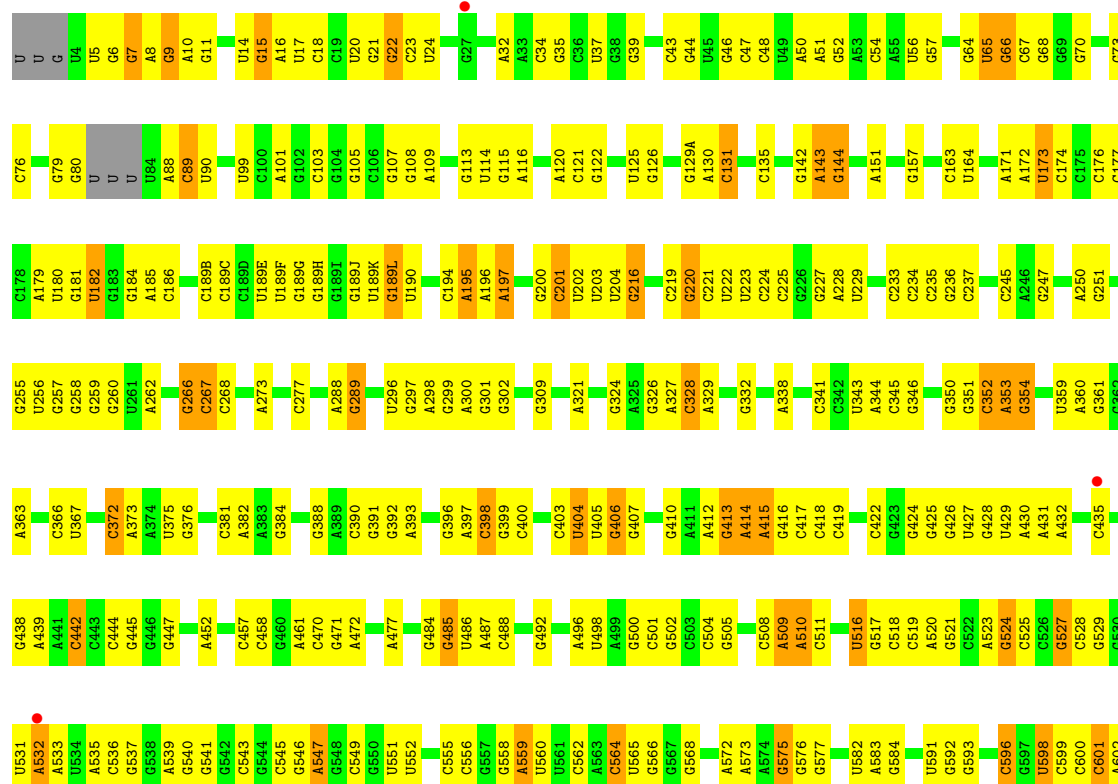


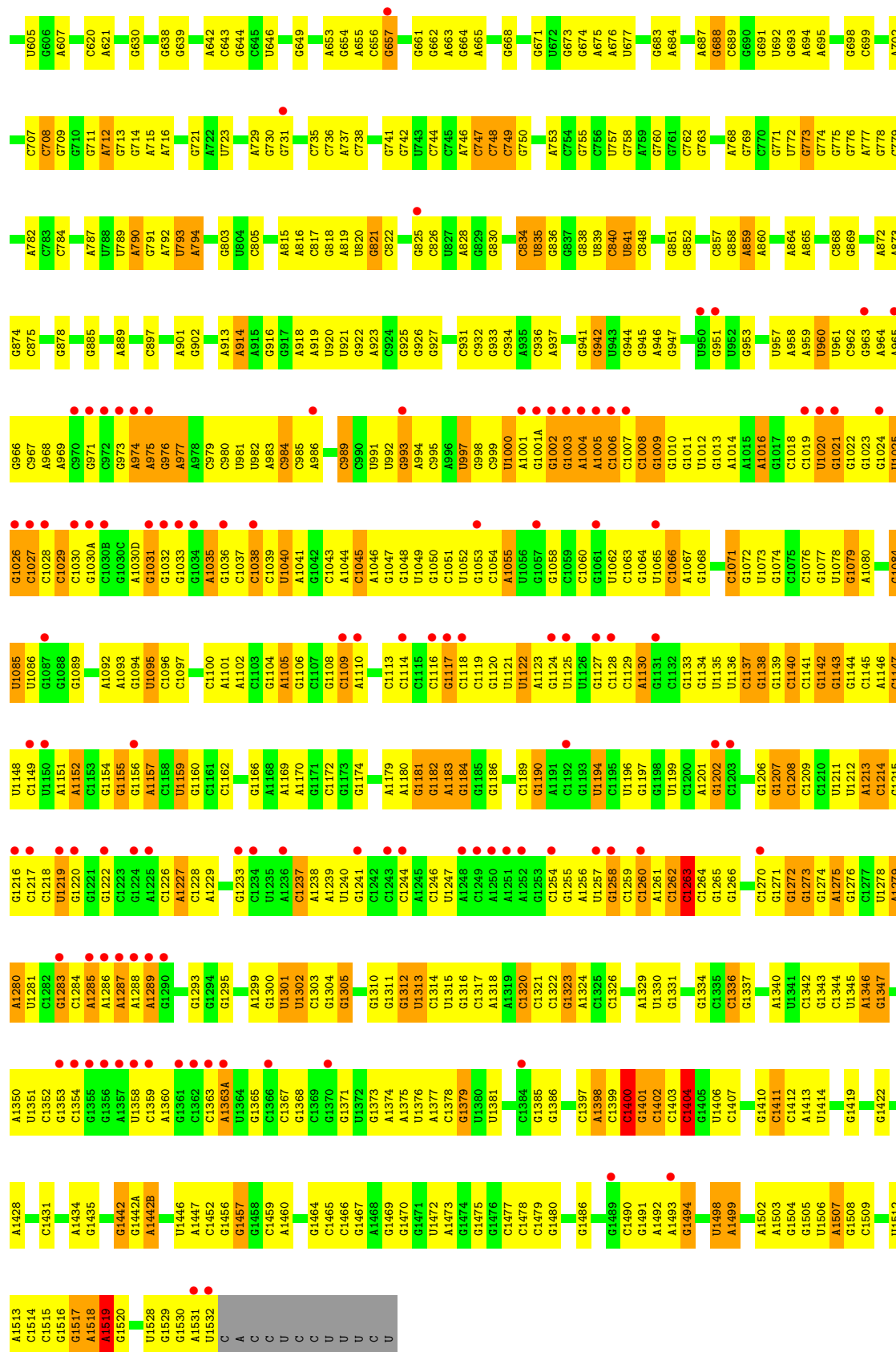
• Molecule 31: 50S ribosomal protein L36



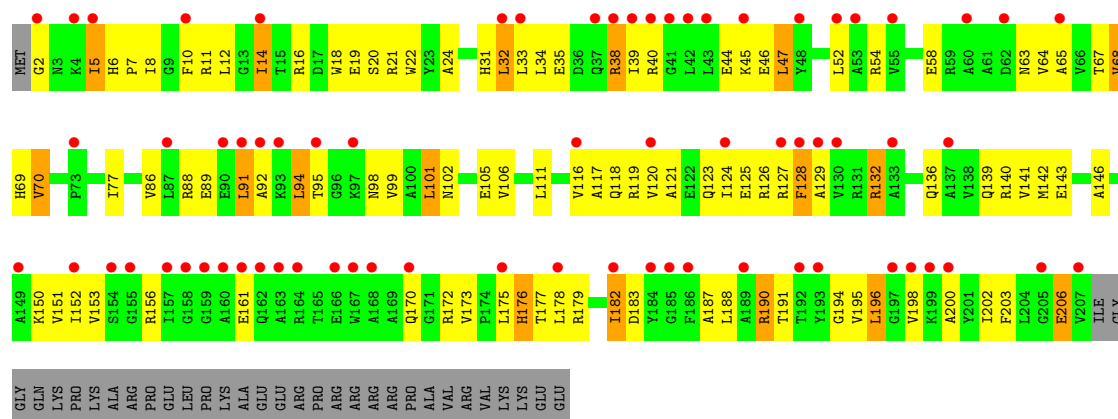
• Molecule 32: 16S Ribosomal RNA





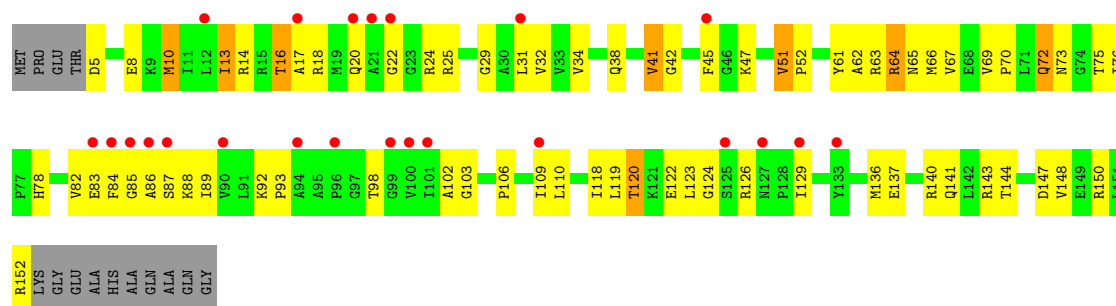








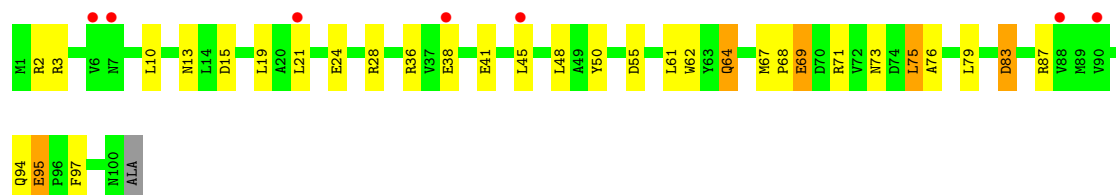
• Molecule 36: 30S ribosomal protein S5



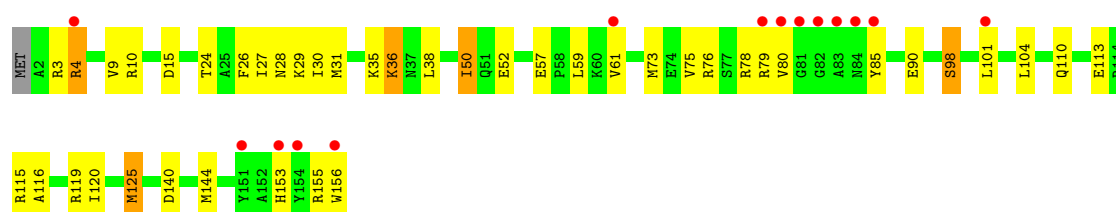
• Molecule 37: 30S ribosomal protein S6



• Molecule 37: 30S ribosomal protein S6

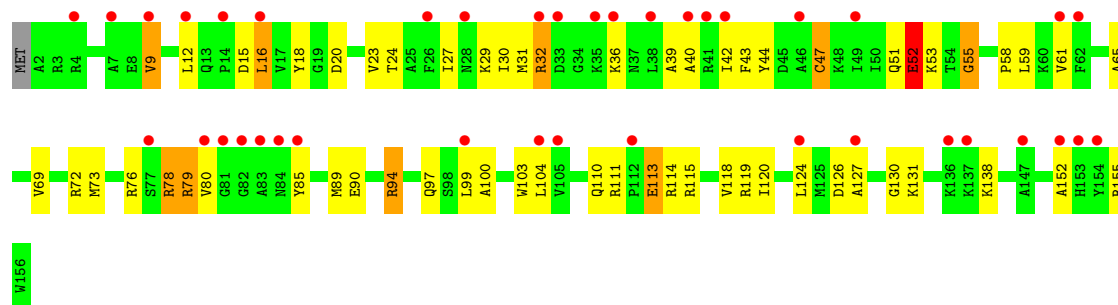


• Molecule 38: 30S ribosomal protein S7

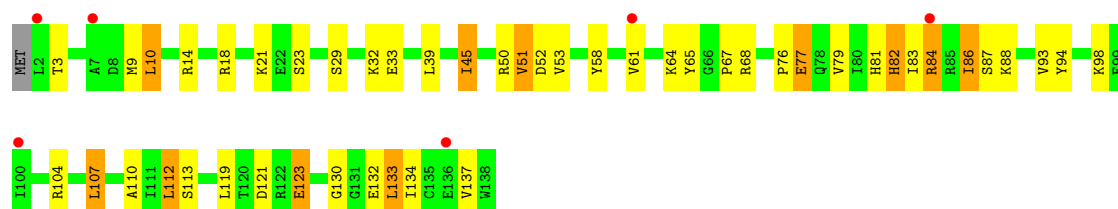


• Molecule 38: 30S ribosomal protein S7

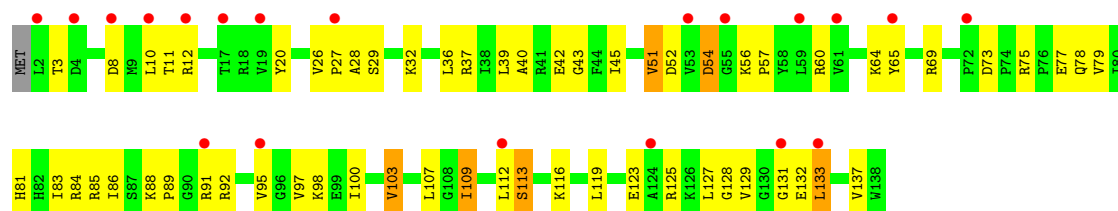




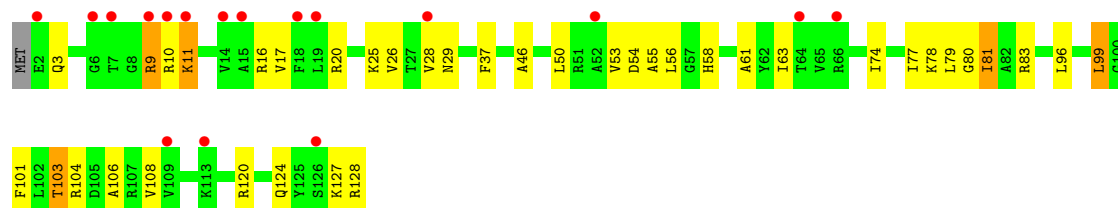
• Molecule 39: 30S ribosomal protein S8



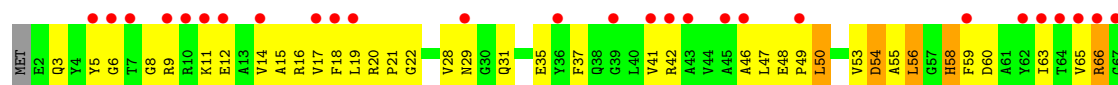
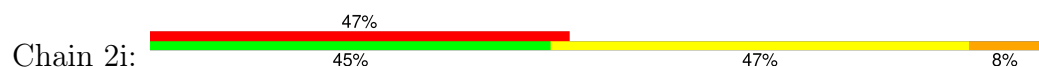
• Molecule 39: 30S ribosomal protein S8



• Molecule 40: 30S ribosomal protein S9

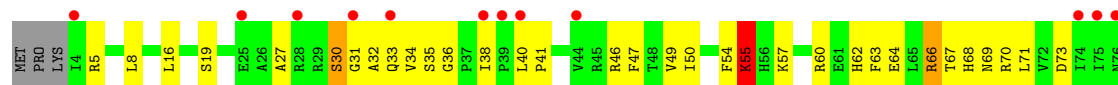


• Molecule 40: 30S ribosomal protein S9

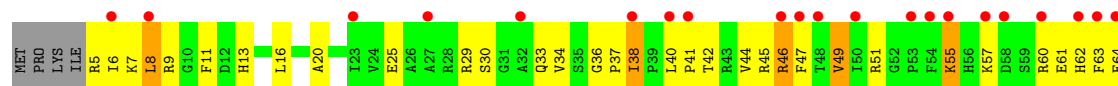




• Molecule 41: 30S ribosomal protein S10



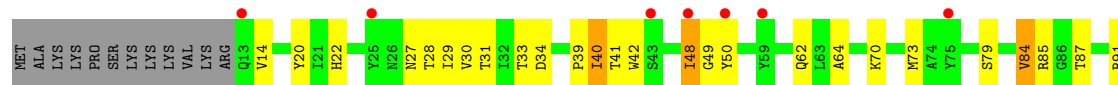
• Molecule 41: 30S ribosomal protein S10



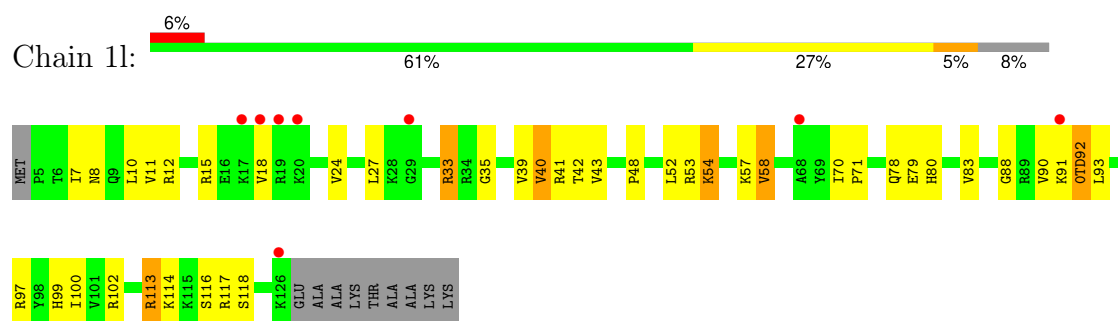
• Molecule 42: 30S ribosomal protein S11



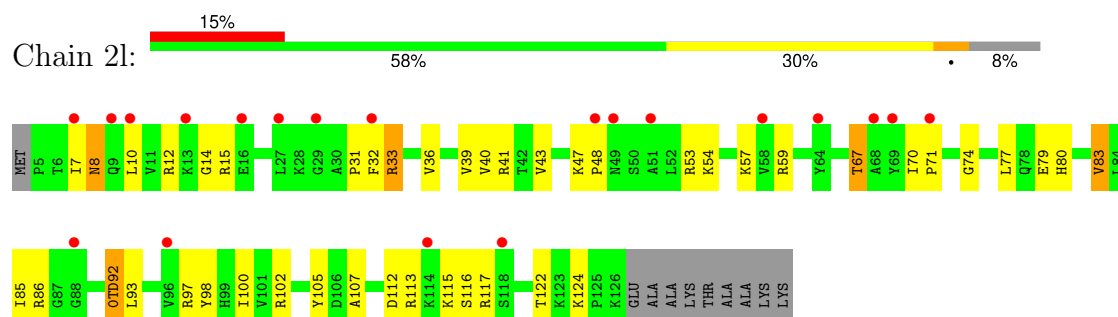
• Molecule 42: 30S ribosomal protein S11



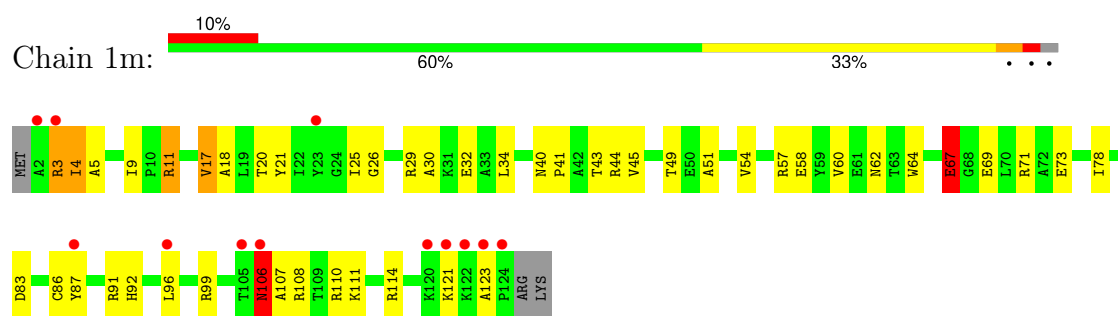
• Molecule 43: 30S ribosomal protein S12



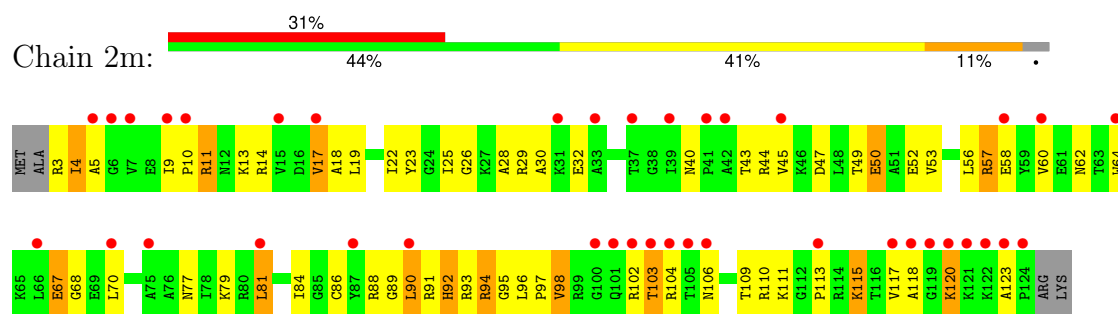
- Molecule 43: 30S ribosomal protein S12



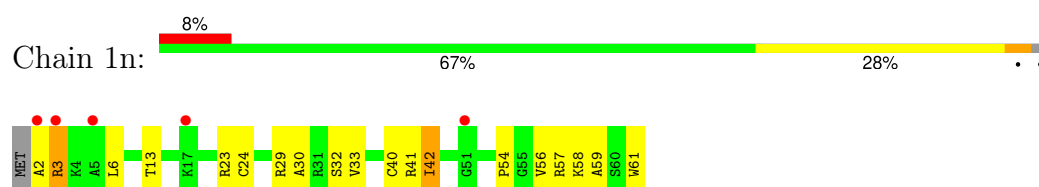
- Molecule 44: 30S ribosomal protein S13



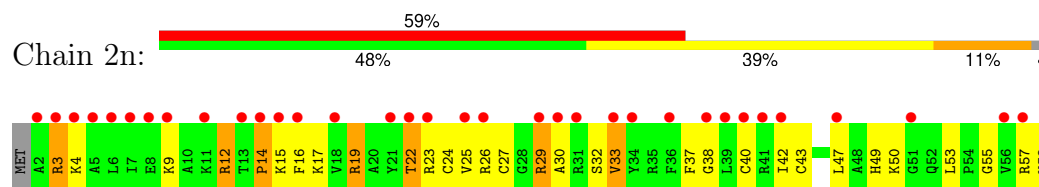
- Molecule 44: 30S ribosomal protein S13



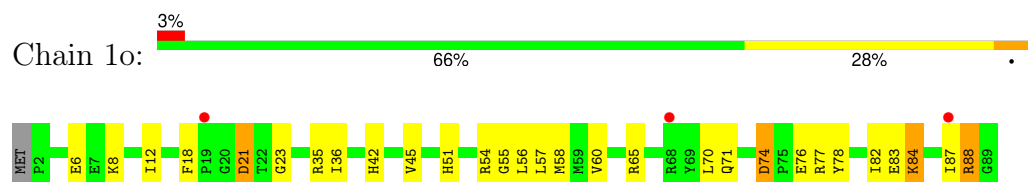
- Molecule 45: 30S ribosomal protein S14 type Z



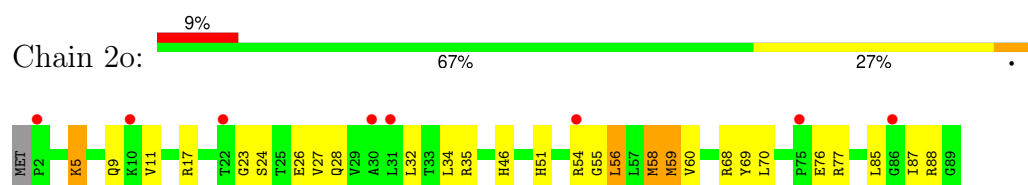
- Molecule 45: 30S ribosomal protein S14 type Z



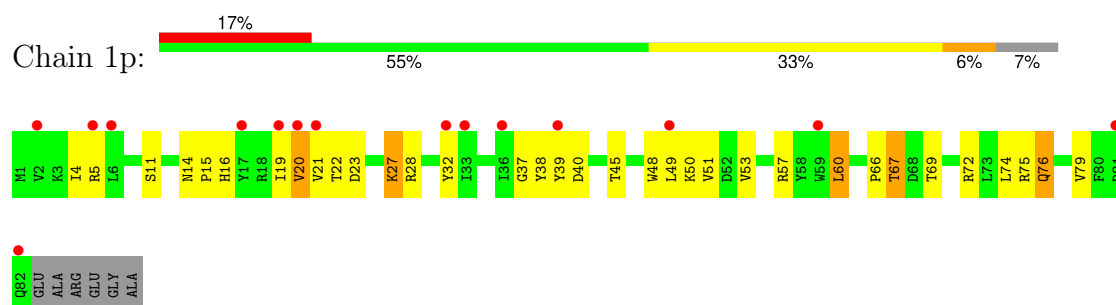
- Molecule 46: 30S ribosomal protein S15



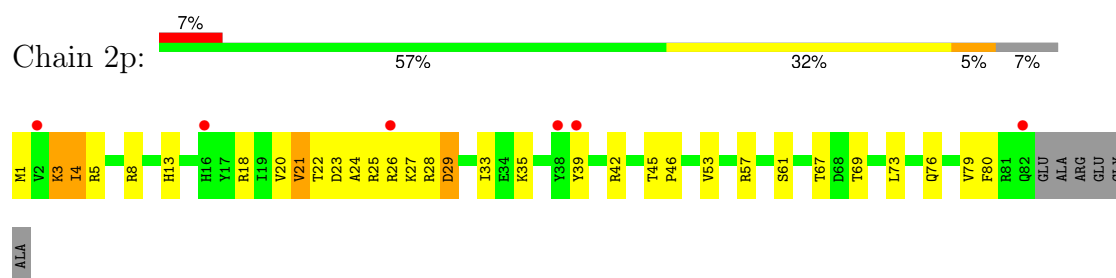
- Molecule 46: 30S ribosomal protein S15



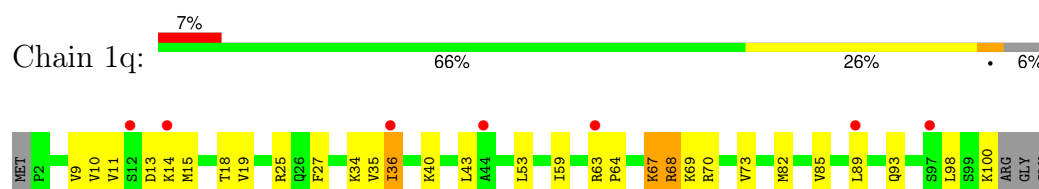
- Molecule 47: 30S ribosomal protein S16



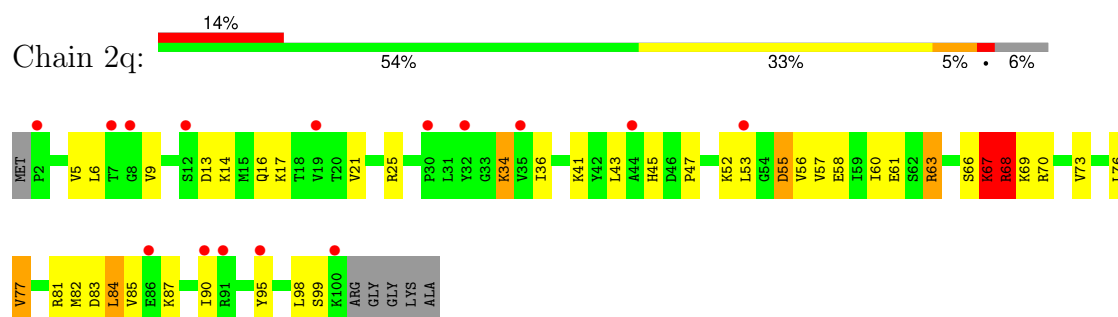
- Molecule 47: 30S ribosomal protein S16



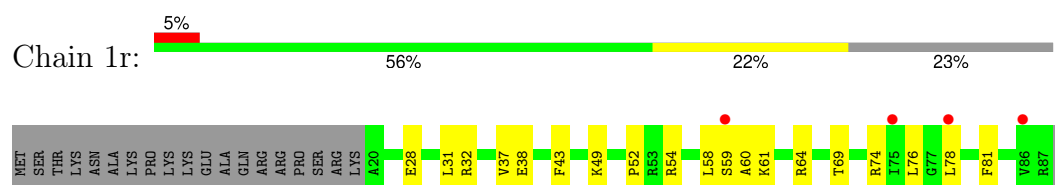
- Molecule 48: 30S ribosomal protein S17



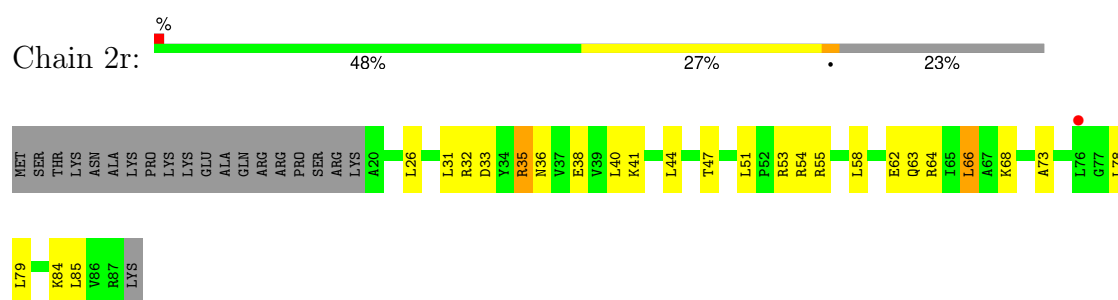
- Molecule 48: 30S ribosomal protein S17



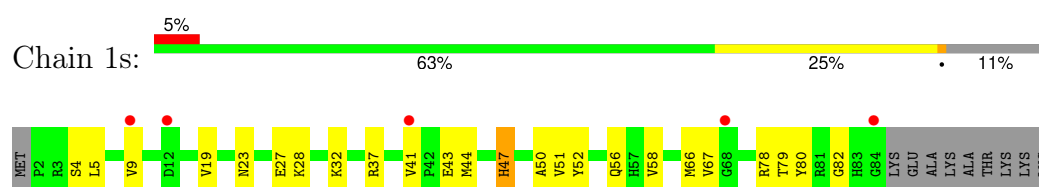
- Molecule 49: 30S ribosomal protein S18



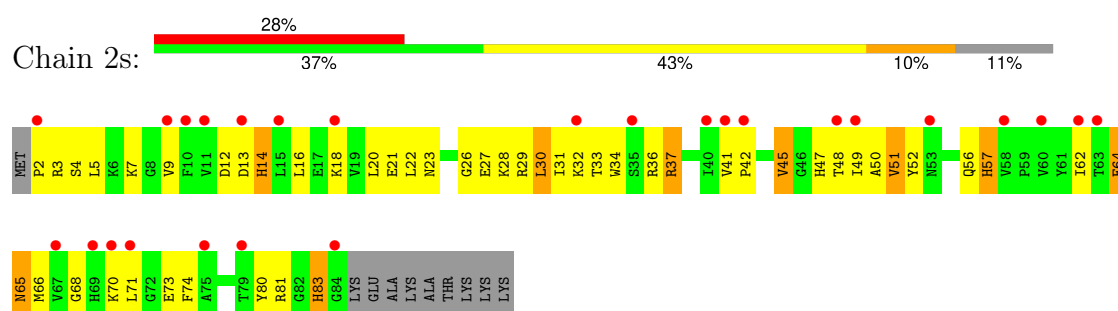
- Molecule 49: 30S ribosomal protein S18



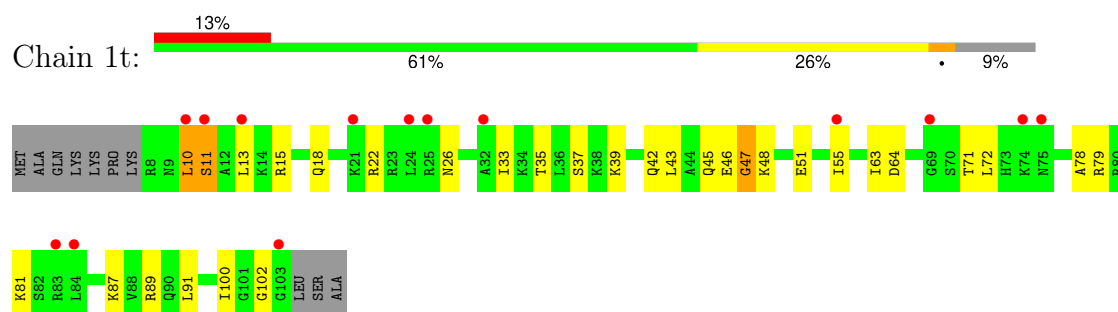
- Molecule 50: 30S ribosomal protein S19



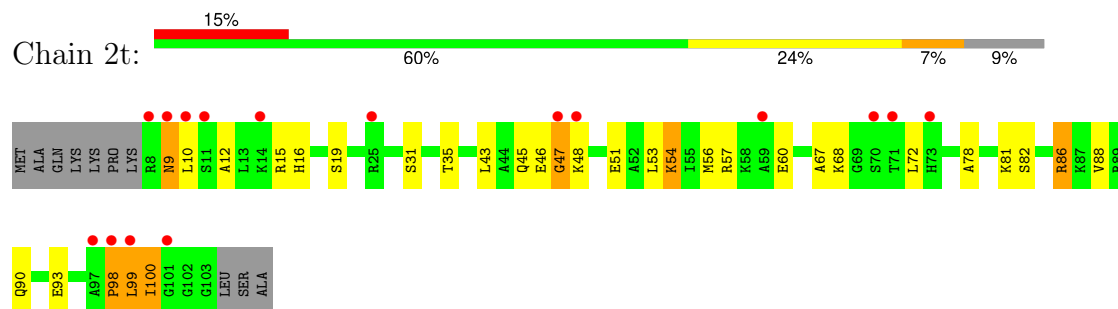
- Molecule 50: 30S ribosomal protein S19



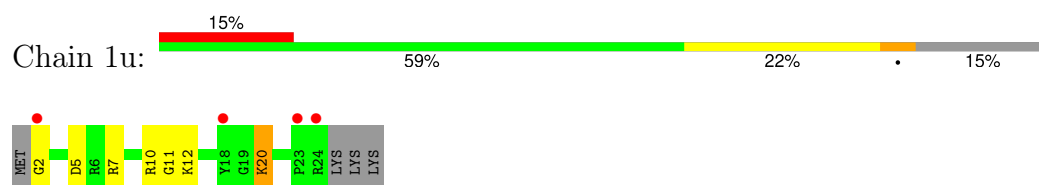
- Molecule 51: 30S ribosomal protein S20



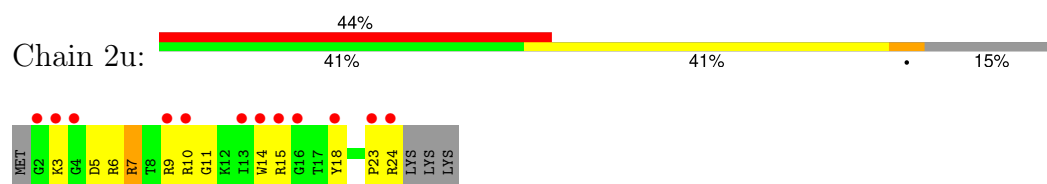
- Molecule 51: 30S ribosomal protein S20



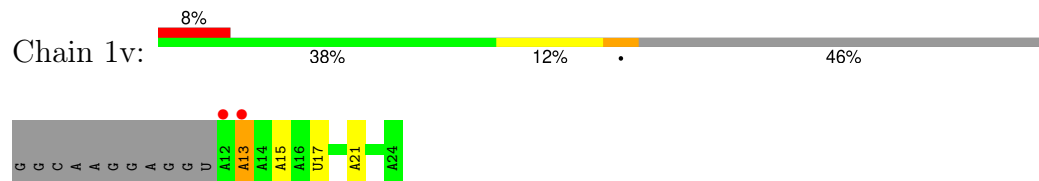
- Molecule 52: 30S ribosomal protein Thx



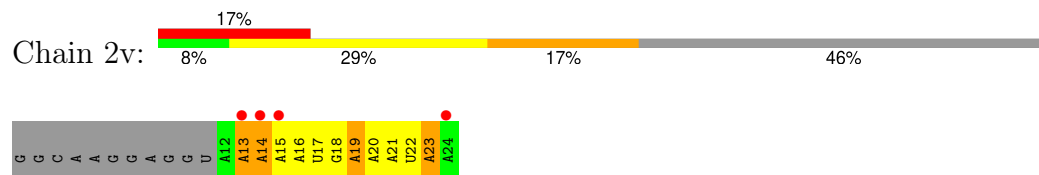
- Molecule 52: 30S ribosomal protein Thx



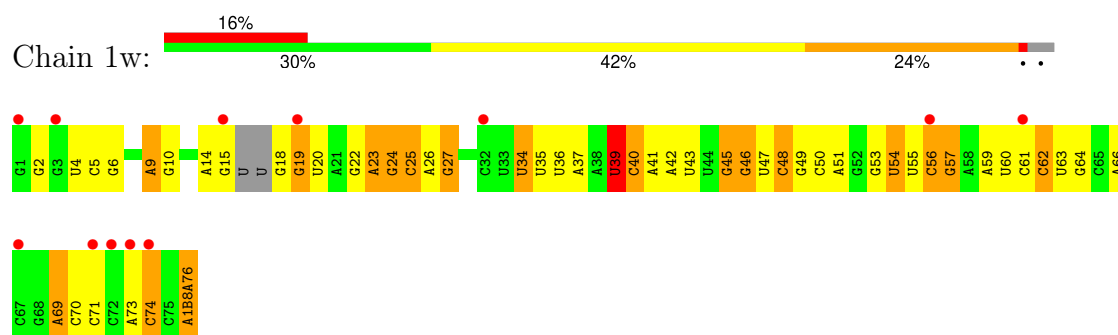
- Molecule 53: MET-LYS-mRNA



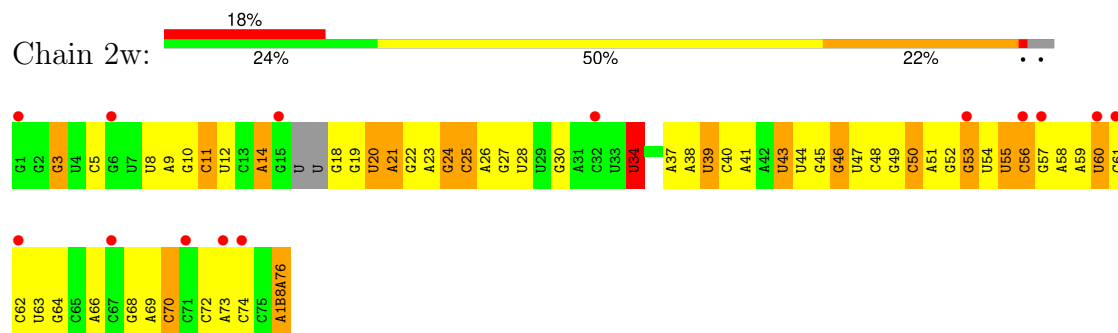
- Molecule 53: MET-LYS-mRNA



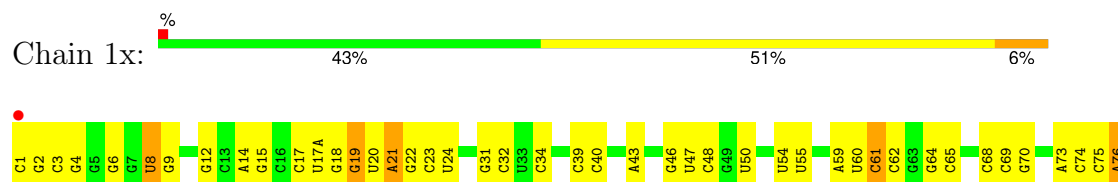
- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys



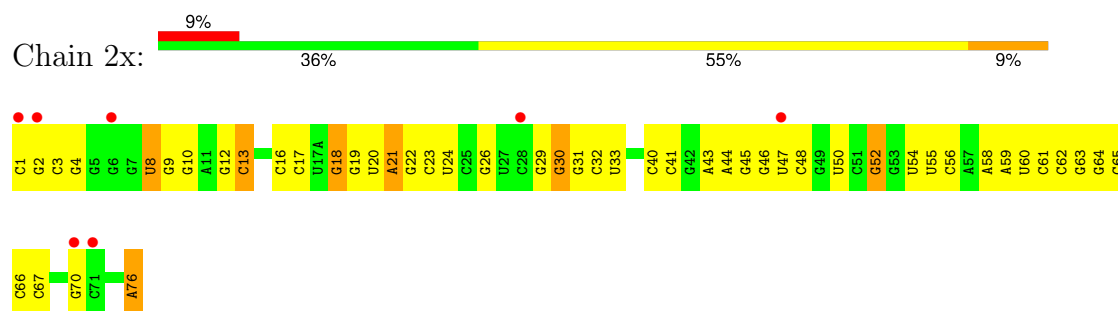
• Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA<sub>Lys</sub>



• Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA<sub>Cys</sub> RNA-part



• Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA<sub>Cys</sub> RNA-part



• Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA<sub>Cys</sub> Peptide-part

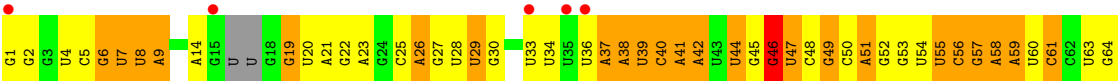
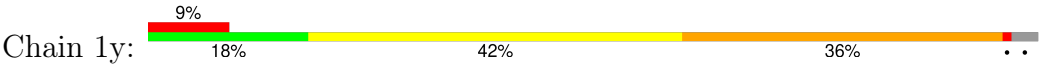


• Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA<sub>Cys</sub> Peptide-part

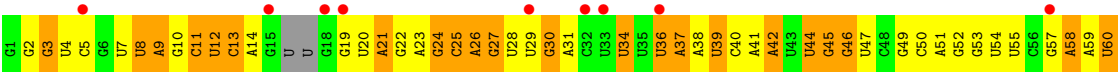
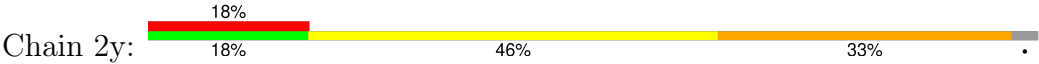




● Molecule 57: E-site Deacylated tRNAlys



● Molecule 57: E-site Deacylated tRNAlys



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.04Å 447.59Å 618.98Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 124.58 – 2.80<br>124.58 – 2.80                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (124.58-2.80)<br>99.2 (124.58-2.80)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.31                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.23 (at 2.82Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1                                               | Depositor        |
| R, $R_{free}$                                                           | 0.229 , 0.281<br>0.229 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 70313 reflections (4.98%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.218                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 54.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 299377                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: 5MU, OMC, A1B8A, TEL, OMG, 2MG, UR3, G7M, ZN, 2MA, M2G, 0TD, MA6, K, 4SU, SF4, OMU, MG, 4OC, T6A, FME, U8U, 5MC, PSU, 8AN

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    | 0.27         | 1/69011 (0.0%) | 0.46        | 1/107720 (0.0%) |
| 1   | 2A    | 0.21         | 0/67295        | 0.40        | 1/105042 (0.0%) |
| 2   | 1B    | 0.21         | 0/2882         | 0.40        | 0/4494          |
| 2   | 2B    | 0.19         | 0/2879         | 0.38        | 0/4487          |
| 3   | 1D    | 0.28         | 0/2186         | 0.52        | 0/2944          |
| 3   | 2D    | 0.23         | 0/2186         | 0.47        | 0/2944          |
| 4   | 1E    | 0.26         | 0/1592         | 0.50        | 0/2149          |
| 4   | 2E    | 0.24         | 0/1592         | 0.45        | 0/2149          |
| 5   | 1F    | 0.24         | 0/1619         | 0.48        | 0/2193          |
| 5   | 2F    | 0.21         | 0/1615         | 0.47        | 0/2188          |
| 6   | 1G    | 0.22         | 0/1448         | 0.46        | 0/1957          |
| 6   | 2G    | 0.20         | 0/1453         | 0.46        | 0/1963          |
| 7   | 1H    | 0.22         | 0/1356         | 0.41        | 0/1834          |
| 7   | 2H    | 0.21         | 0/1356         | 0.41        | 0/1834          |
| 8   | 1I    | 0.20         | 0/1112         | 0.43        | 0/1514          |
| 8   | 2I    | 0.19         | 0/1079         | 0.40        | 0/1475          |
| 9   | 1N    | 0.25         | 0/1144         | 0.45        | 0/1543          |
| 9   | 2N    | 0.19         | 0/1144         | 0.38        | 0/1543          |
| 10  | 1O    | 0.25         | 0/943          | 0.49        | 0/1269          |
| 10  | 2O    | 0.23         | 0/943          | 0.48        | 0/1269          |
| 11  | 1P    | 0.26         | 0/1152         | 0.52        | 0/1533          |
| 11  | 2P    | 0.21         | 0/1152         | 0.51        | 0/1533          |
| 12  | 1Q    | 0.27         | 0/1143         | 0.48        | 0/1527          |
| 12  | 2Q    | 0.21         | 0/1143         | 0.45        | 0/1527          |
| 13  | 1R    | 0.26         | 0/982          | 0.49        | 0/1312          |
| 13  | 2R    | 0.24         | 0/982          | 0.53        | 0/1312          |
| 14  | 1S    | 0.23         | 0/883          | 0.46        | 0/1176          |
| 14  | 2S    | 0.20         | 0/880          | 0.47        | 0/1172          |
| 15  | 1T    | 0.25         | 0/1105         | 0.53        | 1/1477 (0.1%)   |
| 15  | 2T    | 0.20         | 0/1097         | 0.45        | 0/1468          |
| 16  | 1U    | 0.26         | 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          | 0.44        | 0/1049         |
| 17  | 2V    | 0.19         | 0/782          | 0.42        | 0/1049         |
| 18  | 1W    | 0.26         | 0/897          | 0.45        | 0/1205         |
| 18  | 2W    | 0.22         | 0/897          | 0.43        | 0/1205         |
| 19  | 1X    | 0.27         | 0/764          | 0.55        | 0/1025         |
| 19  | 2X    | 0.24         | 0/764          | 0.52        | 0/1025         |
| 20  | 1Y    | 0.22         | 0/819          | 0.48        | 0/1095         |
| 20  | 2Y    | 0.21         | 0/819          | 0.43        | 0/1095         |
| 21  | 1Z    | 0.22         | 0/1267         | 0.47        | 0/1717         |
| 21  | 2Z    | 0.21         | 0/1299         | 0.42        | 0/1763         |
| 22  | 10    | 0.25         | 0/662          | 0.47        | 0/881          |
| 22  | 20    | 0.23         | 0/662          | 0.46        | 0/881          |
| 23  | 11    | 0.24         | 0/762          | 0.43        | 0/1014         |
| 23  | 21    | 0.22         | 0/762          | 0.44        | 0/1014         |
| 24  | 12    | 0.24         | 0/590          | 0.45        | 0/781          |
| 24  | 22    | 0.20         | 0/590          | 0.42        | 0/781          |
| 25  | 13    | 0.23         | 0/474          | 0.45        | 0/635          |
| 25  | 23    | 0.18         | 0/469          | 0.39        | 0/630          |
| 26  | 14    | 0.22         | 0/565          | 0.54        | 0/761          |
| 26  | 24    | 0.22         | 0/545          | 0.55        | 0/737          |
| 27  | 15    | 0.25         | 0/469          | 0.51        | 0/635          |
| 27  | 25    | 0.23         | 0/469          | 0.46        | 0/635          |
| 28  | 16    | 0.26         | 0/460          | 0.44        | 0/613          |
| 28  | 26    | 0.20         | 0/456          | 0.40        | 0/608          |
| 29  | 17    | 0.26         | 0/426          | 0.51        | 0/561          |
| 29  | 27    | 0.24         | 0/426          | 0.50        | 0/561          |
| 30  | 18    | 0.27         | 0/525          | 0.49        | 0/691          |
| 30  | 28    | 0.21         | 0/525          | 0.42        | 0/691          |
| 31  | 19    | 0.26         | 0/310          | 0.53        | 0/407          |
| 31  | 29    | 0.20         | 0/310          | 0.40        | 0/407          |
| 32  | 1a    | 0.20         | 0/35795        | 0.38        | 0/55864        |
| 32  | 2a    | 0.19         | 1/35886 (0.0%) | 0.38        | 1/56005 (0.0%) |
| 33  | 1b    | 0.21         | 0/1881         | 0.48        | 0/2542         |
| 33  | 2b    | 0.29         | 1/1860 (0.1%)  | 0.51        | 0/2518         |
| 34  | 1c    | 0.19         | 0/1572         | 0.38        | 0/2126         |
| 34  | 2c    | 0.25         | 0/1566         | 0.51        | 1/2119 (0.0%)  |
| 35  | 1d    | 0.20         | 0/1685         | 0.44        | 0/2262         |
| 35  | 2d    | 0.20         | 0/1704         | 0.46        | 0/2284         |
| 36  | 1e    | 0.22         | 0/1145         | 0.49        | 0/1543         |
| 36  | 2e    | 0.21         | 0/1149         | 0.49        | 1/1548 (0.1%)  |
| 37  | 1f    | 0.22         | 0/823          | 0.41        | 0/1115         |
| 37  | 2f    | 0.21         | 0/829          | 0.40        | 0/1123         |

| Mol | Chain | Bond lengths |                  | Bond angles |                 |
|-----|-------|--------------|------------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5         |
| 38  | 1g    | 0.19         | 0/1250           | 0.41        | 0/1679          |
| 38  | 2g    | 0.19         | 0/1254           | 0.44        | 0/1683          |
| 39  | 1h    | 0.20         | 0/1108           | 0.42        | 0/1494          |
| 39  | 2h    | 0.19         | 0/1108           | 0.44        | 0/1494          |
| 40  | 1i    | 0.21         | 0/1002           | 0.50        | 0/1346          |
| 40  | 2i    | 0.20         | 0/997            | 0.44        | 0/1343          |
| 41  | 1j    | 0.19         | 0/722            | 0.49        | 0/982           |
| 41  | 2j    | 0.22         | 0/727            | 0.44        | 0/988           |
| 42  | 1k    | 0.20         | 0/844            | 0.44        | 0/1145          |
| 42  | 2k    | 0.17         | 0/848            | 0.42        | 0/1149          |
| 43  | 1l    | 0.21         | 0/937            | 0.44        | 0/1260          |
| 43  | 2l    | 0.21         | 0/937            | 0.45        | 0/1260          |
| 44  | 1m    | 0.21         | 0/969            | 0.47        | 0/1302          |
| 44  | 2m    | 0.26         | 0/961            | 0.50        | 0/1291          |
| 45  | 1n    | 0.18         | 0/501            | 0.44        | 0/664           |
| 45  | 2n    | 0.20         | 0/501            | 0.45        | 0/664           |
| 46  | 1o    | 0.19         | 0/739            | 0.42        | 0/985           |
| 46  | 2o    | 0.19         | 0/739            | 0.41        | 0/985           |
| 47  | 1p    | 0.21         | 0/697            | 0.49        | 0/939           |
| 47  | 2p    | 0.21         | 0/693            | 0.49        | 0/935           |
| 48  | 1q    | 0.18         | 0/836            | 0.41        | 0/1117          |
| 48  | 2q    | 0.21         | 0/836            | 0.47        | 0/1117          |
| 49  | 1r    | 0.19         | 0/560            | 0.42        | 0/746           |
| 49  | 2r    | 0.21         | 0/560            | 0.44        | 0/746           |
| 50  | 1s    | 0.20         | 0/667            | 0.48        | 0/900           |
| 50  | 2s    | 0.24         | 0/661            | 0.56        | 0/893           |
| 51  | 1t    | 0.19         | 0/730            | 0.43        | 0/965           |
| 51  | 2t    | 0.21         | 0/729            | 0.49        | 0/965           |
| 52  | 1u    | 0.20         | 0/203            | 0.51        | 0/266           |
| 52  | 2u    | 0.23         | 0/203            | 0.42        | 0/266           |
| 53  | 1v    | 0.23         | 0/319            | 0.38        | 0/495           |
| 53  | 2v    | 0.24         | 0/319            | 0.44        | 0/495           |
| 54  | 1w    | 0.30         | 2/1593 (0.1%)    | 0.38        | 0/2474          |
| 54  | 2w    | 0.36         | 2/1593 (0.1%)    | 0.54        | 0/2474          |
| 55  | 1x    | 0.25         | 0/1723           | 0.40        | 0/2684          |
| 55  | 2x    | 0.25         | 1/1723 (0.1%)    | 0.39        | 0/2684          |
| 56  | 1z    | 0.50         | 0/16             | 0.68        | 0/19            |
| 56  | 2z    | 0.35         | 0/16             | 0.79        | 0/19            |
| 57  | 1y    | 0.30         | 0/1618           | 0.43        | 0/2513          |
| 57  | 2y    | 0.32         | 2/1618 (0.1%)    | 0.48        | 0/2513          |
| All | All   | 0.23         | 10/316807 (0.0%) | 0.43        | 6/474290 (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 |
|-----|-------|---------------------|---------------------|
| 5   | 2F    | 0                   | 1                   |
| 29  | 27    | 0                   | 1                   |
| 33  | 1b    | 0                   | 2                   |
| All | All   | 0                   | 4                   |

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

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 33  | 2b    | 10  | LEU  | CA-C  | 6.23 | 1.61        | 1.52     |
| 57  | 2y    | 46  | G7M  | O3'-P | 5.51 | 1.61        | 1.56     |
| 54  | 2w    | 46  | G7M  | O3'-P | 5.39 | 1.61        | 1.56     |
| 54  | 1w    | 46  | G7M  | O3'-P | 5.38 | 1.61        | 1.56     |
| 54  | 2w    | 37  | T6A  | O3'-P | 5.26 | 1.61        | 1.56     |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 34  | 2c    | 94   | LEU  | N-CA-C      | -8.65 | 104.76      | 114.62   |
| 36  | 2e    | 109  | ILE  | N-CA-C      | -6.80 | 104.98      | 112.80   |
| 1   | 1A    | 1992 | G    | C2'-C3'-O3' | 6.36  | 119.04      | 109.50   |
| 1   | 2A    | 1992 | G    | C2'-C3'-O3' | 6.10  | 118.65      | 109.50   |
| 15  | 1T    | 129  | ARG  | N-CA-C      | -5.74 | 106.89      | 112.97   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 33  | 1b    | 126 | GLU  | Peptide |
| 33  | 1b    | 130 | ARG  | Peptide |
| 29  | 27    | 46  | VAL  | Peptide |
| 5   | 2F    | 20  | LEU  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1A    | 61852 | 0        | 31193    | 700     | 0            |
| 1   | 2A    | 60322 | 0        | 30424    | 798     | 0            |
| 2   | 1B    | 2577  | 0        | 1304     | 30      | 0            |
| 2   | 2B    | 2575  | 0        | 1303     | 56      | 0            |
| 3   | 1D    | 2136  | 0        | 2218     | 51      | 0            |
| 3   | 2D    | 2136  | 0        | 2218     | 57      | 0            |
| 4   | 1E    | 1559  | 0        | 1618     | 40      | 0            |
| 4   | 2E    | 1559  | 0        | 1618     | 37      | 0            |
| 5   | 1F    | 1584  | 0        | 1625     | 52      | 0            |
| 5   | 2F    | 1580  | 0        | 1619     | 61      | 0            |
| 6   | 1G    | 1423  | 0        | 1436     | 49      | 0            |
| 6   | 2G    | 1428  | 0        | 1438     | 66      | 0            |
| 7   | 1H    | 1330  | 0        | 1407     | 28      | 0            |
| 7   | 2H    | 1330  | 0        | 1407     | 39      | 0            |
| 8   | 1I    | 1097  | 0        | 1140     | 29      | 0            |
| 8   | 2I    | 1064  | 0        | 1082     | 34      | 0            |
| 9   | 1N    | 1117  | 0        | 1184     | 22      | 0            |
| 9   | 2N    | 1117  | 0        | 1184     | 18      | 0            |
| 10  | 1O    | 933   | 0        | 996      | 24      | 0            |
| 10  | 2O    | 933   | 0        | 996      | 24      | 0            |
| 11  | 1P    | 1135  | 0        | 1212     | 37      | 0            |
| 11  | 2P    | 1135  | 0        | 1212     | 38      | 0            |
| 12  | 1Q    | 1122  | 0        | 1179     | 35      | 0            |
| 12  | 2Q    | 1122  | 0        | 1179     | 46      | 0            |
| 13  | 1R    | 968   | 0        | 1033     | 22      | 0            |
| 13  | 2R    | 968   | 0        | 1033     | 24      | 0            |
| 14  | 1S    | 873   | 0        | 927      | 26      | 0            |
| 14  | 2S    | 870   | 0        | 923      | 60      | 0            |
| 15  | 1T    | 1091  | 0        | 1151     | 33      | 0            |
| 15  | 2T    | 1083  | 0        | 1136     | 30      | 0            |
| 16  | 1U    | 959   | 0        | 1018     | 22      | 0            |
| 16  | 2U    | 959   | 0        | 1019     | 31      | 0            |
| 17  | 1V    | 771   | 0        | 829      | 8       | 0            |
| 17  | 2V    | 771   | 0        | 830      | 21      | 0            |
| 18  | 1W    | 886   | 0        | 940      | 27      | 0            |
| 18  | 2W    | 886   | 0        | 940      | 17      | 0            |
| 19  | 1X    | 750   | 0        | 814      | 13      | 0            |
| 19  | 2X    | 750   | 0        | 814      | 25      | 0            |
| 20  | 1Y    | 806   | 0        | 881      | 20      | 0            |
| 20  | 2Y    | 806   | 0        | 881      | 22      | 0            |
| 21  | 1Z    | 1240  | 0        | 1240     | 39      | 0            |
| 21  | 2Z    | 1271  | 0        | 1273     | 49      | 0            |
| 22  | 10    | 653   | 0        | 674      | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | 20    | 653   | 0        | 674      | 20      | 0            |
| 23  | 11    | 755   | 0        | 826      | 17      | 0            |
| 23  | 21    | 755   | 0        | 826      | 23      | 0            |
| 24  | 12    | 588   | 0        | 643      | 9       | 0            |
| 24  | 22    | 588   | 0        | 643      | 22      | 0            |
| 25  | 13    | 469   | 0        | 518      | 15      | 0            |
| 25  | 23    | 464   | 0        | 514      | 16      | 0            |
| 26  | 14    | 552   | 0        | 533      | 18      | 0            |
| 26  | 24    | 532   | 0        | 503      | 27      | 0            |
| 27  | 15    | 455   | 0        | 465      | 6       | 0            |
| 27  | 25    | 455   | 0        | 465      | 10      | 0            |
| 28  | 16    | 453   | 0        | 473      | 13      | 0            |
| 28  | 26    | 449   | 0        | 469      | 14      | 0            |
| 29  | 17    | 418   | 0        | 467      | 11      | 0            |
| 29  | 27    | 418   | 0        | 467      | 15      | 0            |
| 30  | 18    | 517   | 0        | 582      | 14      | 0            |
| 30  | 28    | 517   | 0        | 582      | 18      | 0            |
| 31  | 19    | 307   | 0        | 335      | 6       | 0            |
| 31  | 29    | 307   | 0        | 335      | 10      | 0            |
| 32  | 1a    | 32246 | 0        | 16293    | 454     | 0            |
| 32  | 2a    | 32327 | 0        | 16338    | 577     | 0            |
| 33  | 1b    | 1846  | 0        | 1867     | 53      | 0            |
| 33  | 2b    | 1825  | 0        | 1828     | 81      | 0            |
| 34  | 1c    | 1548  | 0        | 1535     | 40      | 0            |
| 34  | 2c    | 1542  | 0        | 1517     | 75      | 0            |
| 35  | 1d    | 1655  | 0        | 1672     | 56      | 0            |
| 35  | 2d    | 1674  | 0        | 1713     | 71      | 0            |
| 36  | 1e    | 1129  | 0        | 1185     | 35      | 0            |
| 36  | 2e    | 1133  | 0        | 1191     | 47      | 0            |
| 37  | 1f    | 810   | 0        | 804      | 16      | 0            |
| 37  | 2f    | 816   | 0        | 808      | 17      | 0            |
| 38  | 1g    | 1231  | 0        | 1238     | 28      | 0            |
| 38  | 2g    | 1235  | 0        | 1249     | 37      | 0            |
| 39  | 1h    | 1088  | 0        | 1126     | 30      | 0            |
| 39  | 2h    | 1088  | 0        | 1126     | 42      | 0            |
| 40  | 1i    | 983   | 0        | 986      | 28      | 0            |
| 40  | 2i    | 978   | 0        | 966      | 52      | 0            |
| 41  | 1j    | 709   | 0        | 650      | 34      | 0            |
| 41  | 2j    | 714   | 0        | 672      | 35      | 0            |
| 42  | 1k    | 829   | 0        | 825      | 17      | 0            |
| 42  | 2k    | 833   | 0        | 834      | 17      | 0            |
| 43  | 1l    | 932   | 0        | 981      | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | 2l    | 932   | 0        | 981      | 27      | 0            |
| 44  | 1m    | 958   | 0        | 1002     | 30      | 0            |
| 44  | 2m    | 950   | 0        | 988      | 50      | 0            |
| 45  | 1n    | 492   | 0        | 529      | 20      | 0            |
| 45  | 2n    | 492   | 0        | 529      | 25      | 0            |
| 46  | 1o    | 728   | 0        | 760      | 16      | 0            |
| 46  | 2o    | 728   | 0        | 760      | 27      | 0            |
| 47  | 1p    | 681   | 0        | 697      | 27      | 0            |
| 47  | 2p    | 677   | 0        | 686      | 25      | 0            |
| 48  | 1q    | 823   | 0        | 891      | 17      | 0            |
| 48  | 2q    | 823   | 0        | 891      | 26      | 0            |
| 49  | 1r    | 555   | 0        | 618      | 13      | 0            |
| 49  | 2r    | 555   | 0        | 618      | 12      | 0            |
| 50  | 1s    | 652   | 0        | 662      | 10      | 0            |
| 50  | 2s    | 646   | 0        | 644      | 40      | 0            |
| 51  | 1t    | 728   | 0        | 798      | 22      | 0            |
| 51  | 2t    | 727   | 0        | 796      | 19      | 0            |
| 52  | 1u    | 199   | 0        | 208      | 7       | 0            |
| 52  | 2u    | 199   | 0        | 208      | 11      | 0            |
| 53  | 1v    | 283   | 0        | 141      | 6       | 0            |
| 53  | 2v    | 283   | 0        | 141      | 9       | 0            |
| 54  | 1w    | 1599  | 0        | 800      | 31      | 0            |
| 54  | 2w    | 1599  | 0        | 801      | 48      | 0            |
| 55  | 1x    | 1646  | 0        | 839      | 20      | 0            |
| 55  | 2x    | 1646  | 0        | 839      | 32      | 0            |
| 56  | 1z    | 27    | 0        | 28       | 1       | 0            |
| 56  | 2z    | 27    | 0        | 28       | 5       | 0            |
| 57  | 1y    | 1577  | 0        | 799      | 39      | 0            |
| 57  | 2y    | 1577  | 0        | 798      | 38      | 0            |
| 58  | 10    | 11    | 0        | 0        | 0       | 0            |
| 58  | 11    | 5     | 0        | 0        | 0       | 0            |
| 58  | 12    | 2     | 0        | 0        | 0       | 0            |
| 58  | 13    | 4     | 0        | 0        | 0       | 0            |
| 58  | 14    | 1     | 0        | 0        | 0       | 0            |
| 58  | 15    | 8     | 0        | 0        | 0       | 0            |
| 58  | 16    | 2     | 0        | 0        | 0       | 0            |
| 58  | 17    | 7     | 0        | 0        | 0       | 0            |
| 58  | 18    | 6     | 0        | 0        | 0       | 0            |
| 58  | 19    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1A    | 1080  | 0        | 0        | 0       | 0            |
| 58  | 1B    | 40    | 0        | 0        | 0       | 0            |
| 58  | 1D    | 12    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58  | 1E    | 12    | 0        | 0        | 0       | 0            |
| 58  | 1F    | 11    | 0        | 0        | 0       | 0            |
| 58  | 1G    | 5     | 0        | 0        | 0       | 0            |
| 58  | 1N    | 6     | 0        | 0        | 0       | 0            |
| 58  | 1O    | 4     | 0        | 0        | 0       | 0            |
| 58  | 1P    | 9     | 0        | 0        | 0       | 0            |
| 58  | 1Q    | 7     | 0        | 0        | 0       | 0            |
| 58  | 1R    | 7     | 0        | 0        | 0       | 0            |
| 58  | 1S    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1T    | 2     | 0        | 0        | 0       | 0            |
| 58  | 1U    | 10    | 0        | 0        | 0       | 0            |
| 58  | 1V    | 8     | 0        | 0        | 0       | 0            |
| 58  | 1W    | 7     | 0        | 0        | 0       | 0            |
| 58  | 1X    | 5     | 0        | 0        | 0       | 0            |
| 58  | 1Y    | 2     | 0        | 0        | 0       | 0            |
| 58  | 1Z    | 3     | 0        | 0        | 0       | 0            |
| 58  | 1a    | 209   | 0        | 0        | 0       | 0            |
| 58  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1d    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1e    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1f    | 2     | 0        | 0        | 0       | 0            |
| 58  | 1l    | 2     | 0        | 0        | 0       | 0            |
| 58  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1n    | 2     | 0        | 0        | 0       | 0            |
| 58  | 1p    | 2     | 0        | 0        | 0       | 0            |
| 58  | 1t    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1v    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1w    | 5     | 0        | 0        | 0       | 0            |
| 58  | 1x    | 12    | 0        | 0        | 0       | 0            |
| 58  | 20    | 2     | 0        | 0        | 0       | 0            |
| 58  | 21    | 4     | 0        | 0        | 0       | 0            |
| 58  | 23    | 3     | 0        | 0        | 0       | 0            |
| 58  | 25    | 3     | 0        | 0        | 0       | 0            |
| 58  | 27    | 3     | 0        | 0        | 0       | 0            |
| 58  | 28    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2A    | 824   | 0        | 0        | 0       | 0            |
| 58  | 2B    | 19    | 0        | 0        | 0       | 0            |
| 58  | 2D    | 8     | 0        | 0        | 0       | 0            |
| 58  | 2E    | 7     | 0        | 0        | 0       | 0            |
| 58  | 2F    | 6     | 0        | 0        | 0       | 0            |
| 58  | 2G    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2N    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58  | 2O    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2P    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2Q    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2R    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2T    | 3     | 0        | 0        | 0       | 0            |
| 58  | 2U    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2V    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2W    | 4     | 0        | 0        | 0       | 0            |
| 58  | 2X    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2Z    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2a    | 211   | 0        | 0        | 0       | 0            |
| 58  | 2d    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2e    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2f    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2g    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2j    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2k    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2l    | 4     | 0        | 0        | 0       | 0            |
| 58  | 2q    | 2     | 0        | 0        | 1       | 0            |
| 58  | 2r    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2t    | 1     | 0        | 0        | 0       | 0            |
| 58  | 2v    | 3     | 0        | 0        | 0       | 0            |
| 58  | 2w    | 2     | 0        | 0        | 0       | 0            |
| 58  | 2x    | 5     | 0        | 0        | 0       | 0            |
| 59  | 1A    | 1     | 0        | 0        | 0       | 0            |
| 59  | 2A    | 1     | 0        | 0        | 0       | 0            |
| 60  | 1A    | 58    | 0        | 65       | 4       | 0            |
| 60  | 2A    | 58    | 0        | 65       | 4       | 0            |
| 61  | 14    | 1     | 0        | 0        | 0       | 0            |
| 61  | 15    | 1     | 0        | 0        | 0       | 0            |
| 61  | 16    | 1     | 0        | 0        | 0       | 0            |
| 61  | 19    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 61  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 61  | 24    | 1     | 0        | 0        | 0       | 0            |
| 61  | 25    | 1     | 0        | 0        | 0       | 0            |
| 61  | 26    | 1     | 0        | 0        | 0       | 0            |
| 61  | 29    | 1     | 0        | 0        | 0       | 0            |
| 61  | 2Y    | 1     | 0        | 0        | 0       | 0            |
| 61  | 2n    | 1     | 0        | 0        | 0       | 0            |
| 62  | 1d    | 8     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 62  | 2d    | 8     | 0        | 0        | 2       | 0            |
| 63  | 10    | 13    | 0        | 0        | 1       | 0            |
| 63  | 11    | 9     | 0        | 0        | 0       | 0            |
| 63  | 12    | 4     | 0        | 0        | 0       | 0            |
| 63  | 13    | 4     | 0        | 0        | 0       | 0            |
| 63  | 15    | 6     | 0        | 0        | 0       | 0            |
| 63  | 16    | 2     | 0        | 0        | 0       | 0            |
| 63  | 17    | 5     | 0        | 0        | 0       | 0            |
| 63  | 18    | 9     | 0        | 0        | 2       | 0            |
| 63  | 1A    | 1780  | 0        | 0        | 101     | 0            |
| 63  | 1B    | 57    | 0        | 0        | 3       | 0            |
| 63  | 1D    | 24    | 0        | 0        | 1       | 0            |
| 63  | 1E    | 22    | 0        | 0        | 3       | 0            |
| 63  | 1F    | 14    | 0        | 0        | 3       | 0            |
| 63  | 1G    | 2     | 0        | 0        | 0       | 0            |
| 63  | 1H    | 2     | 0        | 0        | 0       | 0            |
| 63  | 1I    | 1     | 0        | 0        | 0       | 0            |
| 63  | 1N    | 7     | 0        | 0        | 0       | 0            |
| 63  | 1O    | 4     | 0        | 0        | 0       | 0            |
| 63  | 1P    | 19    | 0        | 0        | 1       | 0            |
| 63  | 1Q    | 6     | 0        | 0        | 0       | 0            |
| 63  | 1R    | 13    | 0        | 0        | 3       | 0            |
| 63  | 1S    | 4     | 0        | 0        | 0       | 0            |
| 63  | 1T    | 11    | 0        | 0        | 0       | 0            |
| 63  | 1U    | 10    | 0        | 0        | 1       | 0            |
| 63  | 1V    | 9     | 0        | 0        | 0       | 0            |
| 63  | 1W    | 10    | 0        | 0        | 2       | 0            |
| 63  | 1X    | 4     | 0        | 0        | 0       | 0            |
| 63  | 1Y    | 1     | 0        | 0        | 0       | 0            |
| 63  | 1Z    | 1     | 0        | 0        | 0       | 0            |
| 63  | 1a    | 226   | 0        | 0        | 22      | 0            |
| 63  | 1b    | 1     | 0        | 0        | 0       | 0            |
| 63  | 1e    | 2     | 0        | 0        | 0       | 0            |
| 63  | 1l    | 7     | 0        | 0        | 0       | 0            |
| 63  | 1m    | 1     | 0        | 0        | 0       | 0            |
| 63  | 1n    | 1     | 0        | 0        | 0       | 0            |
| 63  | 1q    | 2     | 0        | 0        | 0       | 0            |
| 63  | 1v    | 5     | 0        | 0        | 0       | 0            |
| 63  | 1w    | 5     | 0        | 0        | 1       | 0            |
| 63  | 1x    | 3     | 0        | 0        | 0       | 0            |
| 63  | 1y    | 1     | 0        | 0        | 1       | 0            |
| 63  | 20    | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 63  | 21    | 5      | 0        | 0        | 1       | 0            |
| 63  | 25    | 1      | 0        | 0        | 1       | 0            |
| 63  | 27    | 2      | 0        | 0        | 0       | 0            |
| 63  | 28    | 2      | 0        | 0        | 1       | 0            |
| 63  | 29    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2A    | 850    | 0        | 0        | 79      | 0            |
| 63  | 2B    | 16     | 0        | 0        | 1       | 0            |
| 63  | 2D    | 18     | 0        | 0        | 2       | 0            |
| 63  | 2E    | 10     | 0        | 0        | 1       | 0            |
| 63  | 2F    | 12     | 0        | 0        | 0       | 0            |
| 63  | 2N    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2O    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2P    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2Q    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2R    | 2      | 0        | 0        | 0       | 0            |
| 63  | 2T    | 4      | 0        | 0        | 0       | 0            |
| 63  | 2U    | 2      | 0        | 0        | 0       | 0            |
| 63  | 2W    | 2      | 0        | 0        | 0       | 0            |
| 63  | 2X    | 2      | 0        | 0        | 0       | 0            |
| 63  | 2Z    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2a    | 148    | 0        | 0        | 21      | 0            |
| 63  | 2d    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2e    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2i    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2l    | 5      | 0        | 0        | 0       | 0            |
| 63  | 2p    | 2      | 0        | 0        | 0       | 0            |
| 63  | 2t    | 2      | 0        | 0        | 0       | 0            |
| 63  | 2v    | 1      | 0        | 0        | 0       | 0            |
| 63  | 2w    | 4      | 0        | 0        | 1       | 0            |
| 63  | 2x    | 4      | 0        | 0        | 0       | 0            |
| All | All   | 299377 | 0        | 196882   | 4932    | 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 10.

The worst 5 of 4932 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 | 1.23                     | 1.34              |
| 54:2w:51:A:N6  | 54:2w:63:U:H3  | 1.46                     | 1.14              |
| 57:2y:10:G:H1  | 57:2y:25:C:N4  | 1.47                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2A:2503:2MA:H8 | 56:2z:2:ARG:HH12 | 1.17                     | 1.04              |
| 54:2w:51:A:H3'   | 54:2w:64:G:H21   | 1.17                     | 1.03              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 246 (90%) | 25 (9%)  | 2 (1%)   | 18          | 47  |
| 3   | 2D    | 273/276 (99%) | 245 (90%) | 28 (10%) | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 190 (94%) | 11 (5%)  | 1 (0%)   | 24          | 55  |
| 4   | 2E    | 202/206 (98%) | 182 (90%) | 17 (8%)  | 3 (2%)   | 8           | 28  |
| 5   | 1F    | 201/210 (96%) | 190 (94%) | 10 (5%)  | 1 (0%)   | 24          | 55  |
| 5   | 2F    | 201/210 (96%) | 186 (92%) | 13 (6%)  | 2 (1%)   | 12          | 38  |
| 6   | 1G    | 179/182 (98%) | 152 (85%) | 25 (14%) | 2 (1%)   | 11          | 36  |
| 6   | 2G    | 179/182 (98%) | 155 (87%) | 18 (10%) | 6 (3%)   | 3           | 11  |
| 7   | 1H    | 172/180 (96%) | 158 (92%) | 13 (8%)  | 1 (1%)   | 21          | 51  |
| 7   | 2H    | 172/180 (96%) | 149 (87%) | 21 (12%) | 2 (1%)   | 10          | 34  |
| 8   | 1I    | 144/148 (97%) | 123 (85%) | 20 (14%) | 1 (1%)   | 18          | 47  |
| 8   | 2I    | 144/148 (97%) | 119 (83%) | 22 (15%) | 3 (2%)   | 5           | 20  |
| 9   | 1N    | 138/140 (99%) | 130 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 122 (88%) | 14 (10%) | 2 (1%)   | 9           | 30  |
| 10  | 1O    | 120/122 (98%) | 112 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 10  | 2O    | 120/122 (98%) | 103 (86%) | 15 (12%) | 2 (2%)   | 7           | 25  |
| 11  | 1P    | 147/150 (98%) | 130 (88%) | 14 (10%) | 3 (2%)   | 6           | 21  |
| 11  | 2P    | 147/150 (98%) | 124 (84%) | 19 (13%) | 4 (3%)   | 4           | 15  |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 12  | 1Q    | 139/141 (99%) | 131 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 12  | 2Q    | 139/141 (99%) | 125 (90%)  | 14 (10%) | 0        | 100         | 100 |
| 13  | 1R    | 116/118 (98%) | 111 (96%)  | 4 (3%)   | 1 (1%)   | 14          | 41  |
| 13  | 2R    | 116/118 (98%) | 108 (93%)  | 7 (6%)   | 1 (1%)   | 14          | 41  |
| 14  | 1S    | 108/112 (96%) | 102 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 14  | 2S    | 108/112 (96%) | 93 (86%)   | 11 (10%) | 4 (4%)   | 2           | 9   |
| 15  | 1T    | 129/146 (88%) | 120 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 15  | 2T    | 129/146 (88%) | 116 (90%)  | 11 (8%)  | 2 (2%)   | 7           | 27  |
| 16  | 1U    | 114/118 (97%) | 114 (100%) | 0        | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 111 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 88 (89%)   | 9 (9%)   | 2 (2%)   | 6           | 21  |
| 17  | 2V    | 99/101 (98%)  | 87 (88%)   | 10 (10%) | 2 (2%)   | 6           | 21  |
| 18  | 1W    | 110/113 (97%) | 109 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 107 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 88 (95%)   | 4 (4%)   | 1 (1%)   | 11          | 36  |
| 19  | 2X    | 93/96 (97%)   | 83 (89%)   | 8 (9%)   | 2 (2%)   | 5           | 19  |
| 20  | 1Y    | 105/110 (96%) | 100 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 20  | 2Y    | 105/110 (96%) | 98 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 21  | 1Z    | 148/206 (72%) | 129 (87%)  | 14 (10%) | 5 (3%)   | 3           | 11  |
| 21  | 2Z    | 156/206 (76%) | 128 (82%)  | 22 (14%) | 6 (4%)   | 2           | 9   |
| 22  | 10    | 81/85 (95%)   | 78 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 22  | 20    | 81/85 (95%)   | 73 (90%)   | 7 (9%)   | 1 (1%)   | 10          | 34  |
| 23  | 11    | 95/98 (97%)   | 91 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 23  | 21    | 95/98 (97%)   | 88 (93%)   | 6 (6%)   | 1 (1%)   | 11          | 36  |
| 24  | 12    | 68/72 (94%)   | 65 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 63 (93%)   | 5 (7%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 54 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 25  | 23    | 57/60 (95%)   | 52 (91%)   | 4 (7%)   | 1 (2%)   | 6           | 23  |
| 26  | 14    | 67/71 (94%)   | 49 (73%)   | 15 (22%) | 3 (4%)   | 2           | 7   |
| 26  | 24    | 67/71 (94%)   | 47 (70%)   | 17 (25%) | 3 (4%)   | 2           | 7   |
| 27  | 15    | 57/60 (95%)   | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 27  | 25    | 57/60 (95%)   | 48 (84%)  | 9 (16%)  | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 48 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 45 (88%)  | 5 (10%)  | 1 (2%)   | 6           | 21  |
| 29  | 17    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 60 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 55 (89%)  | 7 (11%)  | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 30 (86%)  | 5 (14%)  | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 195 (85%) | 26 (11%) | 8 (4%)   | 3           | 10  |
| 33  | 2b    | 229/256 (90%) | 177 (77%) | 45 (20%) | 7 (3%)   | 3           | 12  |
| 34  | 1c    | 204/239 (85%) | 184 (90%) | 19 (9%)  | 1 (0%)   | 24          | 55  |
| 34  | 2c    | 204/239 (85%) | 170 (83%) | 32 (16%) | 2 (1%)   | 12          | 38  |
| 35  | 1d    | 206/209 (99%) | 180 (87%) | 24 (12%) | 2 (1%)   | 12          | 38  |
| 35  | 2d    | 206/209 (99%) | 176 (85%) | 29 (14%) | 1 (0%)   | 24          | 55  |
| 36  | 1e    | 146/162 (90%) | 130 (89%) | 12 (8%)  | 4 (3%)   | 4           | 15  |
| 36  | 2e    | 146/162 (90%) | 128 (88%) | 14 (10%) | 4 (3%)   | 4           | 15  |
| 37  | 1f    | 98/101 (97%)  | 91 (93%)  | 6 (6%)   | 1 (1%)   | 12          | 38  |
| 37  | 2f    | 98/101 (97%)  | 90 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/156 (98%) | 130 (85%) | 22 (14%) | 1 (1%)   | 18          | 47  |
| 38  | 2g    | 153/156 (98%) | 133 (87%) | 16 (10%) | 4 (3%)   | 4           | 15  |
| 39  | 1h    | 135/138 (98%) | 125 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 39  | 2h    | 135/138 (98%) | 118 (87%) | 16 (12%) | 1 (1%)   | 18          | 47  |
| 40  | 1i    | 125/128 (98%) | 109 (87%) | 14 (11%) | 2 (2%)   | 7           | 27  |
| 40  | 2i    | 125/128 (98%) | 106 (85%) | 17 (14%) | 2 (2%)   | 7           | 27  |
| 41  | 1j    | 95/105 (90%)  | 78 (82%)  | 11 (12%) | 6 (6%)   | 1           | 3   |
| 41  | 2j    | 94/105 (90%)  | 77 (82%)  | 14 (15%) | 3 (3%)   | 3           | 11  |
| 42  | 1k    | 112/129 (87%) | 100 (89%) | 10 (9%)  | 2 (2%)   | 6           | 23  |
| 42  | 2k    | 112/129 (87%) | 96 (86%)  | 14 (12%) | 2 (2%)   | 6           | 23  |
| 43  | 1l    | 119/132 (90%) | 108 (91%) | 10 (8%)  | 1 (1%)   | 16          | 44  |
| 43  | 2l    | 119/132 (90%) | 107 (90%) | 10 (8%)  | 2 (2%)   | 7           | 25  |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 44  | 1m    | 121/126 (96%)     | 104 (86%)   | 15 (12%)   | 2 (2%)   | 7           | 25  |
| 44  | 2m    | 120/126 (95%)     | 100 (83%)   | 19 (16%)   | 1 (1%)   | 16          | 44  |
| 45  | 1n    | 58/61 (95%)       | 55 (95%)    | 3 (5%)     | 0        | 100         | 100 |
| 45  | 2n    | 58/61 (95%)       | 51 (88%)    | 6 (10%)    | 1 (2%)   | 7           | 25  |
| 46  | 1o    | 86/89 (97%)       | 76 (88%)    | 9 (10%)    | 1 (1%)   | 10          | 34  |
| 46  | 2o    | 86/89 (97%)       | 81 (94%)    | 5 (6%)     | 0        | 100         | 100 |
| 47  | 1p    | 80/88 (91%)       | 68 (85%)    | 12 (15%)   | 0        | 100         | 100 |
| 47  | 2p    | 80/88 (91%)       | 70 (88%)    | 10 (12%)   | 0        | 100         | 100 |
| 48  | 1q    | 97/105 (92%)      | 86 (89%)    | 11 (11%)   | 0        | 100         | 100 |
| 48  | 2q    | 97/105 (92%)      | 85 (88%)    | 10 (10%)   | 2 (2%)   | 5           | 20  |
| 49  | 1r    | 66/88 (75%)       | 59 (89%)    | 7 (11%)    | 0        | 100         | 100 |
| 49  | 2r    | 66/88 (75%)       | 61 (92%)    | 5 (8%)     | 0        | 100         | 100 |
| 50  | 1s    | 81/93 (87%)       | 69 (85%)    | 12 (15%)   | 0        | 100         | 100 |
| 50  | 2s    | 81/93 (87%)       | 63 (78%)    | 15 (18%)   | 3 (4%)   | 2           | 9   |
| 51  | 1t    | 94/106 (89%)      | 86 (92%)    | 5 (5%)     | 3 (3%)   | 3           | 11  |
| 51  | 2t    | 94/106 (89%)      | 81 (86%)    | 9 (10%)    | 4 (4%)   | 2           | 7   |
| 52  | 1u    | 21/27 (78%)       | 18 (86%)    | 3 (14%)    | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 19 (90%)    | 1 (5%)     | 1 (5%)   | 2           | 6   |
| 56  | 1z    | 1/3 (33%)         | 0           | 1 (100%)   | 0        | 100         | 100 |
| 56  | 2z    | 1/3 (33%)         | 0           | 1 (100%)   | 0        | 100         | 100 |
| All | All   | 11372/12134 (94%) | 10129 (89%) | 1098 (10%) | 145 (1%) | 9           | 31  |

