



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2025 – 09:00 PM EDT

PDB ID : 5W4K  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with Klebsazolicin and bound to mRNA and A-, P- and E-site tRNAs at 2.7Å resolution  
Authors : Metelev, M.; Osterman, I.A.; Ghilarov, D.; Khabibullina, N.F.; Yakimov, A.; Shabalin, K.; Utkina, I.; Travin, D.Y.; Komarova, E.S.; Serebryakova, M.; Artamonova, T.; Khodorkovskii, M.; Konevega, A.L.; Sergiev, P.V.; Severinov, K.; Polikanov, Y.S.  
Deposited on : 2017-06-12  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                           |   |  |
|---------------------------|---|--|
| MolProbity                | : | 4.02b-467  |
| Mogul                     | : | 2022.3.0, CSD as543be (2022)                                       |
| Xtriage (Phenix)          | : | 1.21   |
| EDS                       | : | 3.0  |
| Percentile statistics     | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4                      | : | 9.0.004 (Gargrove)   |
| Density-Fitness           | : | 1.0.11   |
| Ideal geometry (proteins) | : | Engh & Huber (2001)  |

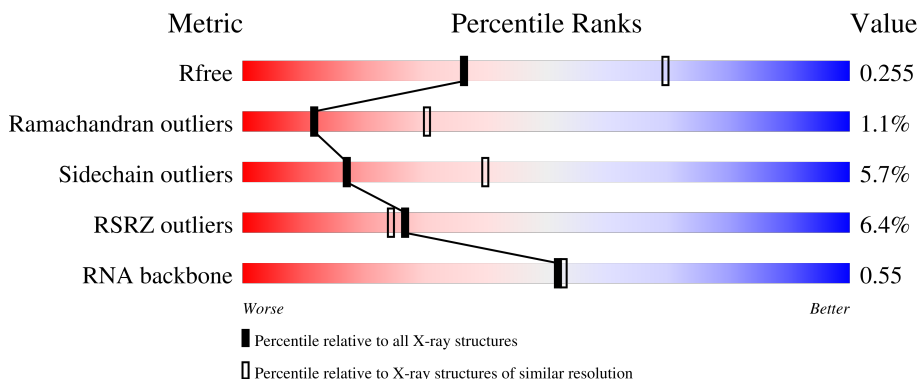
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


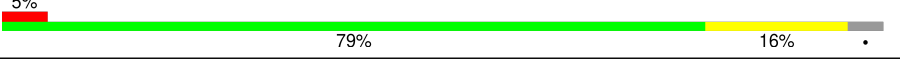

The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 164625                      | 3333 (2.70-2.70)                                      |
| Ramachandran outliers | 177936                      | 3633 (2.70-2.70)                                      |
| Sidechain outliers    | 177891                      | 3633 (2.70-2.70)                                      |
| RSRZ outliers         | 164620                      | 3333 (2.70-2.70)                                      |
| RNA backbone          | 3690                        | 1028 (2.94-2.46)                                      |

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   |  |
| 1   | 2A    | 2915   |  |
| 2   | 1B    | 121    |  |

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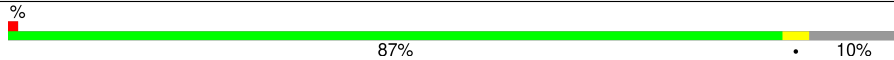
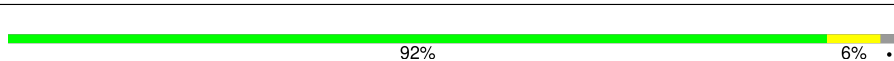
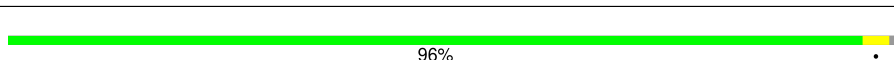
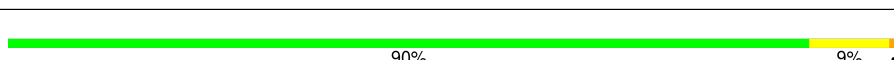
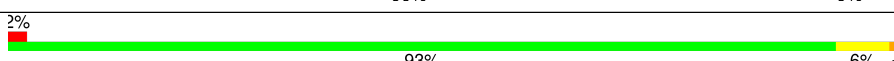
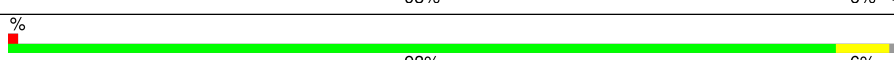
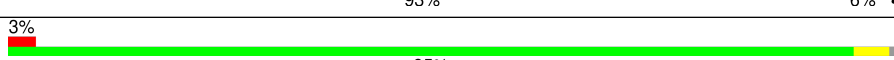
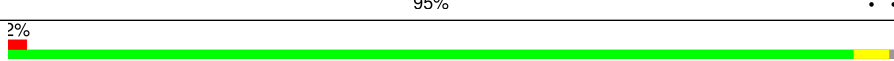
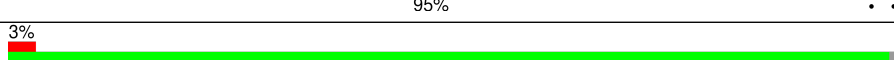
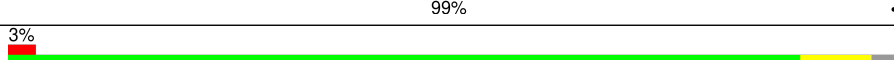
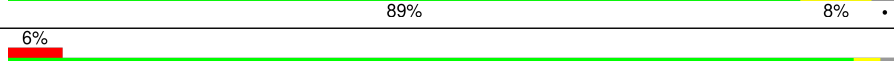
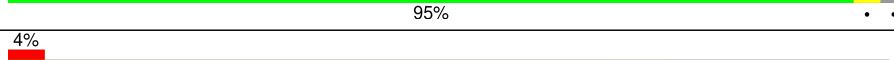


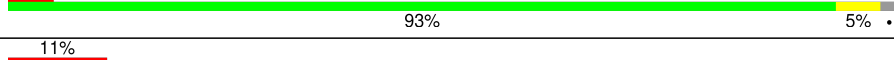
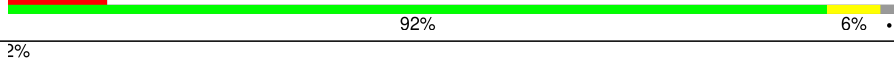
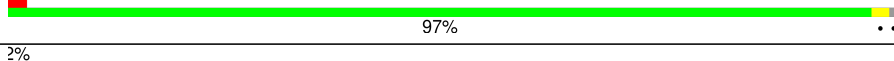
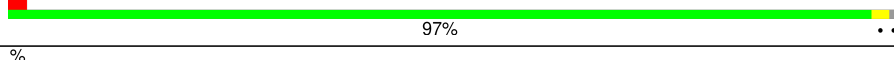
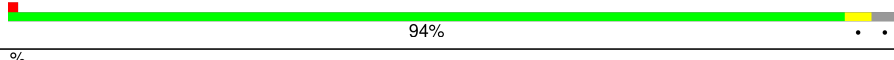
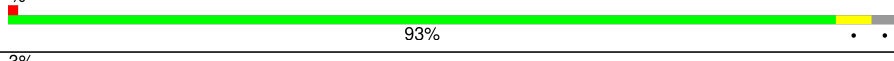
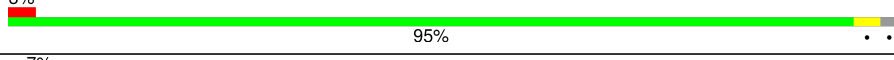
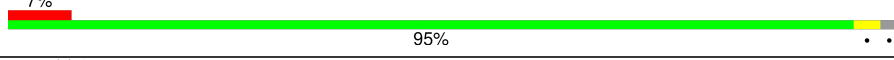

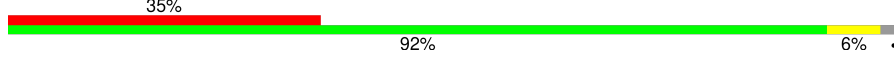
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

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





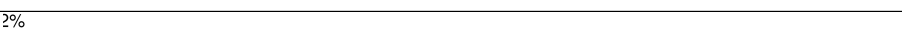


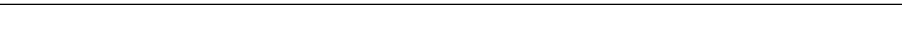
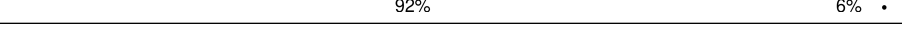
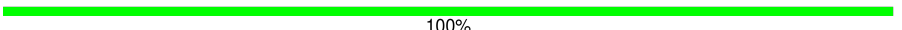

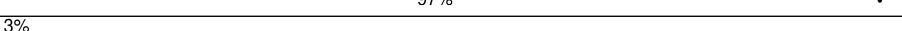


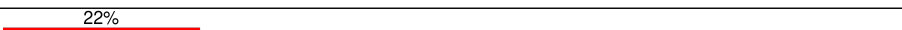




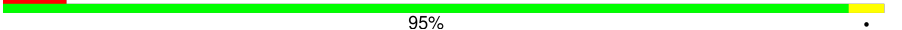





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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | 1T    | 146    |    |
| 15  | 2T    | 146    |    |
| 16  | 1U    | 118    |    |
| 16  | 2U    | 118    |    |
| 17  | 1V    | 101    |    |
| 17  | 2V    | 101    |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

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 27  | 25    | 60     |  92% 7% .       |
| 28  | 16    | 54     |  87% 11% .      |
| 28  | 26    | 54     |  93% 6% .       |
| 29  | 17    | 49     |  2% 88% 10% .   |
| 29  | 27    | 49     |  2% 90% 8% .    |
| 30  | 18    | 65     |  88% 11% .      |
| 30  | 28    | 65     |  92% 6% .       |
| 31  | 19    | 37     |  100%           |
| 31  | 29    | 37     |  8% 97% .       |
| 32  | 1a    | 1521   |  3% 82% 16% ..  |
| 33  | 1b    | 256    |  14% 84% 6% 10% |
| 33  | 2b    | 256    |  22% 83% 7% 10% |
| 34  | 1c    | 239    |  2% 83% . 14%   |
| 34  | 2c    | 239    |  28% 85% . 14%  |
| 35  | 1d    | 209    |  7% 95% .       |
| 35  | 2d    | 209    |  9% 93% 6%     |
| 36  | 1e    | 162    |  % 86% 5% 9%  |
| 36  | 2e    | 162    |  17% 87% . 9% |
| 37  | 1f    | 101    |  96% . .      |
| 37  | 2f    | 101    |  % 96% . .    |
| 38  | 1g    | 156    |  6% 94% 6% .  |
| 38  | 2g    | 156    |  10% 94% 5% . |
| 39  | 1h    | 138    |  2% 96% . .   |
| 39  | 2h    | 138    |  6% 96% . .   |
| 40  | 1i    | 128    |  6% 95% . .   |

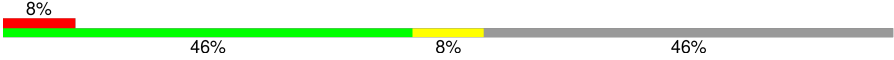
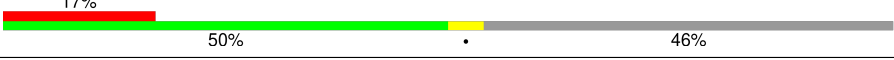


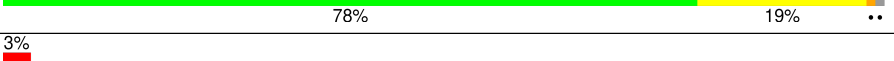
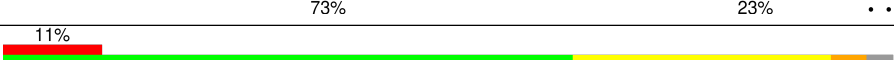
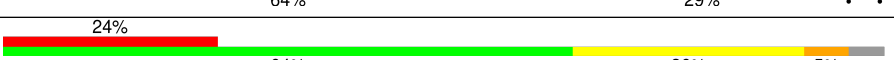
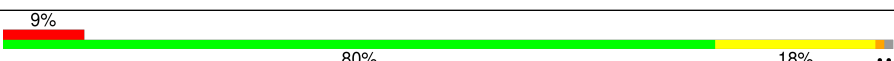
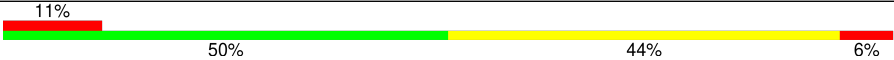

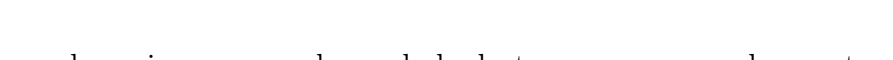
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | 2i    | 128    |                  |
| 41  | 1j    | 105    |                  |
| 41  | 2j    | 105    |                  |
| 42  | 1k    | 129    |   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

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 53  | 1v    | 24     |   |
| 53  | 2v    | 24     |   |
| 54  | 1w    | 76     |   |
| 54  | 2w    | 76     |   |
| 55  | 1x    | 77     |   |
| 55  | 2x    | 77     |   |
| 56  | 1y    | 76     |   |
| 56  | 2y    | 76     |   |
| 57  | 2a    | 1521   |   |
| 58  | A     | 18     |   |
| 58  | B     | 18     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | 1A    | 3515 | -         | -        | -       | X                |
| 59  | MG   | 1a    | 3435 | -         | -        | -       | X                |
| 59  | MG   | 1y    | 104  | -         | -        | -       | X                |
| 59  | MG   | 2a    | 3118 | -         | -        | -       | X                |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 302030 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 |         |         |       |

- 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 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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 |         |         |       |
| 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 mRNA.

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

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

- Molecule 54 is a RNA chain called tRNA, A-site and E-site tRNAs.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 54  | 1w    | 74       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1592  | 713 | 285 | 518 | 74 | 2       |         |       |
| 54  | 2w    | 72       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1544  | 690 | 278 | 502 | 72 | 2       |         |       |

- Molecule 55 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 55  | 1x    | 76       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1       |         |       |
| 55  | 2x    | 76       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1       |         |       |

- Molecule 56 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56  | 1y    | 74       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1585  | 707 | 285 | 518 | 74 | 1       |         |       |
| 56  | 2y    | 73       | Total | C   | N   | O   | P  | S       | 0       | 0     |
|     |       |          | 1565  | 698 | 283 | 510 | 73 | 1       |         |       |

- Molecule 57 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 57  | 2a    | 1503     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32327 | 14396 | 5990 | 10438 | 1503 |         |         |       |

- Molecule 58 is a protein called Klebsazolicin.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 58  | A     | 18       | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 115   | 64 | 23 | 25 | 3 |         |         |       |
| 58  | B     | 18       | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 115   | 64 | 23 | 25 | 3 |         |         |       |

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms         |            | ZeroOcc | AltConf |
|-----|-------|----------|---------------|------------|---------|---------|
| 59  | 1A    | 1229     | Total<br>1229 | Mg<br>1229 | 0       | 0       |
| 59  | 1B    | 38       | Total<br>38   | Mg<br>38   | 0       | 0       |
| 59  | 1D    | 13       | Total<br>13   | Mg<br>13   | 0       | 0       |
| 59  | 1E    | 14       | Total<br>14   | Mg<br>14   | 0       | 0       |
| 59  | 1F    | 10       | Total<br>10   | Mg<br>10   | 0       | 0       |
| 59  | 1G    | 5        | Total<br>5    | Mg<br>5    | 0       | 0       |
| 59  | 1I    | 1        | Total<br>1    | Mg<br>1    | 0       | 0       |
| 59  | 1N    | 9        | Total<br>9    | Mg<br>9    | 0       | 0       |
| 59  | 1O    | 6        | Total<br>6    | Mg<br>6    | 0       | 0       |
| 59  | 1P    | 4        | Total<br>4    | Mg<br>4    | 0       | 0       |
| 59  | 1Q    | 6        | Total<br>6    | Mg<br>6    | 0       | 0       |
| 59  | 1R    | 3        | Total<br>3    | Mg<br>3    | 0       | 0       |
| 59  | 1S    | 3        | Total<br>3    | Mg<br>3    | 0       | 0       |
| 59  | 1T    | 2        | Total<br>2    | Mg<br>2    | 0       | 0       |
| 59  | 1U    | 5        | Total<br>5    | Mg<br>5    | 0       | 0       |
| 59  | 1V    | 2        | Total<br>2    | Mg<br>2    | 0       | 0       |
| 59  | 1W    | 5        | Total<br>5    | Mg<br>5    | 0       | 0       |
| 59  | 1X    | 5        | Total<br>5    | Mg<br>5    | 0       | 0       |
| 59  | 1Y    | 3        | Total<br>3    | Mg<br>3    | 0       | 0       |
| 59  | 1Z    | 4        | Total<br>4    | Mg<br>4    | 0       | 0       |
| 59  | 10    | 8        | Total<br>8    | Mg<br>8    | 0       | 0       |
| 59  | 11    | 3        | Total<br>3    | Mg<br>3    | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 59  | 12    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 13    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 15    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 16    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 17    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 18    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 19    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1a    | 278      | Total<br>278 | Mg<br>278 | 0       | 0       |
| 59  | 1b    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 1d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1f    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 1k    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1l    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 1n    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 1p    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1s    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1v    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 1w    | 12       | Total<br>12  | Mg<br>12  | 0       | 0       |
| 59  | 1x    | 17       | Total<br>17  | Mg<br>17  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 59  | 1y    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 59  | 2A    | 848      | Total<br>848 | Mg<br>848 | 0       | 0       |
| 59  | 2B    | 22       | Total<br>22  | Mg<br>22  | 0       | 0       |
| 59  | 2D    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 59  | 2E    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 59  | 2F    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 59  | 2G    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2N    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2O    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 2P    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2Q    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 59  | 2R    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 2S    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2T    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 2U    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 59  | 2V    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2X    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 2Z    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 20    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | 23    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 25    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |

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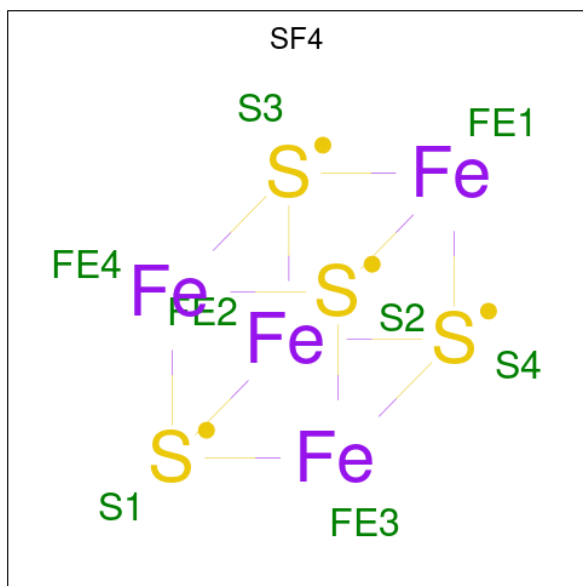
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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 59  | 27    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 28    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 2a    | 239      | Total<br>239 | Mg<br>239 | 0       | 0       |
| 59  | 2d    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 2g    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2j    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 2k    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | 2p    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2q    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 59  | 2r    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | 2v    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 59  | 2w    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 59  | 2x    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 59  | 2y    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 59  | A     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | B     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 60  | 1Y    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 14    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 15    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 16    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 19    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 1n    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 2Y    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 24    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 25    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 26    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 29    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 60  | 2n    | 1        | Total Zn<br>1 1 | 0       | 0       |

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 61  | 1d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 61  | 2d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 62  | 2A    | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 63 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 63  | 1A    | 2636     | Total | O    | 0       | 0       |
|     |       |          | 2636  | 2636 |         |         |
| 63  | 1B    | 71       | Total | O    | 0       | 0       |
|     |       |          | 71    | 71   |         |         |
| 63  | 1D    | 31       | Total | O    | 0       | 0       |
|     |       |          | 31    | 31   |         |         |
| 63  | 1E    | 35       | Total | O    | 0       | 0       |
|     |       |          | 35    | 35   |         |         |
| 63  | 1F    | 18       | Total | O    | 0       | 0       |
|     |       |          | 18    | 18   |         |         |
| 63  | 1G    | 6        | Total | O    | 0       | 0       |
|     |       |          | 6     | 6    |         |         |
| 63  | 1H    | 3        | Total | O    | 0       | 0       |
|     |       |          | 3     | 3    |         |         |
| 63  | 1I    | 2        | Total | O    | 0       | 0       |
|     |       |          | 2     | 2    |         |         |
| 63  | 1N    | 10       | Total | O    | 0       | 0       |
|     |       |          | 10    | 10   |         |         |
| 63  | 1O    | 8        | Total | O    | 0       | 0       |
|     |       |          | 8     | 8    |         |         |
| 63  | 1P    | 23       | Total | O    | 0       | 0       |
|     |       |          | 23    | 23   |         |         |
| 63  | 1Q    | 16       | Total | O    | 0       | 0       |
|     |       |          | 16    | 16   |         |         |
| 63  | 1R    | 14       | Total | O    | 0       | 0       |
|     |       |          | 14    | 14   |         |         |
| 63  | 1S    | 4        | Total | O    | 0       | 0       |
|     |       |          | 4     | 4    |         |         |
| 63  | 1T    | 9        | Total | O    | 0       | 0       |
|     |       |          | 9     | 9    |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 63  | 1U    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 63  | 1V    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 63  | 1W    | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 63  | 1X    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 63  | 1Y    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 63  | 1Z    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 10    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 63  | 11    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 63  | 12    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 63  | 13    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 14    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 15    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 16    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 17    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 63  | 18    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 63  | 19    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 1a    | 523      | Total<br>523 | O<br>523 | 0       | 0       |
| 63  | 1b    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 1d    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 63  | 1e    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 63  | 1g    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 63  | 1k    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 63  | 1l    | 10       | Total<br>10   | O<br>10   | 0       | 0       |
| 63  | 1m    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 63  | 1o    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 63  | 1p    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 63  | 1q    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 63  | 1r    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 63  | 1t    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 63  | 1v    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 63  | 1w    | 26       | Total<br>26   | O<br>26   | 0       | 0       |
| 63  | 1x    | 18       | Total<br>18   | O<br>18   | 0       | 0       |
| 63  | 1y    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 63  | 2A    | 1602     | Total<br>1602 | O<br>1602 | 0       | 0       |
| 63  | 2B    | 28       | Total<br>28   | O<br>28   | 0       | 0       |
| 63  | 2D    | 29       | Total<br>29   | O<br>29   | 0       | 0       |
| 63  | 2E    | 15       | Total<br>15   | O<br>15   | 0       | 0       |
| 63  | 2F    | 20       | Total<br>20   | O<br>20   | 0       | 0       |
| 63  | 2I    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 63  | 2N    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 63  | 2P    | 15       | Total<br>15   | O<br>15   | 0       | 0       |
| 63  | 2Q    | 2        | Total<br>2    | O<br>2    | 0       | 0       |

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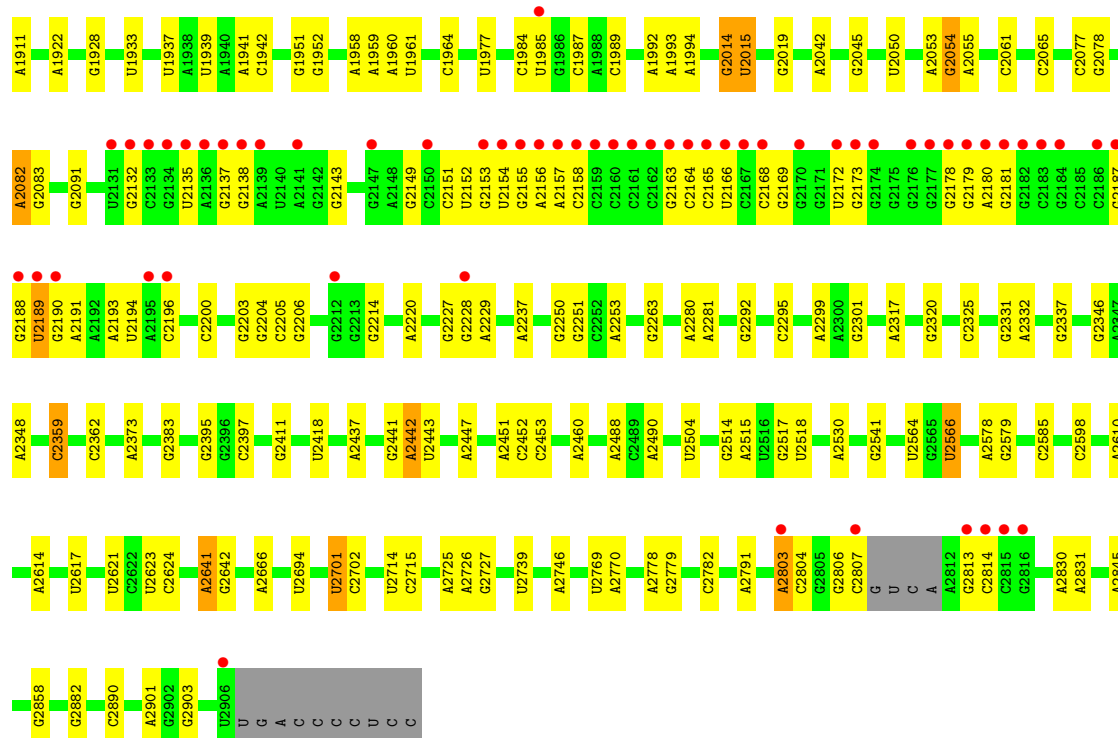
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 63  | 2R    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 2T    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 63  | 2U    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 63  | 2V    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 63  | 2W    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 63  | 2X    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 63  | 2Y    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2Z    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 20    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 63  | 21    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 63  | 22    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 23    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 63  | 25    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 63  | 27    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 63  | 28    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 63  | 29    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2a    | 389      | Total<br>389 | O<br>389 | 0       | 0       |
| 63  | 2d    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 63  | 2e    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 63  | 2f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 63  | 2g    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

*Continued on next page...*

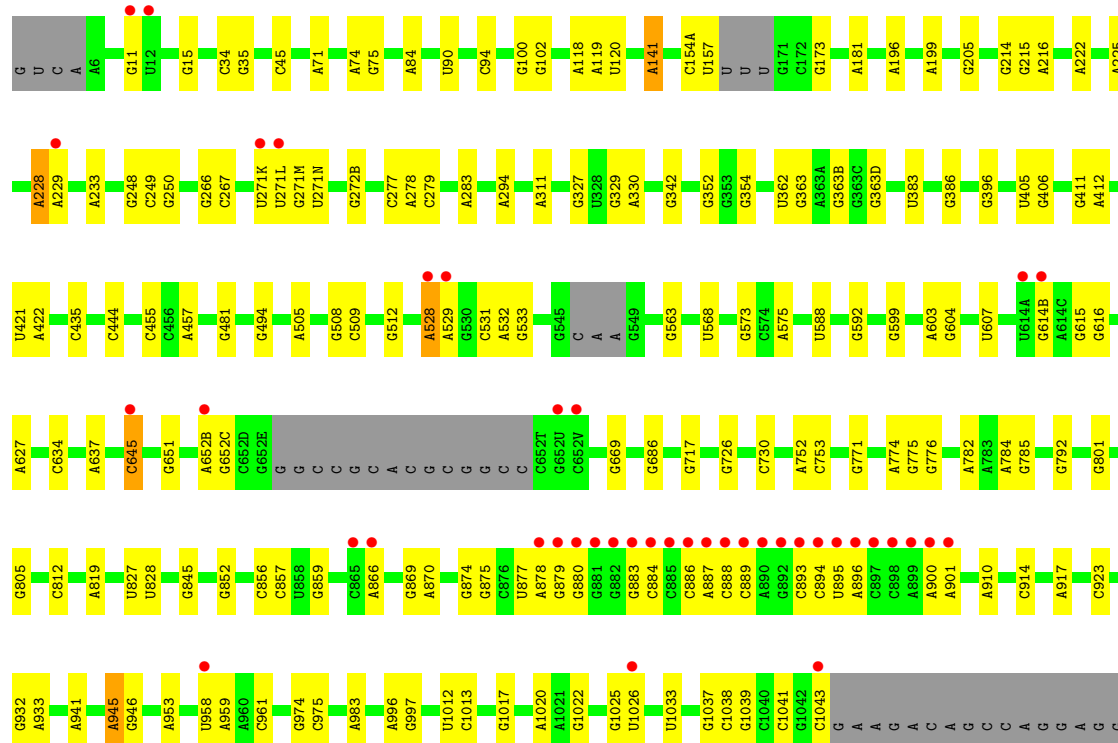
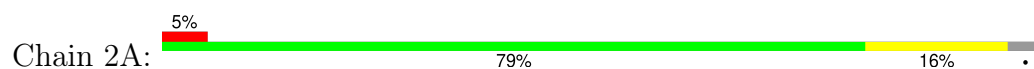
*Continued from previous page...*

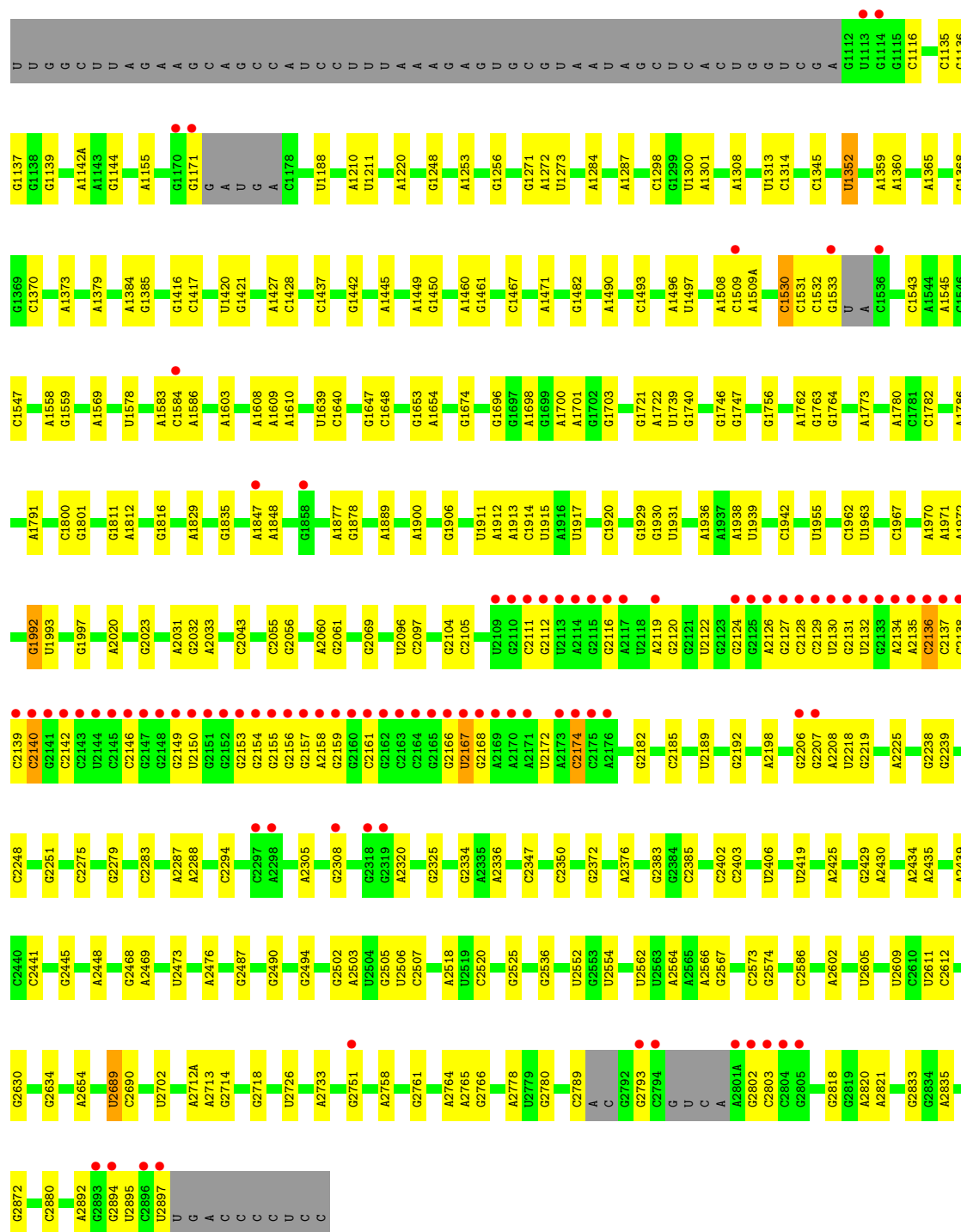
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 63  | 2h    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 63  | 2i    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 2j    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | 2l    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 63  | 2o    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 2p    | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 63  | 2q    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 63  | 2r    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 2t    | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 63  | 2u    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 2v    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 63  | 2w    | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 63  | 2x    | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 63  | 2y    | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 63  | A     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 63  | B     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

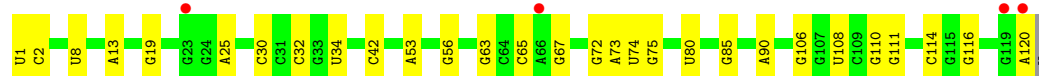
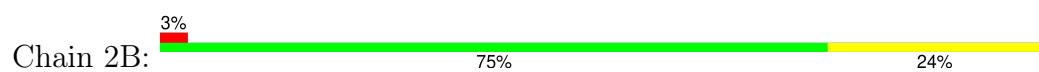




• Molecule 1: 23S Ribosomal RNA



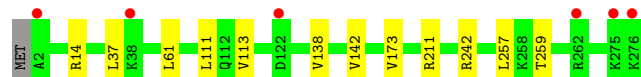




- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



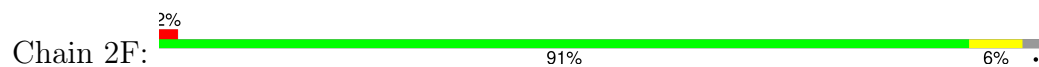
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

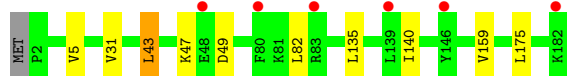


- Molecule 5: 50S ribosomal protein L4

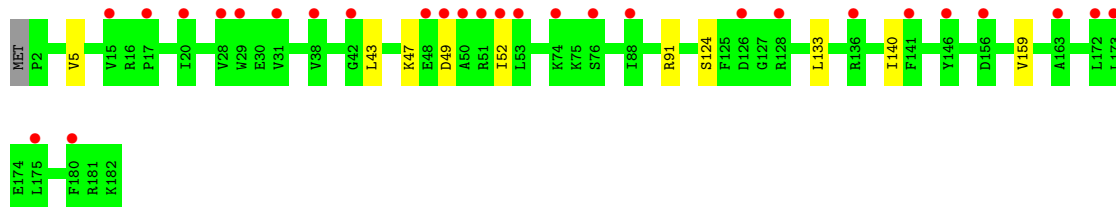


- Molecule 6: 50S ribosomal protein L5





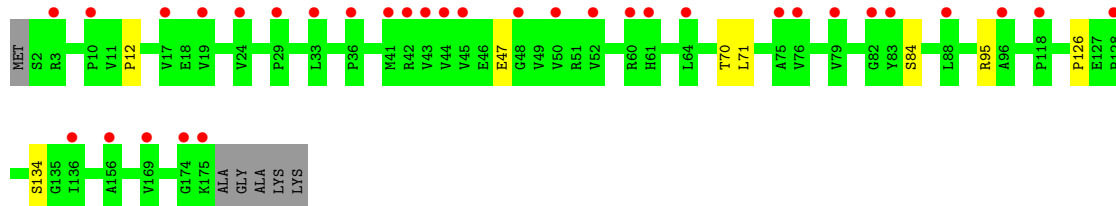
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