5 of 145 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1F    | 130 | ALA  |
| 6   | 1G    | 181 | ARG  |
| 7   | 1H    | 126 | PRO  |
| 21  | 1Z    | 53  | ILE  |
| 26  | 14    | 49  | PHE  |

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | 1D    | 215/218 (99%)  | 204 (95%) | 11 (5%)  | 21          | 54 |
| 3   | 2D    | 215/218 (99%)  | 201 (94%) | 14 (6%)  | 15          | 43 |
| 4   | 1E    | 164/166 (99%)  | 148 (90%) | 16 (10%) | 7           | 25 |
| 4   | 2E    | 164/166 (99%)  | 154 (94%) | 10 (6%)  | 17          | 46 |
| 5   | 1F    | 160/166 (96%)  | 144 (90%) | 16 (10%) | 7           | 24 |
| 5   | 2F    | 159/166 (96%)  | 137 (86%) | 22 (14%) | 3           | 12 |
| 6   | 1G    | 143/156 (92%)  | 126 (88%) | 17 (12%) | 5           | 17 |
| 6   | 2G    | 143/156 (92%)  | 119 (83%) | 24 (17%) | 2           | 8  |
| 7   | 1H    | 144/148 (97%)  | 125 (87%) | 19 (13%) | 4           | 14 |
| 7   | 2H    | 144/148 (97%)  | 125 (87%) | 19 (13%) | 4           | 14 |
| 8   | 1I    | 113/124 (91%)  | 84 (74%)  | 29 (26%) | 0           | 2  |
| 8   | 2I    | 105/124 (85%)  | 81 (77%)  | 24 (23%) | 1           | 3  |
| 9   | 1N    | 118/119 (99%)  | 106 (90%) | 12 (10%) | 7           | 23 |
| 9   | 2N    | 118/119 (99%)  | 107 (91%) | 11 (9%)  | 8           | 27 |
| 10  | 1O    | 100/100 (100%) | 93 (93%)  | 7 (7%)   | 14          | 40 |
| 10  | 2O    | 100/100 (100%) | 92 (92%)  | 8 (8%)   | 11          | 34 |
| 11  | 1P    | 115/116 (99%)  | 105 (91%) | 10 (9%)  | 9           | 30 |
| 11  | 2P    | 115/116 (99%)  | 103 (90%) | 12 (10%) | 7           | 22 |
| 12  | 1Q    | 111/111 (100%) | 101 (91%) | 10 (9%)  | 9           | 28 |
| 12  | 2Q    | 111/111 (100%) | 96 (86%)  | 15 (14%) | 4           | 13 |
| 13  | 1R    | 101/101 (100%) | 94 (93%)  | 7 (7%)   | 14          | 41 |
| 13  | 2R    | 101/101 (100%) | 99 (98%)  | 2 (2%)   | 48          | 80 |
| 14  | 1S    | 86/88 (98%)    | 73 (85%)  | 13 (15%) | 3           | 10 |
| 14  | 2S    | 85/88 (97%)    | 69 (81%)  | 16 (19%) | 1           | 5  |
| 15  | 1T    | 115/127 (91%)  | 108 (94%) | 7 (6%)   | 17          | 46 |
| 15  | 2T    | 113/127 (89%)  | 107 (95%) | 6 (5%)   | 20          | 52 |
| 16  | 1U    | 93/94 (99%)    | 83 (89%)  | 10 (11%) | 6           | 21 |
| 16  | 2U    | 93/94 (99%)    | 87 (94%)  | 6 (6%)   | 15          | 43 |
| 17  | 1V    | 80/82 (98%)    | 74 (92%)  | 6 (8%)   | 12          | 37 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 17  | 2V    | 80/82 (98%)   | 68 (85%)  | 12 (15%) | 3           | 10 |
| 18  | 1W    | 90/92 (98%)   | 86 (96%)  | 4 (4%)   | 25          | 59 |
| 18  | 2W    | 90/92 (98%)   | 81 (90%)  | 9 (10%)  | 7           | 24 |
| 19  | 1X    | 77/78 (99%)   | 72 (94%)  | 5 (6%)   | 15          | 43 |
| 19  | 2X    | 77/78 (99%)   | 70 (91%)  | 7 (9%)   | 9           | 28 |
| 20  | 1Y    | 85/91 (93%)   | 73 (86%)  | 12 (14%) | 3           | 12 |
| 20  | 2Y    | 85/91 (93%)   | 73 (86%)  | 12 (14%) | 3           | 12 |
| 21  | 1Z    | 135/179 (75%) | 113 (84%) | 22 (16%) | 2           | 8  |
| 21  | 2Z    | 137/179 (76%) | 109 (80%) | 28 (20%) | 1           | 4  |
| 22  | 10    | 65/67 (97%)   | 63 (97%)  | 2 (3%)   | 35          | 70 |
| 22  | 20    | 65/67 (97%)   | 64 (98%)  | 1 (2%)   | 57          | 84 |
| 23  | 11    | 80/83 (96%)   | 74 (92%)  | 6 (8%)   | 12          | 37 |
| 23  | 21    | 80/83 (96%)   | 71 (89%)  | 9 (11%)  | 5           | 19 |
| 24  | 12    | 65/67 (97%)   | 58 (89%)  | 7 (11%)  | 6           | 21 |
| 24  | 22    | 65/67 (97%)   | 55 (85%)  | 10 (15%) | 2           | 10 |
| 25  | 13    | 51/52 (98%)   | 44 (86%)  | 7 (14%)  | 3           | 13 |
| 25  | 23    | 50/52 (96%)   | 44 (88%)  | 6 (12%)  | 5           | 17 |
| 26  | 14    | 59/63 (94%)   | 47 (80%)  | 12 (20%) | 1           | 4  |
| 26  | 24    | 53/63 (84%)   | 44 (83%)  | 9 (17%)  | 2           | 7  |
| 27  | 15    | 50/52 (96%)   | 44 (88%)  | 6 (12%)  | 5           | 17 |
| 27  | 25    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 28          | 63 |
| 28  | 16    | 51/52 (98%)   | 47 (92%)  | 4 (8%)   | 11          | 35 |
| 28  | 26    | 50/52 (96%)   | 40 (80%)  | 10 (20%) | 1           | 4  |
| 29  | 17    | 41/42 (98%)   | 38 (93%)  | 3 (7%)   | 13          | 38 |
| 29  | 27    | 41/42 (98%)   | 37 (90%)  | 4 (10%)  | 7           | 25 |
| 30  | 18    | 54/55 (98%)   | 50 (93%)  | 4 (7%)   | 13          | 37 |
| 30  | 28    | 54/55 (98%)   | 51 (94%)  | 3 (6%)   | 19          | 50 |
| 31  | 19    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 37          | 73 |
| 31  | 29    | 34/34 (100%)  | 31 (91%)  | 3 (9%)   | 9           | 29 |
| 33  | 1b    | 192/220 (87%) | 169 (88%) | 23 (12%) | 5           | 17 |
| 33  | 2b    | 187/220 (85%) | 145 (78%) | 42 (22%) | 1           | 3  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 34  | 1c    | 142/188 (76%) | 129 (91%) | 13 (9%)  | 8           | 27 |
| 34  | 2c    | 140/188 (74%) | 114 (81%) | 26 (19%) | 1           | 5  |
| 35  | 1d    | 169/181 (93%) | 147 (87%) | 22 (13%) | 4           | 14 |
| 35  | 2d    | 173/181 (96%) | 148 (86%) | 25 (14%) | 3           | 11 |
| 36  | 1e    | 113/123 (92%) | 99 (88%)  | 14 (12%) | 4           | 16 |
| 36  | 2e    | 114/123 (93%) | 99 (87%)  | 15 (13%) | 4           | 14 |
| 37  | 1f    | 84/90 (93%)   | 73 (87%)  | 11 (13%) | 4           | 14 |
| 37  | 2f    | 85/90 (94%)   | 74 (87%)  | 11 (13%) | 4           | 14 |
| 38  | 1g    | 119/127 (94%) | 101 (85%) | 18 (15%) | 3           | 10 |
| 38  | 2g    | 120/127 (94%) | 104 (87%) | 16 (13%) | 4           | 14 |
| 39  | 1h    | 114/119 (96%) | 98 (86%)  | 16 (14%) | 3           | 12 |
| 39  | 2h    | 114/119 (96%) | 100 (88%) | 14 (12%) | 4           | 16 |
| 40  | 1i    | 90/99 (91%)   | 82 (91%)  | 8 (9%)   | 9           | 29 |
| 40  | 2i    | 89/99 (90%)   | 76 (85%)  | 13 (15%) | 3           | 11 |
| 41  | 1j    | 66/92 (72%)   | 58 (88%)  | 8 (12%)  | 5           | 16 |
| 41  | 2j    | 69/92 (75%)   | 52 (75%)  | 17 (25%) | 1           | 2  |
| 42  | 1k    | 82/99 (83%)   | 69 (84%)  | 13 (16%) | 2           | 9  |
| 42  | 2k    | 83/99 (84%)   | 74 (89%)  | 9 (11%)  | 6           | 21 |
| 43  | 1l    | 96/108 (89%)  | 87 (91%)  | 9 (9%)   | 8           | 27 |
| 43  | 2l    | 96/108 (89%)  | 83 (86%)  | 13 (14%) | 4           | 13 |
| 44  | 1m    | 93/101 (92%)  | 83 (89%)  | 10 (11%) | 6           | 21 |
| 44  | 2m    | 92/101 (91%)  | 72 (78%)  | 20 (22%) | 1           | 3  |
| 45  | 1n    | 49/50 (98%)   | 42 (86%)  | 7 (14%)  | 3           | 11 |
| 45  | 2n    | 49/50 (98%)   | 40 (82%)  | 9 (18%)  | 1           | 6  |
| 46  | 1o    | 78/80 (98%)   | 69 (88%)  | 9 (12%)  | 5           | 18 |
| 46  | 2o    | 78/80 (98%)   | 72 (92%)  | 6 (8%)   | 12          | 36 |
| 47  | 1p    | 69/74 (93%)   | 61 (88%)  | 8 (12%)  | 5           | 18 |
| 47  | 2p    | 68/74 (92%)   | 60 (88%)  | 8 (12%)  | 5           | 17 |
| 48  | 1q    | 94/97 (97%)   | 84 (89%)  | 10 (11%) | 6           | 22 |
| 48  | 2q    | 94/97 (97%)   | 74 (79%)  | 20 (21%) | 1           | 4  |
| 49  | 1r    | 59/77 (77%)   | 56 (95%)  | 3 (5%)   | 21          | 54 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 49  | 2r    | 59/77 (77%)      | 49 (83%)   | 10 (17%)   | 2           | 7  |
| 50  | 1s    | 69/80 (86%)      | 58 (84%)   | 11 (16%)   | 2           | 9  |
| 50  | 2s    | 67/80 (84%)      | 54 (81%)   | 13 (19%)   | 1           | 5  |
| 51  | 1t    | 70/82 (85%)      | 65 (93%)   | 5 (7%)     | 13          | 39 |
| 51  | 2t    | 70/82 (85%)      | 64 (91%)   | 6 (9%)     | 10          | 31 |
| 52  | 1u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)     | 19          | 50 |
| 52  | 2u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)     | 19          | 50 |
| 56  | 1z    | 2/2 (100%)       | 1 (50%)    | 1 (50%)    | 0           | 0  |
| 56  | 2z    | 2/2 (100%)       | 1 (50%)    | 1 (50%)    | 0           | 0  |
| All | All   | 9307/10068 (92%) | 8193 (88%) | 1114 (12%) | 5           | 17 |

5 of 1114 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | 2e    | 150 | ARG  |
| 38  | 2g    | 113 | GLU  |
| 36  | 2e    | 120 | THR  |
| 45  | 2n    | 3   | ARG  |
| 39  | 1h    | 23  | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2d    | 116 | GLN  |
| 51  | 2t    | 16  | HIS  |
| 36  | 2e    | 127 | ASN  |
| 41  | 2j    | 13  | HIS  |
| 38  | 1g    | 28  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2864/2915 (98%) | 527 (18%)         | 24 (0%)         |
| 1   | 2A    | 2791/2915 (95%) | 532 (19%)         | 24 (0%)         |
| 2   | 1B    | 119/121 (98%)   | 15 (12%)          | 0               |
| 2   | 2B    | 118/121 (97%)   | 28 (23%)          | 0               |
| 32  | 1a    | 1497/1521 (98%) | 281 (18%)         | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 32  | 2a    | 1501/1521 (98%) | 364 (24%)         | 0               |
| 53  | 1v    | 12/24 (50%)     | 2 (16%)           | 0               |
| 53  | 2v    | 12/24 (50%)     | 5 (41%)           | 0               |
| 54  | 1w    | 71/76 (93%)     | 33 (46%)          | 0               |
| 54  | 2w    | 71/76 (93%)     | 34 (47%)          | 0               |
| 55  | 1x    | 75/77 (97%)     | 17 (22%)          | 0               |
| 55  | 2x    | 75/77 (97%)     | 17 (22%)          | 0               |
| 57  | 1y    | 72/76 (94%)     | 34 (47%)          | 0               |
| 57  | 2y    | 72/76 (94%)     | 38 (52%)          | 0               |
| All | All   | 9350/9620 (97%) | 1927 (20%)        | 48 (0%)         |

5 of 1927 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 10  | G    |
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 15  | G    |
| 1   | 1A    | 29  | U    |
| 1   | 1A    | 34  | C    |

5 of 48 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 277  | C    |
| 1   | 2A    | 1210 | A    |
| 1   | 2A    | 528  | A    |
| 1   | 2A    | 856  | C    |
| 1   | 2A    | 1442 | G    |

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

86 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 |
| 32  | 5MC   | 2a    | 1404 | 32       | 19,22,23     | 1.70 | 3 (15%)  | 26,32,35    | 1.15 | 2 (7%)   |
| 1   | PSU   | 1A    | 2605 | 58,1     | 18,21,22     | 1.31 | 4 (22%)  | 21,30,33    | 1.92 | 4 (19%)  |
| 57  | G7M   | 1y    | 46   | 57       | 23,26,27     | 1.58 | 3 (13%)  | 34,39,42    | 1.82 | 4 (11%)  |
| 57  | PSU   | 2y    | 55   | 57       | 18,21,22     | 1.32 | 2 (11%)  | 21,30,33    | 2.21 | 4 (19%)  |
| 32  | 2MG   | 1a    | 1207 | 32       | 23,26,27     | 1.26 | 2 (8%)   | 33,38,41    | 2.24 | 9 (27%)  |
| 1   | PSU   | 1A    | 1911 | 1        | 18,21,22     | 1.41 | 3 (16%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 57  | 5MU   | 2y    | 54   | 57       | 19,22,23     | 1.43 | 5 (26%)  | 27,32,35    | 2.12 | 7 (25%)  |
| 54  | PSU   | 2w    | 55   | 58,54    | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.99 | 4 (19%)  |
| 1   | OMC   | 1A    | 1920 | 1        | 19,22,23     | 0.81 | 0        | 25,31,34    | 0.97 | 0        |
| 1   | 5MU   | 2A    | 1939 | 58,1     | 19,22,23     | 1.39 | 4 (21%)  | 27,32,35    | 2.24 | 6 (22%)  |
| 32  | 5MC   | 1a    | 1407 | 32       | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.17 | 2 (7%)   |
| 57  | PSU   | 1y    | 55   | 57       | 18,21,22     | 1.44 | 2 (11%)  | 21,30,33    | 1.89 | 3 (14%)  |
| 1   | PSU   | 2A    | 2605 | 1        | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.01 | 3 (14%)  |
| 32  | MA6   | 1a    | 1518 | 32       | 23,26,27     | 0.40 | 0        | 33,38,41    | 2.01 | 9 (27%)  |
| 32  | MA6   | 1a    | 1519 | 32       | 23,26,27     | 0.42 | 0        | 33,38,41    | 1.99 | 9 (27%)  |
| 43  | 0TD   | 2l    | 92   | 43       | 8,9,10       | 4.49 | 2 (25%)  | 6,11,13     | 7.26 | 2 (33%)  |
| 57  | U8U   | 2y    | 34   | 57,53    | 17,21,25     | 1.64 | 3 (17%)  | 21,30,37    | 1.47 | 3 (14%)  |
| 57  | PSU   | 1y    | 39   | 57       | 18,21,22     | 1.50 | 3 (16%)  | 21,30,33    | 1.73 | 3 (14%)  |
| 32  | G7M   | 2a    | 527  | 32,58    | 23,26,27     | 1.50 | 3 (13%)  | 34,39,42    | 1.70 | 5 (14%)  |
| 32  | 4OC   | 2a    | 1402 | 32,58    | 20,23,24     | 0.76 | 0        | 25,32,35    | 1.06 | 2 (8%)   |
| 1   | 2MA   | 2A    | 2503 | 58,1     | 22,25,26     | 1.49 | 5 (22%)  | 32,37,40    | 2.20 | 7 (21%)  |
| 56  | FME   | 2z    | 1    | 56       | 8,9,10       | 1.00 | 0        | 8,9,11      | 0.78 | 0        |
| 55  | 8AN   | 1x    | 76   | 56,55    | 21,24,25     | 1.59 | 3 (14%)  | 26,35,38    | 2.39 | 6 (23%)  |
| 54  | U8U   | 2w    | 34   | 53,54    | 20,24,25     | 1.40 | 3 (15%)  | 22,34,37    | 1.37 | 4 (18%)  |
| 32  | G7M   | 1a    | 527  | 32,58    | 23,26,27     | 1.51 | 4 (17%)  | 34,39,42    | 1.63 | 4 (11%)  |
| 55  | 5MC   | 2x    | 32   | 55       | 19,22,23     | 1.56 | 3 (15%)  | 26,32,35    | 1.18 | 3 (11%)  |
| 55  | 8AN   | 2x    | 76   | 56,55,58 | 21,24,25     | 1.43 | 3 (14%)  | 26,35,38    | 2.38 | 11 (42%) |
| 55  | PSU   | 1x    | 55   | 55       | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.98 | 3 (14%)  |
| 55  | 5MU   | 2x    | 54   | 55       | 19,22,23     | 1.42 | 6 (31%)  | 27,32,35    | 2.25 | 7 (25%)  |
| 54  | A1B8A | 2w    | 76   | 54       | 30,33,34     | 1.26 | 3 (10%)  | 36,46,49    | 2.16 | 9 (25%)  |
| 32  | 5MC   | 1a    | 967  | 32       | 19,22,23     | 1.44 | 3 (15%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 1   | PSU   | 2A    | 1911 | 1        | 18,21,22     | 1.42 | 3 (16%)  | 21,30,33    | 2.06 | 3 (14%)  |
| 1   | 5MU   | 2A    | 1915 | 1        | 19,22,23     | 1.47 | 5 (26%)  | 27,32,35    | 2.02 | 5 (18%)  |
| 54  | 5MU   | 1w    | 54   | 54       | 19,22,23     | 1.43 | 4 (21%)  | 27,32,35    | 2.24 | 6 (22%)  |
| 54  | A1B8A | 1w    | 76   | 56,54    | 30,33,34     | 1.25 | 3 (10%)  | 36,46,49    | 2.08 | 9 (25%)  |

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 5MC  | 2a    | 967  | 32,58   | 19,22,23     | 1.71 | 3 (15%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 55  | 4SU  | 1x    | 8    | 55      | 18,21,22     | 2.34 | 5 (27%)  | 25,30,33    | 1.59 | 5 (20%)  |
| 1   | 2MA  | 1A    | 2503 | 58,1    | 22,25,26     | 1.39 | 3 (13%)  | 32,37,40    | 2.47 | 10 (31%) |
| 43  | 0TD  | 1l    | 92   | 43      | 8,9,10       | 4.68 | 1 (12%)  | 6,11,13     | 1.85 | 2 (33%)  |
| 1   | PSU  | 2A    | 1917 | 1       | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 2.11 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1407 | 32      | 19,22,23     | 1.65 | 3 (15%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 57  | G7M  | 2y    | 46   | 57      | 23,26,27     | 1.56 | 3 (13%)  | 34,39,42    | 1.88 | 4 (11%)  |
| 1   | 5MC  | 1A    | 1962 | 58,1    | 19,22,23     | 1.64 | 3 (15%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 55  | 5MC  | 1x    | 32   | 55      | 19,22,23     | 1.81 | 3 (15%)  | 26,32,35    | 1.19 | 2 (7%)   |
| 1   | OMU  | 1A    | 2552 | 58,1    | 19,22,23     | 1.22 | 3 (15%)  | 25,31,34    | 1.89 | 5 (20%)  |
| 32  | 5MC  | 1a    | 1404 | 32      | 19,22,23     | 1.74 | 3 (15%)  | 26,32,35    | 1.15 | 3 (11%)  |
| 32  | MA6  | 2a    | 1519 | 32      | 23,26,27     | 0.44 | 0        | 33,38,41    | 2.12 | 9 (27%)  |
| 32  | PSU  | 1a    | 516  | 32,58   | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 54  | 5MU  | 2w    | 54   | 54      | 19,22,23     | 1.52 | 5 (26%)  | 27,32,35    | 1.60 | 7 (25%)  |
| 32  | M2G  | 2a    | 966  | 32      | 24,27,28     | 1.34 | 4 (16%)  | 33,40,43    | 1.88 | 5 (15%)  |
| 57  | T6A  | 1y    | 37   | 57      | 21,24,35     | 1.54 | 4 (19%)  | 30,35,52    | 2.01 | 7 (23%)  |
| 32  | 5MC  | 2a    | 1400 | 32      | 19,22,23     | 1.72 | 3 (15%)  | 26,32,35    | 1.21 | 4 (15%)  |
| 54  | T6A  | 1w    | 37   | 54      | 31,34,35     | 1.40 | 4 (12%)  | 43,49,52    | 1.80 | 10 (23%) |
| 32  | UR3  | 2a    | 1498 | 32,58   | 19,22,23     | 0.98 | 0        | 26,32,35    | 1.77 | 4 (15%)  |
| 1   | 5MC  | 2A    | 1962 | 58,1    | 19,22,23     | 1.54 | 3 (15%)  | 26,32,35    | 1.15 | 2 (7%)   |
| 54  | PSU  | 1w    | 39   | 54      | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 57  | 5MU  | 1y    | 54   | 57      | 19,22,23     | 1.41 | 5 (26%)  | 27,32,35    | 2.25 | 7 (25%)  |
| 1   | OMU  | 2A    | 2552 | 58,1    | 19,22,23     | 1.22 | 3 (15%)  | 25,31,34    | 1.69 | 5 (20%)  |
| 1   | PSU  | 1A    | 1917 | 1       | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.08 | 3 (14%)  |
| 1   | OMG  | 1A    | 2251 | 58,55,1 | 23,26,27     | 1.23 | 3 (13%)  | 32,38,41    | 2.20 | 7 (21%)  |
| 32  | 4OC  | 1a    | 1402 | 32      | 20,23,24     | 0.73 | 0        | 25,32,35    | 1.04 | 2 (8%)   |
| 54  | PSU  | 2w    | 39   | 54      | 18,21,22     | 1.43 | 2 (11%)  | 21,30,33    | 1.70 | 3 (14%)  |
| 1   | 5MC  | 2A    | 1942 | 1       | 19,22,23     | 1.74 | 3 (15%)  | 26,32,35    | 1.18 | 2 (7%)   |
| 57  | T6A  | 2y    | 37   | 57,32   | 21,24,35     | 1.58 | 3 (14%)  | 30,35,52    | 1.98 | 8 (26%)  |
| 56  | FME  | 1z    | 1    | 56      | 8,9,10       | 1.04 | 0        | 8,9,11      | 0.81 | 0        |
| 54  | U8U  | 1w    | 34   | 53,54   | 20,24,25     | 1.40 | 3 (15%)  | 22,34,37    | 1.71 | 4 (18%)  |
| 57  | U8U  | 1y    | 34   | 57      | 17,21,25     | 1.50 | 3 (17%)  | 21,30,37    | 1.45 | 3 (14%)  |
| 55  | 5MU  | 1x    | 54   | 55      | 19,22,23     | 1.48 | 5 (26%)  | 27,32,35    | 1.74 | 5 (18%)  |
| 32  | PSU  | 2a    | 516  | 32,58   | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.17 | 6 (28%)  |
| 1   | OMG  | 2A    | 2251 | 55,1    | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 1.95 | 7 (21%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 54  | T6A  | 2w    | 37   | 53,54 | 31,34,35     | 1.40 | 3 (9%)   | 43,49,52    | 1.95 | 10 (23%) |
| 55  | PSU  | 2x    | 55   | 55    | 18,21,22     | 1.33 | 2 (11%)  | 21,30,33    | 2.13 | 4 (19%)  |
| 32  | 2MG  | 2a    | 1207 | 32    | 23,26,27     | 1.26 | 3 (13%)  | 33,38,41    | 2.10 | 6 (18%)  |
| 32  | MA6  | 2a    | 1518 | 32    | 23,26,27     | 0.40 | 0        | 33,38,41    | 2.06 | 9 (27%)  |
| 54  | G7M  | 1w    | 46   | 54    | 23,26,27     | 1.52 | 3 (13%)  | 34,39,42    | 1.79 | 5 (14%)  |
| 1   | 5MC  | 1A    | 1942 | 1     | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.10 | 2 (7%)   |
| 32  | M2G  | 1a    | 966  | 32    | 24,27,28     | 1.28 | 4 (16%)  | 33,40,43    | 1.86 | 6 (18%)  |
| 32  | 5MC  | 1a    | 1400 | 32    | 19,22,23     | 1.76 | 3 (15%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 55  | 4SU  | 2x    | 8    | 55    | 18,21,22     | 2.20 | 6 (33%)  | 25,30,33    | 1.50 | 7 (28%)  |
| 1   | OMC  | 2A    | 1920 | 1     | 19,22,23     | 0.77 | 0        | 25,31,34    | 0.86 | 1 (4%)   |
| 32  | UR3  | 1a    | 1498 | 32    | 19,22,23     | 1.07 | 1 (5%)   | 26,32,35    | 1.82 | 5 (19%)  |
| 54  | PSU  | 1w    | 55   | 54    | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.94 | 4 (19%)  |
| 1   | 5MU  | 1A    | 1915 | 1     | 19,22,23     | 1.42 | 6 (31%)  | 27,32,35    | 2.16 | 7 (25%)  |
| 1   | 5MU  | 1A    | 1939 | 58,1  | 19,22,23     | 1.41 | 4 (21%)  | 27,32,35    | 2.26 | 6 (22%)  |
| 54  | G7M  | 2w    | 46   | 54    | 23,26,27     | 1.46 | 3 (13%)  | 34,39,42    | 1.73 | 5 (14%)  |
| 57  | PSU  | 2y    | 39   | 57,42 | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.85 | 4 (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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 32  | 5MC  | 2a    | 1404 | 32    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2605 | 58,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | G7M  | 1y    | 46   | 57    | -       | 1/7/25/26  | 0/3/3/3 |
| 57  | PSU  | 2y    | 55   | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | PSU  | 1A    | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | 5MU  | 2y    | 54   | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2w    | 55   | 58,54 | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 1A    | 1920 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 58,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | PSU  | 1y    | 55   | 57    | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 2605 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1518 | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | MA6  | 1a    | 1519 | 32    | -       | 3/11/29/30 | 0/3/3/3 |

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| Mol | Type  | Chain | Res  | Link     | Chirals | Torsions   | Rings   |
|-----|-------|-------|------|----------|---------|------------|---------|
| 43  | 0TD   | 2l    | 92   | 43       | -       | 3/7/12/14  | -       |
| 57  | U8U   | 2y    | 34   | 57,53    | -       | 0/7/25/29  | 0/2/2/2 |
| 57  | PSU   | 1y    | 39   | 57       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | G7M   | 2a    | 527  | 32,58    | -       | 2/7/25/26  | 0/3/3/3 |
| 32  | 4OC   | 2a    | 1402 | 32,58    | -       | 2/9/29/30  | 0/2/2/2 |
| 1   | 2MA   | 2A    | 2503 | 58,1     | -       | 2/7/25/26  | 0/3/3/3 |
| 56  | FME   | 2z    | 1    | 56       | -       | 3/7/9/11   | -       |
| 55  | 8AN   | 1x    | 76   | 56,55    | -       | 3/7/25/26  | 0/3/3/3 |
| 54  | U8U   | 2w    | 34   | 53,54    | -       | 3/10/28/29 | 0/2/2/2 |
| 32  | G7M   | 1a    | 527  | 32,58    | -       | 2/7/25/26  | 0/3/3/3 |
| 55  | 5MC   | 2x    | 32   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 8AN   | 2x    | 76   | 56,55,58 | -       | 3/7/25/26  | 0/3/3/3 |
| 55  | PSU   | 1x    | 55   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU   | 2x    | 54   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | A1B8A | 2w    | 76   | 54       | -       | 3/20/38/39 | 0/3/3/3 |
| 32  | 5MC   | 1a    | 967  | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU   | 2A    | 1911 | 1        | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | 5MU   | 2A    | 1915 | 1        | -       | 1/7/25/26  | 0/2/2/2 |
| 54  | 5MU   | 1w    | 54   | 54       | -       | 2/7/25/26  | 0/2/2/2 |
| 54  | A1B8A | 1w    | 76   | 56,54    | -       | 3/20/38/39 | 0/3/3/3 |
| 32  | 5MC   | 2a    | 967  | 32,58    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 4SU   | 1x    | 8    | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA   | 1A    | 2503 | 58,1     | -       | 3/7/25/26  | 0/3/3/3 |
| 43  | 0TD   | 1l    | 92   | 43       | -       | 4/7/12/14  | -       |
| 1   | PSU   | 2A    | 1917 | 1        | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC   | 2a    | 1407 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | G7M   | 2y    | 46   | 57       | -       | 0/7/25/26  | 0/3/3/3 |
| 1   | 5MC   | 1A    | 1962 | 58,1     | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MC   | 1x    | 32   | 55       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU   | 1A    | 2552 | 58,1     | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | 5MC   | 1a    | 1404 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | MA6   | 2a    | 1519 | 32       | -       | 3/11/29/30 | 0/3/3/3 |
| 32  | PSU   | 1a    | 516  | 32,58    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 5MU   | 2w    | 54   | 54       | -       | 1/7/25/26  | 0/2/2/2 |
| 32  | M2G   | 2a    | 966  | 32       | -       | 0/11/29/30 | 0/3/3/3 |
| 57  | T6A   | 1y    | 37   | 57       | -       | 1/7/25/42  | 0/3/3/3 |
| 32  | 5MC   | 2a    | 1400 | 32       | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | T6A   | 1w    | 37   | 54       | -       | 6/23/41/42 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link    | Chirals | Torsions   | Rings   |
|-----|------|-------|------|---------|---------|------------|---------|
| 32  | UR3  | 2a    | 1498 | 32,58   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 58,1    | -       | 1/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1w    | 39   | 54      | -       | 2/7/25/26  | 0/2/2/2 |
| 57  | 5MU  | 1y    | 54   | 57      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | 2A    | 2552 | 58,1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 1A    | 2251 | 58,55,1 | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | 4OC  | 1a    | 1402 | 32      | -       | 1/9/29/30  | 0/2/2/2 |
| 54  | PSU  | 2w    | 39   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | T6A  | 2y    | 37   | 57,32   | -       | 0/7/25/42  | 0/3/3/3 |
| 56  | FME  | 1z    | 1    | 56      | -       | 5/7/9/11   | -       |
| 54  | U8U  | 1w    | 34   | 53,54   | -       | 2/10/28/29 | 0/2/2/2 |
| 57  | U8U  | 1y    | 34   | 57      | -       | 0/7/25/29  | 0/2/2/2 |
| 55  | 5MU  | 1x    | 54   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 32,58   | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 55,1    | -       | 1/9/27/28  | 0/3/3/3 |
| 54  | T6A  | 2w    | 37   | 53,54   | -       | 7/23/41/42 | 0/3/3/3 |
| 55  | PSU  | 2x    | 55   | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32      | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | MA6  | 2a    | 1518 | 32      | -       | 0/11/29/30 | 0/3/3/3 |
| 54  | G7M  | 1w    | 46   | 54      | -       | 2/7/25/26  | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1942 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32      | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1400 | 32      | -       | 2/7/25/26  | 0/2/2/2 |
| 55  | 4SU  | 2x    | 8    | 55      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 2A    | 1920 | 1       | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | UR3  | 1a    | 1498 | 32      | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1w    | 55   | 54      | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 58,1    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | G7M  | 2w    | 46   | 54      | -       | 3/7/25/26  | 0/3/3/3 |
| 57  | PSU  | 2y    | 39   | 57,42   | -       | 0/7/25/26  | 0/2/2/2 |

The worst 5 of 240 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CB-SB | -12.80 | 1.69        | 1.82     |
| 43  | 2l    | 92   | 0TD  | CB-SB | -12.16 | 1.70        | 1.82     |
| 55  | 1x    | 32   | 5MC  | C5-C4 | 6.59   | 1.49        | 1.44     |
| 32  | 1a    | 1400 | 5MC  | C5-C4 | 6.51   | 1.49        | 1.44     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 32  | 1a    | 1404 | 5MC  | C5-C4 | 6.43 | 1.49        | 1.44     |

The worst 5 of 409 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB  | -17.58 | 70.76       | 102.36   |
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3   | -7.96  | 118.80      | 127.18   |
| 55  | 1x    | 76   | 8AN  | O4'-C1'-N9 | 7.90   | 123.27      | 108.09   |
| 1   | 2A    | 2503 | 2MA  | C5-C4-N3   | -7.35  | 119.43      | 127.18   |
| 1   | 1A    | 2251 | OMG  | C5-C4-N3   | -7.09  | 117.11      | 128.39   |

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 32  | 1a    | 1400 | 5MC  | O4'-C4'-C5'-O5' |
| 32  | 1a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 32  | 1a    | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 43  | 1l    | 92   | 0TD  | O-C-CA-CB       |
| 43  | 1l    | 92   | 0TD  | CG-CB-SB-CSB    |

There are no ring outliers.

48 monomers are involved in 72 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32  | 2a    | 1404 | 5MC  | 2       | 0            |
| 57  | 1y    | 46   | G7M  | 1       | 0            |
| 32  | 1a    | 1207 | 2MG  | 1       | 0            |
| 54  | 2w    | 55   | PSU  | 2       | 0            |
| 1   | 2A    | 1939 | 5MU  | 2       | 0            |
| 57  | 1y    | 55   | PSU  | 2       | 0            |
| 32  | 1a    | 1518 | MA6  | 3       | 0            |
| 32  | 1a    | 1519 | MA6  | 2       | 0            |
| 43  | 2l    | 92   | 0TD  | 1       | 0            |
| 57  | 2y    | 34   | U8U  | 2       | 0            |
| 57  | 1y    | 39   | PSU  | 1       | 0            |
| 32  | 2a    | 1402 | 4OC  | 2       | 0            |
| 1   | 2A    | 2503 | 2MA  | 2       | 0            |
| 56  | 2z    | 1    | FME  | 1       | 0            |
| 55  | 1x    | 76   | 8AN  | 2       | 0            |
| 54  | 2w    | 34   | U8U  | 1       | 0            |

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| Mol | Chain | Res  | Type  | Clashes | Symm-Clashes |
|-----|-------|------|-------|---------|--------------|
| 32  | 1a    | 527  | G7M   | 1       | 0            |
| 55  | 2x    | 76   | 8AN   | 1       | 0            |
| 54  | 2w    | 76   | A1B8A | 2       | 0            |
| 1   | 2A    | 1911 | PSU   | 2       | 0            |
| 54  | 1w    | 76   | A1B8A | 2       | 0            |
| 55  | 1x    | 8    | 4SU   | 1       | 0            |
| 1   | 1A    | 2503 | 2MA   | 1       | 0            |
| 43  | 1l    | 92   | 0TD   | 1       | 0            |
| 57  | 2y    | 46   | G7M   | 5       | 0            |
| 1   | 1A    | 2552 | OMU   | 1       | 0            |
| 32  | 2a    | 1519 | MA6   | 3       | 0            |
| 32  | 1a    | 516  | PSU   | 1       | 0            |
| 57  | 1y    | 37   | T6A   | 1       | 0            |
| 32  | 2a    | 1400 | 5MC   | 2       | 0            |
| 32  | 2a    | 1498 | UR3   | 1       | 0            |
| 54  | 1w    | 39   | PSU   | 1       | 0            |
| 1   | 2A    | 2552 | OMU   | 1       | 0            |
| 1   | 1A    | 1917 | PSU   | 1       | 0            |
| 32  | 1a    | 1402 | 4OC   | 3       | 0            |
| 54  | 2w    | 39   | PSU   | 1       | 0            |
| 1   | 2A    | 1942 | 5MC   | 1       | 0            |
| 57  | 2y    | 37   | T6A   | 1       | 0            |
| 56  | 1z    | 1    | FME   | 1       | 0            |
| 54  | 1w    | 34   | U8U   | 4       | 0            |
| 32  | 2a    | 516  | PSU   | 1       | 0            |
| 32  | 2a    | 1207 | 2MG   | 3       | 0            |
| 32  | 2a    | 1518 | MA6   | 2       | 0            |
| 32  | 1a    | 1400 | 5MC   | 1       | 0            |
| 55  | 2x    | 8    | 4SU   | 1       | 0            |
| 32  | 1a    | 1498 | UR3   | 1       | 0            |
| 1   | 1A    | 1939 | 5MU   | 1       | 0            |
| 57  | 2y    | 39   | PSU   | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2677 ligands modelled in this entry, 2673 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 |
| 60  | TEL  | 1A    | 4082 | -    | 60,62,62     | 1.38 | 5 (8%)   | 78,92,92    | 1.70 | 12 (15%) |
| 60  | TEL  | 2A    | 3826 | -    | 60,62,62     | 1.35 | 4 (6%)   | 78,92,92    | 1.98 | 18 (23%) |
| 62  | SF4  | 1d    | 302  | 35   | 0,12,12      | -    | -        | -           |      |          |
| 62  | SF4  | 2d    | 303  | 35   | 0,12,12      | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions      | Rings   |
|-----|------|-------|------|------|---------|---------------|---------|
| 60  | TEL  | 1A    | 4082 | -    | -       | 10/73/108/108 | 0/4/5/5 |
| 60  | TEL  | 2A    | 3826 | -    | -       | 9/73/108/108  | 0/4/5/5 |
| 62  | SF4  | 1d    | 302  | 35   | -       | -             | 0/6/5/5 |
| 62  | SF4  | 2d    | 303  | 35   | -       | -             | 0/6/5/5 |

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

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 60  | 1A    | 4082 | TEL  | O5-C10  | 5.74  | 1.44        | 1.35     |
| 60  | 2A    | 3826 | TEL  | O5-C10  | 5.43  | 1.44        | 1.35     |
| 60  | 1A    | 4082 | TEL  | O9-C15  | 5.08  | 1.45        | 1.34     |
| 60  | 2A    | 3826 | TEL  | O9-C15  | 5.01  | 1.45        | 1.34     |
| 60  | 2A    | 3826 | TEL  | C40-N41 | -3.71 | 1.34        | 1.38     |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 60  | 2A    | 3826 | TEL  | O9-C15-C21  | 9.28  | 120.09      | 110.93   |
| 60  | 1A    | 4082 | TEL  | O9-C15-C21  | 6.60  | 117.44      | 110.93   |
| 60  | 1A    | 4082 | TEL  | C17-C11-N6  | -5.90 | 104.31      | 113.25   |
| 60  | 2A    | 3826 | TEL  | C17-C11-N6  | -5.71 | 104.59      | 113.25   |
| 60  | 1A    | 4082 | TEL  | N31-C37-N41 | -4.39 | 108.85      | 112.35   |

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

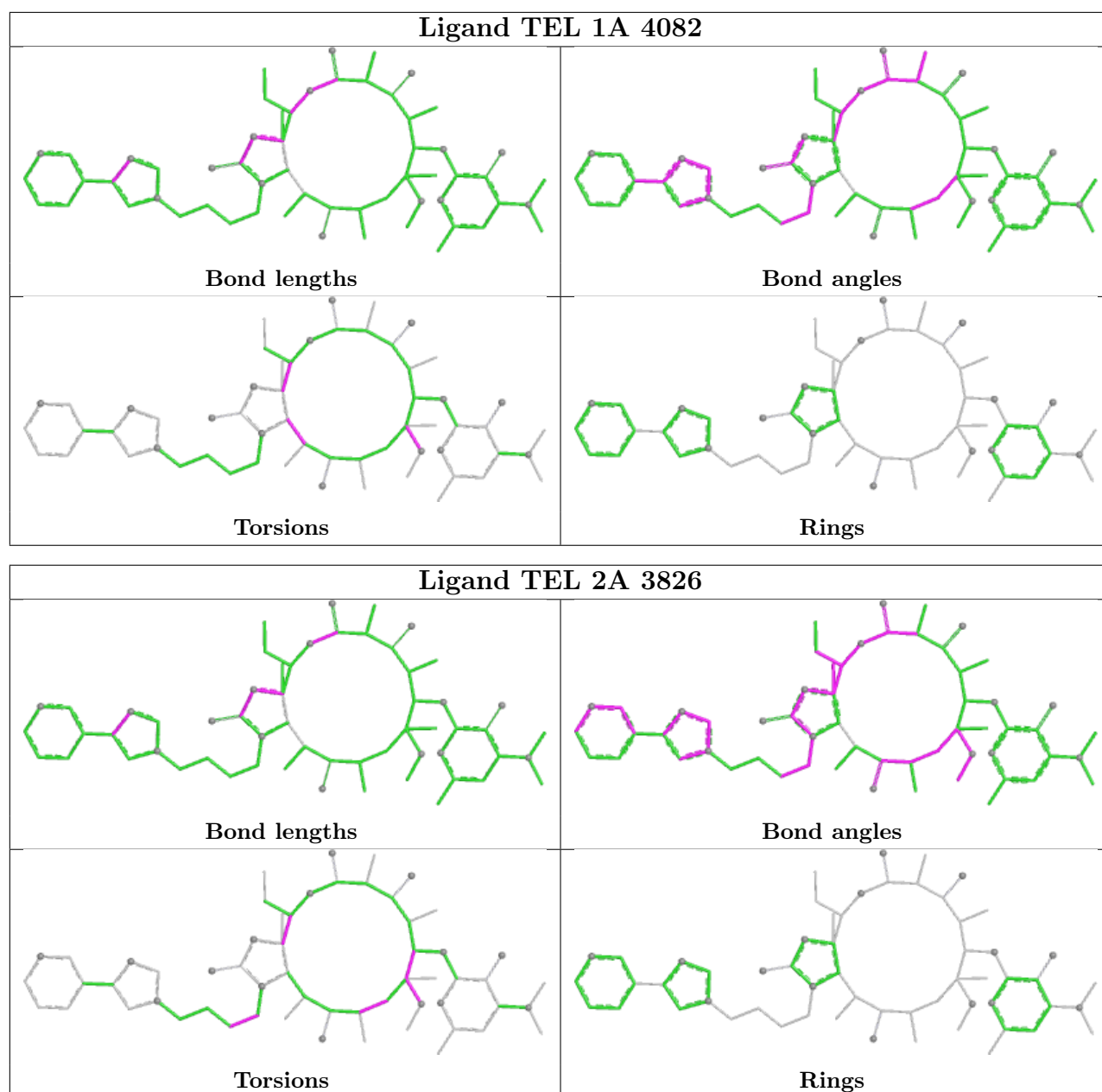
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 60  | 1A    | 4082 | TEL  | C1-C2-C4-C8     |
| 60  | 1A    | 4082 | TEL  | O5-C2-C4-C8     |
| 60  | 1A    | 4082 | TEL  | O5-C2-C4-O9     |
| 60  | 1A    | 4082 | TEL  | C24-C28-O32-C38 |
| 60  | 1A    | 4082 | TEL  | C33-C28-O32-C38 |

There are no ring outliers.