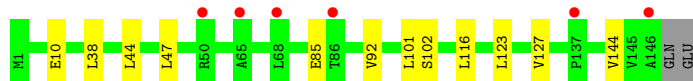
- Molecule 7: 50S ribosomal protein L6



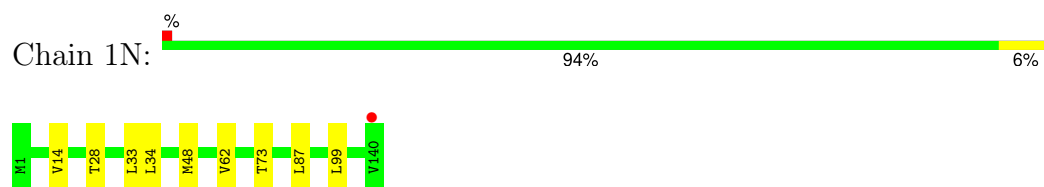
- Molecule 8: 50S ribosomal protein L9



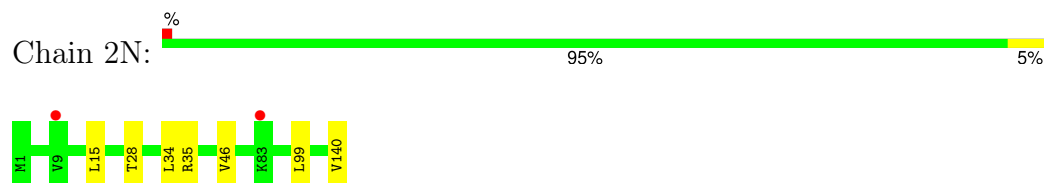
- Molecule 8: 50S ribosomal protein L9



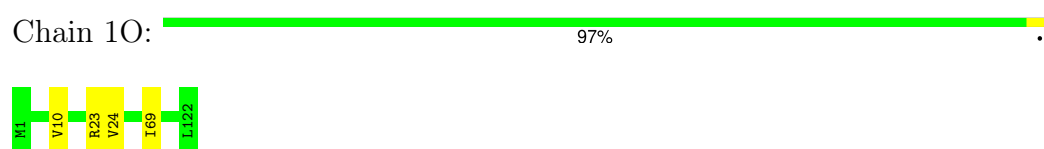
## • Molecule 9: 50S ribosomal protein L13



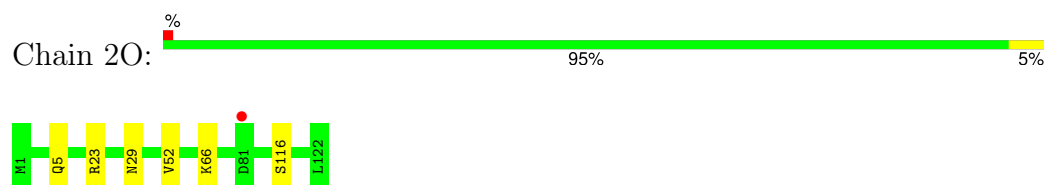
## • Molecule 9: 50S ribosomal protein L13



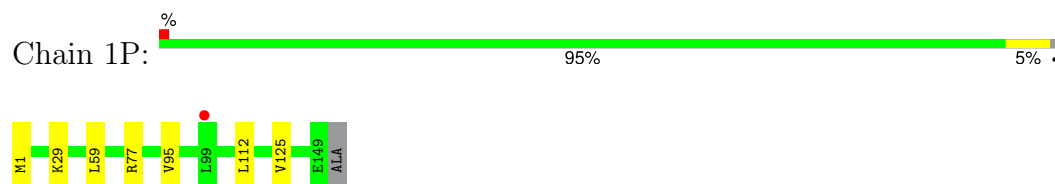
## • Molecule 10: 50S ribosomal protein L14



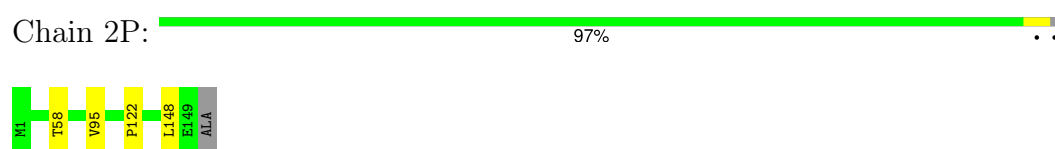
## • Molecule 10: 50S ribosomal protein L14



## • Molecule 11: 50S ribosomal protein L15

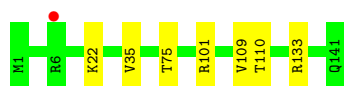


## • Molecule 11: 50S ribosomal protein L15



## • Molecule 12: 50S ribosomal protein L16





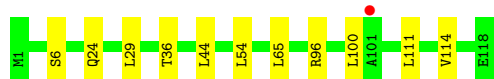
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



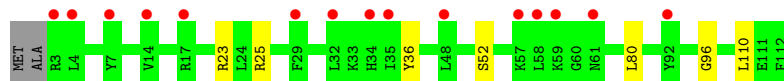
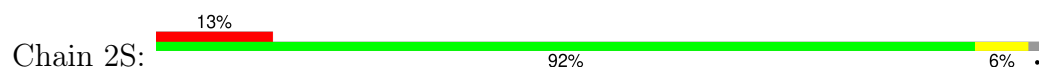
- Molecule 13: 50S ribosomal protein L17



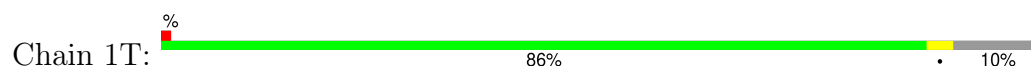
- Molecule 14: 50S ribosomal protein L18



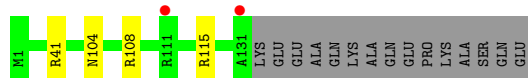
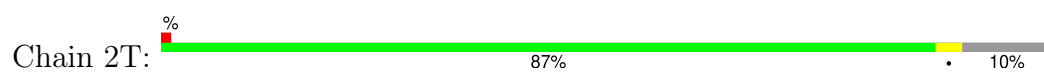
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



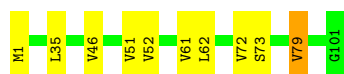
- Molecule 16: 50S ribosomal protein L20



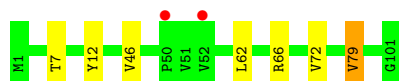
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



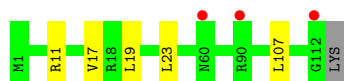
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



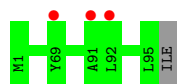
- Molecule 18: 50S ribosomal protein L22



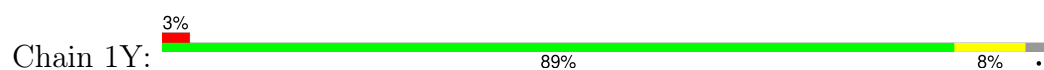
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



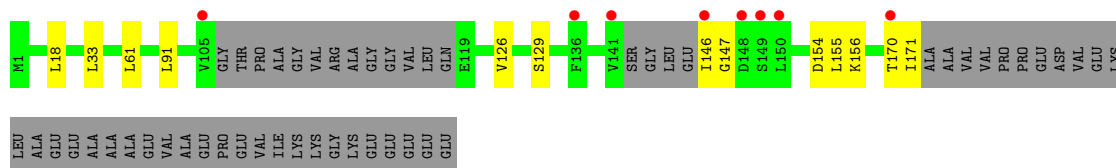
- Molecule 20: 50S ribosomal protein L24



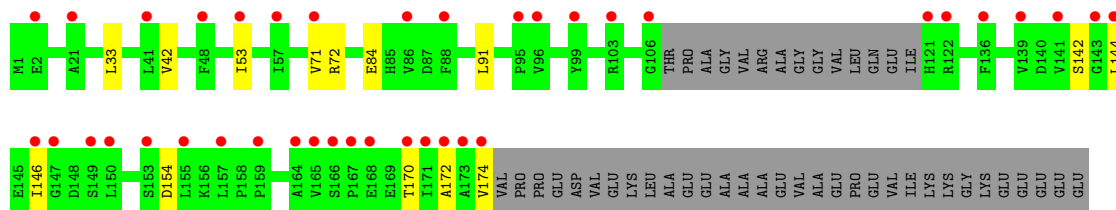
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



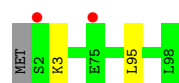
- Molecule 22: 50S ribosomal protein L27



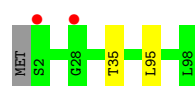
- Molecule 22: 50S ribosomal protein L27



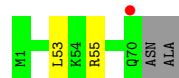
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



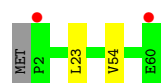
- Molecule 24: 50S ribosomal protein L29



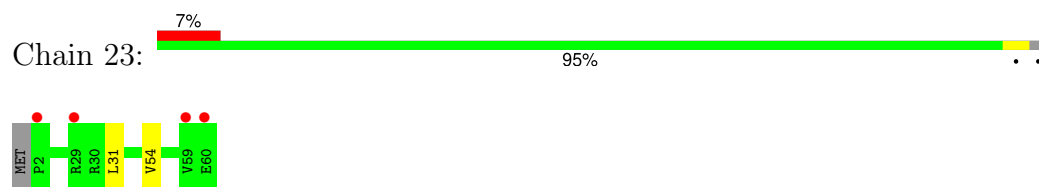
- Molecule 24: 50S ribosomal protein L29



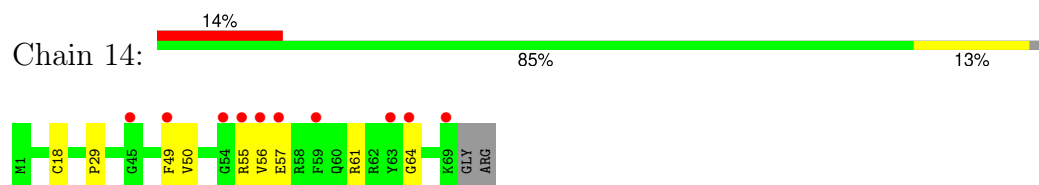
- Molecule 25: 50S ribosomal protein L30



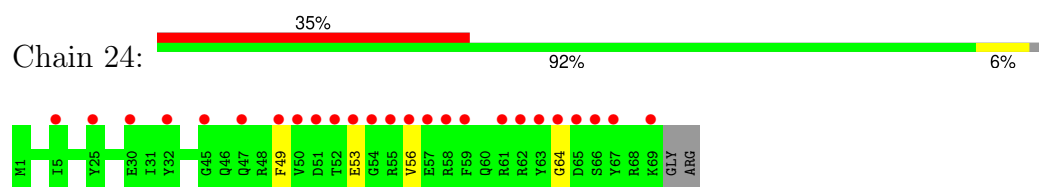
- Molecule 25: 50S ribosomal protein L30



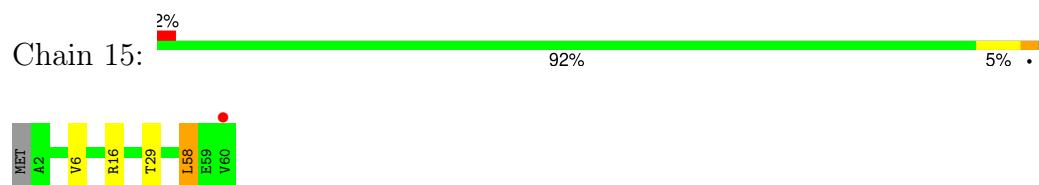
- Molecule 26: 50S ribosomal protein L31



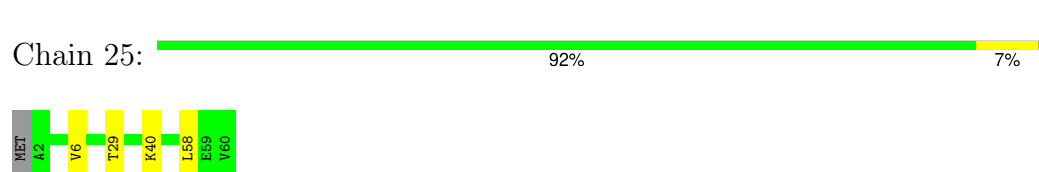
- Molecule 26: 50S ribosomal protein L31



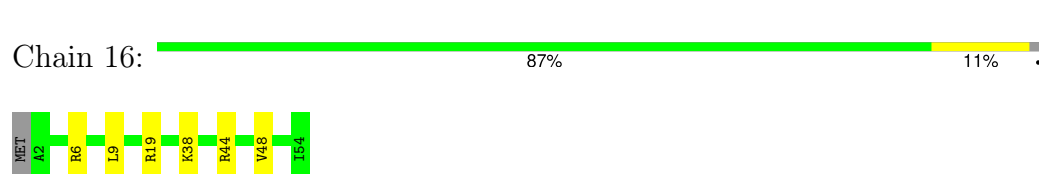
- Molecule 27: 50S ribosomal protein L32



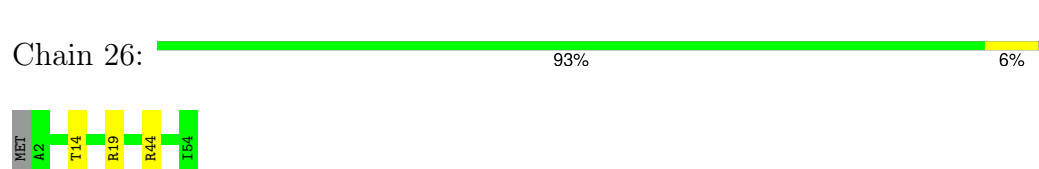
- Molecule 27: 50S ribosomal protein L32



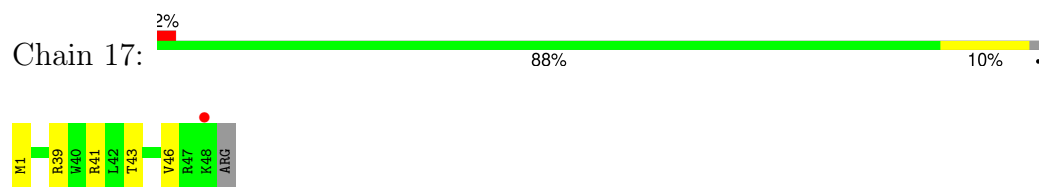
- Molecule 28: 50S ribosomal protein L33



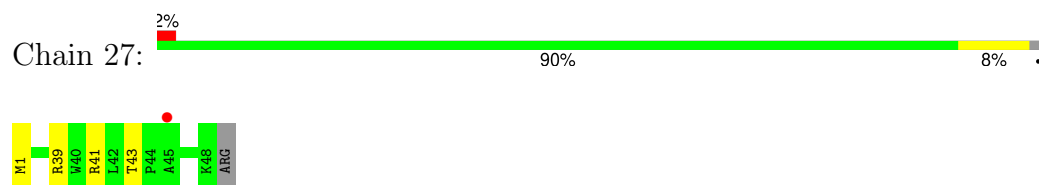
- Molecule 28: 50S ribosomal protein L33



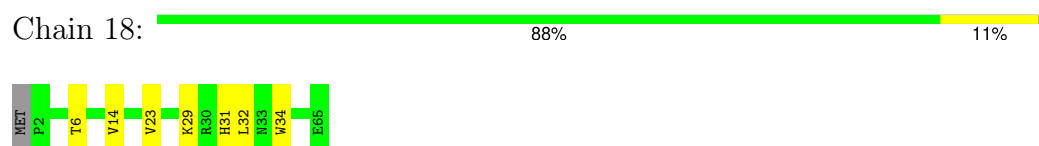
- Molecule 29: 50S ribosomal protein L34



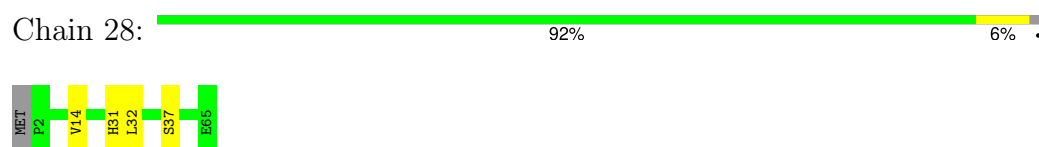
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

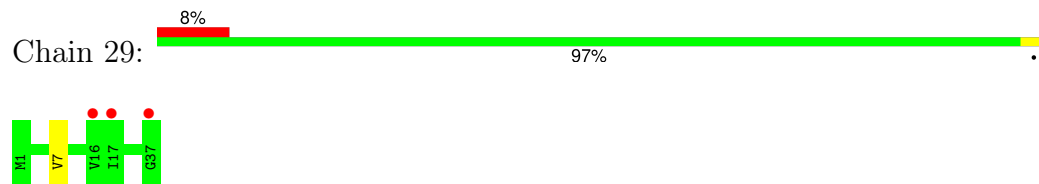


- Molecule 31: 50S ribosomal protein L36

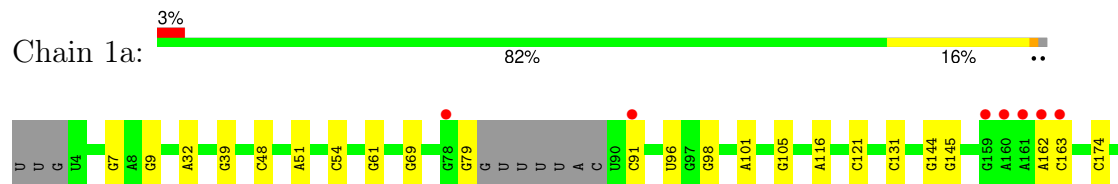


There are no outlier residues recorded for this chain.

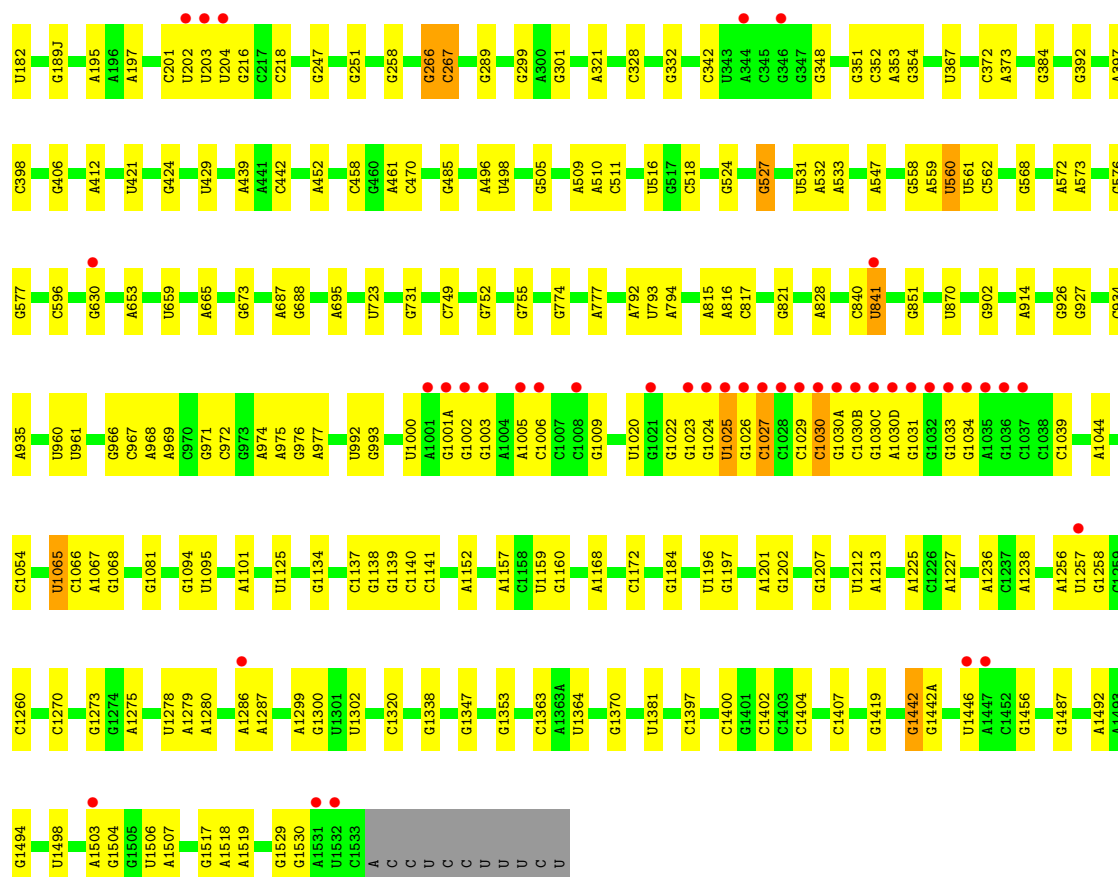
- Molecule 31: 50S ribosomal protein L36



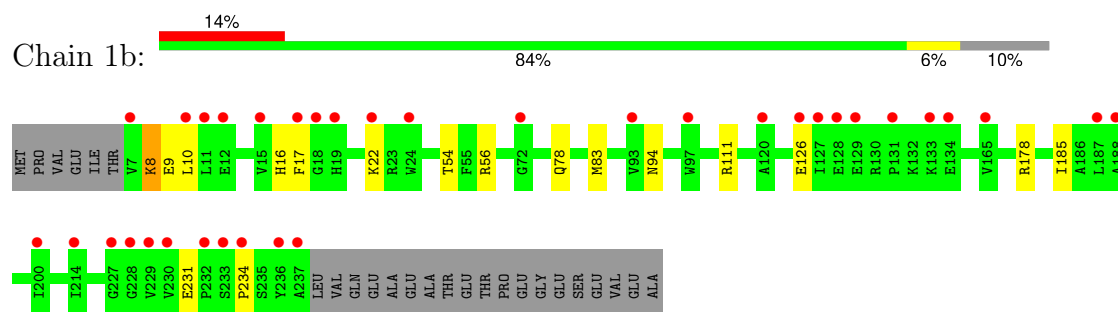
- Molecule 32: 16S Ribosomal RNA



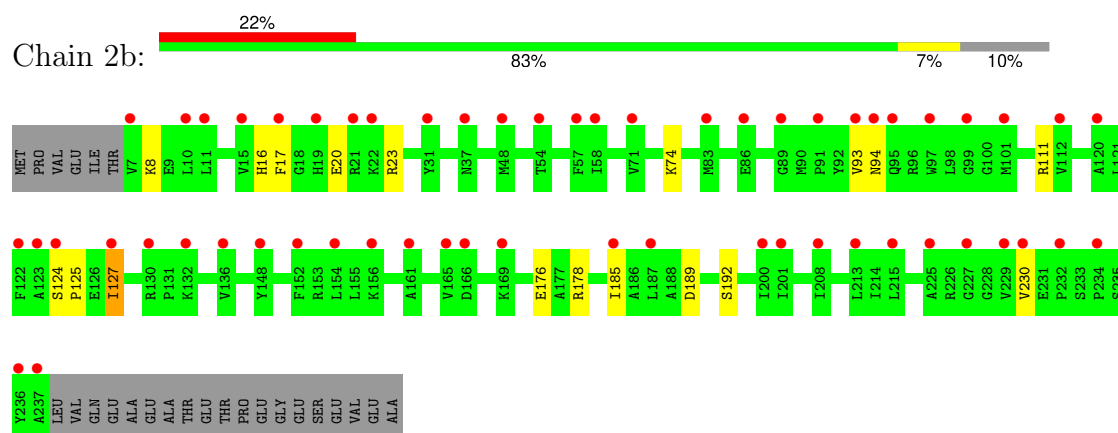




• Molecule 33: 30S ribosomal protein S2

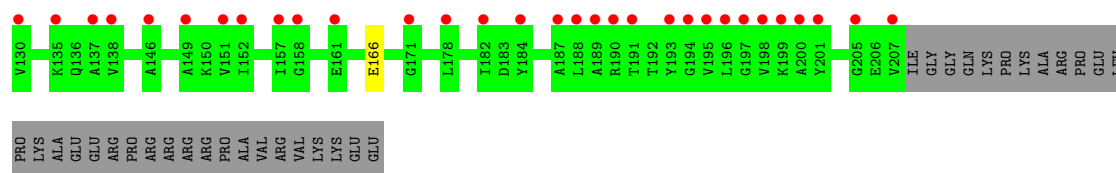


• Molecule 33: 30S ribosomal protein S2



- |      |
|------|
| MET  |
| G2   |
| N3   |
| D62  |
| A65  |
| V66  |
| G81  |
| L87  |
| Q107 |
| S112 |
| L115 |
| P193 |
| G194 |
| V195 |
| E206 |
| V207 |
| ILE  |
| GLY  |
| GLY  |
| GLN  |
| LYS  |
| PRO  |
| LYS  |
| ALA  |
| ARG  |
| PRO  |
| GLU  |
| LEU  |
| PRO  |
| LYS  |
| ALA  |
| GLU  |
| GLU  |
| ARG  |
| PRO  |
| ARG  |
| ARG  |
| ARG  |
| ARG  |
| PRO  |
| ALA  |
| VAL  |
| ARG  |
| VAL  |
| VAL  |
| LYS  |
| LYS  |
| GLU  |

- [illegible]



- | Met  |
|------|
| G2   |
| I5   |
| L19  |
| C31  |
| R59  |
| I70  |
| S83  |
| R107 |
| F110 |
| L135 |
| E150 |
| M154 |
| I158 |
| A164 |
| G167 |
| R168 |
| K169 |
| V170 |
| W173 |
| V178 |
| E179 |
| G180 |
| L194 |
| A195 |
| L196 |
| R209 |

- [illegible]

- [illegible]

- | MET  | PRO | GLU | THR |
|------|-----|-----|-----|
| D5   |     |     |     |
| M10  |     |     |     |
| I11  |     |     |     |
| L12  |     |     |     |
| I13  |     |     |     |
| A17  |     |     |     |
| Q20  |     |     |     |
| A21  |     |     |     |
| G22  |     |     |     |
| R25  |     |     |     |
| L31  |     |     |     |
| V32  |     |     |     |
| V33  |     |     |     |
| V34  |     |     |     |
| V41  |     |     |     |
| V51  |     |     |     |
| A54  |     |     |     |
| E68  |     |     |     |
| G74  |     |     |     |
| T75  |     |     |     |
| I80  |     |     |     |
| G85  |     |     |     |
| A94  |     |     |     |
| V100 |     |     |     |
| I109 |     |     |     |
| L110 |     |     |     |
| E111 |     |     |     |
| L112 |     |     |     |
| A113 |     |     |     |
| G114 |     |     |     |
| V115 |     |     |     |
| I116 |     |     |     |
| L118 |     |     |     |
| T120 |     |     |     |
| S125 |     |     |     |
| V133 |     |     |     |

LYS  
GLY  
GLU  
ALA  
HIS  
ALA  
GLN  
ALA  
GLN  
GLY

- Molecule 37: 30S ribosomal protein S6

Chain 1f:  96% ..

H1  
L21  
V40  
L45  
N100  
ALA

- Molecule 37: 30S ribosomal protein S6

Chain 2f:  96% ..

H1  
L21  
V40  
V72  
S93  
N100  
ALA

- Molecule 38: 30S ribosomal protein S7

Chain 1g:  94% 6% .

MET  
A2  
D15  
L16  
L59  
R79  
G81  
G82  
A83  
N84  
R85  
L104  
R111  
R114  
R115  
H153  
W156

- Molecule 38: 30S ribosomal protein S7

Chain 2g:  94% 5% .

MET  
A2  
R3  
R4  
R5  
R6  
A7  
Q13  
L16  
V17  
R76  
S77  
R78  
R79  
V80  
G81  
G82  
A83  
N84  
Y85  
A152  
W156

- Molecule 39: 30S ribosomal protein S8

Chain 1h:  96% ..

MET  
L2  
T3  
D4  
D25  
V26  
L63  
I80  
R85  
L112  
W138

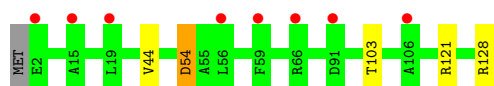
- Molecule 39: 30S ribosomal protein S8

Chain 2h:  96% ..

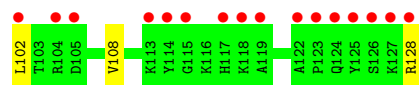
MET  
L2  
T3  
R14  
V51  
D52  
V53  
P67  
R85  
G90  
R102  
G108  
L112  
R122  
E123  
A124  
W138

- Molecule 40: 30S ribosomal protein S9

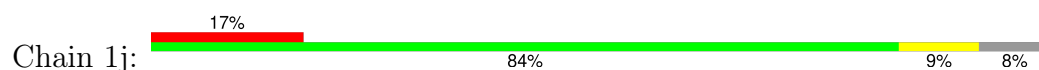
Chain 1i:  95% ..



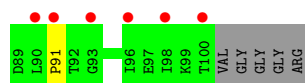
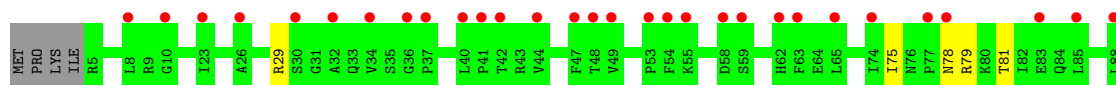
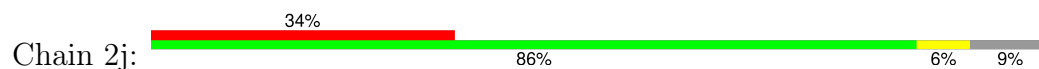
- Molecule 40: 30S ribosomal protein S9



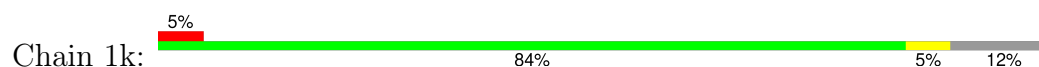
- Molecule 41: 30S ribosomal protein S10



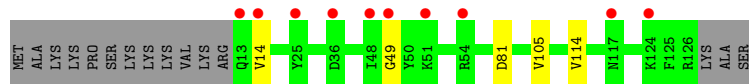
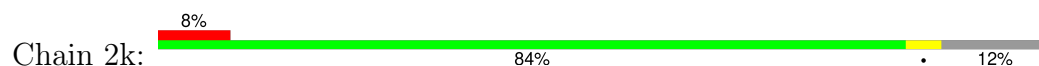
- Molecule 41: 30S ribosomal protein S10



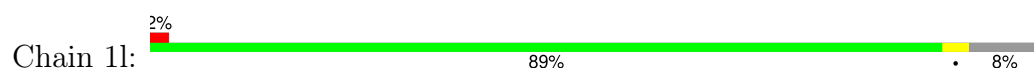
- Molecule 42: 30S ribosomal protein S11



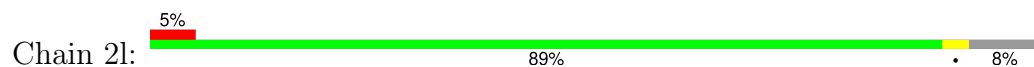
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



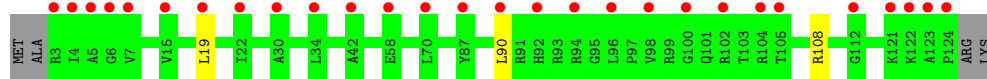
- Molecule 43: 30S ribosomal protein S12



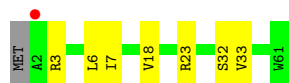
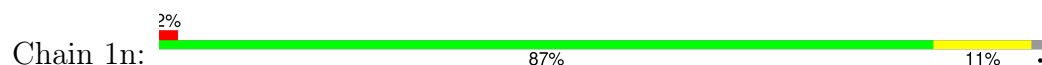
- Molecule 44: 30S ribosomal protein S13



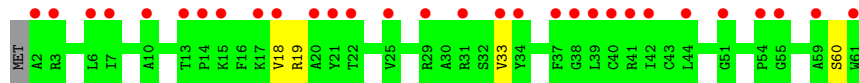
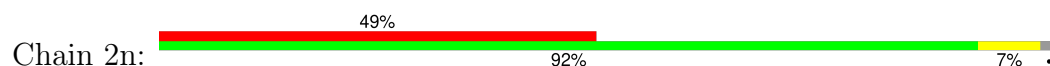
- Molecule 44: 30S ribosomal protein S13



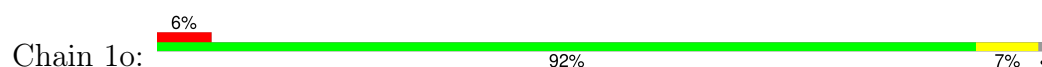
- Molecule 45: 30S ribosomal protein S14 type Z



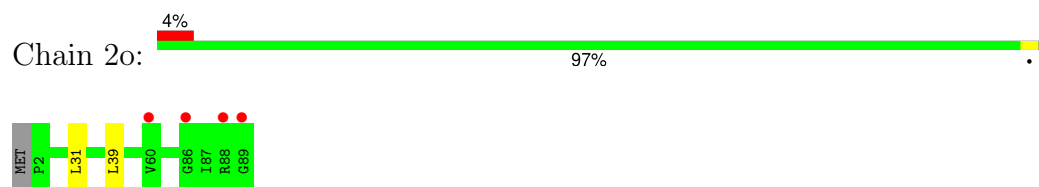
- Molecule 45: 30S ribosomal protein S14 type Z



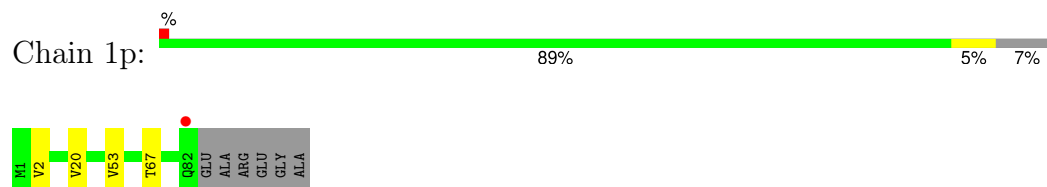
- Molecule 46: 30S ribosomal protein S15



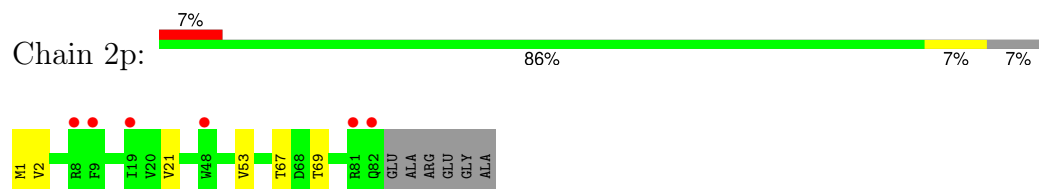
- Molecule 46: 30S ribosomal protein S15