4 monomers are involved in 11 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60  | 1A    | 4082 | TEL  | 4       | 0            |
| 60  | 2A    | 3826 | TEL  | 4       | 0            |
| 62  | 1d    | 302  | SF4  | 1       | 0            |
| 62  | 2d    | 303  | SF4  | 2       | 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    | 2860/2915 (98%) | -0.15  | 107 (3%) 45 36 | 17, 35, 97, 108       | 0     |
| 1   | 2A    | 2789/2915 (95%) | 0.30   | 87 (3%) 51 41  | 30, 58, 93, 107       | 0     |
| 2   | 1B    | 120/121 (99%)   | -0.11  | 1 (0%) 82 75   | 28, 50, 62, 85        | 0     |
| 2   | 2B    | 120/121 (99%)   | 1.20   | 19 (15%) 5 4   | 58, 82, 91, 99        | 0     |
| 3   | 1D    | 275/276 (99%)   | 0.07   | 3 (1%) 78 70   | 17, 34, 49, 76        | 0     |
| 3   | 2D    | 275/276 (99%)   | 0.48   | 7 (2%) 58 48   | 30, 51, 65, 86        | 0     |
| 4   | 1E    | 204/206 (99%)   | 0.14   | 0 100 100      | 18, 42, 62, 80        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.52   | 6 (2%) 53 43   | 29, 56, 70, 83        | 0     |
| 5   | 1F    | 203/210 (96%)   | 0.15   | 0 100 100      | 19, 43, 69, 82        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.60   | 3 (1%) 72 63   | 32, 66, 79, 88        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.55   | 7 (3%) 43 34   | 39, 56, 73, 85        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.48   | 40 (22%) 2 2   | 71, 81, 89, 95        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.30   | 2 (1%) 78 70   | 35, 52, 64, 75        | 0     |
| 7   | 2H    | 174/180 (96%)   | 1.04   | 14 (8%) 18 13  | 68, 81, 89, 95        | 0     |
| 8   | 1I    | 146/148 (98%)   | 0.88   | 5 (3%) 48 39   | 42, 72, 82, 89        | 0     |
| 8   | 2I    | 146/148 (98%)   | 1.03   | 16 (10%) 10 8  | 55, 73, 84, 87        | 0     |
| 9   | 1N    | 140/140 (100%)  | 0.17   | 1 (0%) 84 77   | 25, 40, 60, 75        | 0     |
| 9   | 2N    | 140/140 (100%)  | 1.02   | 11 (7%) 18 13  | 43, 65, 76, 81        | 0     |
| 10  | 1O    | 122/122 (100%)  | 0.09   | 1 (0%) 82 75   | 25, 40, 55, 60        | 0     |
| 10  | 2O    | 122/122 (100%)  | 0.43   | 0 100 100      | 41, 53, 67, 75        | 0     |
| 11  | 1P    | 149/150 (99%)   | 0.41   | 1 (0%) 84 77   | 20, 45, 67, 77        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.77   | 12 (8%) 18 13  | 38, 67, 79, 87        | 0     |
| 12  | 1Q    | 141/141 (100%)  | 0.16   | 2 (1%) 73 64   | 25, 40, 54, 68        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 1.25   | 16 (11%) 10 7  | 47, 66, 77, 82        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | 0.09   | 0 100 100    | 21, 35, 51, 66        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.43   | 0 100 100    | 35, 49, 62, 68        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.31   | 1 (0%) 81 74 | 36, 48, 60, 63        | 0     |
| 14  | 2S    | 110/112 (98%)  | 1.33   | 24 (21%) 2 2 | 63, 74, 83, 86        | 0     |
| 15  | 1T    | 131/146 (89%)  | 0.43   | 3 (2%) 61 51 | 34, 46, 68, 79        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.50   | 2 (1%) 72 63 | 44, 57, 71, 81        | 0     |
| 16  | 1U    | 116/118 (98%)  | 0.06   | 1 (0%) 81 74 | 22, 32, 49, 66        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.77   | 5 (4%) 40 31 | 45, 64, 75, 83        | 0     |
| 17  | 1V    | 101/101 (100%) | 0.08   | 0 100 100    | 22, 43, 60, 70        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.89   | 8 (7%) 18 13 | 43, 73, 81, 85        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.11  | 0 100 100    | 25, 33, 49, 73        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.61   | 2 (1%) 67 58 | 36, 50, 67, 85        | 0     |
| 19  | 1X    | 95/96 (98%)    | 0.08   | 1 (1%) 78 70 | 26, 37, 58, 74        | 0     |
| 19  | 2X    | 95/96 (98%)    | 1.03   | 12 (12%) 8 6 | 48, 59, 73, 79        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.35   | 3 (2%) 55 45 | 36, 48, 67, 77        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 1.37   | 18 (16%) 4 3 | 61, 71, 79, 82        | 0     |
| 21  | 1Z    | 154/206 (74%)  | 0.63   | 8 (5%) 33 25 | 42, 60, 83, 88        | 0     |
| 21  | 2Z    | 160/206 (77%)  | 1.21   | 25 (15%) 5 4 | 70, 80, 89, 95        | 0     |
| 22  | 10    | 83/85 (97%)    | 0.49   | 8 (9%) 13 10 | 26, 36, 62, 78        | 0     |
| 22  | 20    | 83/85 (97%)    | 1.30   | 14 (16%) 4 3 | 51, 65, 75, 91        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.29   | 1 (1%) 79 72 | 25, 42, 65, 70        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.66   | 6 (6%) 26 20 | 36, 56, 74, 78        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.10   | 0 100 100    | 35, 47, 59, 68        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.80   | 1 (1%) 73 64 | 56, 69, 75, 77        | 0     |
| 25  | 13    | 59/60 (98%)    | 0.10   | 0 100 100    | 28, 38, 56, 63        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.72   | 0 100 100    | 54, 67, 77, 82        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.76   | 4 (5%) 29 22 | 52, 74, 88, 94        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.15   | 7 (10%) 12 9 | 74, 87, 93, 99        | 0     |
| 27  | 15    | 59/60 (98%)    | -0.06  | 0 100 100    | 20, 36, 50, 62        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.40   | 0 100 100    | 34, 51, 64, 74        | 0     |
| 28  | 16    | 53/54 (98%)    | 0.14   | 1 (1%) 66 57 | 30, 40, 57, 61        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 1.00   | 5 (9%) 14 10   | 46, 60, 69, 76        | 0     |
| 29  | 17    | 48/49 (97%)     | 0.02   | 1 (2%) 63 54   | 21, 28, 53, 58        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.33   | 3 (6%) 26 19   | 31, 41, 59, 66        | 0     |
| 30  | 18    | 64/65 (98%)     | 0.13   | 1 (1%) 70 61   | 24, 33, 40, 49        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.79   | 2 (3%) 51 41   | 47, 55, 62, 66        | 0     |
| 31  | 19    | 37/37 (100%)    | 0.10   | 1 (2%) 56 46   | 28, 37, 56, 59        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.41   | 5 (13%) 7 5    | 59, 69, 77, 87        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.39   | 31 (2%) 63 54  | 31, 65, 92, 106       | 0     |
| 32  | 2a    | 1491/1521 (98%) | 0.84   | 112 (7%) 20 15 | 50, 80, 97, 106       | 0     |
| 33  | 1b    | 231/256 (90%)   | 0.86   | 22 (9%) 14 10  | 62, 76, 84, 91        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.58   | 64 (27%) 1 1   | 74, 86, 92, 95        | 0     |
| 34  | 1c    | 206/239 (86%)   | 0.53   | 5 (2%) 59 49   | 52, 69, 80, 90        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.60   | 70 (33%) 1 1   | 74, 85, 90, 94        | 0     |
| 35  | 1d    | 208/209 (99%)   | 0.68   | 9 (4%) 40 31   | 55, 67, 77, 80        | 0     |
| 35  | 2d    | 208/209 (99%)   | 1.31   | 35 (16%) 4 3   | 65, 75, 83, 91        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.67   | 3 (2%) 65 56   | 50, 62, 71, 83        | 0     |
| 36  | 2e    | 148/162 (91%)   | 1.16   | 23 (15%) 5 4   | 69, 79, 85, 89        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.49   | 0 100 100      | 49, 64, 75, 79        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.86   | 7 (7%) 22 16   | 60, 72, 80, 83        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.96   | 14 (9%) 15 11  | 57, 70, 84, 99        | 0     |
| 38  | 2g    | 155/156 (99%)   | 1.44   | 39 (25%) 1 1   | 73, 82, 88, 94        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.68   | 6 (4%) 39 31   | 55, 65, 72, 78        | 0     |
| 39  | 2h    | 137/138 (99%)   | 1.29   | 20 (14%) 6 4   | 69, 79, 84, 89        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.16   | 17 (13%) 7 5   | 50, 75, 84, 88        | 0     |
| 40  | 2i    | 127/128 (99%)   | 2.05   | 60 (47%) 0 0   | 74, 86, 91, 93        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.26   | 15 (15%) 5 4   | 51, 74, 85, 90        | 0     |
| 41  | 2j    | 96/105 (91%)    | 1.86   | 34 (35%) 1 0   | 75, 86, 92, 94        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.76   | 7 (6%) 27 20   | 39, 64, 77, 84        | 0     |
| 42  | 2k    | 114/129 (88%)   | 1.03   | 12 (10%) 11 8  | 63, 75, 83, 86        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.71   | 8 (6%) 24 18   | 45, 55, 66, 76        | 0     |
| 43  | 2l    | 121/132 (91%)   | 1.29   | 20 (16%) 4 3   | 53, 71, 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%)     | 0.97   | 12 (9%) 13 9    | 54, 68, 78, 92        | 0     |
| 44  | 2m    | 122/126 (96%)     | 1.71   | 39 (31%) 1 1    | 71, 84, 89, 91        | 0     |
| 45  | 1n    | 60/61 (98%)       | 0.89   | 5 (8%) 17 12    | 56, 65, 75, 81        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.45   | 36 (60%) 0 0    | 77, 85, 89, 94        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.59   | 3 (3%) 48 39    | 50, 61, 73, 84        | 0     |
| 46  | 2o    | 88/89 (98%)       | 1.00   | 8 (9%) 15 11    | 62, 75, 82, 86        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.50   | 15 (18%) 3 2    | 57, 71, 78, 83        | 0     |
| 47  | 2p    | 82/88 (93%)       | 1.17   | 6 (7%) 21 15    | 57, 68, 76, 85        | 0     |
| 48  | 1q    | 99/105 (94%)      | 1.01   | 7 (7%) 22 16    | 53, 67, 75, 80        | 0     |
| 48  | 2q    | 99/105 (94%)      | 1.11   | 15 (15%) 5 4    | 63, 74, 81, 86        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.51   | 4 (5%) 28 21    | 53, 64, 73, 79        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.68   | 1 (1%) 72 63    | 67, 76, 84, 87        | 0     |
| 50  | 1s    | 83/93 (89%)       | 0.84   | 5 (6%) 27 21    | 59, 70, 82, 93        | 0     |
| 50  | 2s    | 83/93 (89%)       | 1.88   | 26 (31%) 1 1    | 79, 86, 92, 93        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.94   | 14 (14%) 6 4    | 59, 70, 78, 86        | 0     |
| 51  | 2t    | 96/106 (90%)      | 1.01   | 16 (16%) 4 3    | 54, 69, 82, 84        | 0     |
| 52  | 1u    | 23/27 (85%)       | 1.35   | 4 (17%) 4 3     | 58, 64, 69, 76        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.31   | 12 (52%) 0 0    | 76, 81, 84, 89        | 0     |
| 53  | 1v    | 13/24 (54%)       | 1.27   | 2 (15%) 5 4     | 41, 77, 94, 95        | 0     |
| 53  | 2v    | 13/24 (54%)       | 1.61   | 4 (30%) 1 1     | 78, 91, 95, 97        | 0     |
| 54  | 1w    | 67/76 (88%)       | 1.22   | 12 (17%) 3 3    | 58, 96, 102, 104      | 0     |
| 54  | 2w    | 67/76 (88%)       | 1.45   | 14 (20%) 2 2    | 78, 99, 105, 106      | 0     |
| 55  | 1x    | 72/77 (93%)       | 0.38   | 1 (1%) 73 64    | 41, 65, 83, 84        | 0     |
| 55  | 2x    | 72/77 (93%)       | 1.03   | 7 (9%) 13 10    | 52, 82, 91, 97        | 0     |
| 56  | 1z    | 2/3 (66%)         | 0.83   | 0 100 100       | 43, 43, 43, 46        | 0     |
| 56  | 2z    | 2/3 (66%)         | 1.70   | 1 (50%) 0 0     | 53, 53, 53, 69        | 0     |
| 57  | 1y    | 68/76 (89%)       | 1.17   | 7 (10%) 12 9    | 54, 99, 105, 107      | 0     |
| 57  | 2y    | 68/76 (89%)       | 1.57   | 14 (20%) 2 2    | 69, 101, 106, 107     | 0     |
| All | All   | 20884/21754 (96%) | 0.57   | 1457 (6%) 22 16 | 17, 63, 91, 108       | 0     |

The worst 5 of 1457 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 44  | 2m    | 123 | ALA  | 8.8  |
| 45  | 1n    | 2   | ALA  | 8.5  |
| 38  | 1g    | 81  | GLY  | 8.3  |
| 44  | 1m    | 123 | ALA  | 7.4  |
| 44  | 1m    | 122 | LYS  | 7.2  |

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

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | PSU  | 2w    | 55   | 20/21 | 0.41 | 0.17 | 94,101,114,114             | 0     |
| 54  | 5MU  | 2w    | 54   | 21/22 | 0.43 | 0.18 | 86,98,102,109              | 0     |
| 57  | G7M  | 2y    | 46   | 24/25 | 0.44 | 0.15 | 93,102,110,121             | 0     |
| 57  | PSU  | 2y    | 55   | 20/21 | 0.51 | 0.16 | 94,102,106,116             | 0     |
| 57  | U8U  | 1y    | 34   | 20/24 | 0.55 | 0.19 | 88,96,101,112              | 0     |
| 57  | G7M  | 1y    | 46   | 24/25 | 0.56 | 0.12 | 91,100,105,115             | 0     |
| 54  | PSU  | 1w    | 55   | 20/21 | 0.57 | 0.18 | 85,97,105,106              | 0     |
| 54  | G7M  | 2w    | 46   | 24/25 | 0.58 | 0.14 | 92,100,105,110             | 0     |
| 57  | T6A  | 1y    | 37   | 22/33 | 0.61 | 0.16 | 79,92,98,108               | 0     |
| 57  | PSU  | 1y    | 39   | 20/21 | 0.64 | 0.13 | 91,97,105,111              | 0     |
| 57  | T6A  | 2y    | 37   | 22/33 | 0.64 | 0.14 | 86,93,102,117              | 0     |
| 54  | G7M  | 1w    | 46   | 24/25 | 0.65 | 0.13 | 86,95,103,104              | 0     |
| 54  | T6A  | 2w    | 37   | 32/33 | 0.66 | 0.20 | 76,92,97,98                | 0     |
| 57  | U8U  | 2y    | 34   | 20/24 | 0.68 | 0.17 | 96,104,112,115             | 0     |
| 57  | PSU  | 2y    | 39   | 20/21 | 0.68 | 0.16 | 89,94,105,106              | 0     |
| 54  | PSU  | 2w    | 39   | 20/21 | 0.69 | 0.17 | 85,93,99,104               | 0     |
| 57  | 5MU  | 2y    | 54   | 21/22 | 0.71 | 0.13 | 87,100,112,125             | 0     |
| 57  | 5MU  | 1y    | 54   | 21/22 | 0.71 | 0.12 | 92,100,102,113             | 0     |
| 57  | PSU  | 1y    | 55   | 20/21 | 0.71 | 0.12 | 95,101,109,118             | 0     |
| 54  | U8U  | 1w    | 34   | 23/24 | 0.72 | 0.22 | 76,83,91,105               | 0     |
| 55  | 5MU  | 2x    | 54   | 21/22 | 0.72 | 0.16 | 84,87,92,107               | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.73 | 0.15 | 79,86,88,93                | 0     |
| 54  | U8U  | 2w    | 34   | 23/24 | 0.73 | 0.20 | 80,92,99,108               | 0     |
| 54  | 5MU  | 1w    | 54   | 21/22 | 0.73 | 0.13 | 78,89,96,98                | 0     |
| 55  | 4SU  | 2x    | 8    | 20/21 | 0.77 | 0.15 | 79,85,90,96                | 0     |
| 55  | PSU  | 2x    | 55   | 20/21 | 0.78 | 0.13 | 77,81,88,100               | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.82 | 0.15 | 80,87,94,99                | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.83 | 0.20 | 74,81,85,86                | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.83 | 0.12 | 80,87,94,94                | 0     |