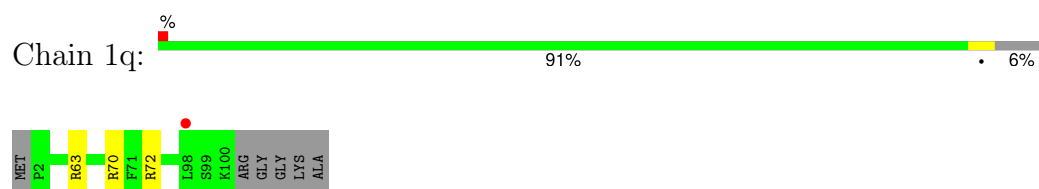
- Molecule 47: 30S ribosomal protein S16



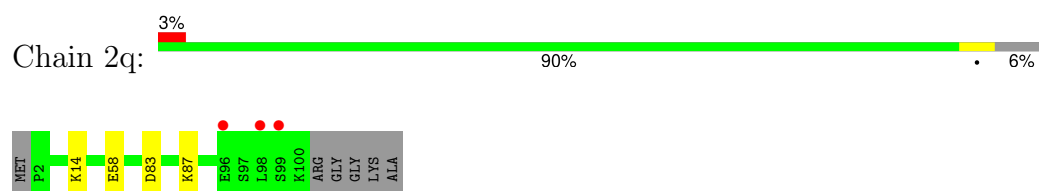
- Molecule 47: 30S ribosomal protein S16



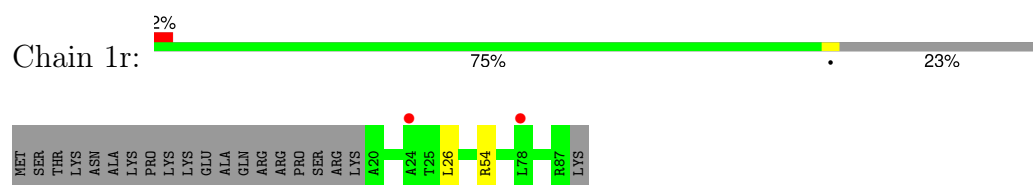
- Molecule 48: 30S ribosomal protein S17



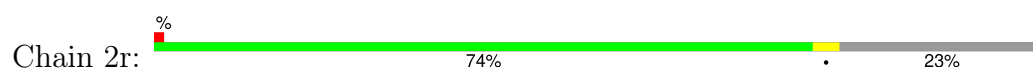
- Molecule 48: 30S ribosomal protein S17

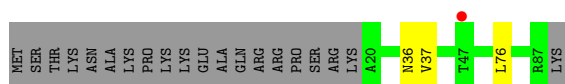


- Molecule 49: 30S ribosomal protein S18

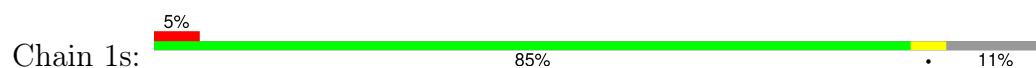


- Molecule 49: 30S ribosomal protein S18

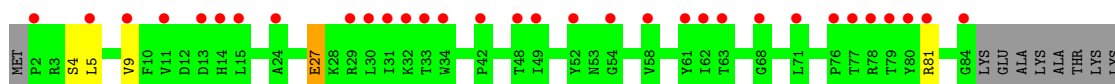
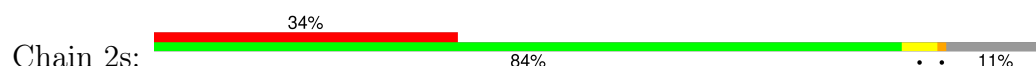




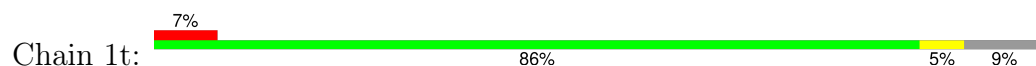
- Molecule 50: 30S ribosomal protein S19



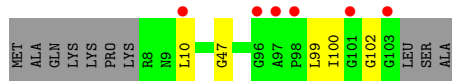
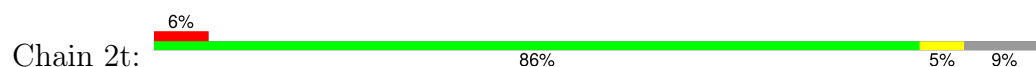
- Molecule 50: 30S ribosomal protein S19



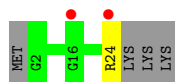
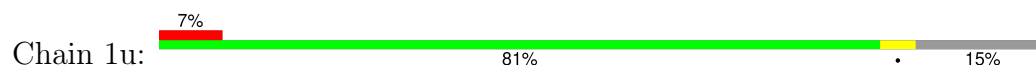
- Molecule 51: 30S ribosomal protein S20



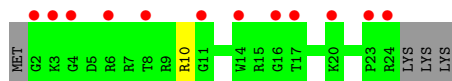
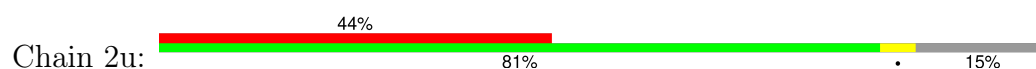
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA



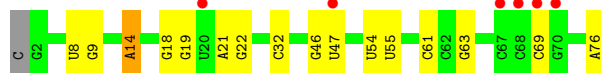
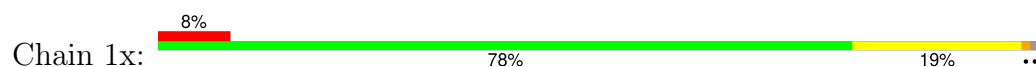
- Molecule 54: tRNA, A-site and E-site tRNAs



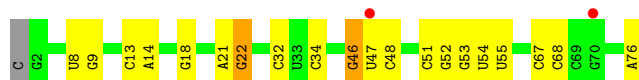
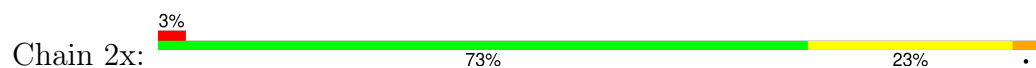
- Molecule 54: tRNA, A-site and E-site tRNAs



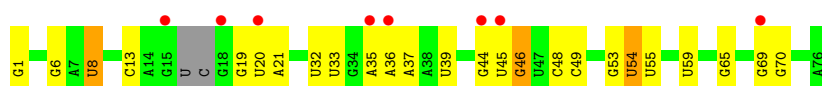
- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA

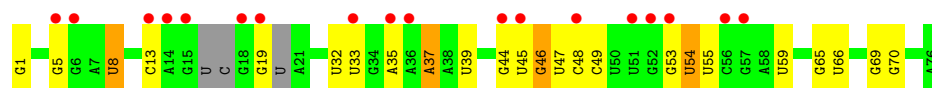


- Molecule 56: tRNA

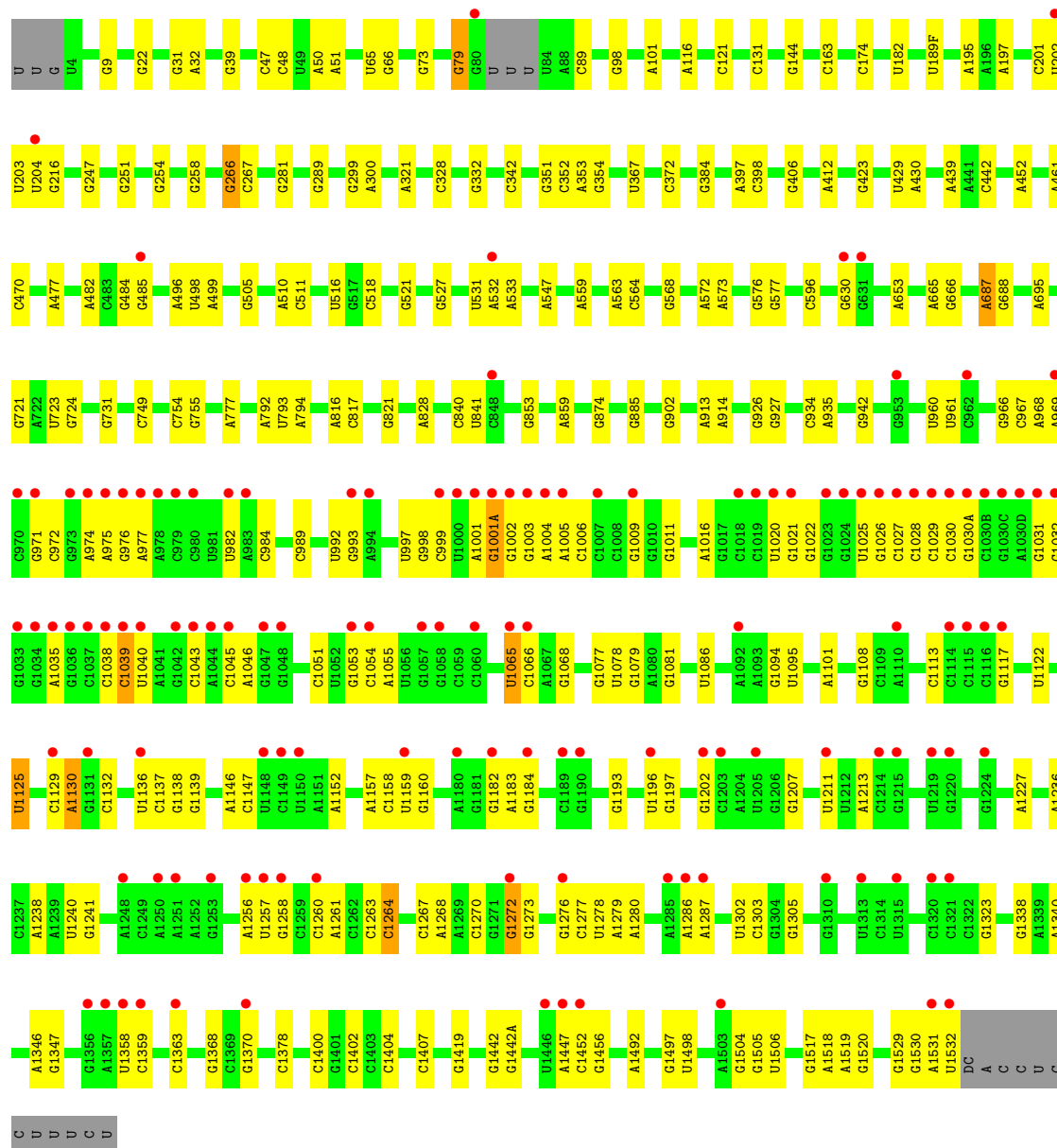
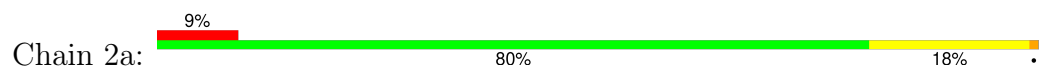




- Molecule 56: tRNA



- Molecule 57: 16S Ribosomal RNA



- Molecule 58: Klebsazolicin





● Molecule 58: Klebsazolicin



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.64Å 449.06Å 622.01Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 155.50 – 2.70<br>155.50 – 2.70                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (155.50-2.70)<br>99.3 (155.50-2.70)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.16  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.25 (at 2.69Å)   | Xtriage          |
| Refinement program  | PHENIX 1.8.2  | Depositor        |
| R, $R_{free}$   | 0.207 , 0.252<br>0.211 , 0.255                              | Depositor<br>DCC |
| $R_{free}$ test set   | 78960 reflections (5.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.0  | Xtriage          |
| Anisotropy  | 0.239   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 70.5   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 302030  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: 2MA, ZN, BB9, SF4, MG, 5MC, UR3, K, M2G, 5MU, 0TD, 4OC, OMG, G7M, 2MG, MIA, 4SU, MA6, PSU, 9VA, 2MU, 9VD

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    | 0.54         | 0/69009       | 0.98        | 82/107712 (0.1%) |
| 1   | 2A    | 0.41         | 0/67293       | 0.88        | 41/105034 (0.0%) |
| 2   | 1B    | 0.46         | 1/2882 (0.0%) | 0.88        | 0/4494           |
| 2   | 2B    | 0.41         | 1/2879 (0.0%) | 0.87        | 1/4487 (0.0%)    |
| 3   | 1D    | 0.36         | 0/2186        | 0.57        | 0/2944           |
| 3   | 2D    | 0.33         | 0/2186        | 0.54        | 0/2944           |
| 4   | 1E    | 0.36         | 0/1592        | 0.54        | 0/2149           |
| 4   | 2E    | 0.31         | 0/1592        | 0.50        | 0/2149           |
| 5   | 1F    | 0.34         | 0/1619        | 0.57        | 0/2193           |
| 5   | 2F    | 0.30         | 0/1615        | 0.49        | 0/2188           |
| 6   | 1G    | 0.29         | 0/1448        | 0.49        | 0/1957           |
| 6   | 2G    | 0.30         | 0/1453        | 0.52        | 0/1963           |
| 7   | 1H    | 0.33         | 0/1356        | 0.50        | 0/1834           |
| 7   | 2H    | 0.29         | 0/1356        | 0.45        | 0/1834           |
| 8   | 1I    | 0.29         | 0/1112        | 0.51        | 0/1514           |
| 8   | 2I    | 0.27         | 0/1079        | 0.50        | 0/1475           |
| 9   | 1N    | 0.34         | 0/1144        | 0.53        | 0/1543           |
| 9   | 2N    | 0.29         | 0/1144        | 0.46        | 0/1543           |
| 10  | 1O    | 0.38         | 0/943         | 0.56        | 0/1269           |
| 10  | 2O    | 0.34         | 0/943         | 0.52        | 0/1269           |
| 11  | 1P    | 0.34         | 0/1152        | 0.56        | 0/1533           |
| 11  | 2P    | 0.31         | 0/1152        | 0.52        | 0/1533           |
| 12  | 1Q    | 0.35         | 0/1143        | 0.54        | 0/1527           |
| 12  | 2Q    | 0.30         | 0/1143        | 0.48        | 0/1527           |
| 13  | 1R    | 0.33         | 0/982         | 0.54        | 0/1312           |
| 13  | 2R    | 0.27         | 0/982         | 0.53        | 0/1312           |
| 14  | 1S    | 0.32         | 0/883         | 0.56        | 0/1176           |
| 14  | 2S    | 0.32         | 0/880         | 0.47        | 0/1172           |
| 15  | 1T    | 0.35         | 0/1105        | 0.54        | 0/1477           |
| 15  | 2T    | 0.29         | 0/1097        | 0.46        | 0/1468           |
| 16  | 1U    | 0.39         | 0/977         | 0.55        | 0/1301           |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 16  | 2U    | 0.31         | 0/977   | 0.46        | 0/1301          |
| 17  | 1V    | 0.38         | 0/782   | 0.57        | 0/1049          |
| 17  | 2V    | 0.30         | 0/782   | 0.51        | 0/1049          |
| 18  | 1W    | 0.35         | 0/897   | 0.54        | 0/1205          |
| 18  | 2W    | 0.32         | 0/897   | 0.49        | 0/1205          |
| 19  | 1X    | 0.38         | 0/764   | 0.57        | 0/1025          |
| 19  | 2X    | 0.31         | 0/764   | 0.48        | 0/1025          |
| 20  | 1Y    | 0.36         | 0/819   | 0.57        | 1/1095 (0.1%)   |
| 20  | 2Y    | 0.32         | 0/819   | 0.53        | 0/1095          |
| 21  | 1Z    | 0.32         | 0/1267  | 0.53        | 0/1717          |
| 21  | 2Z    | 0.30         | 0/1299  | 0.50        | 0/1763          |
| 22  | 10    | 0.37         | 0/662   | 0.58        | 0/881           |
| 22  | 20    | 0.30         | 0/662   | 0.50        | 0/881           |
| 23  | 11    | 0.35         | 0/762   | 0.53        | 0/1014          |
| 23  | 21    | 0.32         | 0/762   | 0.53        | 0/1014          |
| 24  | 12    | 0.32         | 0/590   | 0.49        | 0/781           |
| 24  | 22    | 0.28         | 0/590   | 0.42        | 0/781           |
| 25  | 13    | 0.32         | 0/474   | 0.53        | 0/635           |
| 25  | 23    | 0.28         | 0/469   | 0.46        | 0/630           |
| 26  | 14    | 0.35         | 0/565   | 0.53        | 0/761           |
| 26  | 24    | 0.31         | 0/545   | 0.50        | 0/737           |
| 27  | 15    | 0.35         | 0/469   | 0.59        | 1/635 (0.2%)    |
| 27  | 25    | 0.32         | 0/469   | 0.50        | 0/635           |
| 28  | 16    | 0.35         | 0/460   | 0.55        | 0/613           |
| 28  | 26    | 0.29         | 0/456   | 0.49        | 0/608           |
| 29  | 17    | 0.34         | 0/426   | 0.54        | 0/561           |
| 29  | 27    | 0.31         | 0/426   | 0.52        | 0/561           |
| 30  | 18    | 0.32         | 0/525   | 0.55        | 0/691           |
| 30  | 28    | 0.30         | 0/525   | 0.49        | 0/691           |
| 31  | 19    | 0.34         | 0/310   | 0.53        | 0/407           |
| 31  | 29    | 0.30         | 0/310   | 0.52        | 0/407           |
| 32  | 1a    | 0.39         | 0/35795 | 0.89        | 39/55864 (0.1%) |
| 33  | 1b    | 0.29         | 0/1881  | 0.48        | 0/2542          |
| 33  | 2b    | 0.31         | 0/1860  | 0.47        | 0/2518          |
| 34  | 1c    | 0.29         | 0/1572  | 0.47        | 0/2126          |
| 34  | 2c    | 0.29         | 0/1566  | 0.46        | 0/2119          |
| 35  | 1d    | 0.30         | 0/1685  | 0.49        | 0/2262          |
| 35  | 2d    | 0.29         | 0/1704  | 0.47        | 0/2284          |
| 36  | 1e    | 0.31         | 0/1145  | 0.51        | 0/1543          |
| 36  | 2e    | 0.31         | 0/1149  | 0.51        | 0/1548          |
| 37  | 1f    | 0.30         | 0/823   | 0.47        | 0/1115          |
| 37  | 2f    | 0.31         | 0/829   | 0.48        | 0/1123          |
| 38  | 1g    | 0.28         | 0/1250  | 0.44        | 0/1679          |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | 2g    | 0.28         | 0/1254           | 0.44        | 0/1683            |
| 39  | 1h    | 0.28         | 0/1108           | 0.48        | 0/1494            |
| 39  | 2h    | 0.28         | 0/1108           | 0.46        | 0/1494            |
| 40  | 1i    | 0.29         | 0/1002           | 0.50        | 0/1346            |
| 40  | 2i    | 0.30         | 0/997            | 0.50        | 0/1343            |
| 41  | 1j    | 0.28         | 0/722            | 0.48        | 0/982             |
| 41  | 2j    | 0.30         | 0/727            | 0.52        | 0/988             |
| 42  | 1k    | 0.29         | 0/844            | 0.48        | 0/1145            |
| 42  | 2k    | 0.29         | 0/848            | 0.48        | 0/1149            |
| 43  | 1l    | 0.31         | 0/937            | 0.53        | 0/1260            |
| 43  | 2l    | 0.29         | 0/937            | 0.49        | 0/1260            |
| 44  | 1m    | 0.29         | 0/969            | 0.49        | 0/1302            |
| 44  | 2m    | 0.28         | 0/961            | 0.51        | 0/1291            |
| 45  | 1n    | 0.30         | 0/501            | 0.48        | 0/664             |
| 45  | 2n    | 0.32         | 0/501            | 0.50        | 0/664             |
| 46  | 1o    | 0.28         | 0/739            | 0.43        | 0/985             |
| 46  | 2o    | 0.26         | 0/739            | 0.42        | 0/985             |
| 47  | 1p    | 0.28         | 0/697            | 0.51        | 0/939             |
| 47  | 2p    | 0.29         | 0/693            | 0.50        | 0/935             |
| 48  | 1q    | 0.30         | 0/836            | 0.48        | 0/1117            |
| 48  | 2q    | 0.30         | 0/836            | 0.47        | 0/1117            |
| 49  | 1r    | 0.28         | 0/560            | 0.48        | 0/746             |
| 49  | 2r    | 0.28         | 0/560            | 0.44        | 0/746             |
| 50  | 1s    | 0.28         | 0/667            | 0.54        | 0/900             |
| 50  | 2s    | 0.30         | 0/661            | 0.54        | 0/893             |
| 51  | 1t    | 0.28         | 0/730            | 0.47        | 0/965             |
| 51  | 2t    | 0.28         | 0/729            | 0.43        | 0/965             |
| 52  | 1u    | 0.27         | 0/203            | 0.44        | 0/266             |
| 52  | 2u    | 0.36         | 0/203            | 0.48        | 0/266             |
| 53  | 1v    | 0.42         | 0/310            | 0.86        | 0/480             |
| 53  | 2v    | 0.47         | 0/310            | 0.86        | 0/480             |
| 54  | 1w    | 0.54         | 1/1606 (0.1%)    | 1.09        | 0/2497            |
| 54  | 2w    | 0.51         | 0/1556           | 1.13        | 4/2418 (0.2%)     |
| 55  | 1x    | 0.55         | 1/1725 (0.1%)    | 1.13        | 13/2689 (0.5%)    |
| 55  | 2x    | 0.46         | 0/1725           | 1.06        | 7/2689 (0.3%)     |
| 56  | 1y    | 0.72         | 6/1632 (0.4%)    | 1.22        | 13/2540 (0.5%)    |
| 56  | 2y    | 0.75         | 6/1609 (0.4%)    | 1.24        | 12/2502 (0.5%)    |
| 57  | 2a    | 0.38         | 3/35886 (0.0%)   | 0.90        | 50/56005 (0.1%)   |
| 58  | A     | 2.13         | 4/74 (5.4%)      | 2.00        | 5/97 (5.2%)       |
| 58  | B     | 2.13         | 3/74 (4.1%)      | 2.04        | 4/97 (4.1%)       |
| All | All   | 0.42         | 26/316886 (0.0%) | 0.84        | 273/474393 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 26  | 24    | 0                   | 1                   |
| 33  | 1b    | 0                   | 1                   |
| 50  | 2s    | 0                   | 1                   |
| 58  | A     | 1                   | 0                   |
| 58  | B     | 1                   | 0                   |
| All | All   | 2                   | 3                   |