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| Mol | Type  | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|-------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | M2G   | 2a    | 966  | 25/26 | 0.85 | 0.17 | 61,70,90,94                 | 0     |
| 32  | 5MC   | 2a    | 967  | 21/22 | 0.85 | 0.16 | 71,77,87,89                 | 0     |
| 32  | G7M   | 2a    | 527  | 24/25 | 0.85 | 0.15 | 58,69,76,78                 | 0     |
| 54  | T6A   | 1w    | 37   | 32/33 | 0.85 | 0.14 | 67,76,83,84                 | 0     |
| 1   | PSU   | 2A    | 1911 | 20/21 | 0.86 | 0.12 | 62,70,80,83                 | 0     |
| 54  | A1B8A | 2w    | 76   | 31/32 | 0.86 | 0.16 | 48,67,78,84                 | 0     |
| 55  | PSU   | 1x    | 55   | 20/21 | 0.87 | 0.11 | 57,66,75,81                 | 0     |
| 1   | OMC   | 2A    | 1920 | 21/22 | 0.87 | 0.14 | 54,71,78,78                 | 0     |
| 43  | 0TD   | 2l    | 92   | 10/11 | 0.87 | 0.14 | 63,68,72,89                 | 0     |
| 56  | FME   | 2z    | 1    | 10/11 | 0.87 | 0.23 | 62,66,74,74                 | 0     |
| 32  | 4OC   | 2a    | 1402 | 22/23 | 0.88 | 0.15 | 63,74,79,81                 | 0     |
| 1   | PSU   | 2A    | 1917 | 20/21 | 0.89 | 0.11 | 57,78,83,83                 | 0     |
| 55  | 5MC   | 2x    | 32   | 21/22 | 0.89 | 0.14 | 70,74,79,83                 | 0     |
| 54  | PSU   | 1w    | 39   | 20/21 | 0.89 | 0.10 | 74,85,90,91                 | 0     |
| 1   | 5MU   | 1A    | 1915 | 21/22 | 0.89 | 0.12 | 53,61,71,73                 | 0     |
| 32  | 5MC   | 2a    | 1404 | 21/22 | 0.90 | 0.14 | 57,65,72,78                 | 0     |
| 43  | 0TD   | 1l    | 92   | 10/11 | 0.90 | 0.12 | 50,54,57,66                 | 0     |
| 32  | PSU   | 1a    | 516  | 20/21 | 0.91 | 0.10 | 57,64,69,71                 | 0     |
| 54  | A1B8A | 1w    | 76   | 31/32 | 0.91 | 0.13 | 31,48,58,65                 | 0     |
| 55  | 8AN   | 1x    | 76   | 22/23 | 0.91 | 0.13 | 31,43,54,60                 | 0     |
| 55  | 5MU   | 1x    | 54   | 21/22 | 0.91 | 0.11 | 65,72,79,85                 | 0     |
| 1   | 5MC   | 2A    | 1962 | 21/22 | 0.92 | 0.13 | 40,53,60,70                 | 0     |
| 1   | PSU   | 1A    | 1917 | 20/21 | 0.92 | 0.11 | 41,54,63,66                 | 0     |
| 56  | FME   | 1z    | 1    | 10/11 | 0.92 | 0.20 | 41,52,67,68                 | 0     |
| 55  | 8AN   | 2x    | 76   | 22/23 | 0.92 | 0.11 | 49,55,63,72                 | 0     |
| 32  | M2G   | 1a    | 966  | 25/26 | 0.93 | 0.14 | 37,48,57,61                 | 0     |
| 1   | 5MC   | 2A    | 1942 | 21/22 | 0.93 | 0.12 | 39,62,73,78                 | 0     |
| 55  | 4SU   | 1x    | 8    | 20/21 | 0.93 | 0.10 | 49,56,61,62                 | 0     |
| 55  | 5MC   | 1x    | 32   | 21/22 | 0.93 | 0.13 | 41,52,57,66                 | 0     |
| 32  | 2MG   | 1a    | 1207 | 24/25 | 0.93 | 0.10 | 59,65,73,76                 | 0     |
| 32  | 5MC   | 2a    | 1407 | 21/22 | 0.93 | 0.12 | 59,64,69,72                 | 0     |
| 32  | MA6   | 2a    | 1518 | 24/25 | 0.93 | 0.13 | 58,68,72,77                 | 0     |
| 32  | MA6   | 2a    | 1519 | 24/25 | 0.93 | 0.15 | 60,69,76,78                 | 0     |
| 32  | MA6   | 1a    | 1519 | 24/25 | 0.93 | 0.13 | 36,39,42,51                 | 0     |
| 1   | 5MC   | 1A    | 1942 | 21/22 | 0.94 | 0.10 | 36,46,53,55                 | 0     |
| 32  | UR3   | 2a    | 1498 | 21/22 | 0.94 | 0.11 | 55,65,71,74                 | 0     |
| 32  | G7M   | 1a    | 527  | 24/25 | 0.94 | 0.11 | 48,52,59,60                 | 0     |
| 32  | 4OC   | 1a    | 1402 | 22/23 | 0.94 | 0.11 | 41,47,54,60                 | 0     |
| 1   | OMU   | 2A    | 2552 | 21/22 | 0.95 | 0.09 | 36,43,50,51                 | 0     |
| 1   | PSU   | 2A    | 2605 | 20/21 | 0.95 | 0.09 | 33,38,40,43                 | 0     |
| 32  | 5MC   | 1a    | 1404 | 21/22 | 0.95 | 0.11 | 26,39,42,49                 | 0     |
| 32  | UR3   | 1a    | 1498 | 21/22 | 0.95 | 0.10 | 29,38,41,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.95 | 0.11 | 45,52,57,59                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.95 | 0.10 | 34,39,44,45                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.96 | 0.08 | 38,48,53,56                 | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.96 | 0.10 | 29,48,53,54                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.96 | 0.09 | 32,36,40,43                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.97 | 0.09 | 27,37,42,46                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.97 | 0.10 | 41,47,52,58                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.08 | 27,31,35,36                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.97 | 0.09 | 26,38,41,42                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.97 | 0.07 | 23,36,41,46                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.06 | 23,27,32,36                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.07 | 19,24,29,34                 | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.07 | 16,20,25,26                 | 0     |
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.98 | 0.07 | 21,29,33,37                 | 0     |
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.98 | 0.06 | 17,28,30,31                 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3787 | 1/1   | 0.59 | 0.18 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3797 | 1/1   | 0.60 | 0.25 | 81,81,81,81                 | 0     |
| 58  | MG   | 2a    | 3185 | 1/1   | 0.60 | 0.20 | 89,89,89,89                 | 0     |
| 58  | MG   | 2a    | 3133 | 1/1   | 0.61 | 0.37 | 83,83,83,83                 | 0     |
| 58  | MG   | 2A    | 3758 | 1/1   | 0.61 | 0.15 | 76,76,76,76                 | 0     |
| 58  | MG   | 1a    | 1712 | 1/1   | 0.62 | 0.21 | 78,78,78,78                 | 0     |
| 58  | MG   | 2A    | 3546 | 1/1   | 0.62 | 0.22 | 53,53,53,53                 | 0     |
| 58  | MG   | 2a    | 3146 | 1/1   | 0.62 | 0.10 | 102,102,102,102             | 0     |
| 58  | MG   | 1a    | 1695 | 1/1   | 0.62 | 0.18 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3050 | 1/1   | 0.63 | 0.25 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3190 | 1/1   | 0.63 | 0.16 | 89,89,89,89                 | 0     |
| 58  | MG   | 2A    | 3081 | 1/1   | 0.65 | 0.31 | 59,59,59,59                 | 0     |
| 58  | MG   | 2a    | 3036 | 1/1   | 0.65 | 0.24 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3194 | 1/1   | 0.65 | 0.33 | 81,81,81,81                 | 0     |
| 58  | MG   | 1A    | 3882 | 1/1   | 0.66 | 0.25 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3758 | 1/1   | 0.66 | 0.16 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 4066 | 1/1   | 0.67 | 0.22 | 78,78,78,78                 | 0     |
| 58  | MG   | 2A    | 3749 | 1/1   | 0.67 | 0.17 | 77,77,77,77                 | 0     |
| 58  | MG   | 2A    | 3567 | 1/1   | 0.68 | 0.21 | 82,82,82,82                 | 0     |
| 58  | MG   | 2A    | 3295 | 1/1   | 0.68 | 0.15 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3458 | 1/1   | 0.69 | 0.25 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3770 | 1/1   | 0.69 | 0.24 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3436 | 1/1   | 0.69 | 0.19 | 60,60,60,60                 | 0     |
| 58  | MG   | 2a    | 3173 | 1/1   | 0.70 | 0.25 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3541 | 1/1   | 0.70 | 0.15 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3715 | 1/1   | 0.70 | 0.45 | 48,48,48,48                 | 0     |
| 58  | MG   | 1W    | 207  | 1/1   | 0.70 | 0.17 | 42,42,42,42                 | 0     |
| 58  | MG   | 2l    | 101  | 1/1   | 0.71 | 0.17 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3097 | 1/1   | 0.71 | 0.19 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3515 | 1/1   | 0.71 | 0.13 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3307 | 1/1   | 0.71 | 0.15 | 75,75,75,75                 | 0     |
| 58  | MG   | 2a    | 3098 | 1/1   | 0.72 | 0.18 | 87,87,87,87                 | 0     |
| 58  | MG   | 2a    | 3109 | 1/1   | 0.72 | 0.17 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3323 | 1/1   | 0.72 | 0.29 | 81,81,81,81                 | 0     |
| 58  | MG   | 2A    | 3029 | 1/1   | 0.72 | 0.23 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3163 | 1/1   | 0.72 | 0.19 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3205 | 1/1   | 0.72 | 0.14 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3274 | 1/1   | 0.72 | 0.18 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3456 | 1/1   | 0.72 | 0.16 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3065 | 1/1   | 0.72 | 0.17 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3246 | 1/1   | 0.73 | 0.26 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3649 | 1/1   | 0.73 | 0.19 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3415 | 1/1   | 0.73 | 0.11 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3935 | 1/1   | 0.73 | 0.13 | 74,74,74,74                 | 0     |
| 58  | MG   | 1a    | 1751 | 1/1   | 0.73 | 0.16 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3058 | 1/1   | 0.73 | 0.19 | 54,54,54,54                 | 0     |
| 58  | MG   | 1W    | 202  | 1/1   | 0.74 | 0.19 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3728 | 1/1   | 0.74 | 0.19 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3613 | 1/1   | 0.74 | 0.18 | 44,44,44,44                 | 0     |
| 58  | MG   | 1t    | 201  | 1/1   | 0.74 | 0.32 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3296 | 1/1   | 0.74 | 0.28 | 70,70,70,70                 | 0     |
| 58  | MG   | 2A    | 3010 | 1/1   | 0.74 | 0.16 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3181 | 1/1   | 0.74 | 0.23 | 70,70,70,70                 | 0     |
| 58  | MG   | 1B    | 205  | 1/1   | 0.74 | 0.30 | 68,68,68,68                 | 0     |
| 58  | MG   | 2a    | 3005 | 1/1   | 0.74 | 0.32 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3653 | 1/1   | 0.74 | 0.32 | 85,85,85,85                 | 0     |
| 58  | MG   | 2l    | 202  | 1/1   | 0.74 | 0.26 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 3204 | 1/1   | 0.75 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3220 | 1/1   | 0.75 | 0.24 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3233 | 1/1   | 0.75 | 0.16 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3812 | 1/1   | 0.75 | 0.14 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3266 | 1/1   | 0.75 | 0.30 | 76,76,76,76                 | 0     |
| 58  | MG   | 1x    | 110  | 1/1   | 0.75 | 0.19 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3719 | 1/1   | 0.75 | 0.13 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 4003 | 1/1   | 0.75 | 0.15 | 70,70,70,70                 | 0     |
| 58  | MG   | 1a    | 1643 | 1/1   | 0.75 | 0.25 | 70,70,70,70                 | 0     |
| 58  | MG   | 1a    | 1667 | 1/1   | 0.75 | 0.27 | 68,68,68,68                 | 0     |
| 58  | MG   | 1a    | 1692 | 1/1   | 0.75 | 0.20 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 4019 | 1/1   | 0.75 | 0.14 | 27,27,27,27                 | 0     |
| 58  | MG   | 2a    | 3210 | 1/1   | 0.75 | 0.21 | 80,80,80,80                 | 0     |
| 58  | MG   | 1A    | 3820 | 1/1   | 0.75 | 0.15 | 72,72,72,72                 | 0     |
| 58  | MG   | 2w    | 101  | 1/1   | 0.75 | 0.24 | 85,85,85,85                 | 0     |
| 58  | MG   | 1A    | 3815 | 1/1   | 0.76 | 0.14 | 46,46,46,46                 | 0     |
| 58  | MG   | 2a    | 3139 | 1/1   | 0.76 | 0.29 | 78,78,78,78                 | 0     |
| 58  | MG   | 2A    | 3252 | 1/1   | 0.76 | 0.15 | 61,61,61,61                 | 0     |
| 58  | MG   | 1B    | 213  | 1/1   | 0.76 | 0.19 | 56,56,56,56                 | 0     |
| 58  | MG   | 2a    | 3007 | 1/1   | 0.76 | 0.24 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3647 | 1/1   | 0.76 | 0.19 | 62,62,62,62                 | 0     |
| 58  | MG   | 2a    | 3037 | 1/1   | 0.76 | 0.18 | 71,71,71,71                 | 0     |
| 58  | MG   | 2a    | 3064 | 1/1   | 0.76 | 0.35 | 60,60,60,60                 | 0     |
| 58  | MG   | 1a    | 1704 | 1/1   | 0.76 | 0.29 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 4077 | 1/1   | 0.76 | 0.16 | 39,39,39,39                 | 0     |
| 58  | MG   | 2a    | 3130 | 1/1   | 0.76 | 0.17 | 70,70,70,70                 | 0     |
| 58  | MG   | 2a    | 3132 | 1/1   | 0.76 | 0.09 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3203 | 1/1   | 0.77 | 0.18 | 67,67,67,67                 | 0     |
| 58  | MG   | 2B    | 212  | 1/1   | 0.77 | 0.25 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 3424 | 1/1   | 0.77 | 0.31 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3923 | 1/1   | 0.77 | 0.15 | 62,62,62,62                 | 0     |
| 58  | MG   | 2a    | 3160 | 1/1   | 0.77 | 0.16 | 74,74,74,74                 | 0     |
| 58  | MG   | 1A    | 3599 | 1/1   | 0.77 | 0.23 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3408 | 1/1   | 0.77 | 0.33 | 79,79,79,79                 | 0     |
| 58  | MG   | 2a    | 3177 | 1/1   | 0.77 | 0.15 | 68,68,68,68                 | 0     |
| 58  | MG   | 1n    | 102  | 1/1   | 0.77 | 0.21 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3440 | 1/1   | 0.77 | 0.10 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3035 | 1/1   | 0.77 | 0.10 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3371 | 1/1   | 0.77 | 0.13 | 42,42,42,42                 | 0     |
| 58  | MG   | 2a    | 3121 | 1/1   | 0.77 | 0.22 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3124 | 1/1   | 0.77 | 0.25 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3088 | 1/1   | 0.77 | 0.22 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3279 | 1/1   | 0.78 | 0.23 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3450 | 1/1   | 0.78 | 0.31 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3281 | 1/1   | 0.78 | 0.26 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3227 | 1/1   | 0.78 | 0.14 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3175 | 1/1   | 0.78 | 0.16 | 84,84,84,84                 | 0     |
| 58  | MG   | 1A    | 3946 | 1/1   | 0.78 | 0.21 | 64,64,64,64                 | 0     |
| 58  | MG   | 1Y    | 201  | 1/1   | 0.78 | 0.09 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3637 | 1/1   | 0.78 | 0.14 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3812 | 1/1   | 0.78 | 0.15 | 64,64,64,64                 | 0     |
| 58  | MG   | 2a    | 3193 | 1/1   | 0.78 | 0.14 | 75,75,75,75                 | 0     |
| 58  | MG   | 1x    | 108  | 1/1   | 0.78 | 0.13 | 66,66,66,66                 | 0     |
| 58  | MG   | 20    | 101  | 1/1   | 0.78 | 0.15 | 70,70,70,70                 | 0     |
| 58  | MG   | 1x    | 109  | 1/1   | 0.78 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3164 | 1/1   | 0.78 | 0.34 | 59,59,59,59                 | 0     |
| 58  | MG   | 2x    | 102  | 1/1   | 0.78 | 0.27 | 77,77,77,77                 | 0     |
| 58  | MG   | 1A    | 3130 | 1/1   | 0.79 | 0.11 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3095 | 1/1   | 0.79 | 0.11 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3425 | 1/1   | 0.79 | 0.24 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1608 | 1/1   | 0.79 | 0.19 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 3321 | 1/1   | 0.79 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3346 | 1/1   | 0.79 | 0.20 | 70,70,70,70                 | 0     |
| 58  | MG   | 2a    | 3092 | 1/1   | 0.79 | 0.10 | 82,82,82,82                 | 0     |
| 58  | MG   | 1a    | 1656 | 1/1   | 0.79 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3693 | 1/1   | 0.79 | 0.17 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3244 | 1/1   | 0.79 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3868 | 1/1   | 0.79 | 0.11 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3702 | 1/1   | 0.79 | 0.12 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 3188 | 1/1   | 0.79 | 0.31 | 40,40,40,40                 | 0     |
| 58  | MG   | 1S    | 201  | 1/1   | 0.79 | 0.09 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3777 | 1/1   | 0.79 | 0.19 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3324 | 1/1   | 0.80 | 0.21 | 65,65,65,65                 | 0     |
| 58  | MG   | 1a    | 1615 | 1/1   | 0.80 | 0.22 | 47,47,47,47                 | 0     |
| 58  | MG   | 1a    | 1697 | 1/1   | 0.80 | 0.35 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3358 | 1/1   | 0.80 | 0.29 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3710 | 1/1   | 0.80 | 0.20 | 50,50,50,50                 | 0     |
| 58  | MG   | 2a    | 3170 | 1/1   | 0.80 | 0.32 | 78,78,78,78                 | 0     |
| 58  | MG   | 1A    | 3673 | 1/1   | 0.80 | 0.16 | 67,67,67,67                 | 0     |
| 58  | MG   | 1B    | 229  | 1/1   | 0.80 | 0.25 | 73,73,73,73                 | 0     |
| 58  | MG   | 1A    | 3721 | 1/1   | 0.80 | 0.24 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3489 | 1/1   | 0.80 | 0.11 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3094 | 1/1   | 0.80 | 0.25 | 78,78,78,78                 | 0     |
| 58  | MG   | 2A    | 3302 | 1/1   | 0.80 | 0.15 | 64,64,64,64                 | 0     |
| 58  | MG   | 2a    | 3100 | 1/1   | 0.80 | 0.16 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3101 | 1/1   | 0.80 | 0.11 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3126 | 1/1   | 0.80 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 2j    | 201  | 1/1   | 0.80 | 0.30 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3802 | 1/1   | 0.80 | 0.17 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3625 | 1/1   | 0.80 | 0.30 | 79,79,79,79                 | 0     |
| 58  | MG   | 2B    | 204  | 1/1   | 0.80 | 0.23 | 69,69,69,69                 | 0     |
| 58  | MG   | 2a    | 3097 | 1/1   | 0.81 | 0.35 | 67,67,67,67                 | 0     |
| 58  | MG   | 1a    | 1660 | 1/1   | 0.81 | 0.20 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3569 | 1/1   | 0.81 | 0.14 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3260 | 1/1   | 0.81 | 0.23 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3883 | 1/1   | 0.81 | 0.20 | 78,78,78,78                 | 0     |
| 58  | MG   | 2A    | 3754 | 1/1   | 0.81 | 0.17 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3543 | 1/1   | 0.81 | 0.15 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3466 | 1/1   | 0.81 | 0.18 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3777 | 1/1   | 0.81 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3687 | 1/1   | 0.81 | 0.14 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3192 | 1/1   | 0.81 | 0.20 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3804 | 1/1   | 0.81 | 0.19 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3195 | 1/1   | 0.81 | 0.10 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3559 | 1/1   | 0.81 | 0.17 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3795 | 1/1   | 0.81 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3583 | 1/1   | 0.81 | 0.17 | 59,59,59,59                 | 0     |
| 58  | MG   | 20    | 102  | 1/1   | 0.81 | 0.19 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3609 | 1/1   | 0.81 | 0.08 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3299 | 1/1   | 0.81 | 0.23 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3030 | 1/1   | 0.81 | 0.16 | 51,51,51,51                 | 0     |
| 58  | MG   | 2a    | 3010 | 1/1   | 0.81 | 0.17 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3035 | 1/1   | 0.81 | 0.16 | 51,51,51,51                 | 0     |
| 58  | MG   | 1a    | 1634 | 1/1   | 0.81 | 0.12 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3954 | 1/1   | 0.81 | 0.21 | 68,68,68,68                 | 0     |
| 58  | MG   | 2l    | 201  | 1/1   | 0.81 | 0.16 | 62,62,62,62                 | 0     |
| 58  | MG   | 2a    | 3080 | 1/1   | 0.81 | 0.27 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3696 | 1/1   | 0.81 | 0.19 | 73,73,73,73                 | 0     |
| 58  | MG   | 1A    | 3870 | 1/1   | 0.81 | 0.14 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3534 | 1/1   | 0.82 | 0.20 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3796 | 1/1   | 0.82 | 0.17 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 4014 | 1/1   | 0.82 | 0.10 | 46,46,46,46                 | 0     |
| 58  | MG   | 2a    | 3034 | 1/1   | 0.82 | 0.34 | 77,77,77,77                 | 0     |
| 58  | MG   | 2A    | 3553 | 1/1   | 0.82 | 0.13 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3459 | 1/1   | 0.82 | 0.27 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3040 | 1/1   | 0.82 | 0.37 | 73,73,73,73                 | 0     |
| 58  | MG   | 2a    | 3071 | 1/1   | 0.82 | 0.33 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 4065 | 1/1   | 0.82 | 0.19 | 81,81,81,81                 | 0     |
| 58  | MG   | 2A    | 3584 | 1/1   | 0.82 | 0.18 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3473 | 1/1   | 0.82 | 0.22 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3062 | 1/1   | 0.82 | 0.13 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3691 | 1/1   | 0.82 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3495 | 1/1   | 0.82 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3083 | 1/1   | 0.82 | 0.14 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3701 | 1/1   | 0.82 | 0.16 | 50,50,50,50                 | 0     |
| 58  | MG   | 1B    | 218  | 1/1   | 0.82 | 0.11 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3129 | 1/1   | 0.82 | 0.20 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3096 | 1/1   | 0.82 | 0.11 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3309 | 1/1   | 0.82 | 0.22 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3317 | 1/1   | 0.82 | 0.20 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1735 | 1/1   | 0.82 | 0.14 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3182 | 1/1   | 0.82 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3750 | 1/1   | 0.82 | 0.18 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3388 | 1/1   | 0.82 | 0.11 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3389 | 1/1   | 0.82 | 0.19 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3391 | 1/1   | 0.82 | 0.21 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3406 | 1/1   | 0.82 | 0.16 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3158 | 1/1   | 0.82 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 2a    | 3179 | 1/1   | 0.82 | 0.17 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3027 | 1/1   | 0.82 | 0.29 | 74,74,74,74                 | 0     |
| 58  | MG   | 2a    | 3183 | 1/1   | 0.82 | 0.16 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3595 | 1/1   | 0.82 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 2a    | 3186 | 1/1   | 0.82 | 0.20 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3811 | 1/1   | 0.82 | 0.13 | 74,74,74,74                 | 0     |
| 58  | MG   | 1A    | 3438 | 1/1   | 0.82 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3817 | 1/1   | 0.82 | 0.13 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3197 | 1/1   | 0.82 | 0.23 | 72,72,72,72                 | 0     |
| 58  | MG   | 2a    | 3204 | 1/1   | 0.82 | 0.35 | 72,72,72,72                 | 0     |
| 58  | MG   | 14    | 101  | 1/1   | 0.82 | 0.13 | 63,63,63,63                 | 0     |
| 58  | MG   | 2B    | 205  | 1/1   | 0.82 | 0.09 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3293 | 1/1   | 0.82 | 0.27 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3474 | 1/1   | 0.82 | 0.28 | 73,73,73,73                 | 0     |
| 58  | MG   | 1A    | 3980 | 1/1   | 0.82 | 0.13 | 23,23,23,23                 | 0     |
| 58  | MG   | 2A    | 3505 | 1/1   | 0.82 | 0.17 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3721 | 1/1   | 0.83 | 0.20 | 65,65,65,65                 | 0     |
| 58  | MG   | 1a    | 1677 | 1/1   | 0.83 | 0.24 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3096 | 1/1   | 0.83 | 0.19 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3002 | 1/1   | 0.83 | 0.16 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3008 | 1/1   | 0.83 | 0.18 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3912 | 1/1   | 0.83 | 0.17 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3287 | 1/1   | 0.83 | 0.23 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3120 | 1/1   | 0.83 | 0.19 | 69,69,69,69                 | 0     |
| 58  | MG   | 1B    | 216  | 1/1   | 0.83 | 0.18 | 70,70,70,70                 | 0     |
| 58  | MG   | 2A    | 3526 | 1/1   | 0.83 | 0.13 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3784 | 1/1   | 0.83 | 0.16 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3149 | 1/1   | 0.83 | 0.18 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1613 | 1/1   | 0.83 | 0.18 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3185 | 1/1   | 0.83 | 0.40 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3810 | 1/1   | 0.83 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 2a    | 3141 | 1/1   | 0.83 | 0.18 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3666 | 1/1   | 0.83 | 0.14 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3060 | 1/1   | 0.83 | 0.20 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3046 | 1/1   | 0.83 | 0.21 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3047 | 1/1   | 0.83 | 0.13 | 59,59,59,59                 | 0     |
| 58  | MG   | 1a    | 1744 | 1/1   | 0.83 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3384 | 1/1   | 0.83 | 0.11 | 46,46,46,46                 | 0     |
| 58  | MG   | 2W    | 201  | 1/1   | 0.83 | 0.15 | 57,57,57,57                 | 0     |
| 58  | MG   | 1B    | 232  | 1/1   | 0.83 | 0.11 | 86,86,86,86                 | 0     |
| 58  | MG   | 2A    | 3231 | 1/1   | 0.83 | 0.32 | 66,66,66,66                 | 0     |
| 58  | MG   | 1a    | 1768 | 1/1   | 0.83 | 0.20 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3648 | 1/1   | 0.83 | 0.17 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3399 | 1/1   | 0.83 | 0.20 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3651 | 1/1   | 0.83 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3027 | 1/1   | 0.83 | 0.28 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3368 | 1/1   | 0.83 | 0.20 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3066 | 1/1   | 0.83 | 0.12 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3457 | 1/1   | 0.83 | 0.11 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3051 | 1/1   | 0.83 | 0.10 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3052 | 1/1   | 0.83 | 0.22 | 83,83,83,83                 | 0     |
| 58  | MG   | 2A    | 3712 | 1/1   | 0.83 | 0.15 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3955 | 1/1   | 0.83 | 0.12 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3448 | 1/1   | 0.83 | 0.16 | 59,59,59,59                 | 0     |
| 58  | MG   | 2w    | 102  | 1/1   | 0.83 | 0.19 | 77,77,77,77                 | 0     |
| 58  | MG   | 2a    | 3090 | 1/1   | 0.83 | 0.12 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3285 | 1/1   | 0.84 | 0.20 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3810 | 1/1   | 0.84 | 0.14 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3573 | 1/1   | 0.84 | 0.23 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3040 | 1/1   | 0.84 | 0.23 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3048 | 1/1   | 0.84 | 0.15 | 62,62,62,62                 | 0     |
| 58  | MG   | 1Q    | 204  | 1/1   | 0.84 | 0.07 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3970 | 1/1   | 0.84 | 0.12 | 31,31,31,31                 | 0     |
| 58  | MG   | 2a    | 3060 | 1/1   | 0.84 | 0.21 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3071 | 1/1   | 0.84 | 0.22 | 60,60,60,60                 | 0     |
| 58  | MG   | 2a    | 3065 | 1/1   | 0.84 | 0.15 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3700 | 1/1   | 0.84 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1a    | 1731 | 1/1   | 0.84 | 0.13 | 81,81,81,81                 | 0     |
| 58  | MG   | 2a    | 3084 | 1/1   | 0.84 | 0.18 | 61,61,61,61                 | 0     |
| 58  | MG   | 2a    | 3085 | 1/1   | 0.84 | 0.18 | 77,77,77,77                 | 0     |
| 58  | MG   | 2A    | 3313 | 1/1   | 0.84 | 0.10 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3323 | 1/1   | 0.84 | 0.18 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3332 | 1/1   | 0.84 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3496 | 1/1   | 0.84 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3360 | 1/1   | 0.84 | 0.18 | 68,68,68,68                 | 0     |
| 58  | MG   | 1a    | 1757 | 1/1   | 0.84 | 0.15 | 59,59,59,59                 | 0     |
| 58  | MG   | 1a    | 1760 | 1/1   | 0.84 | 0.21 | 61,61,61,61                 | 0     |
| 58  | MG   | 2a    | 3105 | 1/1   | 0.84 | 0.24 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3420 | 1/1   | 0.84 | 0.14 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1776 | 1/1   | 0.84 | 0.16 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3730 | 1/1   | 0.84 | 0.11 | 67,67,67,67                 | 0     |
| 58  | MG   | 1a    | 1795 | 1/1   | 0.84 | 0.21 | 66,66,66,66                 | 0     |
| 58  | MG   | 1A    | 3671 | 1/1   | 0.84 | 0.17 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 4068 | 1/1   | 0.84 | 0.14 | 79,79,79,79                 | 0     |
| 58  | MG   | 1w    | 101  | 1/1   | 0.84 | 0.10 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3428 | 1/1   | 0.84 | 0.18 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3775 | 1/1   | 0.84 | 0.18 | 39,39,39,39                 | 0     |
| 58  | MG   | 1a    | 1623 | 1/1   | 0.84 | 0.22 | 65,65,65,65                 | 0     |
| 58  | MG   | 2a    | 3145 | 1/1   | 0.84 | 0.11 | 82,82,82,82                 | 0     |
| 58  | MG   | 2A    | 3446 | 1/1   | 0.84 | 0.20 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3270 | 1/1   | 0.84 | 0.21 | 59,59,59,59                 | 0     |
| 58  | MG   | 1a    | 1639 | 1/1   | 0.84 | 0.21 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3561 | 1/1   | 0.84 | 0.10 | 54,54,54,54                 | 0     |
| 58  | MG   | 2a    | 3172 | 1/1   | 0.84 | 0.18 | 71,71,71,71                 | 0     |
| 58  | MG   | 1a    | 1648 | 1/1   | 0.84 | 0.31 | 64,64,64,64                 | 0     |
| 58  | MG   | 2a    | 3174 | 1/1   | 0.84 | 0.21 | 70,70,70,70                 | 0     |
| 58  | MG   | 1a    | 1649 | 1/1   | 0.84 | 0.26 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3481 | 1/1   | 0.84 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 1B    | 209  | 1/1   | 0.84 | 0.30 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3819 | 1/1   | 0.84 | 0.14 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3824 | 1/1   | 0.84 | 0.15 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3502 | 1/1   | 0.84 | 0.20 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3365 | 1/1   | 0.84 | 0.24 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3513 | 1/1   | 0.84 | 0.13 | 54,54,54,54                 | 0     |
| 58  | MG   | 2B    | 215  | 1/1   | 0.84 | 0.23 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3797 | 1/1   | 0.84 | 0.11 | 35,35,35,35                 | 0     |
| 58  | MG   | 1a    | 1675 | 1/1   | 0.84 | 0.17 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3272 | 1/1   | 0.84 | 0.12 | 78,78,78,78                 | 0     |
| 58  | MG   | 1A    | 3947 | 1/1   | 0.84 | 0.15 | 17,17,17,17                 | 0     |
| 58  | MG   | 1a    | 1682 | 1/1   | 0.84 | 0.08 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3052 | 1/1   | 0.84 | 0.16 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3282 | 1/1   | 0.84 | 0.14 | 62,62,62,62                 | 0     |
| 58  | MG   | 2v    | 101  | 1/1   | 0.84 | 0.09 | 60,60,60,60                 | 0     |
| 58  | MG   | 2a    | 3017 | 1/1   | 0.84 | 0.18 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3570 | 1/1   | 0.84 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 2a    | 3032 | 1/1   | 0.84 | 0.19 | 80,80,80,80                 | 0     |
| 58  | MG   | 2x    | 104  | 1/1   | 0.84 | 0.27 | 74,74,74,74                 | 0     |
| 58  | MG   | 1a    | 1631 | 1/1   | 0.85 | 0.27 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3189 | 1/1   | 0.85 | 0.17 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3062 | 1/1   | 0.85 | 0.16 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3581 | 1/1   | 0.85 | 0.16 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3041 | 1/1   | 0.85 | 0.16 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3046 | 1/1   | 0.85 | 0.18 | 81,81,81,81                 | 0     |
| 58  | MG   | 1a    | 1764 | 1/1   | 0.85 | 0.21 | 66,66,66,66                 | 0     |
| 58  | MG   | 1A    | 3871 | 1/1   | 0.85 | 0.12 | 23,23,23,23                 | 0     |
| 58  | MG   | 2A    | 3085 | 1/1   | 0.85 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 1a    | 1773 | 1/1   | 0.85 | 0.16 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3878 | 1/1   | 0.85 | 0.12 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3639 | 1/1   | 0.85 | 0.16 | 55,55,55,55                 | 0     |
| 58  | MG   | 1B    | 226  | 1/1   | 0.85 | 0.17 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3098 | 1/1   | 0.85 | 0.14 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3310 | 1/1   | 0.85 | 0.18 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3311 | 1/1   | 0.85 | 0.17 | 78,78,78,78                 | 0     |
| 58  | MG   | 2A    | 3312 | 1/1   | 0.85 | 0.09 | 63,63,63,63                 | 0     |
| 58  | MG   | 1a    | 1797 | 1/1   | 0.85 | 0.13 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3707 | 1/1   | 0.85 | 0.14 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3318 | 1/1   | 0.85 | 0.13 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3711 | 1/1   | 0.85 | 0.19 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3319 | 1/1   | 0.85 | 0.26 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3986 | 1/1   | 0.85 | 0.09 | 74,74,74,74                 | 0     |
| 58  | MG   | 2A    | 3142 | 1/1   | 0.85 | 0.26 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3340 | 1/1   | 0.85 | 0.17 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3115 | 1/1   | 0.85 | 0.26 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3210 | 1/1   | 0.85 | 0.12 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3158 | 1/1   | 0.85 | 0.19 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3364 | 1/1   | 0.85 | 0.15 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3383 | 1/1   | 0.85 | 0.16 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3170 | 1/1   | 0.85 | 0.11 | 50,50,50,50                 | 0     |
| 58  | MG   | 2a    | 3131 | 1/1   | 0.85 | 0.34 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3040 | 1/1   | 0.85 | 0.18 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3894 | 1/1   | 0.85 | 0.12 | 52,52,52,52                 | 0     |
| 58  | MG   | 1V    | 201  | 1/1   | 0.85 | 0.30 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 4020 | 1/1   | 0.85 | 0.38 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3400 | 1/1   | 0.85 | 0.21 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3007 | 1/1   | 0.85 | 0.19 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 4025 | 1/1   | 0.85 | 0.12 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 4031 | 1/1   | 0.85 | 0.12 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3223 | 1/1   | 0.85 | 0.15 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3353 | 1/1   | 0.85 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3444 | 1/1   | 0.85 | 0.30 | 59,59,59,59                 | 0     |
| 58  | MG   | 19    | 101  | 1/1   | 0.85 | 0.12 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3669 | 1/1   | 0.85 | 0.15 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3242 | 1/1   | 0.85 | 0.11 | 57,57,57,57                 | 0     |
| 58  | MG   | 2B    | 202  | 1/1   | 0.85 | 0.11 | 70,70,70,70                 | 0     |
| 58  | MG   | 2A    | 3037 | 1/1   | 0.85 | 0.15 | 39,39,39,39                 | 0     |
| 58  | MG   | 1a    | 1714 | 1/1   | 0.85 | 0.15 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3251 | 1/1   | 0.85 | 0.23 | 60,60,60,60                 | 0     |
| 58  | MG   | 1a    | 1716 | 1/1   | 0.85 | 0.09 | 47,47,47,47                 | 0     |
| 58  | MG   | 2a    | 3189 | 1/1   | 0.85 | 0.26 | 61,61,61,61                 | 0     |
| 58  | MG   | 2D    | 302  | 1/1   | 0.85 | 0.14 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3258 | 1/1   | 0.85 | 0.08 | 40,40,40,40                 | 0     |
| 58  | MG   | 1a    | 1729 | 1/1   | 0.85 | 0.16 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3026 | 1/1   | 0.85 | 0.24 | 49,49,49,49                 | 0     |
| 58  | MG   | 2a    | 3201 | 1/1   | 0.85 | 0.26 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3268 | 1/1   | 0.85 | 0.23 | 70,70,70,70                 | 0     |
| 58  | MG   | 2a    | 3206 | 1/1   | 0.85 | 0.17 | 69,69,69,69                 | 0     |
| 58  | MG   | 2I    | 103  | 1/1   | 0.85 | 0.23 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3269 | 1/1   | 0.85 | 0.32 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3006 | 1/1   | 0.85 | 0.28 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3753 | 1/1   | 0.85 | 0.10 | 19,19,19,19                 | 0     |
| 58  | MG   | 1a    | 1739 | 1/1   | 0.85 | 0.11 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3570 | 1/1   | 0.85 | 0.11 | 32,32,32,32                 | 0     |
| 58  | MG   | 2a    | 3023 | 1/1   | 0.85 | 0.14 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3552 | 1/1   | 0.85 | 0.17 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3280 | 1/1   | 0.85 | 0.22 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3375 | 1/1   | 0.86 | 0.21 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3038 | 1/1   | 0.86 | 0.23 | 75,75,75,75                 | 0     |
| 58  | MG   | 1W    | 201  | 1/1   | 0.86 | 0.27 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3462 | 1/1   | 0.86 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3629 | 1/1   | 0.86 | 0.17 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3663 | 1/1   | 0.86 | 0.14 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3666 | 1/1   | 0.86 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1779 | 1/1   | 0.86 | 0.22 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3635 | 1/1   | 0.86 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3074 | 1/1   | 0.86 | 0.17 | 65,65,65,65                 | 0     |
| 58  | MG   | 1Z    | 302  | 1/1   | 0.86 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3070 | 1/1   | 0.86 | 0.30 | 73,73,73,73                 | 0     |
| 58  | MG   | 1A    | 3823 | 1/1   | 0.86 | 0.15 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3207 | 1/1   | 0.86 | 0.22 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3716 | 1/1   | 0.86 | 0.11 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3267 | 1/1   | 0.86 | 0.14 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3086 | 1/1   | 0.86 | 0.26 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3417 | 1/1   | 0.86 | 0.14 | 65,65,65,65                 | 0     |
| 58  | MG   | 1a    | 1603 | 1/1   | 0.86 | 0.17 | 57,57,57,57                 | 0     |
| 58  | MG   | 1w    | 104  | 1/1   | 0.86 | 0.26 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3735 | 1/1   | 0.86 | 0.28 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3741 | 1/1   | 0.86 | 0.18 | 56,56,56,56                 | 0     |
| 58  | MG   | 1a    | 1701 | 1/1   | 0.86 | 0.12 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3474 | 1/1   | 0.86 | 0.11 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3275 | 1/1   | 0.86 | 0.23 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3449 | 1/1   | 0.86 | 0.28 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3100 | 1/1   | 0.86 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3482 | 1/1   | 0.86 | 0.30 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3107 | 1/1   | 0.86 | 0.16 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3120 | 1/1   | 0.86 | 0.24 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3788 | 1/1   | 0.86 | 0.13 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3004 | 1/1   | 0.86 | 0.28 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3482 | 1/1   | 0.86 | 0.10 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3486 | 1/1   | 0.86 | 0.23 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3805 | 1/1   | 0.86 | 0.23 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3377 | 1/1   | 0.86 | 0.13 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3291 | 1/1   | 0.86 | 0.12 | 54,54,54,54                 | 0     |
| 58  | MG   | 1a    | 1617 | 1/1   | 0.86 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3815 | 1/1   | 0.86 | 0.24 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3508 | 1/1   | 0.86 | 0.17 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3150 | 1/1   | 0.86 | 0.13 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3821 | 1/1   | 0.86 | 0.15 | 65,65,65,65                 | 0     |
| 58  | MG   | 1a    | 1728 | 1/1   | 0.86 | 0.11 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2B    | 201  | 1/1   | 0.86 | 0.12 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3022 | 1/1   | 0.86 | 0.21 | 54,54,54,54                 | 0     |
| 58  | MG   | 2B    | 203  | 1/1   | 0.86 | 0.15 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3305 | 1/1   | 0.86 | 0.25 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3543 | 1/1   | 0.86 | 0.15 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3181 | 1/1   | 0.86 | 0.29 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3550 | 1/1   | 0.86 | 0.16 | 65,65,65,65                 | 0     |
| 58  | MG   | 1B    | 225  | 1/1   | 0.86 | 0.20 | 45,45,45,45                 | 0     |
| 58  | MG   | 2E    | 305  | 1/1   | 0.86 | 0.10 | 26,26,26,26                 | 0     |
| 58  | MG   | 2P    | 202  | 1/1   | 0.86 | 0.18 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3675 | 1/1   | 0.86 | 0.14 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3686 | 1/1   | 0.86 | 0.09 | 25,25,25,25                 | 0     |
| 58  | MG   | 1a    | 1637 | 1/1   | 0.86 | 0.24 | 70,70,70,70                 | 0     |
| 58  | MG   | 2a    | 3195 | 1/1   | 0.86 | 0.11 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3039 | 1/1   | 0.86 | 0.16 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3574 | 1/1   | 0.86 | 0.21 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3209 | 1/1   | 0.86 | 0.21 | 64,64,64,64                 | 0     |
| 58  | MG   | 2a    | 3205 | 1/1   | 0.86 | 0.21 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3219 | 1/1   | 0.86 | 0.10 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3590 | 1/1   | 0.86 | 0.12 | 19,19,19,19                 | 0     |
| 58  | MG   | 1E    | 308  | 1/1   | 0.86 | 0.11 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3619 | 1/1   | 0.86 | 0.14 | 41,41,41,41                 | 0     |
| 58  | MG   | 2a    | 3018 | 1/1   | 0.86 | 0.20 | 62,62,62,62                 | 0     |
| 58  | MG   | 2l    | 204  | 1/1   | 0.86 | 0.12 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3431 | 1/1   | 0.86 | 0.20 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3806 | 1/1   | 0.86 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3229 | 1/1   | 0.86 | 0.13 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3646 | 1/1   | 0.86 | 0.15 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3170 | 1/1   | 0.86 | 0.13 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1808 | 1/1   | 0.87 | 0.16 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1809 | 1/1   | 0.87 | 0.23 | 70,70,70,70                 | 0     |
| 58  | MG   | 1B    | 203  | 1/1   | 0.87 | 0.14 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3599 | 1/1   | 0.87 | 0.26 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3604 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 58  | MG   | 2a    | 3021 | 1/1   | 0.87 | 0.42 | 73,73,73,73                 | 0     |
| 58  | MG   | 2a    | 3022 | 1/1   | 0.87 | 0.15 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3155 | 1/1   | 0.87 | 0.12 | 43,43,43,43                 | 0     |
| 58  | MG   | 2a    | 3025 | 1/1   | 0.87 | 0.26 | 72,72,72,72                 | 0     |
| 58  | MG   | 2a    | 3026 | 1/1   | 0.87 | 0.13 | 77,77,77,77                 | 0     |
| 58  | MG   | 1A    | 3578 | 1/1   | 0.87 | 0.12 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3010 | 1/1   | 0.87 | 0.08 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3634 | 1/1   | 0.87 | 0.28 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3035 | 1/1   | 0.87 | 0.22 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3636 | 1/1   | 0.87 | 0.18 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3597 | 1/1   | 0.87 | 0.16 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3485 | 1/1   | 0.87 | 0.15 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3641 | 1/1   | 0.87 | 0.12 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3184 | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3042 | 1/1   | 0.87 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3044 | 1/1   | 0.87 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3248 | 1/1   | 0.87 | 0.13 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3929 | 1/1   | 0.87 | 0.14 | 30,30,30,30                 | 0     |
| 58  | MG   | 2a    | 3050 | 1/1   | 0.87 | 0.18 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3931 | 1/1   | 0.87 | 0.18 | 61,61,61,61                 | 0     |
| 58  | MG   | 1a    | 1670 | 1/1   | 0.87 | 0.18 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3357 | 1/1   | 0.87 | 0.27 | 70,70,70,70                 | 0     |
| 58  | MG   | 2A    | 3656 | 1/1   | 0.87 | 0.20 | 63,63,63,63                 | 0     |
| 58  | MG   | 1a    | 1673 | 1/1   | 0.87 | 0.21 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3320 | 1/1   | 0.87 | 0.08 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3368 | 1/1   | 0.87 | 0.13 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3706 | 1/1   | 0.87 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3371 | 1/1   | 0.87 | 0.16 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3508 | 1/1   | 0.87 | 0.16 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3639 | 1/1   | 0.87 | 0.12 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3222 | 1/1   | 0.87 | 0.10 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3713 | 1/1   | 0.87 | 0.14 | 43,43,43,43                 | 0     |
| 58  | MG   | 1a    | 1686 | 1/1   | 0.87 | 0.24 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3225 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 1N    | 204  | 1/1   | 0.87 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 1P    | 207  | 1/1   | 0.87 | 0.14 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3230 | 1/1   | 0.87 | 0.18 | 78,78,78,78                 | 0     |
| 58  | MG   | 2a    | 3102 | 1/1   | 0.87 | 0.10 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3729 | 1/1   | 0.87 | 0.15 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3405 | 1/1   | 0.87 | 0.20 | 51,51,51,51                 | 0     |
| 58  | MG   | 2a    | 3114 | 1/1   | 0.87 | 0.15 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3644 | 1/1   | 0.87 | 0.19 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3653 | 1/1   | 0.87 | 0.13 | 25,25,25,25                 | 0     |
| 58  | MG   | 2A    | 3742 | 1/1   | 0.87 | 0.12 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3743 | 1/1   | 0.87 | 0.11 | 65,65,65,65                 | 0     |
| 58  | MG   | 2a    | 3128 | 1/1   | 0.87 | 0.18 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3409 | 1/1   | 0.87 | 0.20 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3413 | 1/1   | 0.87 | 0.11 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3234 | 1/1   | 0.87 | 0.07 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3239 | 1/1   | 0.87 | 0.18 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3760 | 1/1   | 0.87 | 0.11 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3966 | 1/1   | 0.87 | 0.17 | 62,62,62,62                 | 0     |
| 58  | MG   | 2a    | 3140 | 1/1   | 0.87 | 0.18 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3968 | 1/1   | 0.87 | 0.11 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3800 | 1/1   | 0.87 | 0.13 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3248 | 1/1   | 0.87 | 0.15 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3249 | 1/1   | 0.87 | 0.15 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3792 | 1/1   | 0.87 | 0.09 | 60,60,60,60                 | 0     |
| 58  | MG   | 2a    | 3164 | 1/1   | 0.87 | 0.22 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3258 | 1/1   | 0.87 | 0.15 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3261 | 1/1   | 0.87 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3255 | 1/1   | 0.87 | 0.16 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3544 | 1/1   | 0.87 | 0.12 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3809 | 1/1   | 0.87 | 0.11 | 74,74,74,74                 | 0     |
| 58  | MG   | 2A    | 3468 | 1/1   | 0.87 | 0.09 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3471 | 1/1   | 0.87 | 0.16 | 72,72,72,72                 | 0     |
| 58  | MG   | 10    | 108  | 1/1   | 0.87 | 0.12 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3265 | 1/1   | 0.87 | 0.21 | 68,68,68,68                 | 0     |
| 58  | MG   | 2a    | 3184 | 1/1   | 0.87 | 0.24 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3547 | 1/1   | 0.87 | 0.15 | 44,44,44,44                 | 0     |
| 58  | MG   | 15    | 107  | 1/1   | 0.87 | 0.22 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3324 | 1/1   | 0.87 | 0.17 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1602 | 1/1   | 0.87 | 0.21 | 58,58,58,58                 | 0     |
| 58  | MG   | 1a    | 1756 | 1/1   | 0.87 | 0.09 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3383 | 1/1   | 0.87 | 0.39 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3854 | 1/1   | 0.87 | 0.10 | 31,31,31,31                 | 0     |
| 58  | MG   | 2a    | 3196 | 1/1   | 0.87 | 0.09 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3516 | 1/1   | 0.87 | 0.23 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3387 | 1/1   | 0.87 | 0.14 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 4060 | 1/1   | 0.87 | 0.18 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3105 | 1/1   | 0.87 | 0.13 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3333 | 1/1   | 0.87 | 0.18 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3209 | 1/1   | 0.87 | 0.23 | 70,70,70,70                 | 0     |
| 58  | MG   | 1a    | 1627 | 1/1   | 0.87 | 0.18 | 66,66,66,66                 | 0     |
| 58  | MG   | 2F    | 303  | 1/1   | 0.87 | 0.14 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3104 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3289 | 1/1   | 0.87 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3875 | 1/1   | 0.87 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3577 | 1/1   | 0.87 | 0.20 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3124 | 1/1   | 0.87 | 0.18 | 72,72,72,72                 | 0     |
| 58  | MG   | 1a    | 1806 | 1/1   | 0.87 | 0.31 | 54,54,54,54                 | 0     |
| 58  | MG   | 28    | 102  | 1/1   | 0.87 | 0.23 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3141 | 1/1   | 0.87 | 0.13 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3451 | 1/1   | 0.88 | 0.23 | 43,43,43,43                 | 0     |
| 58  | MG   | 1a    | 1661 | 1/1   | 0.88 | 0.16 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3042 | 1/1   | 0.88 | 0.20 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3874 | 1/1   | 0.88 | 0.09 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3571 | 1/1   | 0.88 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3049 | 1/1   | 0.88 | 0.15 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3339 | 1/1   | 0.88 | 0.15 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3024 | 1/1   | 0.88 | 0.24 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3571 | 1/1   | 0.88 | 0.19 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3019 | 1/1   | 0.88 | 0.13 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3277 | 1/1   | 0.88 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3061 | 1/1   | 0.88 | 0.17 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1681 | 1/1   | 0.88 | 0.17 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3891 | 1/1   | 0.88 | 0.17 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3703 | 1/1   | 0.88 | 0.11 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3911 | 1/1   | 0.88 | 0.14 | 68,68,68,68                 | 0     |
| 58  | MG   | 1a    | 1693 | 1/1   | 0.88 | 0.22 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3713 | 1/1   | 0.88 | 0.10 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3623 | 1/1   | 0.88 | 0.21 | 61,61,61,61                 | 0     |
| 58  | MG   | 1D    | 302  | 1/1   | 0.88 | 0.36 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3630 | 1/1   | 0.88 | 0.16 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3631 | 1/1   | 0.88 | 0.19 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3297 | 1/1   | 0.88 | 0.18 | 64,64,64,64                 | 0     |
| 58  | MG   | 1D    | 306  | 1/1   | 0.88 | 0.10 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3154 | 1/1   | 0.88 | 0.14 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3304 | 1/1   | 0.88 | 0.15 | 63,63,63,63                 | 0     |
| 58  | MG   | 1F    | 308  | 1/1   | 0.88 | 0.09 | 44,44,44,44                 | 0     |
| 58  | MG   | 1F    | 311  | 1/1   | 0.88 | 0.11 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3928 | 1/1   | 0.88 | 0.16 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3463 | 1/1   | 0.88 | 0.15 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3469 | 1/1   | 0.88 | 0.17 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3598 | 1/1   | 0.88 | 0.10 | 17,17,17,17                 | 0     |
| 58  | MG   | 2A    | 3652 | 1/1   | 0.88 | 0.18 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3302 | 1/1   | 0.88 | 0.14 | 37,37,37,37                 | 0     |
| 58  | MG   | 2a    | 3069 | 1/1   | 0.88 | 0.20 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3109 | 1/1   | 0.88 | 0.17 | 48,48,48,48                 | 0     |