The worst 5 of 26 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 56  | 2y    | 37  | A    | C5-C4 | 13.66  | 1.48        | 1.38     |
| 56  | 1y    | 37  | A    | C5-C4 | 13.39  | 1.48        | 1.38     |
| 58  | B     | 12  | SER  | CA-CB | -13.07 | 1.33        | 1.52     |
| 58  | A     | 12  | SER  | CA-CB | -12.57 | 1.34        | 1.52     |
| 56  | 2y    | 1   | G    | OP3-P | -10.39 | 1.48        | 1.61     |

The worst 5 of 273 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 57  | 2a    | 1263 | C    | N1-C2-O2 | 22.88 | 132.63      | 118.90   |
| 57  | 2a    | 1272 | G    | N3-C2-N2 | 20.83 | 134.48      | 119.90   |
| 56  | 2y    | 37   | A    | C2-N3-C4 | 20.81 | 121.00      | 110.60   |
| 56  | 1y    | 37   | A    | C2-N3-C4 | 20.56 | 120.88      | 110.60   |
| 57  | 2a    | 1272 | G    | C5-C6-O6 | 20.05 | 140.63      | 128.60   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 58  | A     | 12  | SER  | CA   |
| 58  | B     | 12  | SER  | CA   |

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 33  | 1b    | 8   | LYS  | Peptide |
| 26  | 24    | 56  | VAL  | Peptide |
| 50  | 2s    | 27  | GLU  | Peptide |

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 261 (96%) | 12 (4%) | 0        | 100         | 100 |
| 3   | 2D    | 273/276 (99%) | 259 (95%) | 14 (5%) | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 194 (96%) | 7 (4%)  | 1 (0%)   | 25          | 49  |
| 4   | 2E    | 202/206 (98%) | 193 (96%) | 8 (4%)  | 1 (0%)   | 25          | 49  |
| 5   | 1F    | 201/210 (96%) | 195 (97%) | 5 (2%)  | 1 (0%)   | 25          | 49  |
| 5   | 2F    | 201/210 (96%) | 193 (96%) | 7 (4%)  | 1 (0%)   | 25          | 49  |
| 6   | 1G    | 179/182 (98%) | 168 (94%) | 8 (4%)  | 3 (2%)   | 7           | 20  |
| 6   | 2G    | 179/182 (98%) | 162 (90%) | 13 (7%) | 4 (2%)   | 5           | 15  |
| 7   | 1H    | 172/180 (96%) | 161 (94%) | 10 (6%) | 1 (1%)   | 22          | 45  |
| 7   | 2H    | 172/180 (96%) | 156 (91%) | 13 (8%) | 3 (2%)   | 7           | 20  |
| 8   | 1I    | 144/148 (97%) | 130 (90%) | 13 (9%) | 1 (1%)   | 19          | 42  |
| 8   | 2I    | 144/148 (97%) | 129 (90%) | 13 (9%) | 2 (1%)   | 9           | 24  |
| 9   | 1N    | 138/140 (99%) | 133 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 132 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 10  | 1O    | 120/122 (98%) | 115 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 10  | 2O    | 120/122 (98%) | 112 (93%) | 6 (5%)  | 2 (2%)   | 7           | 20  |
| 11  | 1P    | 147/150 (98%) | 134 (91%) | 12 (8%) | 1 (1%)   | 19          | 42  |
| 11  | 2P    | 147/150 (98%) | 137 (93%) | 9 (6%)  | 1 (1%)   | 19          | 42  |
| 12  | 1Q    | 139/141 (99%) | 130 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 12  | 2Q    | 139/141 (99%) | 130 (94%) | 6 (4%)  | 3 (2%)   | 5           | 15  |
| 13  | 1R    | 116/118 (98%) | 109 (94%) | 7 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 13  | 2R    | 116/118 (98%) | 108 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 14  | 1S    | 108/112 (96%) | 102 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 14  | 2S    | 108/112 (96%) | 102 (94%)  | 5 (5%)   | 1 (1%)   | 14          | 35  |
| 15  | 1T    | 129/146 (88%) | 123 (95%)  | 5 (4%)   | 1 (1%)   | 16          | 38  |
| 15  | 2T    | 129/146 (88%) | 124 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 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%)  | 96 (97%)   | 2 (2%)   | 1 (1%)   | 13          | 33  |
| 17  | 2V    | 99/101 (98%)  | 92 (93%)   | 6 (6%)   | 1 (1%)   | 13          | 33  |
| 18  | 1W    | 110/113 (97%) | 109 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 110 (100%) | 0        | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 91 (98%)   | 1 (1%)   | 1 (1%)   | 12          | 30  |
| 19  | 2X    | 93/96 (97%)   | 89 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 20  | 1Y    | 105/110 (96%) | 97 (92%)   | 7 (7%)   | 1 (1%)   | 13          | 33  |
| 20  | 2Y    | 105/110 (96%) | 100 (95%)  | 4 (4%)   | 1 (1%)   | 13          | 33  |
| 21  | 1Z    | 148/206 (72%) | 134 (90%)  | 12 (8%)  | 2 (1%)   | 9           | 24  |
| 21  | 2Z    | 156/206 (76%) | 138 (88%)  | 15 (10%) | 3 (2%)   | 6           | 17  |
| 22  | 10    | 81/85 (95%)   | 79 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 22  | 20    | 81/85 (95%)   | 76 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 23  | 11    | 95/98 (97%)   | 92 (97%)   | 2 (2%)   | 1 (1%)   | 12          | 30  |
| 23  | 21    | 95/98 (97%)   | 94 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 24  | 12    | 68/72 (94%)   | 67 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 66 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 57 (100%)  | 0        | 0        | 100         | 100 |
| 25  | 23    | 57/60 (95%)   | 54 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 26  | 14    | 67/71 (94%)   | 53 (79%)   | 9 (13%)  | 5 (8%)   | 1           | 1   |
| 26  | 24    | 67/71 (94%)   | 53 (79%)   | 13 (19%) | 1 (2%)   | 8           | 22  |
| 27  | 15    | 57/60 (95%)   | 55 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 56 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 49 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 50 (98%)   | 1 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 29  | 17    | 46/49 (94%)   | 46 (100%) | 0        | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 62 (100%) | 0        | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 59 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 31  | 19    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 34 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 194 (85%) | 26 (11%) | 9 (4%)   | 2           | 5   |
| 33  | 2b    | 229/256 (90%) | 201 (88%) | 21 (9%)  | 7 (3%)   | 3           | 8   |
| 34  | 1c    | 204/239 (85%) | 188 (92%) | 13 (6%)  | 3 (2%)   | 8           | 22  |
| 34  | 2c    | 204/239 (85%) | 178 (87%) | 24 (12%) | 2 (1%)   | 13          | 33  |
| 35  | 1d    | 206/209 (99%) | 193 (94%) | 11 (5%)  | 2 (1%)   | 13          | 33  |
| 35  | 2d    | 206/209 (99%) | 189 (92%) | 14 (7%)  | 3 (2%)   | 8           | 22  |
| 36  | 1e    | 146/162 (90%) | 135 (92%) | 8 (6%)   | 3 (2%)   | 5           | 15  |
| 36  | 2e    | 146/162 (90%) | 134 (92%) | 10 (7%)  | 2 (1%)   | 9           | 24  |
| 37  | 1f    | 98/101 (97%)  | 94 (96%)  | 3 (3%)   | 1 (1%)   | 13          | 33  |
| 37  | 2f    | 98/101 (97%)  | 94 (96%)  | 3 (3%)   | 1 (1%)   | 13          | 33  |
| 38  | 1g    | 153/156 (98%) | 142 (93%) | 10 (6%)  | 1 (1%)   | 19          | 42  |
| 38  | 2g    | 153/156 (98%) | 140 (92%) | 9 (6%)   | 4 (3%)   | 4           | 11  |
| 39  | 1h    | 135/138 (98%) | 130 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 39  | 2h    | 135/138 (98%) | 118 (87%) | 17 (13%) | 0        | 100         | 100 |
| 40  | 1i    | 125/128 (98%) | 109 (87%) | 14 (11%) | 2 (2%)   | 8           | 21  |
| 40  | 2i    | 125/128 (98%) | 110 (88%) | 15 (12%) | 0        | 100         | 100 |
| 41  | 1j    | 95/105 (90%)  | 84 (88%)  | 6 (6%)   | 5 (5%)   | 1           | 3   |
| 41  | 2j    | 94/105 (90%)  | 79 (84%)  | 10 (11%) | 5 (5%)   | 1           | 3   |
| 42  | 1k    | 112/129 (87%) | 105 (94%) | 6 (5%)   | 1 (1%)   | 14          | 35  |
| 42  | 2k    | 112/129 (87%) | 105 (94%) | 5 (4%)   | 2 (2%)   | 7           | 18  |
| 43  | 1l    | 119/132 (90%) | 114 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 43  | 2l    | 119/132 (90%) | 110 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 44  | 1m    | 121/126 (96%) | 111 (92%) | 9 (7%)   | 1 (1%)   | 16          | 38  |
| 44  | 2m    | 120/126 (95%) | 108 (90%) | 12 (10%) | 0        | 100         | 100 |
| 45  | 1n    | 58/61 (95%)   | 56 (97%)  | 2 (3%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 45  | 2n    | 58/61 (95%)       | 51 (88%)    | 5 (9%)   | 2 (3%)   | 3           | 7   |
| 46  | 1o    | 86/89 (97%)       | 83 (96%)    | 2 (2%)   | 1 (1%)   | 11          | 28  |
| 46  | 2o    | 86/89 (97%)       | 83 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 47  | 1p    | 80/88 (91%)       | 72 (90%)    | 7 (9%)   | 1 (1%)   | 10          | 26  |
| 47  | 2p    | 80/88 (91%)       | 70 (88%)    | 9 (11%)  | 1 (1%)   | 10          | 26  |
| 48  | 1q    | 97/105 (92%)      | 91 (94%)    | 6 (6%)   | 0        | 100         | 100 |
| 48  | 2q    | 97/105 (92%)      | 90 (93%)    | 7 (7%)   | 0        | 100         | 100 |
| 49  | 1r    | 66/88 (75%)       | 63 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 49  | 2r    | 66/88 (75%)       | 63 (96%)    | 2 (3%)   | 1 (2%)   | 8           | 22  |
| 50  | 1s    | 81/93 (87%)       | 72 (89%)    | 8 (10%)  | 1 (1%)   | 11          | 28  |
| 50  | 2s    | 81/93 (87%)       | 68 (84%)    | 10 (12%) | 3 (4%)   | 2           | 6   |
| 51  | 1t    | 94/106 (89%)      | 85 (90%)    | 5 (5%)   | 4 (4%)   | 2           | 4   |
| 51  | 2t    | 94/106 (89%)      | 85 (90%)    | 4 (4%)   | 5 (5%)   | 1           | 3   |
| 52  | 1u    | 21/27 (78%)       | 19 (90%)    | 2 (10%)  | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 15 (71%)    | 6 (29%)  | 0        | 100         | 100 |
| 58  | A     | 12/18 (67%)       | 5 (42%)     | 5 (42%)  | 2 (17%)  | 0           | 0   |
| 58  | B     | 12/18 (67%)       | 6 (50%)     | 4 (33%)  | 2 (17%)  | 0           | 0   |
| All | All   | 11394/12164 (94%) | 10597 (93%) | 676 (6%) | 121 (1%) | 12          | 30  |

5 of 121 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 1G    | 47  | LYS  |
| 7   | 1H    | 126 | PRO  |
| 8   | 1I    | 10  | GLU  |
| 20  | 1Y    | 55  | TYR  |
| 23  | 1I    | 3   | LYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | 1D    | 215/218 (99%)  | 197 (92%) | 18 (8%)  | 9           | 22 |
| 3   | 2D    | 215/218 (99%)  | 203 (94%) | 12 (6%)  | 17          | 41 |
| 4   | 1E    | 164/166 (99%)  | 149 (91%) | 15 (9%)  | 7           | 19 |
| 4   | 2E    | 164/166 (99%)  | 153 (93%) | 11 (7%)  | 13          | 33 |
| 5   | 1F    | 160/166 (96%)  | 147 (92%) | 13 (8%)  | 9           | 23 |
| 5   | 2F    | 159/166 (96%)  | 148 (93%) | 11 (7%)  | 13          | 31 |
| 6   | 1G    | 143/156 (92%)  | 135 (94%) | 8 (6%)   | 17          | 41 |
| 6   | 2G    | 143/156 (92%)  | 137 (96%) | 6 (4%)   | 25          | 53 |
| 7   | 1H    | 144/148 (97%)  | 138 (96%) | 6 (4%)   | 25          | 53 |
| 7   | 2H    | 144/148 (97%)  | 139 (96%) | 5 (4%)   | 31          | 60 |
| 8   | 1I    | 113/124 (91%)  | 103 (91%) | 10 (9%)  | 8           | 20 |
| 8   | 2I    | 105/124 (85%)  | 95 (90%)  | 10 (10%) | 7           | 17 |
| 9   | 1N    | 118/119 (99%)  | 109 (92%) | 9 (8%)   | 11          | 27 |
| 9   | 2N    | 118/119 (99%)  | 111 (94%) | 7 (6%)   | 16          | 38 |
| 10  | 1O    | 100/100 (100%) | 96 (96%)  | 4 (4%)   | 27          | 55 |
| 10  | 2O    | 100/100 (100%) | 96 (96%)  | 4 (4%)   | 27          | 55 |
| 11  | 1P    | 115/116 (99%)  | 109 (95%) | 6 (5%)   | 19          | 44 |
| 11  | 2P    | 115/116 (99%)  | 112 (97%) | 3 (3%)   | 41          | 70 |
| 12  | 1Q    | 111/111 (100%) | 104 (94%) | 7 (6%)   | 15          | 35 |
| 12  | 2Q    | 111/111 (100%) | 103 (93%) | 8 (7%)   | 12          | 30 |
| 13  | 1R    | 101/101 (100%) | 89 (88%)  | 12 (12%) | 4           | 10 |
| 13  | 2R    | 101/101 (100%) | 90 (89%)  | 11 (11%) | 5           | 13 |
| 14  | 1S    | 86/88 (98%)    | 78 (91%)  | 8 (9%)   | 7           | 18 |
| 14  | 2S    | 85/88 (97%)    | 79 (93%)  | 6 (7%)   | 12          | 30 |
| 15  | 1T    | 115/127 (91%)  | 111 (96%) | 4 (4%)   | 31          | 60 |
| 15  | 2T    | 113/127 (89%)  | 109 (96%) | 4 (4%)   | 31          | 60 |
| 16  | 1U    | 93/94 (99%)    | 86 (92%)  | 7 (8%)   | 11          | 28 |
| 16  | 2U    | 93/94 (99%)    | 90 (97%)  | 3 (3%)   | 34          | 63 |
| 17  | 1V    | 80/82 (98%)    | 70 (88%)  | 10 (12%) | 3           | 9  |
| 17  | 2V    | 80/82 (98%)    | 73 (91%)  | 7 (9%)   | 8           | 20 |
| 18  | 1W    | 90/92 (98%)    | 83 (92%)  | 7 (8%)   | 10          | 26 |
| 18  | 2W    | 90/92 (98%)    | 85 (94%)  | 5 (6%)   | 17          | 41 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 19  | 1X    | 77/78 (99%)   | 74 (96%)  | 3 (4%)   | 27          | 56  |
| 19  | 2X    | 77/78 (99%)   | 77 (100%) | 0        | 100         | 100 |
| 20  | 1Y    | 85/91 (93%)   | 78 (92%)  | 7 (8%)   | 9           | 23  |
| 20  | 2Y    | 85/91 (93%)   | 83 (98%)  | 2 (2%)   | 44          | 73  |
| 21  | 1Z    | 135/179 (75%) | 124 (92%) | 11 (8%)  | 9           | 23  |
| 21  | 2Z    | 137/179 (76%) | 126 (92%) | 11 (8%)  | 10          | 24  |
| 22  | 10    | 65/67 (97%)   | 61 (94%)  | 4 (6%)   | 15          | 36  |
| 22  | 20    | 65/67 (97%)   | 60 (92%)  | 5 (8%)   | 10          | 26  |
| 23  | 11    | 80/83 (96%)   | 79 (99%)  | 1 (1%)   | 65          | 85  |
| 23  | 21    | 80/83 (96%)   | 78 (98%)  | 2 (2%)   | 42          | 72  |
| 24  | 12    | 65/67 (97%)   | 63 (97%)  | 2 (3%)   | 35          | 64  |
| 24  | 22    | 65/67 (97%)   | 62 (95%)  | 3 (5%)   | 23          | 49  |
| 25  | 13    | 51/52 (98%)   | 49 (96%)  | 2 (4%)   | 27          | 56  |
| 25  | 23    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 27          | 55  |
| 26  | 14    | 59/63 (94%)   | 55 (93%)  | 4 (7%)   | 13          | 32  |
| 26  | 24    | 53/63 (84%)   | 51 (96%)  | 2 (4%)   | 28          | 56  |
| 27  | 15    | 50/52 (96%)   | 46 (92%)  | 4 (8%)   | 10          | 24  |
| 27  | 25    | 50/52 (96%)   | 46 (92%)  | 4 (8%)   | 10          | 24  |
| 28  | 16    | 51/52 (98%)   | 45 (88%)  | 6 (12%)  | 4           | 10  |
| 28  | 26    | 50/52 (96%)   | 47 (94%)  | 3 (6%)   | 16          | 38  |
| 29  | 17    | 41/42 (98%)   | 36 (88%)  | 5 (12%)  | 4           | 9   |
| 29  | 27    | 41/42 (98%)   | 37 (90%)  | 4 (10%)  | 6           | 16  |
| 30  | 18    | 54/55 (98%)   | 47 (87%)  | 7 (13%)  | 3           | 8   |
| 30  | 28    | 54/55 (98%)   | 50 (93%)  | 4 (7%)   | 11          | 28  |
| 31  | 19    | 34/34 (100%)  | 34 (100%) | 0        | 100         | 100 |
| 31  | 29    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 37          | 67  |
| 33  | 1b    | 192/220 (87%) | 184 (96%) | 8 (4%)   | 25          | 53  |
| 33  | 2b    | 187/220 (85%) | 175 (94%) | 12 (6%)  | 14          | 34  |
| 34  | 1c    | 142/188 (76%) | 137 (96%) | 5 (4%)   | 31          | 60  |
| 34  | 2c    | 140/188 (74%) | 138 (99%) | 2 (1%)   | 62          | 84  |
| 35  | 1d    | 169/181 (93%) | 160 (95%) | 9 (5%)   | 19          | 43  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 35  | 2d    | 173/181 (96%) | 161 (93%) | 12 (7%)  | 13          | 31 |
| 36  | 1e    | 113/123 (92%) | 108 (96%) | 5 (4%)   | 24          | 51 |
| 36  | 2e    | 114/123 (93%) | 109 (96%) | 5 (4%)   | 24          | 51 |
| 37  | 1f    | 84/90 (93%)   | 82 (98%)  | 2 (2%)   | 44          | 73 |
| 37  | 2f    | 85/90 (94%)   | 83 (98%)  | 2 (2%)   | 44          | 73 |
| 38  | 1g    | 119/127 (94%) | 111 (93%) | 8 (7%)   | 13          | 33 |
| 38  | 2g    | 120/127 (94%) | 116 (97%) | 4 (3%)   | 33          | 62 |
| 39  | 1h    | 114/119 (96%) | 109 (96%) | 5 (4%)   | 24          | 51 |
| 39  | 2h    | 114/119 (96%) | 109 (96%) | 5 (4%)   | 24          | 51 |
| 40  | 1i    | 90/99 (91%)   | 86 (96%)  | 4 (4%)   | 24          | 51 |
| 40  | 2i    | 89/99 (90%)   | 80 (90%)  | 9 (10%)  | 6           | 15 |
| 41  | 1j    | 66/92 (72%)   | 62 (94%)  | 4 (6%)   | 15          | 36 |
| 41  | 2j    | 69/92 (75%)   | 68 (99%)  | 1 (1%)   | 62          | 84 |
| 42  | 1k    | 82/99 (83%)   | 77 (94%)  | 5 (6%)   | 15          | 36 |
| 42  | 2k    | 83/99 (84%)   | 80 (96%)  | 3 (4%)   | 30          | 59 |
| 43  | 1l    | 96/108 (89%)  | 93 (97%)  | 3 (3%)   | 35          | 64 |
| 43  | 2l    | 96/108 (89%)  | 93 (97%)  | 3 (3%)   | 35          | 64 |
| 44  | 1m    | 93/101 (92%)  | 84 (90%)  | 9 (10%)  | 6           | 17 |
| 44  | 2m    | 92/101 (91%)  | 89 (97%)  | 3 (3%)   | 33          | 62 |
| 45  | 1n    | 49/50 (98%)   | 42 (86%)  | 7 (14%)  | 2           | 7  |
| 45  | 2n    | 49/50 (98%)   | 47 (96%)  | 2 (4%)   | 26          | 54 |
| 46  | 1o    | 78/80 (98%)   | 73 (94%)  | 5 (6%)   | 14          | 34 |
| 46  | 2o    | 78/80 (98%)   | 76 (97%)  | 2 (3%)   | 41          | 70 |
| 47  | 1p    | 69/74 (93%)   | 66 (96%)  | 3 (4%)   | 25          | 52 |
| 47  | 2p    | 68/74 (92%)   | 63 (93%)  | 5 (7%)   | 11          | 28 |
| 48  | 1q    | 94/97 (97%)   | 91 (97%)  | 3 (3%)   | 34          | 63 |
| 48  | 2q    | 94/97 (97%)   | 90 (96%)  | 4 (4%)   | 25          | 52 |
| 49  | 1r    | 59/77 (77%)   | 57 (97%)  | 2 (3%)   | 32          | 61 |
| 49  | 2r    | 59/77 (77%)   | 57 (97%)  | 2 (3%)   | 32          | 61 |
| 50  | 1s    | 69/80 (86%)   | 66 (96%)  | 3 (4%)   | 25          | 52 |
| 50  | 2s    | 67/80 (84%)   | 65 (97%)  | 2 (3%)   | 36          | 65 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 51  | 1t    | 70/82 (85%)      | 69 (99%)   | 1 (1%)   | 62          | 84  |
| 51  | 2t    | 70/82 (85%)      | 70 (100%)  | 0        | 100         | 100 |
| 52  | 1u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)   | 17          | 41  |
| 52  | 2u    | 18/22 (82%)      | 17 (94%)   | 1 (6%)   | 17          | 41  |
| 58  | A     | 9/9 (100%)       | 7 (78%)    | 2 (22%)  | 1           | 2   |
| 58  | B     | 9/9 (100%)       | 7 (78%)    | 2 (22%)  | 1           | 2   |
| All | All   | 9321/10082 (92%) | 8790 (94%) | 531 (6%) | 17          | 40  |

5 of 531 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2d    | 83  | SER  |
| 36  | 2e    | 75  | THR  |
| 35  | 2d    | 31  | CYS  |
| 48  | 2q    | 83  | ASP  |
| 30  | 18    | 14  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 2c    | 102 | ASN  |
| 49  | 2r    | 63  | GLN  |
| 36  | 2e    | 78  | HIS  |
| 40  | 2i    | 3   | GLN  |
| 50  | 2s    | 83  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2861/2915 (98%) | 407 (14%)         | 38 (1%)         |
| 1   | 2A    | 2788/2915 (95%) | 458 (16%)         | 25 (0%)         |
| 2   | 1B    | 120/121 (99%)   | 10 (8%)           | 1 (0%)          |
| 2   | 2B    | 118/121 (97%)   | 27 (22%)          | 0               |
| 32  | 1a    | 1494/1521 (98%) | 227 (15%)         | 0               |
| 53  | 1v    | 12/24 (50%)     | 2 (16%)           | 0               |
| 53  | 2v    | 12/24 (50%)     | 1 (8%)            | 0               |
| 54  | 1w    | 71/76 (93%)     | 23 (32%)          | 0               |
| 54  | 2w    | 68/76 (89%)     | 22 (32%)          | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 55  | 1x    | 75/77 (97%)     | 10 (13%)          | 0               |
| 55  | 2x    | 75/77 (97%)     | 14 (18%)          | 0               |
| 56  | 1y    | 72/76 (94%)     | 19 (26%)          | 0               |
| 56  | 2y    | 70/76 (92%)     | 18 (25%)          | 0               |
| 57  | 2a    | 1498/1521 (98%) | 260 (17%)         | 0               |
| All | All   | 9334/9620 (97%) | 1498 (16%)        | 64 (0%)         |

5 of 1498 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 12  | U    |
| 1   | 1A    | 34  | C    |
| 1   | 1A    | 45  | C    |
| 1   | 1A    | 54  | G    |
| 1   | 1A    | 70  | A    |

5 of 64 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1608 | A    |
| 1   | 2A    | 1913 | A    |
| 1   | 1A    | 1554 | A    |
| 1   | 1A    | 1425 | A    |
| 1   | 2A    | 1992 | G    |

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

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

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | G7M  | 1a    | 527  | 59,32 | 20,26,27     | 2.75 | 3 (15%)  | 16,39,42    | 0.89 | 1 (6%)   |
| 55  | PSU  | 2x    | 55   | 55    | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 2.02 | 4 (19%)  |
| 1   | 4OC  | 2A    | 1920 | 1     | 19,22,24     | 0.76 | 0        | 25,31,35    | 0.88 | 1 (4%)   |



| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 43  | 0TD  | 2l    | 92   | 43      | 8,9,10       | 4.58 | 1 (12%)  | 6,11,13     | 3.35 | 3 (50%)  |
| 55  | 4SU  | 2x    | 8    | 55,59   | 18,21,22     | 2.08 | 4 (22%)  | 25,30,33    | 1.47 | 6 (24%)  |
| 1   | PSU  | 2A    | 1917 | 1       | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 2.04 | 3 (14%)  |
| 54  | PSU  | 2w    | 32   | 54      | 18,21,22     | 1.32 | 2 (11%)  | 21,30,33    | 1.95 | 4 (19%)  |
| 55  | 5MC  | 1x    | 32   | 55      | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.22 | 2 (7%)   |
| 1   | 5MC  | 1A    | 1984 | 59,1    | 19,22,23     | 1.61 | 3 (15%)  | 26,32,35    | 1.10 | 2 (7%)   |
| 1   | OMG  | 2A    | 2251 | 55,59,1 | 19,26,27     | 0.92 | 1 (5%)   | 21,38,41    | 1.10 | 2 (9%)   |
| 56  | 4SU  | 1y    | 8    | 56      | 18,21,22     | 1.75 | 5 (27%)  | 25,30,33    | 1.99 | 5 (20%)  |
| 1   | 2MU  | 1A    | 2564 | 59,1    | 19,22,24     | 1.22 | 2 (10%)  | 25,31,36    | 2.05 | 6 (24%)  |
| 32  | 5MC  | 1a    | 1404 | 32      | 19,22,23     | 1.73 | 3 (15%)  | 26,32,35    | 1.20 | 4 (15%)  |
| 32  | PSU  | 1a    | 516  | 59,32   | 18,21,22     | 1.35 | 3 (16%)  | 21,30,33    | 1.97 | 5 (23%)  |
| 58  | BB9  | A     | 6    | 58      | 2,5,6        | 4.24 | 1 (50%)  | 1,5,7       | 2.55 | 1 (100%) |
| 54  | MIA  | 2w    | 37   | 54      | 19,27,32     | 1.94 | 2 (10%)  | 18,39,47    | 1.51 | 4 (22%)  |
| 1   | PSU  | 1A    | 1939 | 1       | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 2.07 | 3 (14%)  |
| 1   | 5MU  | 1A    | 1961 | 1       | 19,22,23     | 1.41 | 5 (26%)  | 27,32,35    | 2.38 | 6 (22%)  |
| 32  | M2G  | 1a    | 966  | 32      | 20,27,28     | 1.33 | 2 (10%)  | 19,40,43    | 1.06 | 2 (10%)  |
| 57  | 5MC  | 2a    | 1404 | 57      | 19,22,23     | 1.70 | 3 (15%)  | 26,32,35    | 1.22 | 3 (11%)  |
| 54  | MIA  | 1w    | 37   | 54      | 24,31,32     | 2.22 | 3 (12%)  | 22,44,47    | 2.47 | 6 (27%)  |
| 57  | UR3  | 2a    | 1498 | 57      | 19,22,23     | 1.02 | 1 (5%)   | 26,32,35    | 1.79 | 3 (11%)  |
| 58  | BB9  | A     | 9    | 58      | 2,5,6        | 4.61 | 1 (50%)  | 1,5,7       | 2.56 | 1 (100%) |
| 1   | 2MA  | 2A    | 2503 | 59,1    | 18,25,26     | 0.72 | 0        | 20,37,40    | 1.86 | 4 (20%)  |
| 1   | 5MC  | 1A    | 1964 | 59,1    | 19,22,23     | 1.46 | 3 (15%)  | 26,32,35    | 1.12 | 2 (7%)   |
| 32  | 5MC  | 1a    | 1400 | 32      | 19,22,23     | 1.61 | 3 (15%)  | 26,32,35    | 1.15 | 3 (11%)  |
| 58  | BB9  | B     | 17   | 58      | 2,5,6        | 4.30 | 1 (50%)  | 1,5,7       | 4.14 | 1 (100%) |
| 54  | PSU  | 1w    | 32   | 59,54   | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.93 | 3 (14%)  |
| 56  | 5MU  | 2y    | 54   | 56      | 19,22,23     | 1.52 | 5 (26%)  | 27,32,35    | 2.02 | 9 (33%)  |
| 32  | 4OC  | 1a    | 1402 | 32      | 20,23,24     | 0.75 | 0        | 25,32,35    | 1.06 | 1 (4%)   |
| 32  | 5MC  | 1a    | 967  | 32      | 19,22,23     | 1.58 | 2 (10%)  | 26,32,35    | 1.05 | 2 (7%)   |
| 57  | G7M  | 2a    | 527  | 57,59   | 20,26,27     | 2.68 | 4 (20%)  | 16,39,42    | 0.90 | 1 (6%)   |
| 32  | 2MG  | 1a    | 1207 | 32      | 18,26,27     | 0.92 | 1 (5%)   | 16,38,41    | 1.63 | 4 (25%)  |
| 57  | MA6  | 2a    | 1519 | 57      | 19,26,27     | 1.21 | 2 (10%)  | 18,38,41    | 2.03 | 4 (22%)  |
| 32  | MA6  | 1a    | 1518 | 32      | 19,26,27     | 1.11 | 2 (10%)  | 18,38,41    | 2.19 | 5 (27%)  |
| 1   | 2MU  | 2A    | 2552 | 59,1    | 19,22,24     | 1.29 | 2 (10%)  | 25,31,36    | 2.02 | 6 (24%)  |
| 57  | 5MC  | 2a    | 1407 | 57      | 19,22,23     | 1.50 | 3 (15%)  | 26,32,35    | 1.22 | 3 (11%)  |
| 57  | 5MC  | 2a    | 967  | 57      | 19,22,23     | 1.74 | 3 (15%)  | 26,32,35    | 1.09 | 2 (7%)   |