| 58  | MG   | 1V    | 203  | 1/1   | 0.88 | 0.75 | 36,36,36,36                 | 0     |
| 58  | MG   | 2a    | 3072 | 1/1   | 0.88 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3311 | 1/1   | 0.88 | 0.12 | 39,39,39,39                 | 0     |
| 58  | MG   | 2a    | 3083 | 1/1   | 0.88 | 0.24 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3671 | 1/1   | 0.88 | 0.08 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3692 | 1/1   | 0.88 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1750 | 1/1   | 0.88 | 0.18 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3698 | 1/1   | 0.88 | 0.17 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3315 | 1/1   | 0.88 | 0.11 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3222 | 1/1   | 0.88 | 0.16 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3348 | 1/1   | 0.88 | 0.16 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3959 | 1/1   | 0.88 | 0.12 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3358 | 1/1   | 0.88 | 0.10 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3099 | 1/1   | 0.88 | 0.13 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3075 | 1/1   | 0.88 | 0.14 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3362 | 1/1   | 0.88 | 0.10 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3399 | 1/1   | 0.88 | 0.14 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3156 | 1/1   | 0.88 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 13    | 104  | 1/1   | 0.88 | 0.16 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3159 | 1/1   | 0.88 | 0.15 | 74,74,74,74                 | 0     |
| 58  | MG   | 2A    | 3161 | 1/1   | 0.88 | 0.18 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3249 | 1/1   | 0.88 | 0.11 | 51,51,51,51                 | 0     |
| 58  | MG   | 2a    | 3123 | 1/1   | 0.88 | 0.27 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3175 | 1/1   | 0.88 | 0.23 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3740 | 1/1   | 0.88 | 0.10 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3179 | 1/1   | 0.88 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3979 | 1/1   | 0.88 | 0.10 | 20,20,20,20                 | 0     |
| 58  | MG   | 18    | 102  | 1/1   | 0.88 | 0.08 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3183 | 1/1   | 0.88 | 0.14 | 66,66,66,66                 | 0     |
| 58  | MG   | 1a    | 1793 | 1/1   | 0.88 | 0.18 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1794 | 1/1   | 0.88 | 0.18 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3757 | 1/1   | 0.88 | 0.16 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3322 | 1/1   | 0.88 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3981 | 1/1   | 0.88 | 0.13 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3767 | 1/1   | 0.88 | 0.16 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3158 | 1/1   | 0.88 | 0.28 | 77,77,77,77                 | 0     |
| 58  | MG   | 2A    | 3412 | 1/1   | 0.88 | 0.24 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3533 | 1/1   | 0.88 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3251 | 1/1   | 0.88 | 0.15 | 49,49,49,49                 | 0     |
| 58  | MG   | 2a    | 3169 | 1/1   | 0.88 | 0.27 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 4010 | 1/1   | 0.88 | 0.16 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3211 | 1/1   | 0.88 | 0.22 | 57,57,57,57                 | 0     |
| 58  | MG   | 1n    | 101  | 1/1   | 0.88 | 0.31 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3197 | 1/1   | 0.88 | 0.21 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3445 | 1/1   | 0.88 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3840 | 1/1   | 0.88 | 0.14 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3846 | 1/1   | 0.88 | 0.26 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1w    | 102  | 1/1   | 0.88 | 0.10 | 78,78,78,78                 | 0     |
| 58  | MG   | 1A    | 3852 | 1/1   | 0.88 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 1x    | 105  | 1/1   | 0.88 | 0.25 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3463 | 1/1   | 0.88 | 0.26 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3813 | 1/1   | 0.88 | 0.09 | 53,53,53,53                 | 0     |
| 58  | MG   | 2a    | 3187 | 1/1   | 0.88 | 0.29 | 68,68,68,68                 | 0     |
| 58  | MG   | 2a    | 3188 | 1/1   | 0.88 | 0.26 | 61,61,61,61                 | 0     |
| 58  | MG   | 1a    | 1628 | 1/1   | 0.88 | 0.13 | 64,64,64,64                 | 0     |
| 58  | MG   | 1a    | 1630 | 1/1   | 0.88 | 0.11 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 4029 | 1/1   | 0.88 | 0.16 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3001 | 1/1   | 0.88 | 0.30 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3853 | 1/1   | 0.88 | 0.09 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3005 | 1/1   | 0.88 | 0.16 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3006 | 1/1   | 0.88 | 0.16 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3112 | 1/1   | 0.88 | 0.10 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3490 | 1/1   | 0.88 | 0.18 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3498 | 1/1   | 0.88 | 0.11 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3864 | 1/1   | 0.88 | 0.14 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1641 | 1/1   | 0.88 | 0.14 | 51,51,51,51                 | 0     |
| 58  | MG   | 2B    | 219  | 1/1   | 0.88 | 0.13 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3866 | 1/1   | 0.88 | 0.12 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3027 | 1/1   | 0.88 | 0.12 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1644 | 1/1   | 0.88 | 0.24 | 66,66,66,66                 | 0     |
| 58  | MG   | 2O    | 201  | 1/1   | 0.88 | 0.22 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3267 | 1/1   | 0.88 | 0.23 | 62,62,62,62                 | 0     |
| 58  | MG   | 2T    | 202  | 1/1   | 0.88 | 0.23 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3449 | 1/1   | 0.88 | 0.27 | 55,55,55,55                 | 0     |
| 58  | MG   | 2x    | 101  | 1/1   | 0.88 | 0.24 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3539 | 1/1   | 0.88 | 0.16 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 4080 | 1/1   | 0.88 | 0.16 | 41,41,41,41                 | 0     |
| 58  | MG   | 2a    | 3031 | 1/1   | 0.89 | 0.30 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3664 | 1/1   | 0.89 | 0.20 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3129 | 1/1   | 0.89 | 0.15 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3404 | 1/1   | 0.89 | 0.18 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3683 | 1/1   | 0.89 | 0.09 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3689 | 1/1   | 0.89 | 0.10 | 59,59,59,59                 | 0     |
| 58  | MG   | 11    | 102  | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 58  | MG   | 2a    | 3039 | 1/1   | 0.89 | 0.24 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3181 | 1/1   | 0.89 | 0.22 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3089 | 1/1   | 0.89 | 0.23 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3701 | 1/1   | 0.89 | 0.24 | 45,45,45,45                 | 0     |
| 58  | MG   | 2a    | 3043 | 1/1   | 0.89 | 0.30 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3702 | 1/1   | 0.89 | 0.15 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3134 | 1/1   | 0.89 | 0.11 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3592 | 1/1   | 0.89 | 0.12 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 4035 | 1/1   | 0.89 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3055 | 1/1   | 0.89 | 0.17 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3416 | 1/1   | 0.89 | 0.28 | 46,46,46,46                 | 0     |
| 58  | MG   | 2a    | 3056 | 1/1   | 0.89 | 0.17 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4038 | 1/1   | 0.89 | 0.10 | 34,34,34,34                 | 0     |
| 58  | MG   | 2a    | 3061 | 1/1   | 0.89 | 0.15 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3423 | 1/1   | 0.89 | 0.22 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3426 | 1/1   | 0.89 | 0.25 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3066 | 1/1   | 0.89 | 0.25 | 69,69,69,69                 | 0     |
| 58  | MG   | 2a    | 3068 | 1/1   | 0.89 | 0.11 | 76,76,76,76                 | 0     |
| 58  | MG   | 1A    | 3877 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3259 | 1/1   | 0.89 | 0.14 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3442 | 1/1   | 0.89 | 0.11 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3063 | 1/1   | 0.89 | 0.18 | 49,49,49,49                 | 0     |
| 58  | MG   | 2a    | 3078 | 1/1   | 0.89 | 0.22 | 65,65,65,65                 | 0     |
| 58  | MG   | 1a    | 1609 | 1/1   | 0.89 | 0.15 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3733 | 1/1   | 0.89 | 0.16 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3059 | 1/1   | 0.89 | 0.12 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3073 | 1/1   | 0.89 | 0.12 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1759 | 1/1   | 0.89 | 0.08 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 4074 | 1/1   | 0.89 | 0.19 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3747 | 1/1   | 0.89 | 0.10 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3082 | 1/1   | 0.89 | 0.18 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3887 | 1/1   | 0.89 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3753 | 1/1   | 0.89 | 0.13 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1624 | 1/1   | 0.89 | 0.23 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3263 | 1/1   | 0.89 | 0.19 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3091 | 1/1   | 0.89 | 0.14 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3759 | 1/1   | 0.89 | 0.13 | 65,65,65,65                 | 0     |
| 58  | MG   | 2a    | 3103 | 1/1   | 0.89 | 0.17 | 68,68,68,68                 | 0     |
| 58  | MG   | 2a    | 3104 | 1/1   | 0.89 | 0.11 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3478 | 1/1   | 0.89 | 0.07 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3418 | 1/1   | 0.89 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 2a    | 3112 | 1/1   | 0.89 | 0.25 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1629 | 1/1   | 0.89 | 0.22 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1783 | 1/1   | 0.89 | 0.12 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3119 | 1/1   | 0.89 | 0.40 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3099 | 1/1   | 0.89 | 0.16 | 44,44,44,44                 | 0     |
| 58  | MG   | 1a    | 1787 | 1/1   | 0.89 | 0.17 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3607 | 1/1   | 0.89 | 0.09 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3054 | 1/1   | 0.89 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 2a    | 3125 | 1/1   | 0.89 | 0.21 | 61,61,61,61                 | 0     |
| 58  | MG   | 2a    | 3126 | 1/1   | 0.89 | 0.20 | 47,47,47,47                 | 0     |
| 58  | MG   | 1B    | 211  | 1/1   | 0.89 | 0.15 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3286 | 1/1   | 0.89 | 0.17 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3625 | 1/1   | 0.89 | 0.12 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3515 | 1/1   | 0.89 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3113 | 1/1   | 0.89 | 0.11 | 68,68,68,68                 | 0     |
| 58  | MG   | 1B    | 215  | 1/1   | 0.89 | 0.16 | 67,67,67,67                 | 0     |
| 58  | MG   | 2a    | 3134 | 1/1   | 0.89 | 0.23 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3626 | 1/1   | 0.89 | 0.12 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3798 | 1/1   | 0.89 | 0.12 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3325 | 1/1   | 0.89 | 0.26 | 48,48,48,48                 | 0     |
| 58  | MG   | 2a    | 3144 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3934 | 1/1   | 0.89 | 0.09 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3803 | 1/1   | 0.89 | 0.11 | 49,49,49,49                 | 0     |
| 58  | MG   | 2a    | 3154 | 1/1   | 0.89 | 0.21 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3329 | 1/1   | 0.89 | 0.20 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3509 | 1/1   | 0.89 | 0.08 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3948 | 1/1   | 0.89 | 0.09 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3558 | 1/1   | 0.89 | 0.20 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3166 | 1/1   | 0.89 | 0.13 | 61,61,61,61                 | 0     |
| 58  | MG   | 1x    | 101  | 1/1   | 0.89 | 0.27 | 65,65,65,65                 | 0     |
| 58  | MG   | 1x    | 103  | 1/1   | 0.89 | 0.15 | 56,56,56,56                 | 0     |
| 58  | MG   | 1a    | 1663 | 1/1   | 0.89 | 0.13 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3163 | 1/1   | 0.89 | 0.07 | 43,43,43,43                 | 0     |
| 58  | MG   | 2B    | 210  | 1/1   | 0.89 | 0.14 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3164 | 1/1   | 0.89 | 0.13 | 68,68,68,68                 | 0     |
| 58  | MG   | 2B    | 214  | 1/1   | 0.89 | 0.26 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3314 | 1/1   | 0.89 | 0.10 | 58,58,58,58                 | 0     |
| 58  | MG   | 1a    | 1664 | 1/1   | 0.89 | 0.16 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3426 | 1/1   | 0.89 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 2D    | 308  | 1/1   | 0.89 | 0.20 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3592 | 1/1   | 0.89 | 0.15 | 56,56,56,56                 | 0     |
| 58  | MG   | 1a    | 1668 | 1/1   | 0.89 | 0.14 | 52,52,52,52                 | 0     |
| 58  | MG   | 2F    | 306  | 1/1   | 0.89 | 0.14 | 64,64,64,64                 | 0     |
| 58  | MG   | 2G    | 201  | 1/1   | 0.89 | 0.26 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3522 | 1/1   | 0.89 | 0.29 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3338 | 1/1   | 0.89 | 0.09 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3162 | 1/1   | 0.89 | 0.44 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3345 | 1/1   | 0.89 | 0.27 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3542 | 1/1   | 0.89 | 0.15 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3829 | 1/1   | 0.89 | 0.11 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3084 | 1/1   | 0.89 | 0.17 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3187 | 1/1   | 0.89 | 0.21 | 54,54,54,54                 | 0     |
| 58  | MG   | 2a    | 3203 | 1/1   | 0.89 | 0.19 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3188 | 1/1   | 0.89 | 0.20 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3335 | 1/1   | 0.89 | 0.15 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3169 | 1/1   | 0.89 | 0.17 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3450 | 1/1   | 0.89 | 0.11 | 37,37,37,37                 | 0     |
| 58  | MG   | 2a    | 3008 | 1/1   | 0.89 | 0.25 | 64,64,64,64                 | 0     |
| 58  | MG   | 2a    | 3211 | 1/1   | 0.89 | 0.18 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3204 | 1/1   | 0.89 | 0.25 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3985 | 1/1   | 0.89 | 0.12 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3300 | 1/1   | 0.89 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3861 | 1/1   | 0.89 | 0.30 | 40,40,40,40                 | 0     |
| 58  | MG   | 2t    | 201  | 1/1   | 0.89 | 0.19 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3650 | 1/1   | 0.89 | 0.10 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3356 | 1/1   | 0.89 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1a    | 1703 | 1/1   | 0.89 | 0.09 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3038 | 1/1   | 0.89 | 0.14 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3398 | 1/1   | 0.89 | 0.21 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3228 | 1/1   | 0.89 | 0.08 | 38,38,38,38                 | 0     |
| 58  | MG   | 2a    | 3016 | 1/1   | 0.90 | 0.12 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3099 | 1/1   | 0.90 | 0.20 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3621 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1X    | 105  | 1/1   | 0.90 | 0.08 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3807 | 1/1   | 0.90 | 0.09 | 23,23,23,23                 | 0     |
| 58  | MG   | 2A    | 3608 | 1/1   | 0.90 | 0.14 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3306 | 1/1   | 0.90 | 0.12 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3489 | 1/1   | 0.90 | 0.08 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3110 | 1/1   | 0.90 | 0.29 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3491 | 1/1   | 0.90 | 0.16 | 52,52,52,52                 | 0     |
| 58  | MG   | 2a    | 3029 | 1/1   | 0.90 | 0.18 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3117 | 1/1   | 0.90 | 0.10 | 67,67,67,67                 | 0     |
| 58  | MG   | 1a    | 1771 | 1/1   | 0.90 | 0.20 | 75,75,75,75                 | 0     |
| 58  | MG   | 2a    | 3033 | 1/1   | 0.90 | 0.18 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3400 | 1/1   | 0.90 | 0.15 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3001 | 1/1   | 0.90 | 0.08 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3138 | 1/1   | 0.90 | 0.24 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3132 | 1/1   | 0.90 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3827 | 1/1   | 0.90 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3644 | 1/1   | 0.90 | 0.14 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3146 | 1/1   | 0.90 | 0.22 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3335 | 1/1   | 0.90 | 0.11 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1785 | 1/1   | 0.90 | 0.20 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3107 | 1/1   | 0.90 | 0.14 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3990 | 1/1   | 0.90 | 0.11 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3995 | 1/1   | 0.90 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 2a    | 3047 | 1/1   | 0.90 | 0.14 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3830 | 1/1   | 0.90 | 0.10 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3351 | 1/1   | 0.90 | 0.18 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3353 | 1/1   | 0.90 | 0.16 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3832 | 1/1   | 0.90 | 0.09 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1800 | 1/1   | 0.90 | 0.31 | 66,66,66,66                 | 0     |
| 58  | MG   | 1a    | 1801 | 1/1   | 0.90 | 0.16 | 73,73,73,73                 | 0     |
| 58  | MG   | 2A    | 3667 | 1/1   | 0.90 | 0.08 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3668 | 1/1   | 0.90 | 0.14 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3647 | 1/1   | 0.90 | 0.09 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3681 | 1/1   | 0.90 | 0.17 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3363 | 1/1   | 0.90 | 0.12 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3684 | 1/1   | 0.90 | 0.07 | 71,71,71,71                 | 0     |
| 58  | MG   | 2A    | 3168 | 1/1   | 0.90 | 0.09 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3264 | 1/1   | 0.90 | 0.12 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3173 | 1/1   | 0.90 | 0.09 | 31,31,31,31                 | 0     |
| 58  | MG   | 2a    | 3077 | 1/1   | 0.90 | 0.18 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3657 | 1/1   | 0.90 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 4022 | 1/1   | 0.90 | 0.17 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1622 | 1/1   | 0.90 | 0.08 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3385 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3227 | 1/1   | 0.90 | 0.17 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3524 | 1/1   | 0.90 | 0.12 | 41,41,41,41                 | 0     |
| 58  | MG   | 2a    | 3088 | 1/1   | 0.90 | 0.09 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3856 | 1/1   | 0.90 | 0.09 | 39,39,39,39                 | 0     |
| 58  | MG   | 2a    | 3091 | 1/1   | 0.90 | 0.11 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3393 | 1/1   | 0.90 | 0.21 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3141 | 1/1   | 0.90 | 0.11 | 18,18,18,18                 | 0     |
| 58  | MG   | 1w    | 105  | 1/1   | 0.90 | 0.14 | 80,80,80,80                 | 0     |
| 58  | MG   | 1A    | 3432 | 1/1   | 0.90 | 0.26 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 4046 | 1/1   | 0.90 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3720 | 1/1   | 0.90 | 0.23 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3193 | 1/1   | 0.90 | 0.22 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3194 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 4048 | 1/1   | 0.90 | 0.14 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3196 | 1/1   | 0.90 | 0.15 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3411 | 1/1   | 0.90 | 0.11 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3199 | 1/1   | 0.90 | 0.16 | 69,69,69,69                 | 0     |
| 58  | MG   | 2a    | 3111 | 1/1   | 0.90 | 0.07 | 79,79,79,79                 | 0     |
| 58  | MG   | 1A    | 3271 | 1/1   | 0.90 | 0.14 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 4064 | 1/1   | 0.90 | 0.09 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3867 | 1/1   | 0.90 | 0.13 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3745 | 1/1   | 0.90 | 0.09 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3235 | 1/1   | 0.90 | 0.10 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3288 | 1/1   | 0.90 | 0.11 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3552 | 1/1   | 0.90 | 0.07 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3237 | 1/1   | 0.90 | 0.14 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3430 | 1/1   | 0.90 | 0.13 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3435 | 1/1   | 0.90 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 4079 | 1/1   | 0.90 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3297 | 1/1   | 0.90 | 0.26 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3452 | 1/1   | 0.90 | 0.14 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3764 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3454 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3023 | 1/1   | 0.90 | 0.16 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3149 | 1/1   | 0.90 | 0.27 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3098 | 1/1   | 0.90 | 0.11 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3714 | 1/1   | 0.90 | 0.13 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3456 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3888 | 1/1   | 0.90 | 0.09 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3793 | 1/1   | 0.90 | 0.12 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 3575 | 1/1   | 0.90 | 0.26 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3152 | 1/1   | 0.90 | 0.10 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3892 | 1/1   | 0.90 | 0.35 | 36,36,36,36                 | 0     |
| 58  | MG   | 2a    | 3155 | 1/1   | 0.90 | 0.12 | 61,61,61,61                 | 0     |
| 58  | MG   | 2a    | 3156 | 1/1   | 0.90 | 0.10 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3467 | 1/1   | 0.90 | 0.07 | 60,60,60,60                 | 0     |
| 58  | MG   | 1a    | 1674 | 1/1   | 0.90 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3250 | 1/1   | 0.90 | 0.21 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3472 | 1/1   | 0.90 | 0.17 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3247 | 1/1   | 0.90 | 0.08 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3749 | 1/1   | 0.90 | 0.08 | 16,16,16,16                 | 0     |
| 58  | MG   | 1A    | 3460 | 1/1   | 0.90 | 0.16 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3814 | 1/1   | 0.90 | 0.14 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3918 | 1/1   | 0.90 | 0.08 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1685 | 1/1   | 0.90 | 0.26 | 39,39,39,39                 | 0     |
| 58  | MG   | 1B    | 234  | 1/1   | 0.90 | 0.12 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3256 | 1/1   | 0.90 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3493 | 1/1   | 0.90 | 0.13 | 65,65,65,65                 | 0     |
| 58  | MG   | 1a    | 1689 | 1/1   | 0.90 | 0.28 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3501 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1B    | 235  | 1/1   | 0.90 | 0.10 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3263 | 1/1   | 0.90 | 0.08 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3582 | 1/1   | 0.90 | 0.24 | 60,60,60,60                 | 0     |
| 58  | MG   | 1a    | 1694 | 1/1   | 0.90 | 0.41 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3768 | 1/1   | 0.90 | 0.15 | 54,54,54,54                 | 0     |
| 58  | MG   | 1E    | 301  | 1/1   | 0.90 | 0.20 | 43,43,43,43                 | 0     |
| 58  | MG   | 1E    | 305  | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3590 | 1/1   | 0.90 | 0.20 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3536 | 1/1   | 0.90 | 0.15 | 38,38,38,38                 | 0     |
| 58  | MG   | 1E    | 312  | 1/1   | 0.90 | 0.07 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3072 | 1/1   | 0.90 | 0.39 | 63,63,63,63                 | 0     |
| 58  | MG   | 1F    | 306  | 1/1   | 0.90 | 0.15 | 27,27,27,27                 | 0     |
| 58  | MG   | 2a    | 3200 | 1/1   | 0.90 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3124 | 1/1   | 0.90 | 0.28 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3788 | 1/1   | 0.90 | 0.10 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1719 | 1/1   | 0.90 | 0.13 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3253 | 1/1   | 0.90 | 0.09 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3319 | 1/1   | 0.90 | 0.13 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3385 | 1/1   | 0.90 | 0.08 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3254 | 1/1   | 0.90 | 0.11 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3568 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 2g    | 201  | 1/1   | 0.90 | 0.19 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3290 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 2k    | 201  | 1/1   | 0.90 | 0.10 | 73,73,73,73                 | 0     |
| 58  | MG   | 1U    | 205  | 1/1   | 0.90 | 0.25 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3579 | 1/1   | 0.90 | 0.10 | 24,24,24,24                 | 0     |
| 58  | MG   | 2l    | 203  | 1/1   | 0.90 | 0.14 | 74,74,74,74                 | 0     |
| 58  | MG   | 1A    | 3949 | 1/1   | 0.90 | 0.09 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3582 | 1/1   | 0.90 | 0.21 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3952 | 1/1   | 0.90 | 0.11 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3394 | 1/1   | 0.90 | 0.16 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3589 | 1/1   | 0.90 | 0.11 | 71,71,71,71                 | 0     |
| 58  | MG   | 2a    | 3011 | 1/1   | 0.90 | 0.29 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3012 | 1/1   | 0.90 | 0.30 | 71,71,71,71                 | 0     |
| 58  | MG   | 2a    | 3015 | 1/1   | 0.90 | 0.19 | 70,70,70,70                 | 0     |
| 59  | K    | 2A    | 3418 | 1/1   | 0.90 | 0.12 | 74,74,74,74                 | 0     |
| 61  | ZN   | 24    | 501  | 1/1   | 0.90 | 0.14 | 128,128,128,128             | 0     |
| 58  | MG   | 1A    | 3600 | 1/1   | 0.91 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3600 | 1/1   | 0.91 | 0.11 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3602 | 1/1   | 0.91 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3256 | 1/1   | 0.91 | 0.14 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3715 | 1/1   | 0.91 | 0.09 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3320 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3322 | 1/1   | 0.91 | 0.16 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3620 | 1/1   | 0.91 | 0.18 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3608 | 1/1   | 0.91 | 0.14 | 77,77,77,77                 | 0     |
| 58  | MG   | 2A    | 3152 | 1/1   | 0.91 | 0.10 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3332 | 1/1   | 0.91 | 0.15 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3333 | 1/1   | 0.91 | 0.10 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3967 | 1/1   | 0.91 | 0.10 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3336 | 1/1   | 0.91 | 0.07 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3859 | 1/1   | 0.91 | 0.17 | 40,40,40,40                 | 0     |
| 58  | MG   | 1B    | 228  | 1/1   | 0.91 | 0.13 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3343 | 1/1   | 0.91 | 0.21 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3727 | 1/1   | 0.91 | 0.10 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3160 | 1/1   | 0.91 | 0.28 | 51,51,51,51                 | 0     |
| 58  | MG   | 1b    | 301  | 1/1   | 0.91 | 0.15 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 3974 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3312 | 1/1   | 0.91 | 0.13 | 54,54,54,54                 | 0     |
| 58  | MG   | 1a    | 1642 | 1/1   | 0.91 | 0.11 | 73,73,73,73                 | 0     |
| 58  | MG   | 1v    | 101  | 1/1   | 0.91 | 0.11 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3359 | 1/1   | 0.91 | 0.09 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3738 | 1/1   | 0.91 | 0.08 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 3011 | 1/1   | 0.91 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3662 | 1/1   | 0.91 | 0.15 | 59,59,59,59                 | 0     |
| 58  | MG   | 1a    | 1645 | 1/1   | 0.91 | 0.19 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3180 | 1/1   | 0.91 | 0.26 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3623 | 1/1   | 0.91 | 0.10 | 23,23,23,23                 | 0     |
| 58  | MG   | 2a    | 3055 | 1/1   | 0.91 | 0.26 | 60,60,60,60                 | 0     |
| 58  | MG   | 1D    | 312  | 1/1   | 0.91 | 0.10 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3373 | 1/1   | 0.91 | 0.22 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3398 | 1/1   | 0.91 | 0.10 | 39,39,39,39                 | 0     |
| 58  | MG   | 2a    | 3062 | 1/1   | 0.91 | 0.24 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3673 | 1/1   | 0.91 | 0.17 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3378 | 1/1   | 0.91 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3273 | 1/1   | 0.91 | 0.13 | 35,35,35,35                 | 0     |
| 58  | MG   | 1x    | 106  | 1/1   | 0.91 | 0.20 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3994 | 1/1   | 0.91 | 0.07 | 34,34,34,34                 | 0     |
| 58  | MG   | 1E    | 310  | 1/1   | 0.91 | 0.14 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3693 | 1/1   | 0.91 | 0.12 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3189 | 1/1   | 0.91 | 0.17 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3073 | 1/1   | 0.91 | 0.09 | 64,64,64,64                 | 0     |
| 58  | MG   | 2a    | 3076 | 1/1   | 0.91 | 0.21 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3191 | 1/1   | 0.91 | 0.13 | 57,57,57,57                 | 0     |
| 58  | MG   | 1E    | 311  | 1/1   | 0.91 | 0.20 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3395 | 1/1   | 0.91 | 0.35 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3705 | 1/1   | 0.91 | 0.09 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3776 | 1/1   | 0.91 | 0.10 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3343 | 1/1   | 0.91 | 0.14 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3409 | 1/1   | 0.91 | 0.15 | 66,66,66,66                 | 0     |
| 58  | MG   | 1a    | 1671 | 1/1   | 0.91 | 0.26 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3410 | 1/1   | 0.91 | 0.09 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3643 | 1/1   | 0.91 | 0.17 | 35,35,35,35                 | 0     |
| 58  | MG   | 1P    | 206  | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3014 | 1/1   | 0.91 | 0.17 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3718 | 1/1   | 0.91 | 0.21 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3555 | 1/1   | 0.91 | 0.09 | 29,29,29,29                 | 0     |
| 58  | MG   | 1a    | 1679 | 1/1   | 0.91 | 0.17 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3217 | 1/1   | 0.91 | 0.15 | 28,28,28,28                 | 0     |
| 58  | MG   | 1P    | 208  | 1/1   | 0.91 | 0.14 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3028 | 1/1   | 0.91 | 0.17 | 78,78,78,78                 | 0     |
| 58  | MG   | 1Q    | 201  | 1/1   | 0.91 | 0.23 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3413 | 1/1   | 0.91 | 0.25 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3736 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3349 | 1/1   | 0.91 | 0.13 | 39,39,39,39                 | 0     |
| 58  | MG   | 1a    | 1687 | 1/1   | 0.91 | 0.28 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3429 | 1/1   | 0.91 | 0.24 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 4027 | 1/1   | 0.91 | 0.09 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3433 | 1/1   | 0.91 | 0.13 | 65,65,65,65                 | 0     |
| 58  | MG   | 2a    | 3118 | 1/1   | 0.91 | 0.15 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3200 | 1/1   | 0.91 | 0.15 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3438 | 1/1   | 0.91 | 0.11 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3439 | 1/1   | 0.91 | 0.14 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3471 | 1/1   | 0.91 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3441 | 1/1   | 0.91 | 0.07 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 4032 | 1/1   | 0.91 | 0.16 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3286 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3235 | 1/1   | 0.91 | 0.08 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3236 | 1/1   | 0.91 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3762 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3898 | 1/1   | 0.91 | 0.22 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3241 | 1/1   | 0.91 | 0.16 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3260 | 1/1   | 0.91 | 0.22 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3774 | 1/1   | 0.91 | 0.10 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3243 | 1/1   | 0.91 | 0.14 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3364 | 1/1   | 0.91 | 0.31 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3780 | 1/1   | 0.91 | 0.17 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3461 | 1/1   | 0.91 | 0.17 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 4052 | 1/1   | 0.91 | 0.06 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3054 | 1/1   | 0.91 | 0.17 | 58,58,58,58                 | 0     |
| 58  | MG   | 2a    | 3148 | 1/1   | 0.91 | 0.21 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1707 | 1/1   | 0.91 | 0.23 | 54,54,54,54                 | 0     |
| 58  | MG   | 1a    | 1708 | 1/1   | 0.91 | 0.13 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3059 | 1/1   | 0.91 | 0.12 | 58,58,58,58                 | 0     |
| 58  | MG   | 10    | 104  | 1/1   | 0.91 | 0.24 | 39,39,39,39                 | 0     |
| 58  | MG   | 10    | 105  | 1/1   | 0.91 | 0.13 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3427 | 1/1   | 0.91 | 0.12 | 66,66,66,66                 | 0     |
| 58  | MG   | 10    | 109  | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 10    | 110  | 1/1   | 0.91 | 0.12 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3684 | 1/1   | 0.91 | 0.07 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3819 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3488 | 1/1   | 0.91 | 0.05 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1736 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 58  | MG   | 15    | 105  | 1/1   | 0.91 | 0.07 | 56,56,56,56                 | 0     |
| 58  | MG   | 15    | 106  | 1/1   | 0.91 | 0.20 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3430 | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3503 | 1/1   | 0.91 | 0.10 | 56,56,56,56                 | 0     |
| 58  | MG   | 16    | 101  | 1/1   | 0.91 | 0.11 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3180 | 1/1   | 0.91 | 0.17 | 71,71,71,71                 | 0     |
| 58  | MG   | 1a    | 1752 | 1/1   | 0.91 | 0.08 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3089 | 1/1   | 0.91 | 0.12 | 52,52,52,52                 | 0     |
| 58  | MG   | 17    | 107  | 1/1   | 0.91 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 4069 | 1/1   | 0.91 | 0.10 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3518 | 1/1   | 0.91 | 0.08 | 43,43,43,43                 | 0     |
| 58  | MG   | 2B    | 211  | 1/1   | 0.91 | 0.20 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3521 | 1/1   | 0.91 | 0.16 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3522 | 1/1   | 0.91 | 0.12 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3115 | 1/1   | 0.91 | 0.11 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3528 | 1/1   | 0.91 | 0.12 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3284 | 1/1   | 0.91 | 0.09 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 4075 | 1/1   | 0.91 | 0.20 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3295 | 1/1   | 0.91 | 0.15 | 52,52,52,52                 | 0     |
| 58  | MG   | 2E    | 307  | 1/1   | 0.91 | 0.17 | 59,59,59,59                 | 0     |
| 58  | MG   | 2a    | 3199 | 1/1   | 0.91 | 0.20 | 68,68,68,68                 | 0     |
| 58  | MG   | 2F    | 301  | 1/1   | 0.91 | 0.20 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1a    | 1765 | 1/1   | 0.91 | 0.14 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3288 | 1/1   | 0.91 | 0.10 | 81,81,81,81                 | 0     |
| 58  | MG   | 1A    | 3072 | 1/1   | 0.91 | 0.11 | 20,20,20,20                 | 0     |
| 58  | MG   | 1a    | 1769 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3133 | 1/1   | 0.91 | 0.09 | 43,43,43,43                 | 0     |
| 58  | MG   | 2Q    | 202  | 1/1   | 0.91 | 0.19 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3292 | 1/1   | 0.91 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 2V    | 202  | 1/1   | 0.91 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1611 | 1/1   | 0.91 | 0.19 | 68,68,68,68                 | 0     |
| 58  | MG   | 1B    | 201  | 1/1   | 0.91 | 0.14 | 40,40,40,40                 | 0     |
| 58  | MG   | 1a    | 1777 | 1/1   | 0.91 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3114 | 1/1   | 0.91 | 0.15 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3837 | 1/1   | 0.91 | 0.13 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3447 | 1/1   | 0.91 | 0.22 | 59,59,59,59                 | 0     |
| 58  | MG   | 2a    | 3003 | 1/1   | 0.91 | 0.07 | 72,72,72,72                 | 0     |
| 58  | MG   | 2a    | 3004 | 1/1   | 0.91 | 0.23 | 54,54,54,54                 | 0     |
| 58  | MG   | 1a    | 1619 | 1/1   | 0.91 | 0.20 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3246 | 1/1   | 0.91 | 0.13 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3127 | 1/1   | 0.91 | 0.14 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3130 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3132 | 1/1   | 0.91 | 0.15 | 64,64,64,64                 | 0     |
| 58  | MG   | 1a    | 1791 | 1/1   | 0.91 | 0.08 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3139 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3953 | 1/1   | 0.91 | 0.14 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3962 | 1/1   | 0.92 | 0.09 | 74,74,74,74                 | 0     |
| 58  | MG   | 2B    | 206  | 1/1   | 0.92 | 0.14 | 79,79,79,79                 | 0     |
| 58  | MG   | 2B    | 207  | 1/1   | 0.92 | 0.10 | 61,61,61,61                 | 0     |
| 58  | MG   | 2B    | 209  | 1/1   | 0.92 | 0.12 | 62,62,62,62                 | 0     |
| 58  | MG   | 10    | 111  | 1/1   | 0.92 | 0.07 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3750 | 1/1   | 0.92 | 0.08 | 30,30,30,30                 | 0     |
| 58  | MG   | 11    | 103  | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 58  | MG   | 2B    | 213  | 1/1   | 0.92 | 0.15 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3163 | 1/1   | 0.92 | 0.16 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3464 | 1/1   | 0.92 | 0.20 | 51,51,51,51                 | 0     |
| 58  | MG   | 2B    | 216  | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 58  | MG   | 2B    | 217  | 1/1   | 0.92 | 0.11 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3755 | 1/1   | 0.92 | 0.11 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3210 | 1/1   | 0.92 | 0.22 | 42,42,42,42                 | 0     |
| 58  | MG   | 2D    | 304  | 1/1   | 0.92 | 0.22 | 48,48,48,48                 | 0     |
| 58  | MG   | 2D    | 305  | 1/1   | 0.92 | 0.24 | 67,67,67,67                 | 0     |
| 58  | MG   | 1f    | 202  | 1/1   | 0.92 | 0.08 | 65,65,65,65                 | 0     |
| 58  | MG   | 2E    | 302  | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2E    | 304  | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3470 | 1/1   | 0.92 | 0.20 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3212 | 1/1   | 0.92 | 0.17 | 59,59,59,59                 | 0     |
| 58  | MG   | 15    | 103  | 1/1   | 0.92 | 0.32 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3757 | 1/1   | 0.92 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3564 | 1/1   | 0.92 | 0.17 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3278 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3771 | 1/1   | 0.92 | 0.06 | 53,53,53,53                 | 0     |
| 58  | MG   | 2P    | 201  | 1/1   | 0.92 | 0.10 | 54,54,54,54                 | 0     |
| 58  | MG   | 16    | 102  | 1/1   | 0.92 | 0.25 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3488 | 1/1   | 0.92 | 0.16 | 72,72,72,72                 | 0     |
| 58  | MG   | 1A    | 3344 | 1/1   | 0.92 | 0.23 | 54,54,54,54                 | 0     |
| 58  | MG   | 2T    | 203  | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3228 | 1/1   | 0.92 | 0.24 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3491 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 58  | MG   | 2W    | 202  | 1/1   | 0.92 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3492 | 1/1   | 0.92 | 0.20 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3441 | 1/1   | 0.92 | 0.09 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3497 | 1/1   | 0.92 | 0.16 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3783 | 1/1   | 0.92 | 0.11 | 17,17,17,17                 | 0     |
| 58  | MG   | 23    | 102  | 1/1   | 0.92 | 0.11 | 65,65,65,65                 | 0     |
| 58  | MG   | 1x    | 102  | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3346 | 1/1   | 0.92 | 0.08 | 37,37,37,37                 | 0     |
| 58  | MG   | 1x    | 104  | 1/1   | 0.92 | 0.14 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3282 | 1/1   | 0.92 | 0.18 | 22,22,22,22                 | 0     |
| 58  | MG   | 1a    | 1606 | 1/1   | 0.92 | 0.07 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3237 | 1/1   | 0.92 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3350 | 1/1   | 0.92 | 0.09 | 52,52,52,52                 | 0     |
| 58  | MG   | 2a    | 3009 | 1/1   | 0.92 | 0.20 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3240 | 1/1   | 0.92 | 0.32 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 4002 | 1/1   | 0.92 | 0.14 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3233 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 58  | MG   | 2a    | 3013 | 1/1   | 0.92 | 0.13 | 58,58,58,58                 | 0     |
| 58  | MG   | 1x    | 111  | 1/1   | 0.92 | 0.27 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3018 | 1/1   | 0.92 | 0.17 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3579 | 1/1   | 0.92 | 0.07 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3530 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4017 | 1/1   | 0.92 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 2a    | 3020 | 1/1   | 0.92 | 0.10 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3580 | 1/1   | 0.92 | 0.06 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3453 | 1/1   | 0.92 | 0.15 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3291 | 1/1   | 0.92 | 0.13 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2a    | 3024 | 1/1   | 0.92 | 0.15 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 3361 | 1/1   | 0.92 | 0.26 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3594 | 1/1   | 0.92 | 0.11 | 23,23,23,23                 | 0     |
| 58  | MG   | 2A    | 3018 | 1/1   | 0.92 | 0.13 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3020 | 1/1   | 0.92 | 0.17 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3168 | 1/1   | 0.92 | 0.08 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3458 | 1/1   | 0.92 | 0.15 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3026 | 1/1   | 0.92 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3563 | 1/1   | 0.92 | 0.13 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3566 | 1/1   | 0.92 | 0.15 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3817 | 1/1   | 0.92 | 0.21 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3818 | 1/1   | 0.92 | 0.19 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1633 | 1/1   | 0.92 | 0.36 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3238 | 1/1   | 0.92 | 0.23 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3578 | 1/1   | 0.92 | 0.07 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3270 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3580 | 1/1   | 0.92 | 0.16 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3034 | 1/1   | 0.92 | 0.15 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 4039 | 1/1   | 0.92 | 0.12 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 4041 | 1/1   | 0.92 | 0.10 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3036 | 1/1   | 0.92 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3370 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3602 | 1/1   | 0.92 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 4056 | 1/1   | 0.92 | 0.13 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3044 | 1/1   | 0.92 | 0.14 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3017 | 1/1   | 0.92 | 0.18 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3374 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3609 | 1/1   | 0.92 | 0.13 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3605 | 1/1   | 0.92 | 0.16 | 48,48,48,48                 | 0     |
| 58  | MG   | 1a    | 1651 | 1/1   | 0.92 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3470 | 1/1   | 0.92 | 0.09 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3613 | 1/1   | 0.92 | 0.24 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3615 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 4067 | 1/1   | 0.92 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3839 | 1/1   | 0.92 | 0.22 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3057 | 1/1   | 0.92 | 0.17 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3293 | 1/1   | 0.92 | 0.17 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3173 | 1/1   | 0.92 | 0.12 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3472 | 1/1   | 0.92 | 0.15 | 48,48,48,48                 | 0     |
| 58  | MG   | 2a    | 3074 | 1/1   | 0.92 | 0.29 | 72,72,72,72                 | 0     |
| 58  | MG   | 2A    | 3632 | 1/1   | 0.92 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3060 | 1/1   | 0.92 | 0.13 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3298 | 1/1   | 0.92 | 0.45 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3847 | 1/1   | 0.92 | 0.30 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3849 | 1/1   | 0.92 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3381 | 1/1   | 0.92 | 0.13 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3174 | 1/1   | 0.92 | 0.14 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3480 | 1/1   | 0.92 | 0.13 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3067 | 1/1   | 0.92 | 0.31 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3068 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3041 | 1/1   | 0.92 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3313 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3047 | 1/1   | 0.92 | 0.06 | 26,26,26,26                 | 0     |
| 58  | MG   | 2a    | 3095 | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3862 | 1/1   | 0.92 | 0.15 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3077 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3654 | 1/1   | 0.92 | 0.18 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3316 | 1/1   | 0.92 | 0.07 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3108 | 1/1   | 0.92 | 0.13 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3649 | 1/1   | 0.92 | 0.07 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3650 | 1/1   | 0.92 | 0.09 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3086 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3492 | 1/1   | 0.92 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3328 | 1/1   | 0.92 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3191 | 1/1   | 0.92 | 0.11 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3662 | 1/1   | 0.92 | 0.13 | 20,20,20,20                 | 0     |
| 58  | MG   | 2A    | 3677 | 1/1   | 0.92 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3679 | 1/1   | 0.92 | 0.13 | 58,58,58,58                 | 0     |
| 58  | MG   | 2a    | 3116 | 1/1   | 0.92 | 0.22 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3664 | 1/1   | 0.92 | 0.09 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3405 | 1/1   | 0.92 | 0.14 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3337 | 1/1   | 0.92 | 0.28 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3685 | 1/1   | 0.92 | 0.11 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3497 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3881 | 1/1   | 0.92 | 0.08 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3498 | 1/1   | 0.92 | 0.09 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3344 | 1/1   | 0.92 | 0.27 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3503 | 1/1   | 0.92 | 0.07 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3103 | 1/1   | 0.92 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3408 | 1/1   | 0.92 | 0.13 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3703 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3677 | 1/1   | 0.92 | 0.09 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3680 | 1/1   | 0.92 | 0.10 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3354 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1a    | 1710 | 1/1   | 0.92 | 0.22 | 40,40,40,40                 | 0     |
| 58  | MG   | 1a    | 1711 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3030 | 1/1   | 0.92 | 0.11 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3116 | 1/1   | 0.92 | 0.21 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3685 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3152 | 1/1   | 0.92 | 0.13 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3717 | 1/1   | 0.92 | 0.20 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3899 | 1/1   | 0.92 | 0.23 | 26,26,26,26                 | 0     |
| 58  | MG   | 2A    | 3366 | 1/1   | 0.92 | 0.09 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3904 | 1/1   | 0.92 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3370 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3910 | 1/1   | 0.92 | 0.09 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3372 | 1/1   | 0.92 | 0.23 | 44,44,44,44                 | 0     |
| 58  | MG   | 1a    | 1730 | 1/1   | 0.92 | 0.13 | 45,45,45,45                 | 0     |
| 58  | MG   | 1F    | 309  | 1/1   | 0.92 | 0.16 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3376 | 1/1   | 0.92 | 0.16 | 55,55,55,55                 | 0     |
| 58  | MG   | 2a    | 3168 | 1/1   | 0.92 | 0.18 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3377 | 1/1   | 0.92 | 0.23 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3136 | 1/1   | 0.92 | 0.24 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3380 | 1/1   | 0.92 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3382 | 1/1   | 0.92 | 0.35 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3519 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3521 | 1/1   | 0.92 | 0.24 | 47,47,47,47                 | 0     |
| 58  | MG   | 2a    | 3176 | 1/1   | 0.92 | 0.25 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3748 | 1/1   | 0.92 | 0.15 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3140 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 58  | MG   | 1O    | 203  | 1/1   | 0.92 | 0.11 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3752 | 1/1   | 0.92 | 0.16 | 45,45,45,45                 | 0     |
| 58  | MG   | 2a    | 3182 | 1/1   | 0.92 | 0.22 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3916 | 1/1   | 0.92 | 0.08 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1749 | 1/1   | 0.92 | 0.19 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3153 | 1/1   | 0.92 | 0.19 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3699 | 1/1   | 0.92 | 0.09 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3087 | 1/1   | 0.92 | 0.10 | 25,25,25,25                 | 0     |
| 58  | MG   | 2A    | 3153 | 1/1   | 0.92 | 0.35 | 63,63,63,63                 | 0     |
| 58  | MG   | 1a    | 1754 | 1/1   | 0.92 | 0.08 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3402 | 1/1   | 0.92 | 0.15 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3156 | 1/1   | 0.92 | 0.32 | 43,43,43,43                 | 0     |
| 58  | MG   | 1R    | 205  | 1/1   | 0.92 | 0.20 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3930 | 1/1   | 0.92 | 0.08 | 62,62,62,62                 | 0     |
| 58  | MG   | 1U    | 201  | 1/1   | 0.92 | 0.17 | 35,35,35,35                 | 0     |
| 58  | MG   | 1a    | 1761 | 1/1   | 0.92 | 0.16 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3534 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3539 | 1/1   | 0.92 | 0.35 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3167 | 1/1   | 0.92 | 0.14 | 61,61,61,61                 | 0     |
| 58  | MG   | 2a    | 3202 | 1/1   | 0.92 | 0.16 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3704 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 58  | MG   | 1V    | 206  | 1/1   | 0.92 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3712 | 1/1   | 0.92 | 0.12 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3799 | 1/1   | 0.92 | 0.15 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3420 | 1/1   | 0.92 | 0.26 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3219 | 1/1   | 0.92 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3055 | 1/1   | 0.92 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 2e    | 201  | 1/1   | 0.92 | 0.06 | 67,67,67,67                 | 0     |
| 58  | MG   | 1X    | 104  | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3330 | 1/1   | 0.92 | 0.09 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3223 | 1/1   | 0.92 | 0.09 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1784 | 1/1   | 0.92 | 0.11 | 67,67,67,67                 | 0     |
| 58  | MG   | 1A    | 3225 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1786 | 1/1   | 0.92 | 0.17 | 54,54,54,54                 | 0     |
| 58  | MG   | 10    | 103  | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 58  | MG   | 1a    | 1790 | 1/1   | 0.92 | 0.14 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3818 | 1/1   | 0.92 | 0.13 | 66,66,66,66                 | 0     |
| 58  | MG   | 2v    | 102  | 1/1   | 0.92 | 0.21 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 3554 | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3190 | 1/1   | 0.92 | 0.27 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3125 | 1/1   | 0.92 | 0.08 | 32,32,32,32                 | 0     |
| 58  | MG   | 10    | 107  | 1/1   | 0.92 | 0.09 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3956 | 1/1   | 0.92 | 0.11 | 64,64,64,64                 | 0     |
| 58  | MG   | 2x    | 105  | 1/1   | 0.92 | 0.15 | 61,61,61,61                 | 0     |
| 58  | MG   | 1a    | 1796 | 1/1   | 0.92 | 0.28 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3560 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3116 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3860 | 1/1   | 0.93 | 0.07 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3238 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3244 | 1/1   | 0.93 | 0.26 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3011 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 4059 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3016 | 1/1   | 0.93 | 0.19 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3122 | 1/1   | 0.93 | 0.25 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3247 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3865 | 1/1   | 0.93 | 0.17 | 26,26,26,26                 | 0     |
| 58  | MG   | 1a    | 1638 | 1/1   | 0.93 | 0.14 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3697 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3461 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 2E    | 306  | 1/1   | 0.93 | 0.13 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3386 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3326 | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 2F    | 302  | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 4071 | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3467 | 1/1   | 0.93 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3514 | 1/1   | 0.93 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1a    | 1647 | 1/1   | 0.93 | 0.06 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3259 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3036 | 1/1   | 0.93 | 0.18 | 49,49,49,49                 | 0     |
| 58  | MG   | 2Q    | 201  | 1/1   | 0.93 | 0.20 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3519 | 1/1   | 0.93 | 0.12 | 48,48,48,48                 | 0     |
| 58  | MG   | 2R    | 201  | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 58  | MG   | 2T    | 201  | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3261 | 1/1   | 0.93 | 0.07 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3262 | 1/1   | 0.93 | 0.07 | 72,72,72,72                 | 0     |
| 58  | MG   | 2V    | 201  | 1/1   | 0.93 | 0.28 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3328 | 1/1   | 0.93 | 0.15 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3093 | 1/1   | 0.93 | 0.13 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3705 | 1/1   | 0.93 | 0.11 | 61,61,61,61                 | 0     |
| 58  | MG   | 2X    | 101  | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 58  | MG   | 2Z    | 301  | 1/1   | 0.93 | 0.16 | 80,80,80,80                 | 0     |
| 58  | MG   | 1a    | 1654 | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 58  | MG   | 1a    | 1655 | 1/1   | 0.93 | 0.20 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3043 | 1/1   | 0.93 | 0.06 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3708 | 1/1   | 0.93 | 0.07 | 26,26,26,26                 | 0     |
| 58  | MG   | 2A    | 3542 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 58  | MG   | 27    | 101  | 1/1   | 0.93 | 0.27 | 42,42,42,42                 | 0     |
| 58  | MG   | 27    | 103  | 1/1   | 0.93 | 0.15 | 41,41,41,41                 | 0     |
| 58  | MG   | 1a    | 1658 | 1/1   | 0.93 | 0.15 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3273 | 1/1   | 0.93 | 0.09 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 4081 | 1/1   | 0.93 | 0.21 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3048 | 1/1   | 0.93 | 0.11 | 67,67,67,67                 | 0     |
| 58  | MG   | 2A    | 3278 | 1/1   | 0.93 | 0.25 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3557 | 1/1   | 0.93 | 0.12 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3064 | 1/1   | 0.93 | 0.18 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3331 | 1/1   | 0.93 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3561 | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3051 | 1/1   | 0.93 | 0.18 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3128 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1666 | 1/1   | 0.93 | 0.22 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3885 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 58  | MG   | 1B    | 210  | 1/1   | 0.93 | 0.09 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3069 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3577 | 1/1   | 0.93 | 0.12 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3587 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3889 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3724 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3589 | 1/1   | 0.93 | 0.15 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1676 | 1/1   | 0.93 | 0.19 | 47,47,47,47                 | 0     |
| 58  | MG   | 1B    | 221  | 1/1   | 0.93 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3893 | 1/1   | 0.93 | 0.17 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1680 | 1/1   | 0.93 | 0.23 | 74,74,74,74                 | 0     |
| 58  | MG   | 1A    | 3477 | 1/1   | 0.93 | 0.13 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3591 | 1/1   | 0.93 | 0.16 | 23,23,23,23                 | 0     |
| 58  | MG   | 2a    | 3030 | 1/1   | 0.93 | 0.25 | 68,68,68,68                 | 0     |
| 58  | MG   | 2A    | 3070 | 1/1   | 0.93 | 0.14 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3596 | 1/1   | 0.93 | 0.11 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3597 | 1/1   | 0.93 | 0.15 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3209 | 1/1   | 0.93 | 0.07 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3300 | 1/1   | 0.93 | 0.13 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3746 | 1/1   | 0.93 | 0.10 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3747 | 1/1   | 0.93 | 0.15 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3481 | 1/1   | 0.93 | 0.21 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3336 | 1/1   | 0.93 | 0.07 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3080 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3612 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3308 | 1/1   | 0.93 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1690 | 1/1   | 0.93 | 0.28 | 49,49,49,49                 | 0     |
| 58  | MG   | 1B    | 239  | 1/1   | 0.93 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3752 | 1/1   | 0.93 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3084 | 1/1   | 0.93 | 0.12 | 39,39,39,39                 | 0     |
| 58  | MG   | 1D    | 303  | 1/1   | 0.93 | 0.13 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3628 | 1/1   | 0.93 | 0.29 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3629 | 1/1   | 0.93 | 0.25 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3914 | 1/1   | 0.93 | 0.14 | 53,53,53,53                 | 0     |
| 58  | MG   | 1D    | 310  | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 58  | MG   | 1a    | 1698 | 1/1   | 0.93 | 0.11 | 53,53,53,53                 | 0     |
| 58  | MG   | 2a    | 3057 | 1/1   | 0.93 | 0.07 | 58,58,58,58                 | 0     |
| 58  | MG   | 2a    | 3059 | 1/1   | 0.93 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1700 | 1/1   | 0.93 | 0.08 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3321 | 1/1   | 0.93 | 0.12 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3046 | 1/1   | 0.93 | 0.06 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3104 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3097 | 1/1   | 0.93 | 0.20 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3325 | 1/1   | 0.93 | 0.16 | 56,56,56,56                 | 0     |
| 58  | MG   | 2a    | 3067 | 1/1   | 0.93 | 0.14 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3645 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3327 | 1/1   | 0.93 | 0.13 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3922 | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3331 | 1/1   | 0.93 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3756 | 1/1   | 0.93 | 0.16 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3301 | 1/1   | 0.93 | 0.13 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3422 | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3028 | 1/1   | 0.93 | 0.11 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3769 | 1/1   | 0.93 | 0.16 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3105 | 1/1   | 0.93 | 0.14 | 45,45,45,45                 | 0     |
| 58  | MG   | 2a    | 3079 | 1/1   | 0.93 | 0.13 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3339 | 1/1   | 0.93 | 0.09 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3657 | 1/1   | 0.93 | 0.12 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3106 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3347 | 1/1   | 0.93 | 0.15 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3348 | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3936 | 1/1   | 0.93 | 0.17 | 58,58,58,58                 | 0     |
| 58  | MG   | 1a    | 1725 | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 58  | MG   | 1a    | 1726 | 1/1   | 0.93 | 0.07 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3937 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3940 | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 58  | MG   | 1O    | 204  | 1/1   | 0.93 | 0.09 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3356 | 1/1   | 0.93 | 0.46 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3305 | 1/1   | 0.93 | 0.10 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3310 | 1/1   | 0.93 | 0.09 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3784 | 1/1   | 0.93 | 0.10 | 12,12,12,12                 | 0     |
| 58  | MG   | 2A    | 3128 | 1/1   | 0.93 | 0.39 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3687 | 1/1   | 0.93 | 0.10 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3688 | 1/1   | 0.93 | 0.08 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3129 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3050 | 1/1   | 0.93 | 0.23 | 41,41,41,41                 | 0     |
| 58  | MG   | 2a    | 3106 | 1/1   | 0.93 | 0.20 | 65,65,65,65                 | 0     |
| 58  | MG   | 1Q    | 202  | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 58  | MG   | 2a    | 3110 | 1/1   | 0.93 | 0.26 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3694 | 1/1   | 0.93 | 0.12 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3365 | 1/1   | 0.93 | 0.06 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1745 | 1/1   | 0.93 | 0.08 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3700 | 1/1   | 0.93 | 0.10 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3950 | 1/1   | 0.93 | 0.12 | 49,49,49,49                 | 0     |
| 58  | MG   | 1Q    | 207  | 1/1   | 0.93 | 0.10 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3504 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3624 | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3505 | 1/1   | 0.93 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3506 | 1/1   | 0.93 | 0.10 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3147 | 1/1   | 0.93 | 0.15 | 42,42,42,42                 | 0     |
| 58  | MG   | 1U    | 206  | 1/1   | 0.93 | 0.20 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3627 | 1/1   | 0.93 | 0.08 | 21,21,21,21                 | 0     |
| 58  | MG   | 1V    | 202  | 1/1   | 0.93 | 0.37 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3381 | 1/1   | 0.93 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3016 | 1/1   | 0.93 | 0.12 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3801 | 1/1   | 0.93 | 0.10 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 3964 | 1/1   | 0.93 | 0.12 | 69,69,69,69                 | 0     |
| 58  | MG   | 1A    | 3630 | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3386 | 1/1   | 0.93 | 0.24 | 51,51,51,51                 | 0     |
| 58  | MG   | 2a    | 3136 | 1/1   | 0.93 | 0.20 | 58,58,58,58                 | 0     |
| 58  | MG   | 1W    | 203  | 1/1   | 0.93 | 0.11 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3723 | 1/1   | 0.93 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3433 | 1/1   | 0.93 | 0.29 | 34,34,34,34                 | 0     |
| 58  | MG   | 2a    | 3142 | 1/1   | 0.93 | 0.11 | 81,81,81,81                 | 0     |
| 58  | MG   | 1A    | 3636 | 1/1   | 0.93 | 0.07 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3638 | 1/1   | 0.93 | 0.13 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3733 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3734 | 1/1   | 0.93 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3971 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3396 | 1/1   | 0.93 | 0.15 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3738 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1778 | 1/1   | 0.93 | 0.21 | 59,59,59,59                 | 0     |
| 58  | MG   | 1Y    | 202  | 1/1   | 0.93 | 0.27 | 46,46,46,46                 | 0     |
| 58  | MG   | 2a    | 3159 | 1/1   | 0.93 | 0.06 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3973 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 2a    | 3161 | 1/1   | 0.93 | 0.11 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 3143 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3403 | 1/1   | 0.93 | 0.18 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3360 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3176 | 1/1   | 0.93 | 0.09 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3439 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3440 | 1/1   | 0.93 | 0.11 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3314 | 1/1   | 0.93 | 0.08 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3525 | 1/1   | 0.93 | 0.09 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3988 | 1/1   | 0.93 | 0.06 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3756 | 1/1   | 0.93 | 0.13 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3651 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3527 | 1/1   | 0.93 | 0.25 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3828 | 1/1   | 0.93 | 0.18 | 48,48,48,48                 | 0     |
| 58  | MG   | 1I    | 105  | 1/1   | 0.93 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3419 | 1/1   | 0.93 | 0.20 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3656 | 1/1   | 0.93 | 0.12 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3530 | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3768 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3424 | 1/1   | 0.93 | 0.13 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3425 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 58  | MG   | 1a    | 1802 | 1/1   | 0.93 | 0.22 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4004 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 4006 | 1/1   | 0.93 | 0.10 | 61,61,61,61                 | 0     |
| 58  | MG   | 2A    | 3781 | 1/1   | 0.93 | 0.17 | 39,39,39,39                 | 0     |
| 58  | MG   | 2a    | 3191 | 1/1   | 0.93 | 0.18 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 4009 | 1/1   | 0.93 | 0.10 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3431 | 1/1   | 0.93 | 0.13 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3791 | 1/1   | 0.93 | 0.19 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3432 | 1/1   | 0.93 | 0.14 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3442 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3833 | 1/1   | 0.93 | 0.10 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3798 | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3834 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3446 | 1/1   | 0.93 | 0.46 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3063 | 1/1   | 0.93 | 0.26 | 51,51,51,51                 | 0     |
| 58  | MG   | 18    | 106  | 1/1   | 0.93 | 0.23 | 66,66,66,66                 | 0     |
| 58  | MG   | 1A    | 4021 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3232 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4023 | 1/1   | 0.93 | 0.16 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3184 | 1/1   | 0.93 | 0.05 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3447 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 58  | MG   | 2d    | 301  | 1/1   | 0.93 | 0.28 | 61,61,61,61                 | 0     |
| 58  | MG   | 2d    | 302  | 1/1   | 0.93 | 0.10 | 73,73,73,73                 | 0     |
| 58  | MG   | 1A    | 3187 | 1/1   | 0.93 | 0.11 | 27,27,27,27                 | 0     |
| 58  | MG   | 2f    | 201  | 1/1   | 0.93 | 0.10 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3218 | 1/1   | 0.93 | 0.19 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3090 | 1/1   | 0.93 | 0.14 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3454 | 1/1   | 0.93 | 0.15 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3851 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3221 | 1/1   | 0.93 | 0.14 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3373 | 1/1   | 0.93 | 0.10 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1a    | 1614 | 1/1   | 0.93 | 0.11 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3272 | 1/1   | 0.93 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 4037 | 1/1   | 0.93 | 0.08 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3376 | 1/1   | 0.93 | 0.16 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3556 | 1/1   | 0.93 | 0.36 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3857 | 1/1   | 0.93 | 0.11 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 4045 | 1/1   | 0.93 | 0.13 | 14,14,14,14                 | 0     |
| 58  | MG   | 2B    | 208  | 1/1   | 0.93 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1625 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1626 | 1/1   | 0.93 | 0.34 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3858 | 1/1   | 0.93 | 0.18 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3480 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 1Z    | 303  | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |
| 58  | MG   | 10    | 101  | 1/1   | 0.94 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3403 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 58  | MG   | 1a    | 1753 | 1/1   | 0.94 | 0.17 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3475 | 1/1   | 0.94 | 0.40 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3585 | 1/1   | 0.94 | 0.10 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3587 | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |
| 58  | MG   | 2W    | 203  | 1/1   | 0.94 | 0.06 | 35,35,35,35                 | 0     |
| 58  | MG   | 2W    | 204  | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 58  | MG   | 1a    | 1755 | 1/1   | 0.94 | 0.12 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 4026 | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3020 | 1/1   | 0.94 | 0.08 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3123 | 1/1   | 0.94 | 0.07 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3593 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1758 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3478 | 1/1   | 0.94 | 0.19 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3479 | 1/1   | 0.94 | 0.06 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3032 | 1/1   | 0.94 | 0.09 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3720 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 58  | MG   | 2a    | 3002 | 1/1   | 0.94 | 0.20 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3081 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3340 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3606 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 11    | 104  | 1/1   | 0.94 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1770 | 1/1   | 0.94 | 0.15 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3611 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3483 | 1/1   | 0.94 | 0.18 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3731 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3412 | 1/1   | 0.94 | 0.20 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3616 | 1/1   | 0.94 | 0.15 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 15    | 102  | 1/1   | 0.94 | 0.19 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3144 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3145 | 1/1   | 0.94 | 0.06 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3352 | 1/1   | 0.94 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3342 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3886 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3147 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3056 | 1/1   | 0.94 | 0.09 | 30,30,30,30                 | 0     |
| 58  | MG   | 15    | 108  | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 4057 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3154 | 1/1   | 0.94 | 0.16 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3151 | 1/1   | 0.94 | 0.23 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3638 | 1/1   | 0.94 | 0.08 | 36,36,36,36                 | 0     |
| 58  | MG   | 17    | 101  | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3157 | 1/1   | 0.94 | 0.07 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3643 | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3890 | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3192 | 1/1   | 0.94 | 0.47 | 41,41,41,41                 | 0     |
| 58  | MG   | 18    | 104  | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3193 | 1/1   | 0.94 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3086 | 1/1   | 0.94 | 0.18 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1601 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3166 | 1/1   | 0.94 | 0.16 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3306 | 1/1   | 0.94 | 0.10 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3351 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3618 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 58  | MG   | 1a    | 1803 | 1/1   | 0.94 | 0.21 | 58,58,58,58                 | 0     |
| 58  | MG   | 2A    | 3174 | 1/1   | 0.94 | 0.11 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1805 | 1/1   | 0.94 | 0.39 | 54,54,54,54                 | 0     |
| 58  | MG   | 1a    | 1607 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 58  | MG   | 2a    | 3045 | 1/1   | 0.94 | 0.16 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3178 | 1/1   | 0.94 | 0.13 | 56,56,56,56                 | 0     |
| 58  | MG   | 1a    | 1807 | 1/1   | 0.94 | 0.30 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3902 | 1/1   | 0.94 | 0.08 | 22,22,22,22                 | 0     |
| 58  | MG   | 2a    | 3049 | 1/1   | 0.94 | 0.20 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3352 | 1/1   | 0.94 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3906 | 1/1   | 0.94 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | 1d    | 301  | 1/1   | 0.94 | 0.25 | 63,63,63,63                 | 0     |
| 58  | MG   | 2a    | 3054 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3390 | 1/1   | 0.94 | 0.18 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1612 | 1/1   | 0.94 | 0.15 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3678 | 1/1   | 0.94 | 0.10 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3392 | 1/1   | 0.94 | 0.14 | 54,54,54,54                 | 0     |
| 58  | MG   | 2A    | 3680 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 58  | MG   | 1m    | 3001 | 1/1   | 0.94 | 0.11 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3394 | 1/1   | 0.94 | 0.14 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3308 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3198 | 1/1   | 0.94 | 0.06 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3397 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 58  | MG   | 1p    | 102  | 1/1   | 0.94 | 0.14 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3357 | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3691 | 1/1   | 0.94 | 0.11 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3437 | 1/1   | 0.94 | 0.07 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3113 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3628 | 1/1   | 0.94 | 0.08 | 13,13,13,13                 | 0     |
| 58  | MG   | 1w    | 103  | 1/1   | 0.94 | 0.06 | 81,81,81,81                 | 0     |
| 58  | MG   | 1A    | 3359 | 1/1   | 0.94 | 0.29 | 46,46,46,46                 | 0     |
| 58  | MG   | 2a    | 3075 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 58  | MG   | 1B    | 207  | 1/1   | 0.94 | 0.21 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3197 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3042 | 1/1   | 0.94 | 0.11 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3410 | 1/1   | 0.94 | 0.21 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3704 | 1/1   | 0.94 | 0.07 | 68,68,68,68                 | 0     |
| 58  | MG   | 1A    | 3926 | 1/1   | 0.94 | 0.14 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3632 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3792 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3709 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3414 | 1/1   | 0.94 | 0.16 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3155 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3362 | 1/1   | 0.94 | 0.10 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3443 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3714 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 58  | MG   | 1B    | 219  | 1/1   | 0.94 | 0.08 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3208 | 1/1   | 0.94 | 0.15 | 34,34,34,34                 | 0     |
| 58  | MG   | 1a    | 1636 | 1/1   | 0.94 | 0.18 | 43,43,43,43                 | 0     |
| 58  | MG   | 1B    | 222  | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3002 | 1/1   | 0.94 | 0.29 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3642 | 1/1   | 0.94 | 0.10 | 36,36,36,36                 | 0     |
| 58  | MG   | 2a    | 3101 | 1/1   | 0.94 | 0.25 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3427 | 1/1   | 0.94 | 0.24 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3529 | 1/1   | 0.94 | 0.24 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3034 | 1/1   | 0.94 | 0.33 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3941 | 1/1   | 0.94 | 0.11 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3226 | 1/1   | 0.94 | 0.14 | 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  | MG   | 2A    | 3731 | 1/1   | 0.94 | 0.28 | 59,59,59,59                 | 0     |
| 58  | MG   | 1B    | 231  | 1/1   | 0.94 | 0.06 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3646 | 1/1   | 0.94 | 0.08 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3531 | 1/1   | 0.94 | 0.07 | 46,46,46,46                 | 0     |
| 58  | MG   | 2a    | 3113 | 1/1   | 0.94 | 0.19 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3436 | 1/1   | 0.94 | 0.09 | 63,63,63,63                 | 0     |
| 58  | MG   | 1a    | 1646 | 1/1   | 0.94 | 0.23 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3809 | 1/1   | 0.94 | 0.15 | 41,41,41,41                 | 0     |
| 58  | MG   | 2a    | 3117 | 1/1   | 0.94 | 0.24 | 49,49,49,49                 | 0     |
| 58  | MG   | 1B    | 236  | 1/1   | 0.94 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3532 | 1/1   | 0.94 | 0.08 | 67,67,67,67                 | 0     |
| 58  | MG   | 1B    | 240  | 1/1   | 0.94 | 0.13 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3744 | 1/1   | 0.94 | 0.08 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3366 | 1/1   | 0.94 | 0.23 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3021 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3816 | 1/1   | 0.94 | 0.16 | 46,46,46,46                 | 0     |
| 58  | MG   | 1D    | 309  | 1/1   | 0.94 | 0.26 | 47,47,47,47                 | 0     |
| 58  | MG   | 2a    | 3127 | 1/1   | 0.94 | 0.19 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3214 | 1/1   | 0.94 | 0.06 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3751 | 1/1   | 0.94 | 0.16 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3540 | 1/1   | 0.94 | 0.06 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3031 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3007 | 1/1   | 0.94 | 0.08 | 43,43,43,43                 | 0     |
| 58  | MG   | 1E    | 302  | 1/1   | 0.94 | 0.13 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3457 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1665 | 1/1   | 0.94 | 0.22 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3265 | 1/1   | 0.94 | 0.16 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3462 | 1/1   | 0.94 | 0.13 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3961 | 1/1   | 0.94 | 0.09 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3822 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 58  | MG   | 2a    | 3143 | 1/1   | 0.94 | 0.07 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3250 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3963 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3041 | 1/1   | 0.94 | 0.14 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3096 | 1/1   | 0.94 | 0.06 | 47,47,47,47                 | 0     |
| 58  | MG   | 2a    | 3149 | 1/1   | 0.94 | 0.14 | 66,66,66,66                 | 0     |
| 58  | MG   | 2a    | 3150 | 1/1   | 0.94 | 0.22 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3455 | 1/1   | 0.94 | 0.14 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3268 | 1/1   | 0.94 | 0.15 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3473 | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3553 | 1/1   | 0.94 | 0.06 | 21,21,21,21                 | 0     |
| 58  | MG   | 2A    | 3476 | 1/1   | 0.94 | 0.21 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3051 | 1/1   | 0.94 | 0.21 | 28,28,28,28                 | 0     |
| 58  | MG   | 1N    | 203  | 1/1   | 0.94 | 0.12 | 47,47,47,47                 | 0     |
| 58  | MG   | 1a    | 1678 | 1/1   | 0.94 | 0.07 | 56,56,56,56                 | 0     |
| 58  | MG   | 2a    | 3162 | 1/1   | 0.94 | 0.09 | 75,75,75,75                 | 0     |
| 58  | MG   | 1A    | 3674 | 1/1   | 0.94 | 0.06 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3264 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 58  | MG   | 1O    | 201  | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 58  | MG   | 2a    | 3167 | 1/1   | 0.94 | 0.21 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3972 | 1/1   | 0.94 | 0.08 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3380 | 1/1   | 0.94 | 0.27 | 26,26,26,26                 | 0     |
| 58  | MG   | 2A    | 3803 | 1/1   | 0.94 | 0.13 | 56,56,56,56                 | 0     |
| 58  | MG   | 1P    | 204  | 1/1   | 0.94 | 0.35 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3066 | 1/1   | 0.94 | 0.13 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3806 | 1/1   | 0.94 | 0.09 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3835 | 1/1   | 0.94 | 0.11 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3495 | 1/1   | 0.94 | 0.20 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3496 | 1/1   | 0.94 | 0.05 | 27,27,27,27                 | 0     |
| 58  | MG   | 1a    | 1688 | 1/1   | 0.94 | 0.28 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3557 | 1/1   | 0.94 | 0.16 | 30,30,30,30                 | 0     |
| 58  | MG   | 1P    | 209  | 1/1   | 0.94 | 0.11 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3681 | 1/1   | 0.94 | 0.08 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3982 | 1/1   | 0.94 | 0.13 | 16,16,16,16                 | 0     |
| 58  | MG   | 1A    | 3382 | 1/1   | 0.94 | 0.28 | 41,41,41,41                 | 0     |
| 58  | MG   | 1Q    | 206  | 1/1   | 0.94 | 0.08 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3226 | 1/1   | 0.94 | 0.25 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3823 | 1/1   | 0.94 | 0.16 | 58,58,58,58                 | 0     |
| 58  | MG   | 1R    | 202  | 1/1   | 0.94 | 0.07 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3283 | 1/1   | 0.94 | 0.13 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3562 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3053 | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 58  | MG   | 2a    | 3192 | 1/1   | 0.94 | 0.12 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3690 | 1/1   | 0.94 | 0.08 | 19,19,19,19                 | 0     |
| 58  | MG   | 2A    | 3520 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 1U    | 202  | 1/1   | 0.94 | 0.17 | 34,34,34,34                 | 0     |
| 58  | MG   | 1U    | 204  | 1/1   | 0.94 | 0.12 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3274 | 1/1   | 0.94 | 0.15 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3527 | 1/1   | 0.94 | 0.09 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3079 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 4000 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 58  | MG   | 1U    | 207  | 1/1   | 0.94 | 0.38 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3535 | 1/1   | 0.94 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 1U    | 210  | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3294 | 1/1   | 0.94 | 0.11 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3540 | 1/1   | 0.94 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 2a    | 3207 | 1/1   | 0.94 | 0.11 | 65,65,65,65                 | 0     |
| 58  | MG   | 2a    | 3208 | 1/1   | 0.94 | 0.08 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3275 | 1/1   | 0.94 | 0.10 | 31,31,31,31                 | 0     |
| 58  | MG   | 1a    | 1715 | 1/1   | 0.94 | 0.17 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3695 | 1/1   | 0.94 | 0.16 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3696 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1724 | 1/1   | 0.94 | 0.07 | 52,52,52,52                 | 0     |
| 58  | MG   | 2D    | 307  | 1/1   | 0.94 | 0.27 | 42,42,42,42                 | 0     |
| 58  | MG   | 1V    | 205  | 1/1   | 0.94 | 0.29 | 31,31,31,31                 | 0     |
| 58  | MG   | 2E    | 301  | 1/1   | 0.94 | 0.14 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3131 | 1/1   | 0.94 | 0.29 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3555 | 1/1   | 0.94 | 0.18 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3556 | 1/1   | 0.94 | 0.17 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3092 | 1/1   | 0.94 | 0.17 | 62,62,62,62                 | 0     |
| 58  | MG   | 1V    | 207  | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3698 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 58  | MG   | 2q    | 202  | 1/1   | 0.94 | 0.07 | 71,71,71,71                 | 0     |
| 58  | MG   | 1A    | 3572 | 1/1   | 0.94 | 0.11 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3102 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3103 | 1/1   | 0.94 | 0.09 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 4018 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 2N    | 201  | 1/1   | 0.94 | 0.07 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3175 | 1/1   | 0.94 | 0.16 | 31,31,31,31                 | 0     |
| 58  | MG   | 1a    | 1743 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3863 | 1/1   | 0.94 | 0.33 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3576 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3316 | 1/1   | 0.94 | 0.12 | 62,62,62,62                 | 0     |
| 60  | TEL  | 2A    | 3826 | 58/58 | 0.94 | 0.14 | 27,41,47,55                 | 0     |
| 58  | MG   | 1A    | 3401 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1a    | 1717 | 1/1   | 0.95 | 0.17 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3554 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3136 | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 58  | MG   | 1a    | 1721 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 1a    | 1722 | 1/1   | 0.95 | 0.06 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 4049 | 1/1   | 0.95 | 0.06 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 4051 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3560 | 1/1   | 0.95 | 0.11 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3138 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3562 | 1/1   | 0.95 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 2R    | 202  | 1/1   | 0.95 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3372 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3444 | 1/1   | 0.95 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3224 | 1/1   | 0.95 | 0.17 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3905 | 1/1   | 0.95 | 0.15 | 49,49,49,49                 | 0     |
| 58  | MG   | 1a    | 1732 | 1/1   | 0.95 | 0.13 | 50,50,50,50                 | 0     |
| 58  | MG   | 1a    | 1733 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3573 | 1/1   | 0.95 | 0.15 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3574 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 4063 | 1/1   | 0.95 | 0.18 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3139 | 1/1   | 0.95 | 0.09 | 31,31,31,31                 | 0     |
| 58  | MG   | 1a    | 1738 | 1/1   | 0.95 | 0.19 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3778 | 1/1   | 0.95 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 1a    | 1740 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3315 | 1/1   | 0.95 | 0.08 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1741 | 1/1   | 0.95 | 0.14 | 35,35,35,35                 | 0     |
| 58  | MG   | 23    | 101  | 1/1   | 0.95 | 0.18 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3317 | 1/1   | 0.95 | 0.16 | 36,36,36,36                 | 0     |
| 58  | MG   | 25    | 103  | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3781 | 1/1   | 0.95 | 0.07 | 16,16,16,16                 | 0     |
| 58  | MG   | 27    | 102  | 1/1   | 0.95 | 0.16 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3633 | 1/1   | 0.95 | 0.10 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3913 | 1/1   | 0.95 | 0.06 | 39,39,39,39                 | 0     |
| 58  | MG   | 1a    | 1748 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3528 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3108 | 1/1   | 0.95 | 0.06 | 47,47,47,47                 | 0     |
| 58  | MG   | 11    | 101  | 1/1   | 0.95 | 0.30 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3594 | 1/1   | 0.95 | 0.19 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3915 | 1/1   | 0.95 | 0.08 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3326 | 1/1   | 0.95 | 0.15 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3598 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3111 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3785 | 1/1   | 0.95 | 0.13 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3601 | 1/1   | 0.95 | 0.08 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3329 | 1/1   | 0.95 | 0.09 | 58,58,58,58                 | 0     |
| 58  | MG   | 2a    | 3014 | 1/1   | 0.95 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3330 | 1/1   | 0.95 | 0.06 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3070 | 1/1   | 0.95 | 0.15 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3115 | 1/1   | 0.95 | 0.23 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3637 | 1/1   | 0.95 | 0.12 | 60,60,60,60                 | 0     |
| 58  | MG   | 12    | 101  | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3118 | 1/1   | 0.95 | 0.17 | 58,58,58,58                 | 0     |
| 58  | MG   | 12    | 102  | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 13    | 102  | 1/1   | 0.95 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3178 | 1/1   | 0.95 | 0.10 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3125 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3617 | 1/1   | 0.95 | 0.19 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3341 | 1/1   | 0.95 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3180 | 1/1   | 0.95 | 0.05 | 30,30,30,30                 | 0     |
| 58  | MG   | 2a    | 3028 | 1/1   | 0.95 | 0.13 | 77,77,77,77                 | 0     |
| 58  | MG   | 2A    | 3622 | 1/1   | 0.95 | 0.11 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3641 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3229 | 1/1   | 0.95 | 0.15 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3627 | 1/1   | 0.95 | 0.06 | 30,30,30,30                 | 0     |
| 58  | MG   | 1a    | 1762 | 1/1   | 0.95 | 0.16 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3347 | 1/1   | 0.95 | 0.07 | 56,56,56,56                 | 0     |
| 58  | MG   | 15    | 104  | 1/1   | 0.95 | 0.21 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3349 | 1/1   | 0.95 | 0.15 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3350 | 1/1   | 0.95 | 0.09 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3633 | 1/1   | 0.95 | 0.10 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3131 | 1/1   | 0.95 | 0.12 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3276 | 1/1   | 0.95 | 0.11 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3135 | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 58  | MG   | 1a    | 1766 | 1/1   | 0.95 | 0.15 | 59,59,59,59                 | 0     |
| 58  | MG   | 1a    | 1767 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3142 | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 58  | MG   | 1B    | 206  | 1/1   | 0.95 | 0.06 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3536 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 58  | MG   | 1B    | 208  | 1/1   | 0.95 | 0.17 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3143 | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3537 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3805 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 58  | MG   | 17    | 105  | 1/1   | 0.95 | 0.13 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3384 | 1/1   | 0.95 | 0.09 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3367 | 1/1   | 0.95 | 0.08 | 59,59,59,59                 | 0     |
| 58  | MG   | 1B    | 212  | 1/1   | 0.95 | 0.20 | 52,52,52,52                 | 0     |
| 58  | MG   | 1a    | 1782 | 1/1   | 0.95 | 0.09 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3151 | 1/1   | 0.95 | 0.16 | 55,55,55,55                 | 0     |
| 58  | MG   | 2a    | 3058 | 1/1   | 0.95 | 0.21 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3091 | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 58  | MG   | 18    | 105  | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3658 | 1/1   | 0.95 | 0.07 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3659 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3660 | 1/1   | 0.95 | 0.06 | 64,64,64,64                 | 0     |
| 58  | MG   | 2A    | 3374 | 1/1   | 0.95 | 0.20 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3005 | 1/1   | 0.95 | 0.10 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3944 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3665 | 1/1   | 0.95 | 0.07 | 72,72,72,72                 | 0     |
| 58  | MG   | 1B    | 217  | 1/1   | 0.95 | 0.20 | 46,46,46,46                 | 0     |
| 58  | MG   | 1a    | 1788 | 1/1   | 0.95 | 0.11 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3284 | 1/1   | 0.95 | 0.39 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3669 | 1/1   | 0.95 | 0.05 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3390 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 1a    | 1604 | 1/1   | 0.95 | 0.10 | 60,60,60,60                 | 0     |
| 58  | MG   | 1a    | 1605 | 1/1   | 0.95 | 0.16 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3162 | 1/1   | 0.95 | 0.06 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3391 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3658 | 1/1   | 0.95 | 0.08 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3387 | 1/1   | 0.95 | 0.22 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3165 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 58  | MG   | 2a    | 3081 | 1/1   | 0.95 | 0.17 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3550 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 58  | MG   | 1a    | 1798 | 1/1   | 0.95 | 0.19 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3686 | 1/1   | 0.95 | 0.11 | 36,36,36,36                 | 0     |
| 58  | MG   | 1a    | 1799 | 1/1   | 0.95 | 0.23 | 55,55,55,55                 | 0     |
| 58  | MG   | 2A    | 3169 | 1/1   | 0.95 | 0.08 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3551 | 1/1   | 0.95 | 0.25 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3171 | 1/1   | 0.95 | 0.10 | 50,50,50,50                 | 0     |
| 58  | MG   | 1a    | 1610 | 1/1   | 0.95 | 0.13 | 34,34,34,34                 | 0     |
| 58  | MG   | 2a    | 3093 | 1/1   | 0.95 | 0.07 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3665 | 1/1   | 0.95 | 0.06 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3236 | 1/1   | 0.95 | 0.29 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1804 | 1/1   | 0.95 | 0.35 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3395 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3396 | 1/1   | 0.95 | 0.20 | 59,59,59,59                 | 0     |
| 58  | MG   | 1B    | 233  | 1/1   | 0.95 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3957 | 1/1   | 0.95 | 0.08 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3958 | 1/1   | 0.95 | 0.11 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3397 | 1/1   | 0.95 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3337 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3338 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3186 | 1/1   | 0.95 | 0.12 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3708 | 1/1   | 0.95 | 0.13 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3022 | 1/1   | 0.95 | 0.07 | 18,18,18,18                 | 0     |
| 58  | MG   | 1A    | 3118 | 1/1   | 0.95 | 0.14 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3242 | 1/1   | 0.95 | 0.17 | 38,38,38,38                 | 0     |
| 58  | MG   | 1p    | 101  | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3682 | 1/1   | 0.95 | 0.09 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3120 | 1/1   | 0.95 | 0.10 | 29,29,29,29                 | 0     |
| 58  | MG   | 1D    | 311  | 1/1   | 0.95 | 0.16 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3078 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3476 | 1/1   | 0.95 | 0.21 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3079 | 1/1   | 0.95 | 0.05 | 29,29,29,29                 | 0     |
| 58  | MG   | 1E    | 303  | 1/1   | 0.95 | 0.05 | 21,21,21,21                 | 0     |
| 58  | MG   | 1A    | 3196 | 1/1   | 0.95 | 0.26 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3200 | 1/1   | 0.95 | 0.11 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3201 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3724 | 1/1   | 0.95 | 0.22 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3202 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3006 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3975 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 58  | MG   | 1a    | 1640 | 1/1   | 0.95 | 0.21 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3208 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3848 | 1/1   | 0.95 | 0.07 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3082 | 1/1   | 0.95 | 0.16 | 34,34,34,34                 | 0     |
| 58  | MG   | 1F    | 304  | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3417 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3215 | 1/1   | 0.95 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3157 | 1/1   | 0.95 | 0.11 | 24,24,24,24                 | 0     |
| 58  | MG   | 2a    | 3137 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3984 | 1/1   | 0.95 | 0.06 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3419 | 1/1   | 0.95 | 0.16 | 54,54,54,54                 | 0     |
| 58  | MG   | 1x    | 112  | 1/1   | 0.95 | 0.20 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3443 | 1/1   | 0.95 | 0.22 | 31,31,31,31                 | 0     |
| 58  | MG   | 1G    | 201  | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 58  | MG   | 1G    | 203  | 1/1   | 0.95 | 0.06 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3003 | 1/1   | 0.95 | 0.17 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3224 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 58  | MG   | 1G    | 204  | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 58  | MG   | 1G    | 205  | 1/1   | 0.95 | 0.13 | 47,47,47,47                 | 0     |
| 58  | MG   | 1N    | 201  | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 58  | MG   | 1N    | 202  | 1/1   | 0.95 | 0.07 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3455 | 1/1   | 0.95 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1657 | 1/1   | 0.95 | 0.06 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3307 | 1/1   | 0.95 | 0.19 | 54,54,54,54                 | 0     |
| 58  | MG   | 2a    | 3157 | 1/1   | 0.95 | 0.10 | 66,66,66,66                 | 0     |
| 58  | MG   | 1A    | 3486 | 1/1   | 0.95 | 0.28 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3459 | 1/1   | 0.95 | 0.13 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3013 | 1/1   | 0.95 | 0.22 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1N    | 205  | 1/1   | 0.95 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3015 | 1/1   | 0.95 | 0.11 | 68,68,68,68                 | 0     |
| 58  | MG   | 1a    | 1662 | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3487 | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3581 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3421 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3776 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 58  | MG   | 1P    | 201  | 1/1   | 0.95 | 0.14 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3025 | 1/1   | 0.95 | 0.22 | 42,42,42,42                 | 0     |
| 58  | MG   | 2a    | 3171 | 1/1   | 0.95 | 0.15 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3019 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3309 | 1/1   | 0.95 | 0.20 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3206 | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3255 | 1/1   | 0.95 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3477 | 1/1   | 0.95 | 0.20 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3043 | 1/1   | 0.95 | 0.31 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3479 | 1/1   | 0.95 | 0.24 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3044 | 1/1   | 0.95 | 0.16 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3033 | 1/1   | 0.95 | 0.06 | 60,60,60,60                 | 0     |
| 58  | MG   | 2A    | 3800 | 1/1   | 0.95 | 0.10 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3596 | 1/1   | 0.95 | 0.12 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3485 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3088 | 1/1   | 0.95 | 0.13 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3487 | 1/1   | 0.95 | 0.10 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 4015 | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 4016 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 58  | MG   | 1R    | 201  | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3257 | 1/1   | 0.95 | 0.10 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3716 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 58  | MG   | 1R    | 203  | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 58  | MG   | 1R    | 204  | 1/1   | 0.95 | 0.31 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3502 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 58  | MG   | 1R    | 207  | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3165 | 1/1   | 0.95 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 1T    | 202  | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 58  | MG   | 2a    | 3198 | 1/1   | 0.95 | 0.11 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3872 | 1/1   | 0.95 | 0.08 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3211 | 1/1   | 0.95 | 0.08 | 31,31,31,31                 | 0     |
| 58  | MG   | 1a    | 1691 | 1/1   | 0.95 | 0.14 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3004 | 1/1   | 0.95 | 0.06 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3509 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3512 | 1/1   | 0.95 | 0.17 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3604 | 1/1   | 0.95 | 0.10 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3732 | 1/1   | 0.95 | 0.08 | 19,19,19,19                 | 0     |
| 58  | MG   | 2A    | 3271 | 1/1   | 0.95 | 0.15 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3318 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 58  | MG   | 1a    | 1696 | 1/1   | 0.95 | 0.24 | 50,50,50,50                 | 0     |
| 58  | MG   | 1U    | 208  | 1/1   | 0.95 | 0.13 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3507 | 1/1   | 0.95 | 0.17 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3745 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3111 | 1/1   | 0.95 | 0.41 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3525 | 1/1   | 0.95 | 0.09 | 40,40,40,40                 | 0     |
| 58  | MG   | 1a    | 1702 | 1/1   | 0.95 | 0.17 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3611 | 1/1   | 0.95 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 1V    | 204  | 1/1   | 0.95 | 0.07 | 27,27,27,27                 | 0     |
| 58  | MG   | 1a    | 1705 | 1/1   | 0.95 | 0.19 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3367 | 1/1   | 0.95 | 0.19 | 50,50,50,50                 | 0     |
| 58  | MG   | 2D    | 301  | 1/1   | 0.95 | 0.18 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3616 | 1/1   | 0.95 | 0.05 | 23,23,23,23                 | 0     |
| 58  | MG   | 2D    | 303  | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 0     |
| 58  | MG   | 2q    | 201  | 1/1   | 0.95 | 0.07 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3510 | 1/1   | 0.95 | 0.08 | 42,42,42,42                 | 0     |
| 58  | MG   | 2r    | 101  | 1/1   | 0.95 | 0.14 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3537 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3069 | 1/1   | 0.95 | 0.09 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3513 | 1/1   | 0.95 | 0.16 | 33,33,33,33                 | 0     |
| 58  | MG   | 2v    | 103  | 1/1   | 0.95 | 0.17 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3221 | 1/1   | 0.95 | 0.07 | 33,33,33,33                 | 0     |
| 58  | MG   | 1a    | 1713 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 58  | MG   | 2E    | 303  | 1/1   | 0.95 | 0.18 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3516 | 1/1   | 0.95 | 0.15 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3518 | 1/1   | 0.95 | 0.25 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3547 | 1/1   | 0.95 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3549 | 1/1   | 0.95 | 0.14 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3076 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 58  | MG   | 1X    | 102  | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 4072 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4073 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3740 | 1/1   | 0.96 | 0.09 | 31,31,31,31                 | 0     |
| 58  | MG   | 1a    | 1772 | 1/1   | 0.96 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3355 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3603 | 1/1   | 0.96 | 0.21 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3744 | 1/1   | 0.96 | 0.18 | 43,43,43,43                 | 0     |
| 58  | MG   | 1a    | 1774 | 1/1   | 0.96 | 0.11 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2Y    | 201  | 1/1   | 0.96 | 0.16 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 4076 | 1/1   | 0.96 | 0.19 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3607 | 1/1   | 0.96 | 0.10 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3517 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 4078 | 1/1   | 0.96 | 0.06 | 23,23,23,23                 | 0     |
| 58  | MG   | 2I    | 102  | 1/1   | 0.96 | 0.22 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3614 | 1/1   | 0.96 | 0.07 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 3077 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 58  | MG   | 17    | 106  | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 58  | MG   | 25    | 102  | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3614 | 1/1   | 0.96 | 0.12 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3617 | 1/1   | 0.96 | 0.06 | 30,30,30,30                 | 0     |
| 58  | MG   | 18    | 101  | 1/1   | 0.96 | 0.09 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3901 | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 58  | MG   | 18    | 103  | 1/1   | 0.96 | 0.10 | 32,32,32,32                 | 0     |
| 58  | MG   | 2a    | 3001 | 1/1   | 0.96 | 0.10 | 57,57,57,57                 | 0     |
| 58  | MG   | 1B    | 202  | 1/1   | 0.96 | 0.12 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3621 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3378 | 1/1   | 0.96 | 0.18 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3903 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3327 | 1/1   | 0.96 | 0.05 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3622 | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3754 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3094 | 1/1   | 0.96 | 0.10 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3031 | 1/1   | 0.96 | 0.17 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3177 | 1/1   | 0.96 | 0.10 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3526 | 1/1   | 0.96 | 0.17 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3760 | 1/1   | 0.96 | 0.07 | 12,12,12,12                 | 0     |
| 58  | MG   | 1B    | 214  | 1/1   | 0.96 | 0.18 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3635 | 1/1   | 0.96 | 0.06 | 79,79,79,79                 | 0     |
| 58  | MG   | 1A    | 3765 | 1/1   | 0.96 | 0.10 | 21,21,21,21                 | 0     |
| 58  | MG   | 1A    | 3767 | 1/1   | 0.96 | 0.07 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3145 | 1/1   | 0.96 | 0.20 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3919 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3008 | 1/1   | 0.96 | 0.08 | 17,17,17,17                 | 0     |
| 58  | MG   | 1B    | 220  | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3148 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 58  | MG   | 1a    | 1616 | 1/1   | 0.96 | 0.08 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3775 | 1/1   | 0.96 | 0.05 | 34,34,34,34                 | 0     |
| 58  | MG   | 1B    | 224  | 1/1   | 0.96 | 0.09 | 47,47,47,47                 | 0     |
| 58  | MG   | 1e    | 201  | 1/1   | 0.96 | 0.09 | 57,57,57,57                 | 0     |
| 58  | MG   | 1f    | 201  | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1a    | 1620 | 1/1   | 0.96 | 0.10 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3927 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3334 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 58  | MG   | 1B    | 227  | 1/1   | 0.96 | 0.09 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3631 | 1/1   | 0.96 | 0.14 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3655 | 1/1   | 0.96 | 0.05 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3388 | 1/1   | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3780 | 1/1   | 0.96 | 0.10 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3932 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3933 | 1/1   | 0.96 | 0.08 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3279 | 1/1   | 0.96 | 0.34 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3230 | 1/1   | 0.96 | 0.06 | 29,29,29,29                 | 0     |
| 58  | MG   | 1a    | 1632 | 1/1   | 0.96 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3037 | 1/1   | 0.96 | 0.09 | 21,21,21,21                 | 0     |
| 58  | MG   | 1B    | 237  | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1635 | 1/1   | 0.96 | 0.07 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3535 | 1/1   | 0.96 | 0.27 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3938 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3786 | 1/1   | 0.96 | 0.05 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3670 | 1/1   | 0.96 | 0.12 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3185 | 1/1   | 0.96 | 0.06 | 63,63,63,63                 | 0     |
| 58  | MG   | 2A    | 3672 | 1/1   | 0.96 | 0.12 | 54,54,54,54                 | 0     |
| 58  | MG   | 1x    | 107  | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3674 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3943 | 1/1   | 0.96 | 0.08 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3207 | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3234 | 1/1   | 0.96 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3421 | 1/1   | 0.96 | 0.09 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3422 | 1/1   | 0.96 | 0.18 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3945 | 1/1   | 0.96 | 0.05 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3790 | 1/1   | 0.96 | 0.09 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3290 | 1/1   | 0.96 | 0.13 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3794 | 1/1   | 0.96 | 0.28 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3150 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3541 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3039 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 58  | MG   | 1E    | 306  | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 58  | MG   | 1E    | 307  | 1/1   | 0.96 | 0.27 | 56,56,56,56                 | 0     |
| 58  | MG   | 1a    | 1652 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1653 | 1/1   | 0.96 | 0.20 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3695 | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3434 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3645 | 1/1   | 0.96 | 0.15 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3699 | 1/1   | 0.96 | 0.06 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3100 | 1/1   | 0.96 | 0.15 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3465 | 1/1   | 0.96 | 0.10 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3545 | 1/1   | 0.96 | 0.21 | 42,42,42,42                 | 0     |
| 58  | MG   | 1F    | 302  | 1/1   | 0.96 | 0.10 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3466 | 1/1   | 0.96 | 0.18 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3017 | 1/1   | 0.96 | 0.07 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3548 | 1/1   | 0.96 | 0.10 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3345 | 1/1   | 0.96 | 0.12 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3232 | 1/1   | 0.96 | 0.10 | 75,75,75,75                 | 0     |
| 58  | MG   | 2A    | 3021 | 1/1   | 0.96 | 0.11 | 62,62,62,62                 | 0     |
| 58  | MG   | 1A    | 3808 | 1/1   | 0.96 | 0.05 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3468 | 1/1   | 0.96 | 0.04 | 44,44,44,44                 | 0     |
| 58  | MG   | 2a    | 3087 | 1/1   | 0.96 | 0.16 | 66,66,66,66                 | 0     |
| 58  | MG   | 1A    | 3402 | 1/1   | 0.96 | 0.12 | 35,35,35,35                 | 0     |
| 58  | MG   | 2a    | 3089 | 1/1   | 0.96 | 0.12 | 61,61,61,61                 | 0     |
| 58  | MG   | 1G    | 202  | 1/1   | 0.96 | 0.15 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3451 | 1/1   | 0.96 | 0.08 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3453 | 1/1   | 0.96 | 0.11 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3811 | 1/1   | 0.96 | 0.08 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3190 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 1a    | 1669 | 1/1   | 0.96 | 0.32 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3660 | 1/1   | 0.96 | 0.05 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3661 | 1/1   | 0.96 | 0.10 | 14,14,14,14                 | 0     |
| 58  | MG   | 1a    | 1672 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3404 | 1/1   | 0.96 | 0.11 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3245 | 1/1   | 0.96 | 0.15 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3726 | 1/1   | 0.96 | 0.08 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3127 | 1/1   | 0.96 | 0.29 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3406 | 1/1   | 0.96 | 0.05 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3465 | 1/1   | 0.96 | 0.05 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3407 | 1/1   | 0.96 | 0.15 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3732 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |
| 58  | MG   | 2a    | 3108 | 1/1   | 0.96 | 0.12 | 70,70,70,70                 | 0     |
| 58  | MG   | 1N    | 206  | 1/1   | 0.96 | 0.04 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3821 | 1/1   | 0.96 | 0.22 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3558 | 1/1   | 0.96 | 0.05 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3976 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3253 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3559 | 1/1   | 0.96 | 0.20 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3825 | 1/1   | 0.96 | 0.10 | 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  | MG   | 1a    | 1684 | 1/1   | 0.96 | 0.15 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3045 | 1/1   | 0.96 | 0.15 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3826 | 1/1   | 0.96 | 0.13 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3083 | 1/1   | 0.96 | 0.14 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3067 | 1/1   | 0.96 | 0.09 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3304 | 1/1   | 0.96 | 0.20 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3676 | 1/1   | 0.96 | 0.12 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3483 | 1/1   | 0.96 | 0.10 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3411 | 1/1   | 0.96 | 0.09 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3567 | 1/1   | 0.96 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 1Q    | 205  | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3991 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3056 | 1/1   | 0.96 | 0.10 | 65,65,65,65                 | 0     |
| 58  | MG   | 1A    | 3568 | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3194 | 1/1   | 0.96 | 0.19 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3997 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3999 | 1/1   | 0.96 | 0.06 | 69,69,69,69                 | 0     |
| 58  | MG   | 2A    | 3761 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3836 | 1/1   | 0.96 | 0.11 | 57,57,57,57                 | 0     |
| 58  | MG   | 2A    | 3763 | 1/1   | 0.96 | 0.14 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3683 | 1/1   | 0.96 | 0.12 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3838 | 1/1   | 0.96 | 0.05 | 19,19,19,19                 | 0     |
| 58  | MG   | 2A    | 3277 | 1/1   | 0.96 | 0.13 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3769 | 1/1   | 0.96 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3064 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3195 | 1/1   | 0.96 | 0.08 | 17,17,17,17                 | 0     |
| 58  | MG   | 1A    | 4005 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3415 | 1/1   | 0.96 | 0.08 | 29,29,29,29                 | 0     |
| 58  | MG   | 2a    | 3147 | 1/1   | 0.96 | 0.08 | 76,76,76,76                 | 0     |
| 58  | MG   | 2A    | 3506 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3778 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 4007 | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 3842 | 1/1   | 0.96 | 0.07 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3782 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 58  | MG   | 2A    | 3783 | 1/1   | 0.96 | 0.12 | 56,56,56,56                 | 0     |
| 58  | MG   | 2A    | 3510 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3786 | 1/1   | 0.96 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3845 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3789 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1709 | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3416 | 1/1   | 0.96 | 0.14 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3085 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3795 | 1/1   | 0.96 | 0.08 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3688 | 1/1   | 0.96 | 0.07 | 27,27,27,27                 | 0     |
| 58  | MG   | 2a    | 3165 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3517 | 1/1   | 0.96 | 0.16 | 42,42,42,42                 | 0     |
| 58  | MG   | 1U    | 209  | 1/1   | 0.96 | 0.28 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3689 | 1/1   | 0.96 | 0.09 | 16,16,16,16                 | 0     |
| 58  | MG   | 2A    | 3801 | 1/1   | 0.96 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3850 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3033 | 1/1   | 0.96 | 0.36 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3057 | 1/1   | 0.96 | 0.19 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3524 | 1/1   | 0.96 | 0.09 | 27,27,27,27                 | 0     |
| 58  | MG   | 1a    | 1718 | 1/1   | 0.96 | 0.16 | 60,60,60,60                 | 0     |
| 58  | MG   | 1A    | 3199 | 1/1   | 0.96 | 0.29 | 42,42,42,42                 | 0     |
| 58  | MG   | 1a    | 1720 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3159 | 1/1   | 0.96 | 0.07 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3160 | 1/1   | 0.96 | 0.09 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3087 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 58  | MG   | 1a    | 1723 | 1/1   | 0.96 | 0.07 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 4024 | 1/1   | 0.96 | 0.09 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3090 | 1/1   | 0.96 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3423 | 1/1   | 0.96 | 0.18 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3161 | 1/1   | 0.96 | 0.05 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3820 | 1/1   | 0.96 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3093 | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 58  | MG   | 2A    | 3094 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 1a    | 1727 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3544 | 1/1   | 0.96 | 0.12 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3493 | 1/1   | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 58  | MG   | 1W    | 204  | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3548 | 1/1   | 0.96 | 0.12 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3048 | 1/1   | 0.96 | 0.05 | 24,24,24,24                 | 0     |
| 58  | MG   | 1X    | 101  | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3551 | 1/1   | 0.96 | 0.10 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3110 | 1/1   | 0.96 | 0.06 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3588 | 1/1   | 0.96 | 0.10 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 4033 | 1/1   | 0.96 | 0.06 | 15,15,15,15                 | 0     |
| 58  | MG   | 1A    | 3135 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3429 | 1/1   | 0.96 | 0.16 | 36,36,36,36                 | 0     |
| 58  | MG   | 1Z    | 301  | 1/1   | 0.96 | 0.07 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3500 | 1/1   | 0.96 | 0.13 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3593 | 1/1   | 0.96 | 0.10 | 54,54,54,54                 | 0     |
| 58  | MG   | 1a    | 1742 | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3711 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 2B    | 218  | 1/1   | 0.96 | 0.14 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3073 | 1/1   | 0.96 | 0.17 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3167 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1a    | 1747 | 1/1   | 0.96 | 0.12 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3213 | 1/1   | 0.96 | 0.16 | 29,29,29,29                 | 0     |
| 58  | MG   | 10    | 106  | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 58  | MG   | 2A    | 3569 | 1/1   | 0.96 | 0.07 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3015 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3434 | 1/1   | 0.96 | 0.15 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3119 | 1/1   | 0.96 | 0.18 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3717 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3576 | 1/1   | 0.96 | 0.10 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 4054 | 1/1   | 0.96 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3334 | 1/1   | 0.96 | 0.09 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 4055 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3876 | 1/1   | 0.96 | 0.09 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3435 | 1/1   | 0.96 | 0.17 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3266 | 1/1   | 0.96 | 0.11 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3722 | 1/1   | 0.96 | 0.09 | 52,52,52,52                 | 0     |
| 58  | MG   | 2F    | 304  | 1/1   | 0.96 | 0.28 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3215 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3076 | 1/1   | 0.96 | 0.05 | 23,23,23,23                 | 0     |
| 58  | MG   | 2A    | 3342 | 1/1   | 0.96 | 0.17 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3588 | 1/1   | 0.96 | 0.12 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3729 | 1/1   | 0.96 | 0.10 | 16,16,16,16                 | 0     |
| 58  | MG   | 1A    | 3511 | 1/1   | 0.96 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3133 | 1/1   | 0.96 | 0.21 | 43,43,43,43                 | 0     |
| 58  | MG   | 13    | 103  | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3140 | 1/1   | 0.96 | 0.10 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3375 | 1/1   | 0.96 | 0.19 | 55,55,55,55                 | 0     |
| 60  | TEL  | 1A    | 4082 | 58/58 | 0.96 | 0.10 | 18,25,33,38                 | 0     |
| 58  | MG   | 1A    | 3735 | 1/1   | 0.96 | 0.16 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3171 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3252 | 1/1   | 0.97 | 0.14 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3292 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3220 | 1/1   | 0.97 | 0.11 | 43,43,43,43                 | 0     |
| 58  | MG   | 2a    | 3053 | 1/1   | 0.97 | 0.13 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3765 | 1/1   | 0.97 | 0.04 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3694 | 1/1   | 0.97 | 0.08 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3586 | 1/1   | 0.97 | 0.09 | 48,48,48,48                 | 0     |
| 58  | MG   | 1W    | 205  | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3873 | 1/1   | 0.97 | 0.11 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3773 | 1/1   | 0.97 | 0.08 | 55,55,55,55                 | 0     |
| 58  | MG   | 1A    | 3106 | 1/1   | 0.97 | 0.11 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3058 | 1/1   | 0.97 | 0.04 | 28,28,28,28                 | 0     |
| 58  | MG   | 1X    | 103  | 1/1   | 0.97 | 0.13 | 42,42,42,42                 | 0     |
| 58  | MG   | 2a    | 3063 | 1/1   | 0.97 | 0.13 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3298 | 1/1   | 0.97 | 0.12 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3978 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3299 | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3563 | 1/1   | 0.97 | 0.15 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3879 | 1/1   | 0.97 | 0.05 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3121 | 1/1   | 0.97 | 0.12 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3122 | 1/1   | 0.97 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3785 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3880 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 58  | MG   | 1a    | 1683 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3038 | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3565 | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 10    | 102  | 1/1   | 0.97 | 0.29 | 48,48,48,48                 | 0     |
| 58  | MG   | 1A    | 3566 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3987 | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3884 | 1/1   | 0.97 | 0.10 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3989 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 58  | MG   | 1A    | 3514 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | 2a    | 3082 | 1/1   | 0.97 | 0.11 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3109 | 1/1   | 0.97 | 0.05 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3134 | 1/1   | 0.97 | 0.11 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3176 | 1/1   | 0.97 | 0.20 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3802 | 1/1   | 0.97 | 0.05 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3137 | 1/1   | 0.97 | 0.10 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3996 | 1/1   | 0.97 | 0.10 | 28,28,28,28                 | 0     |
| 58  | MG   | 1A    | 3707 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3998 | 1/1   | 0.97 | 0.09 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3804 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3303 | 1/1   | 0.97 | 0.15 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 4001 | 1/1   | 0.97 | 0.10 | 56,56,56,56                 | 0     |
| 58  | MG   | 1B    | 238  | 1/1   | 0.97 | 0.06 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3624 | 1/1   | 0.97 | 0.10 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3710 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3816 | 1/1   | 0.97 | 0.09 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3003 | 1/1   | 0.97 | 0.09 | 24,24,24,24                 | 0     |
| 58  | MG   | 1D    | 301  | 1/1   | 0.97 | 0.15 | 22,22,22,22                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3148 | 1/1   | 0.97 | 0.10 | 55,55,55,55                 | 0     |
| 58  | MG   | 1a    | 1706 | 1/1   | 0.97 | 0.14 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3144 | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3822 | 1/1   | 0.97 | 0.18 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3896 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3301 | 1/1   | 0.97 | 0.20 | 51,51,51,51                 | 0     |
| 58  | MG   | 2A    | 3825 | 1/1   | 0.97 | 0.10 | 49,49,49,49                 | 0     |
| 58  | MG   | 2a    | 3107 | 1/1   | 0.97 | 0.28 | 48,48,48,48                 | 0     |
| 58  | MG   | 1D    | 304  | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3303 | 1/1   | 0.97 | 0.15 | 48,48,48,48                 | 0     |
| 58  | MG   | 1D    | 305  | 1/1   | 0.97 | 0.06 | 17,17,17,17                 | 0     |
| 58  | MG   | 2A    | 3009 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3897 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 58  | MG   | 1D    | 308  | 1/1   | 0.97 | 0.13 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3012 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3642 | 1/1   | 0.97 | 0.08 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3061 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 4008 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3201 | 1/1   | 0.97 | 0.08 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3428 | 1/1   | 0.97 | 0.13 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3469 | 1/1   | 0.97 | 0.07 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 4013 | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 58  | MG   | 2a    | 3122 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3202 | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 0     |
| 58  | MG   | 17    | 104  | 1/1   | 0.97 | 0.15 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3813 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3203 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3475 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3052 | 1/1   | 0.97 | 0.21 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3024 | 1/1   | 0.97 | 0.09 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3389 | 1/1   | 0.97 | 0.20 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3909 | 1/1   | 0.97 | 0.06 | 29,29,29,29                 | 0     |
| 58  | MG   | 1E    | 309  | 1/1   | 0.97 | 0.08 | 23,23,23,23                 | 0     |
| 58  | MG   | 2D    | 306  | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3172 | 1/1   | 0.97 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 2a    | 3135 | 1/1   | 0.97 | 0.14 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 3182 | 1/1   | 0.97 | 0.16 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3661 | 1/1   | 0.97 | 0.04 | 50,50,50,50                 | 0     |
| 58  | MG   | 2a    | 3138 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3723 | 1/1   | 0.97 | 0.11 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3045 | 1/1   | 0.97 | 0.12 | 30,30,30,30                 | 0     |
| 58  | MG   | 1F    | 301  | 1/1   | 0.97 | 0.15 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 2A    | 3177 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3032 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3725 | 1/1   | 0.97 | 0.05 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3392 | 1/1   | 0.97 | 0.04 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3728 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3824 | 1/1   | 0.97 | 0.05 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3917 | 1/1   | 0.97 | 0.05 | 17,17,17,17                 | 0     |
| 58  | MG   | 1F    | 310  | 1/1   | 0.97 | 0.04 | 47,47,47,47                 | 0     |
| 58  | MG   | 1a    | 1737 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 58  | MG   | 2a    | 3151 | 1/1   | 0.97 | 0.21 | 52,52,52,52                 | 0     |
| 58  | MG   | 1A    | 4028 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 58  | MG   | 2a    | 3153 | 1/1   | 0.97 | 0.07 | 83,83,83,83                 | 0     |
| 58  | MG   | 2A    | 3676 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3584 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3730 | 1/1   | 0.97 | 0.17 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3585 | 1/1   | 0.97 | 0.05 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3586 | 1/1   | 0.97 | 0.16 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 4034 | 1/1   | 0.97 | 0.11 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3924 | 1/1   | 0.97 | 0.05 | 45,45,45,45                 | 0     |
| 58  | MG   | 2A    | 3507 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3654 | 1/1   | 0.97 | 0.07 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3734 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 58  | MG   | 2U    | 201  | 1/1   | 0.97 | 0.17 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3393 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3511 | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3009 | 1/1   | 0.97 | 0.04 | 23,23,23,23                 | 0     |
| 58  | MG   | 1a    | 1618 | 1/1   | 0.97 | 0.10 | 66,66,66,66                 | 0     |
| 58  | MG   | 2A    | 3198 | 1/1   | 0.97 | 0.22 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 4042 | 1/1   | 0.97 | 0.12 | 57,57,57,57                 | 0     |
| 58  | MG   | 1A    | 4044 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 58  | MG   | 1a    | 1621 | 1/1   | 0.97 | 0.25 | 54,54,54,54                 | 0     |
| 58  | MG   | 1O    | 202  | 1/1   | 0.97 | 0.12 | 50,50,50,50                 | 0     |
| 58  | MG   | 2A    | 3697 | 1/1   | 0.97 | 0.11 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3186 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3741 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3013 | 1/1   | 0.97 | 0.17 | 25,25,25,25                 | 0     |
| 58  | MG   | 2a    | 3178 | 1/1   | 0.97 | 0.13 | 48,48,48,48                 | 0     |
| 58  | MG   | 2A    | 3206 | 1/1   | 0.97 | 0.15 | 42,42,42,42                 | 0     |
| 58  | MG   | 2I    | 104  | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 58  | MG   | 2A    | 3523 | 1/1   | 0.97 | 0.17 | 52,52,52,52                 | 0     |
| 58  | MG   | 1P    | 202  | 1/1   | 0.97 | 0.14 | 36,36,36,36                 | 0     |
| 58  | MG   | 25    | 101  | 1/1   | 0.97 | 0.30 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3591 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 58  | MG   | 1P    | 205  | 1/1   | 0.97 | 0.28 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3361 | 1/1   | 0.97 | 0.12 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3240 | 1/1   | 0.97 | 0.18 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3529 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | 28    | 101  | 1/1   | 0.97 | 0.10 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3355 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 58  | MG   | 1a    | 1763 | 1/1   | 0.97 | 0.08 | 62,62,62,62                 | 0     |
| 58  | MG   | 2A    | 3214 | 1/1   | 0.97 | 0.21 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3538 | 1/1   | 0.97 | 0.19 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3841 | 1/1   | 0.97 | 0.04 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3166 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 58  | MG   | 2A    | 3369 | 1/1   | 0.97 | 0.13 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3843 | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 58  | MG   | 1Q    | 203  | 1/1   | 0.97 | 0.18 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3667 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3668 | 1/1   | 0.97 | 0.05 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3545 | 1/1   | 0.97 | 0.09 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4062 | 1/1   | 0.97 | 0.10 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3722 | 1/1   | 0.97 | 0.08 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3243 | 1/1   | 0.97 | 0.18 | 21,21,21,21                 | 0     |
| 58  | MG   | 2A    | 3075 | 1/1   | 0.97 | 0.11 | 49,49,49,49                 | 0     |
| 58  | MG   | 2A    | 3725 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3490 | 1/1   | 0.97 | 0.04 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3727 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3212 | 1/1   | 0.97 | 0.15 | 36,36,36,36                 | 0     |
| 58  | MG   | 1a    | 1775 | 1/1   | 0.97 | 0.09 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3245 | 1/1   | 0.97 | 0.10 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3117 | 1/1   | 0.97 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3280 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 1R    | 206  | 1/1   | 0.97 | 0.13 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3762 | 1/1   | 0.97 | 0.07 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 4070 | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3014 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3855 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3605 | 1/1   | 0.97 | 0.20 | 11,11,11,11                 | 0     |
| 58  | MG   | 1U    | 203  | 1/1   | 0.97 | 0.17 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3049 | 1/1   | 0.97 | 0.10 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3549 | 1/1   | 0.97 | 0.13 | 18,18,18,18                 | 0     |
| 58  | MG   | 2A    | 3564 | 1/1   | 0.97 | 0.20 | 65,65,65,65                 | 0     |
| 58  | MG   | 2A    | 3565 | 1/1   | 0.97 | 0.04 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3746 | 1/1   | 0.97 | 0.05 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3770 | 1/1   | 0.97 | 0.11 | 18,18,18,18                 | 0     |
| 58  | MG   | 1A    | 3285 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3773 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3960 | 1/1   | 0.97 | 0.06 | 60,60,60,60                 | 0     |
| 58  | MG   | 1a    | 1659 | 1/1   | 0.97 | 0.28 | 64,64,64,64                 | 0     |
| 58  | MG   | 1A    | 3499 | 1/1   | 0.97 | 0.29 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 3612 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3216 | 1/1   | 0.97 | 0.16 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3218 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3965 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 59  | K    | 1A    | 3546 | 1/1   | 0.97 | 0.08 | 75,75,75,75                 | 0     |
| 58  | MG   | 1B    | 204  | 1/1   | 0.97 | 0.04 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3121 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3369 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 61  | ZN   | 14    | 102  | 1/1   | 0.97 | 0.07 | 110,110,110,110             | 0     |
| 61  | ZN   | 2Y    | 202  | 1/1   | 0.97 | 0.05 | 100,100,100,100             | 0     |
| 58  | MG   | 2A    | 3407 | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 61  | ZN   | 29    | 501  | 1/1   | 0.97 | 0.05 | 79,79,79,79                 | 0     |
| 61  | ZN   | 2n    | 501  | 1/1   | 0.97 | 0.05 | 84,84,84,84                 | 0     |
| 62  | SF4  | 2d    | 303  | 8/8   | 0.97 | 0.05 | 72,78,84,91                 | 0     |
| 58  | MG   | 2A    | 3766 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3799 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 58  | MG   | 23    | 103  | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 0     |
| 58  | MG   | 1A    | 3678 | 1/1   | 0.98 | 0.05 | 11,11,11,11                 | 0     |
| 58  | MG   | 1A    | 3679 | 1/1   | 0.98 | 0.06 | 20,20,20,20                 | 0     |
| 58  | MG   | 2A    | 3112 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3771 | 1/1   | 0.98 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3281 | 1/1   | 0.98 | 0.09 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3241 | 1/1   | 0.98 | 0.20 | 34,34,34,34                 | 0     |
| 58  | MG   | 2A    | 3532 | 1/1   | 0.98 | 0.08 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3213 | 1/1   | 0.98 | 0.13 | 54,54,54,54                 | 0     |
| 58  | MG   | 1A    | 3283 | 1/1   | 0.98 | 0.21 | 30,30,30,30                 | 0     |
| 58  | MG   | 1P    | 203  | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 58  | MG   | 2A    | 3216 | 1/1   | 0.98 | 0.08 | 33,33,33,33                 | 0     |
| 58  | MG   | 2A    | 3019 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3736 | 1/1   | 0.98 | 0.03 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3023 | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3634 | 1/1   | 0.98 | 0.05 | 26,26,26,26                 | 0     |
| 58  | MG   | 17    | 102  | 1/1   | 0.98 | 0.04 | 28,28,28,28                 | 0     |
| 58  | MG   | 17    | 103  | 1/1   | 0.98 | 0.09 | 23,23,23,23                 | 0     |
| 58  | MG   | 2A    | 3787 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 4011 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3869 | 1/1   | 0.98 | 0.12 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3790 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3484 | 1/1   | 0.98 | 0.12 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3939 | 1/1   | 0.98 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3742 | 1/1   | 0.98 | 0.06 | 29,29,29,29                 | 0     |
| 58  | MG   | 2A    | 3794 | 1/1   | 0.98 | 0.04 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3743 | 1/1   | 0.98 | 0.10 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3796 | 1/1   | 0.98 | 0.10 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3942 | 1/1   | 0.98 | 0.04 | 40,40,40,40                 | 0     |
| 58  | MG   | 2A    | 3437 | 1/1   | 0.98 | 0.05 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 3262 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3068 | 1/1   | 0.98 | 0.10 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3523 | 1/1   | 0.98 | 0.10 | 21,21,21,21                 | 0     |
| 58  | MG   | 1A    | 3012 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 58  | MG   | 1a    | 1781 | 1/1   | 0.98 | 0.08 | 53,53,53,53                 | 0     |
| 58  | MG   | 1B    | 223  | 1/1   | 0.98 | 0.05 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3640 | 1/1   | 0.98 | 0.06 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3289 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3807 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3808 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3751 | 1/1   | 0.98 | 0.04 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3341 | 1/1   | 0.98 | 0.28 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3137 | 1/1   | 0.98 | 0.13 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3172 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 58  | MG   | 1a    | 1789 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 58  | MG   | 1B    | 230  | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3452 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3114 | 1/1   | 0.98 | 0.04 | 22,22,22,22                 | 0     |
| 58  | MG   | 1a    | 1792 | 1/1   | 0.98 | 0.19 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 4030 | 1/1   | 0.98 | 0.04 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3603 | 1/1   | 0.98 | 0.06 | 13,13,13,13                 | 0     |
| 58  | MG   | 1A    | 3095 | 1/1   | 0.98 | 0.14 | 18,18,18,18                 | 0     |
| 58  | MG   | 1A    | 3648 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3575 | 1/1   | 0.98 | 0.08 | 44,44,44,44                 | 0     |
| 58  | MG   | 1A    | 3294 | 1/1   | 0.98 | 0.11 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3460 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 58  | MG   | 2A    | 3053 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 58  | MG   | 1A    | 3269 | 1/1   | 0.98 | 0.04 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3764 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3254 | 1/1   | 0.98 | 0.07 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3464 | 1/1   | 0.98 | 0.17 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3766 | 1/1   | 0.98 | 0.04 | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3831 | 1/1   | 0.98 | 0.10 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3652 | 1/1   | 0.98 | 0.09 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 4043 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3231 | 1/1   | 0.98 | 0.12 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3895 | 1/1   | 0.98 | 0.04 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3610 | 1/1   | 0.98 | 0.07 | 25,25,25,25                 | 0     |
| 58  | MG   | 1D    | 307  | 1/1   | 0.98 | 0.04 | 28,28,28,28                 | 0     |
| 58  | MG   | 1V    | 208  | 1/1   | 0.98 | 0.04 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 3706 | 1/1   | 0.98 | 0.15 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3969 | 1/1   | 0.98 | 0.06 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 4050 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3595 | 1/1   | 0.98 | 0.06 | 37,37,37,37                 | 0     |
| 58  | MG   | 1A    | 3655 | 1/1   | 0.98 | 0.07 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 3772 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 58  | MG   | 1I    | 201  | 1/1   | 0.98 | 0.03 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3025 | 1/1   | 0.98 | 0.04 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3217 | 1/1   | 0.98 | 0.12 | 31,31,31,31                 | 0     |
| 58  | MG   | 1A    | 3501 | 1/1   | 0.98 | 0.08 | 31,31,31,31                 | 0     |
| 58  | MG   | 2A    | 3484 | 1/1   | 0.98 | 0.07 | 65,65,65,65                 | 0     |
| 58  | MG   | 1E    | 304  | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 58  | MG   | 1A    | 3659 | 1/1   | 0.98 | 0.07 | 21,21,21,21                 | 0     |
| 58  | MG   | 2A    | 3276 | 1/1   | 0.98 | 0.13 | 45,45,45,45                 | 0     |
| 58  | MG   | 1A    | 4058 | 1/1   | 0.98 | 0.10 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3078 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3379 | 1/1   | 0.98 | 0.14 | 22,22,22,22                 | 0     |
| 58  | MG   | 1A    | 3977 | 1/1   | 0.98 | 0.04 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3610 | 1/1   | 0.98 | 0.07 | 51,51,51,51                 | 0     |
| 58  | MG   | 1A    | 4061 | 1/1   | 0.98 | 0.05 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3615 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3907 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 58  | MG   | 1A    | 3908 | 1/1   | 0.98 | 0.04 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3844 | 1/1   | 0.98 | 0.18 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3071 | 1/1   | 0.98 | 0.08 | 21,21,21,21                 | 0     |
| 58  | MG   | 2F    | 305  | 1/1   | 0.98 | 0.08 | 46,46,46,46                 | 0     |
| 58  | MG   | 2A    | 3500 | 1/1   | 0.98 | 0.11 | 59,59,59,59                 | 0     |
| 58  | MG   | 2A    | 3618 | 1/1   | 0.98 | 0.14 | 39,39,39,39                 | 0     |
| 58  | MG   | 2A    | 3739 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 58  | MG   | 1F    | 303  | 1/1   | 0.98 | 0.21 | 28,28,28,28                 | 0     |
| 58  | MG   | 2O    | 202  | 1/1   | 0.98 | 0.04 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 3080 | 1/1   | 0.98 | 0.11 | 31,31,31,31                 | 0     |
| 58  | MG   | 1F    | 305  | 1/1   | 0.98 | 0.10 | 41,41,41,41                 | 0     |
| 58  | MG   | 2A    | 3504 | 1/1   | 0.98 | 0.17 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3205 | 1/1   | 0.98 | 0.16 | 23,23,23,23                 | 0     |
| 58  | MG   | 1a    | 1650 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3619 | 1/1   | 0.98 | 0.05 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3626 | 1/1   | 0.98 | 0.14 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3354 | 1/1   | 0.98 | 0.04 | 40,40,40,40                 | 0     |
| 58  | MG   | 1A    | 3065 | 1/1   | 0.98 | 0.10 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3179 | 1/1   | 0.98 | 0.04 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3789 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 58  | MG   | 1a    | 1746 | 1/1   | 0.98 | 0.06 | 53,53,53,53                 | 0     |
| 58  | MG   | 2A    | 3401 | 1/1   | 0.98 | 0.27 | 40,40,40,40                 | 0     |
| 58  | MG   | 2x    | 103  | 1/1   | 0.98 | 0.13 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3414 | 1/1   | 0.98 | 0.12 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3755 | 1/1   | 0.98 | 0.11 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3992 | 1/1   | 0.98 | 0.05 | 13,13,13,13                 | 0     |
| 58  | MG   | 1A    | 3257 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3921 | 1/1   | 0.98 | 0.03 | 22,22,22,22                 | 0     |
| 58  | MG   | 2A    | 3102 | 1/1   | 0.98 | 0.05 | 38,38,38,38                 | 0     |
| 61  | ZN   | 1Y    | 203  | 1/1   | 0.98 | 0.04 | 61,61,61,61                 | 0     |
| 58  | MG   | 1A    | 3726 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3239 | 1/1   | 0.98 | 0.07 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3512 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 61  | ZN   | 26    | 501  | 1/1   | 0.98 | 0.07 | 66,66,66,66                 | 0     |
| 58  | MG   | 1A    | 3925 | 1/1   | 0.98 | 0.07 | 53,53,53,53                 | 0     |
| 58  | MG   | 1A    | 3029 | 1/1   | 0.98 | 0.07 | 26,26,26,26                 | 0     |
| 62  | SF4  | 1d    | 302  | 8/8   | 0.98 | 0.05 | 58,60,65,70                 | 0     |
| 58  | MG   | 1A    | 3448 | 1/1   | 0.98 | 0.21 | 53,53,53,53                 | 0     |
| 58  | MG   | 1a    | 1699 | 1/1   | 0.99 | 0.05 | 46,46,46,46                 | 0     |
| 58  | MG   | 1A    | 3287 | 1/1   | 0.99 | 0.07 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 3183 | 1/1   | 0.99 | 0.12 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3737 | 1/1   | 0.99 | 0.07 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3123 | 1/1   | 0.99 | 0.15 | 28,28,28,28                 | 0     |
| 58  | MG   | 2A    | 3772 | 1/1   | 0.99 | 0.06 | 32,32,32,32                 | 0     |
| 58  | MG   | 2A    | 3531 | 1/1   | 0.99 | 0.11 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3739 | 1/1   | 0.99 | 0.04 | 37,37,37,37                 | 0     |
| 58  | MG   | 2A    | 3533 | 1/1   | 0.99 | 0.16 | 36,36,36,36                 | 0     |
| 58  | MG   | 1A    | 3119 | 1/1   | 0.99 | 0.15 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3670 | 1/1   | 0.99 | 0.06 | 18,18,18,18                 | 0     |
| 58  | MG   | 1A    | 3692 | 1/1   | 0.99 | 0.04 | 25,25,25,25                 | 0     |
| 58  | MG   | 2A    | 3779 | 1/1   | 0.99 | 0.06 | 25,25,25,25                 | 0     |
| 58  | MG   | 1T    | 201  | 1/1   | 0.99 | 0.05 | 30,30,30,30                 | 0     |
| 58  | MG   | 2A    | 3538 | 1/1   | 0.99 | 0.08 | 30,30,30,30                 | 0     |
| 58  | MG   | 1F    | 307  | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 58  | MG   | 1A    | 3983 | 1/1   | 0.99 | 0.05 | 24,24,24,24                 | 0     |
| 58  | MG   | 2A    | 3379 | 1/1   | 0.99 | 0.06 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3583 | 1/1   | 0.99 | 0.07 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3774 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 58  | MG   | 1A    | 3672 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 58  | MG   | 1A    | 3719 | 1/1   | 0.99 | 0.04 | 17,17,17,17                 | 0     |
| 58  | MG   | 1A    | 3101 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 58  | MG   | 1I    | 202  | 1/1   | 0.99 | 0.06 | 39,39,39,39                 | 0     |
| 58  | MG   | 1A    | 3951 | 1/1   | 0.99 | 0.10 | 16,16,16,16                 | 0     |
| 58  | MG   | 13    | 101  | 1/1   | 0.99 | 0.05 | 32,32,32,32                 | 0     |
| 58  | MG   | 1A    | 3126 | 1/1   | 0.99 | 0.03 | 25,25,25,25                 | 0     |
| 58  | MG   | 2A    | 3494 | 1/1   | 0.99 | 0.07 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3779 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3814 | 1/1   | 0.99 | 0.06 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 3601 | 1/1   | 0.99 | 0.10 | 33,33,33,33                 | 0     |
| 58  | MG   | 15    | 101  | 1/1   | 0.99 | 0.08 | 35,35,35,35                 | 0     |
| 58  | MG   | 2A    | 3499 | 1/1   | 0.99 | 0.07 | 42,42,42,42                 | 0     |
| 58  | MG   | 1A    | 3363 | 1/1   | 0.99 | 0.04 | 36,36,36,36                 | 0     |
| 58  | MG   | 2A    | 3737 | 1/1   | 0.99 | 0.04 | 43,43,43,43                 | 0     |
| 58  | MG   | 1A    | 3920 | 1/1   | 0.99 | 0.04 | 22,22,22,22                 | 0     |
| 58  | MG   | 1A    | 4036 | 1/1   | 0.99 | 0.05 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3620 | 1/1   | 0.99 | 0.07 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3074 | 1/1   | 0.99 | 0.02 | 11,11,11,11                 | 0     |
| 58  | MG   | 1A    | 3146 | 1/1   | 0.99 | 0.04 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 4040 | 1/1   | 0.99 | 0.04 | 25,25,25,25                 | 0     |
| 58  | MG   | 2A    | 3682 | 1/1   | 0.99 | 0.05 | 33,33,33,33                 | 0     |
| 58  | MG   | 1a    | 1780 | 1/1   | 0.99 | 0.04 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3092 | 1/1   | 0.99 | 0.05 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3606 | 1/1   | 0.99 | 0.07 | 25,25,25,25                 | 0     |
| 58  | MG   | 1A    | 3296 | 1/1   | 0.99 | 0.09 | 23,23,23,23                 | 0     |
| 58  | MG   | 1A    | 3445 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 58  | MG   | 1A    | 3663 | 1/1   | 0.99 | 0.04 | 19,19,19,19                 | 0     |
| 58  | MG   | 1W    | 206  | 1/1   | 0.99 | 0.06 | 17,17,17,17                 | 0     |
| 58  | MG   | 2A    | 3690 | 1/1   | 0.99 | 0.06 | 41,41,41,41                 | 0     |
| 58  | MG   | 1A    | 3791 | 1/1   | 0.99 | 0.07 | 19,19,19,19                 | 0     |
| 58  | MG   | 2A    | 3572 | 1/1   | 0.99 | 0.07 | 35,35,35,35                 | 0     |
| 58  | MG   | 1A    | 4047 | 1/1   | 0.99 | 0.05 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 3759 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 58  | MG   | 1A    | 3793 | 1/1   | 0.99 | 0.04 | 19,19,19,19                 | 0     |
| 58  | MG   | 1A    | 3520 | 1/1   | 0.99 | 0.14 | 37,37,37,37                 | 0     |
| 58  | MG   | 2X    | 102  | 1/1   | 0.99 | 0.04 | 63,63,63,63                 | 0     |
| 58  | MG   | 1A    | 3761 | 1/1   | 0.99 | 0.07 | 13,13,13,13                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 61  | ZN   | 19    | 102  | 1/1   | 0.99 | 0.05 | 43,43,43,43                 | 0     |
| 61  | ZN   | 1n    | 103  | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |
| 58  | MG   | 1A    | 3494 | 1/1   | 0.99 | 0.11 | 30,30,30,30                 | 0     |
| 58  | MG   | 1A    | 4053 | 1/1   | 0.99 | 0.03 | 27,27,27,27                 | 0     |
| 61  | ZN   | 25    | 104  | 1/1   | 0.99 | 0.04 | 70,70,70,70                 | 0     |
| 58  | MG   | 1A    | 3763 | 1/1   | 0.99 | 0.04 | 58,58,58,58                 | 0     |
| 58  | MG   | 1A    | 4012 | 1/1   | 0.99 | 0.03 | 16,16,16,16                 | 0     |
| 58  | MG   | 2A    | 3640 | 1/1   | 0.99 | 0.05 | 59,59,59,59                 | 0     |
| 58  | MG   | 1A    | 3900 | 1/1   | 0.99 | 0.03 | 24,24,24,24                 | 0     |
| 58  | MG   | 1A    | 3709 | 1/1   | 0.99 | 0.07 | 22,22,22,22                 | 0     |
| 58  | MG   | 1A    | 3993 | 1/1   | 1.00 | 0.03 | 27,27,27,27                 | 0     |
| 58  | MG   | 1A    | 3748 | 1/1   | 1.00 | 0.09 | 34,34,34,34                 | 0     |
| 58  | MG   | 1A    | 3718 | 1/1   | 1.00 | 0.01 | 20,20,20,20                 | 0     |
| 58  | MG   | 1A    | 3782 | 1/1   | 1.00 | 0.06 | 15,15,15,15                 | 0     |
| 61  | ZN   | 15    | 109  | 1/1   | 1.00 | 0.01 | 42,42,42,42                 | 0     |
| 61  | ZN   | 16    | 103  | 1/1   | 1.00 | 0.04 | 38,38,38,38                 | 0     |
| 58  | MG   | 2A    | 3675 | 1/1   | 1.00 | 0.06 | 19,19,19,19                 | 0     |
| 58  | MG   | 1a    | 1734 | 1/1   | 1.00 | 0.09 | 24,24,24,24                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.