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 5MC  | 2A    | 1942 | 1       | 19,22,23     | 1.64 | 3 (15%)  | 26,32,35    | 1.16 | 2 (7%)   |
| 56  | PSU  | 1y    | 32   | 56      | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.96 | 3 (14%)  |
| 57  | 2MG  | 2a    | 1207 | 57      | 18,26,27     | 0.91 | 1 (5%)   | 16,38,41    | 1.41 | 3 (18%)  |
| 54  | 5MU  | 1w    | 54   | 54      | 19,22,23     | 1.36 | 5 (26%)  | 27,32,35    | 2.11 | 7 (25%)  |
| 54  | PSU  | 2w    | 39   | 54      | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.76 | 3 (14%)  |
| 54  | 5MU  | 2w    | 54   | 54      | 19,22,23     | 1.38 | 5 (26%)  | 27,32,35    | 1.72 | 6 (22%)  |
| 56  | G7M  | 1y    | 46   | 56      | 20,26,27     | 2.70 | 4 (20%)  | 16,39,42    | 0.84 | 1 (6%)   |
| 1   | 2MA  | 1A    | 2515 | 59,1    | 18,25,26     | 0.70 | 0        | 20,37,40    | 2.10 | 4 (20%)  |
| 58  | BB9  | B     | 9    | 58      | 2,5,6        | 4.94 | 1 (50%)  | 1,5,7       | 2.89 | 1 (100%) |
| 56  | PSU  | 1y    | 55   | 56      | 18,21,22     | 1.41 | 2 (11%)  | 21,30,33    | 2.07 | 3 (14%)  |
| 54  | PSU  | 1w    | 39   | 54      | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 1.92 | 3 (14%)  |
| 55  | 5MU  | 2x    | 54   | 55      | 19,22,23     | 1.42 | 5 (26%)  | 27,32,35    | 2.18 | 6 (22%)  |
| 1   | 5MU  | 2A    | 1915 | 1       | 19,22,23     | 1.45 | 6 (31%)  | 27,32,35    | 2.20 | 5 (18%)  |
| 1   | PSU  | 1A    | 2617 | 59,1    | 18,21,22     | 1.39 | 3 (16%)  | 21,30,33    | 2.12 | 4 (19%)  |
| 1   | 4OC  | 1A    | 1942 | 1       | 19,22,24     | 0.78 | 0        | 25,31,35    | 0.95 | 1 (4%)   |
| 54  | PSU  | 2w    | 55   | 54      | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 2.05 | 3 (14%)  |
| 58  | BB9  | A     | 17   | 58      | 2,5,6        | 4.59 | 1 (50%)  | 1,5,7       | 4.29 | 1 (100%) |
| 55  | PSU  | 1x    | 55   | 55,59   | 18,21,22     | 1.31 | 2 (11%)  | 21,30,33    | 2.04 | 4 (19%)  |
| 56  | PSU  | 2y    | 39   | 56      | 18,21,22     | 1.29 | 2 (11%)  | 21,30,33    | 2.00 | 3 (14%)  |
| 54  | PSU  | 1w    | 55   | 54      | 18,21,22     | 1.43 | 2 (11%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 32  | UR3  | 1a    | 1498 | 32      | 19,22,23     | 1.07 | 1 (5%)   | 26,32,35    | 1.79 | 4 (15%)  |
| 56  | G7M  | 2y    | 46   | 56      | 20,26,27     | 2.76 | 4 (20%)  | 16,39,42    | 0.83 | 1 (6%)   |
| 1   | 5MU  | 2A    | 1939 | 59,1    | 19,22,23     | 1.43 | 5 (26%)  | 27,32,35    | 2.38 | 6 (22%)  |
| 1   | OMG  | 1A    | 2263 | 55,59,1 | 19,26,27     | 0.91 | 1 (5%)   | 21,38,41    | 1.04 | 1 (4%)   |
| 57  | PSU  | 2a    | 516  | 57      | 18,21,22     | 1.31 | 2 (11%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 1   | PSU  | 2A    | 1911 | 1       | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 54  | G7M  | 1w    | 46   | 54      | 20,26,27     | 2.73 | 4 (20%)  | 16,39,42    | 0.87 | 1 (6%)   |
| 56  | PSU  | 2y    | 32   | 56      | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.92 | 4 (19%)  |
| 56  | 5MU  | 1y    | 54   | 56      | 19,22,23     | 1.49 | 5 (26%)  | 27,32,35    | 1.81 | 5 (18%)  |
| 1   | 5MU  | 1A    | 1937 | 1       | 19,22,23     | 1.39 | 4 (21%)  | 27,32,35    | 2.28 | 6 (22%)  |
| 56  | PSU  | 2y    | 55   | 56      | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.04 | 3 (14%)  |
| 54  | G7M  | 2w    | 46   | 54      | 20,26,27     | 2.69 | 3 (15%)  | 16,39,42    | 1.18 | 1 (6%)   |
| 55  | 5MU  | 1x    | 54   | 55,59   | 19,22,23     | 1.44 | 6 (31%)  | 27,32,35    | 2.00 | 7 (25%)  |
| 55  | 5MC  | 2x    | 32   | 55      | 19,22,23     | 1.64 | 2 (10%)  | 26,32,35    | 1.19 | 3 (11%)  |
| 58  | BB9  | B     | 6    | 58      | 2,5,6        | 4.08 | 1 (50%)  | 1,5,7       | 2.75 | 1 (100%) |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | 4SU  | 2y    | 8    | 56,59 | 18,21,22     | 1.75 | 4 (22%)  | 25,30,33    | 2.11 | 4 (16%)  |
| 54  | 4SU  | 2w    | 8    | 54    | 18,21,22     | 1.68 | 4 (22%)  | 25,30,33    | 2.49 | 5 (20%)  |
| 57  | M2G  | 2a    | 966  | 57    | 20,27,28     | 1.37 | 3 (15%)  | 19,40,43    | 1.08 | 2 (10%)  |
| 57  | 5MC  | 2a    | 1400 | 57    | 19,22,23     | 1.71 | 3 (15%)  | 26,32,35    | 1.25 | 3 (11%)  |
| 55  | 4SU  | 1x    | 8    | 55    | 18,21,22     | 2.12 | 5 (27%)  | 25,30,33    | 1.66 | 6 (24%)  |
| 32  | MA6  | 1a    | 1519 | 32    | 19,26,27     | 1.11 | 2 (10%)  | 18,38,41    | 1.99 | 5 (27%)  |
| 1   | PSU  | 1A    | 1933 | 1     | 18,21,22     | 1.43 | 2 (11%)  | 21,30,33    | 2.06 | 3 (14%)  |
| 56  | PSU  | 1y    | 39   | 56    | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 54  | 4SU  | 1w    | 8    | 54    | 18,21,22     | 1.76 | 5 (27%)  | 25,30,33    | 1.89 | 4 (16%)  |
| 32  | 5MC  | 1a    | 1407 | 32    | 19,22,23     | 1.48 | 3 (15%)  | 26,32,35    | 1.13 | 2 (7%)   |
| 57  | MA6  | 2a    | 1518 | 57    | 19,26,27     | 1.17 | 2 (10%)  | 18,38,41    | 2.27 | 5 (27%)  |
| 57  | 4OC  | 2a    | 1402 | 57    | 20,23,24     | 0.77 | 0        | 25,32,35    | 1.06 | 2 (8%)   |
| 1   | 5MC  | 2A    | 1962 | 59,1  | 19,22,23     | 1.70 | 3 (15%)  | 26,32,35    | 1.18 | 3 (11%)  |
| 43  | 0TD  | 1l    | 92   | 43    | 8,9,10       | 4.50 | 1 (12%)  | 6,11,13     | 2.36 | 2 (33%)  |
| 1   | PSU  | 2A    | 2605 | 1     | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 2.10 | 5 (23%)  |

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  | G7M  | 1a    | 527  | 59,32   | -       | 3/3/25/26 | 0/3/3/3 |
| 55  | PSU  | 2x    | 55   | 55      | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 4OC  | 2A    | 1920 | 1       | -       | 0/9/27/30 | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43      | -       | 1/7/12/14 | -       |
| 55  | 4SU  | 2x    | 8    | 55,59   | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 2A    | 1917 | 1       | -       | 1/7/25/26 | 0/2/2/2 |
| 54  | PSU  | 2w    | 32   | 54      | -       | 0/7/25/26 | 0/2/2/2 |
| 55  | 5MC  | 1x    | 32   | 55      | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1984 | 59,1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 55,59,1 | -       | 0/5/27/28 | 0/3/3/3 |
| 56  | 4SU  | 1y    | 8    | 56      | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 2MU  | 1A    | 2564 | 59,1    | -       | 0/9/27/28 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1404 | 32      | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | PSU  | 1a    | 516  | 59,32   | -       | 0/7/25/26 | 0/2/2/2 |
| 58  | BB9  | A     | 6    | 58      | -       | 0/0/4/6   | -       |
| 54  | MIA  | 2w    | 37   | 54      | -       | 2/7/29/34 | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 1   | PSU  | 1A    | 1939 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1961 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32    | -       | 0/7/29/30  | 0/3/3/3 |
| 57  | 5MC  | 2a    | 1404 | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | MIA  | 1w    | 37   | 54    | -       | 2/11/33/34 | 0/3/3/3 |
| 57  | UR3  | 2a    | 1498 | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | BB9  | A     | 9    | 58    | -       | 0/0/4/6    | -       |
| 1   | 2MA  | 2A    | 2503 | 59,1  | -       | 1/3/25/26  | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1964 | 59,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1400 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | BB9  | B     | 17   | 58    | -       | 0/0/4/6    | -       |
| 54  | PSU  | 1w    | 32   | 59,54 | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | 5MU  | 2y    | 54   | 56    | -       | 3/7/25/26  | 0/2/2/2 |
| 32  | 4OC  | 1a    | 1402 | 32    | -       | 2/9/29/30  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 967  | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | G7M  | 2a    | 527  | 57,59 | -       | 3/3/25/26  | 0/3/3/3 |
| 32  | 2MG  | 1a    | 1207 | 32    | -       | 0/5/27/28  | 0/3/3/3 |
| 57  | MA6  | 2a    | 1519 | 57    | -       | 4/7/29/30  | 0/3/3/3 |
| 32  | MA6  | 1a    | 1518 | 32    | -       | 0/7/29/30  | 0/3/3/3 |
| 1   | 2MU  | 2A    | 2552 | 59,1  | -       | 0/9/27/28  | 0/2/2/2 |
| 57  | 5MC  | 2a    | 1407 | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | 5MC  | 2a    | 967  | 57    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | PSU  | 1y    | 32   | 56    | -       | 0/7/25/26  | 0/2/2/2 |
| 57  | 2MG  | 2a    | 1207 | 57    | -       | 2/5/27/28  | 0/3/3/3 |
| 54  | 5MU  | 1w    | 54   | 54    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 2w    | 39   | 54    | -       | 0/7/25/26  | 0/2/2/2 |
| 54  | 5MU  | 2w    | 54   | 54    | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | G7M  | 1y    | 46   | 56    | -       | 1/3/25/26  | 0/3/3/3 |
| 1   | 2MA  | 1A    | 2515 | 59,1  | -       | 1/3/25/26  | 0/3/3/3 |
| 58  | BB9  | B     | 9    | 58    | -       | 0/0/4/6    | -       |
| 56  | PSU  | 1y    | 55   | 56    | -       | 1/7/25/26  | 0/2/2/2 |
| 54  | PSU  | 1w    | 39   | 54    | -       | 0/7/25/26  | 0/2/2/2 |
| 55  | 5MU  | 2x    | 54   | 55    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1915 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2617 | 59,1  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4OC  | 1A    | 1942 | 1     | -       | 1/9/27/30  | 0/2/2/2 |
| 54  | PSU  | 2w    | 55   | 54    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | BB9  | A     | 17   | 58    | -       | 0/0/4/6    | -       |
| 55  | PSU  | 1x    | 55   | 55,59 | -       | 0/7/25/26  | 0/2/2/2 |
| 56  | PSU  | 2y    | 39   | 56    | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link    | Chirals | Torsions  | Rings   |
|-----|------|-------|------|---------|---------|-----------|---------|
| 54  | PSU  | 1w    | 55   | 54      | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | UR3  | 1a    | 1498 | 32      | -       | 0/7/25/26 | 0/2/2/2 |
| 56  | G7M  | 2y    | 46   | 56      | -       | 1/3/25/26 | 0/3/3/3 |
| 1   | 5MU  | 2A    | 1939 | 59,1    | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMG  | 1A    | 2263 | 55,59,1 | -       | 0/5/27/28 | 0/3/3/3 |
| 57  | PSU  | 2a    | 516  | 57      | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1       | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | G7M  | 1w    | 46   | 54      | -       | 3/3/25/26 | 0/3/3/3 |
| 56  | PSU  | 2y    | 32   | 56      | -       | 0/7/25/26 | 0/2/2/2 |
| 56  | 5MU  | 1y    | 54   | 56      | -       | 2/7/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1937 | 1       | -       | 0/7/25/26 | 0/2/2/2 |
| 56  | PSU  | 2y    | 55   | 56      | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | G7M  | 2w    | 46   | 54      | -       | 3/3/25/26 | 0/3/3/3 |
| 55  | 5MU  | 1x    | 54   | 55,59   | -       | 0/7/25/26 | 0/2/2/2 |
| 55  | 5MC  | 2x    | 32   | 55      | -       | 0/7/25/26 | 0/2/2/2 |
| 58  | BB9  | B     | 6    | 58      | -       | 0/0/4/6   | -       |
| 56  | 4SU  | 2y    | 8    | 56,59   | -       | 2/7/25/26 | 0/2/2/2 |
| 54  | 4SU  | 2w    | 8    | 54      | -       | 0/7/25/26 | 0/2/2/2 |
| 57  | M2G  | 2a    | 966  | 57      | -       | 0/7/29/30 | 0/3/3/3 |
| 57  | 5MC  | 2a    | 1400 | 57      | -       | 4/7/25/26 | 0/2/2/2 |
| 55  | 4SU  | 1x    | 8    | 55      | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | MA6  | 1a    | 1519 | 32      | -       | 3/7/29/30 | 0/3/3/3 |
| 1   | PSU  | 1A    | 1933 | 1       | -       | 0/7/25/26 | 0/2/2/2 |
| 56  | PSU  | 1y    | 39   | 56      | -       | 0/7/25/26 | 0/2/2/2 |
| 54  | 4SU  | 1w    | 8    | 54      | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32      | -       | 0/7/25/26 | 0/2/2/2 |
| 57  | MA6  | 2a    | 1518 | 57      | -       | 3/7/29/30 | 0/3/3/3 |
| 57  | 4OC  | 2a    | 1402 | 57      | -       | 2/9/29/30 | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 59,1    | -       | 0/7/25/26 | 0/2/2/2 |
| 43  | 0TD  | 1l    | 92   | 43      | -       | 2/7/12/14 | -       |
| 1   | PSU  | 2A    | 2605 | 1       | -       | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 222 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 43  | 2l    | 92  | 0TD  | CB-SB | -12.66 | 1.69        | 1.82     |
| 43  | 1l    | 92  | 0TD  | CB-SB | -12.29 | 1.69        | 1.82     |
| 32  | 1a    | 527 | G7M  | C8-N9 | 7.96   | 1.47        | 1.33     |
| 56  | 2y    | 46  | G7M  | C8-N9 | 7.79   | 1.47        | 1.33     |
| 54  | 1w    | 46  | G7M  | C8-N9 | 7.78   | 1.47        | 1.33     |

The worst 5 of 300 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54  | 1w    | 37   | MIA  | C12-C13-C14 | -9.00 | 110.85      | 127.01   |
| 54  | 2w    | 8    | 4SU  | C4-N3-C2    | -7.73 | 119.90      | 127.31   |
| 57  | 2a    | 1498 | UR3  | C4-N3-C2    | -7.14 | 118.83      | 124.58   |
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB   | -7.10 | 89.59       | 102.36   |
| 1   | 1A    | 2515 | 2MA  | C2-N3-C4    | 7.02  | 121.13      | 115.46   |

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | 1l    | 92  | 0TD  | CA-CB-SB-CSB    |
| 43  | 1l    | 92  | 0TD  | CG-CB-SB-CSB    |
| 54  | 1w    | 37  | MIA  | C12-C13-C14-C15 |
| 54  | 1w    | 37  | MIA  | C12-C13-C14-C16 |
| 56  | 1y    | 8   | 4SU  | O4'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2940 ligands modelled in this entry, 2938 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 61  | SF4  | 2d    | 501 | 35   | 0,12,12      | -    | -           | -           |      |             |
| 61  | SF4  | 1d    | 501 | 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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 61  | SF4  | 2d    | 501 | 35   | -       | -        | 0/6/5/5 |
| 61  | SF4  | 1d    | 501 | 35   | -       | -        | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%) | -0.62  | 128 (4%) 39 37 | 13, 29, 85, 99        | 0     |
| 1   | 2A    | 2789/2915 (95%) | -0.02  | 132 (4%) 37 35 | 25, 51, 87, 102       | 0     |
| 2   | 1B    | 120/121 (99%)   | -0.52  | 0 100 100      | 23, 41, 55, 80        | 0     |
| 2   | 2B    | 120/121 (99%)   | 0.94   | 4 (3%) 49 47   | 55, 72, 80, 89        | 0     |
| 3   | 1D    | 275/276 (99%)   | -0.37  | 3 (1%) 77 77   | 14, 29, 45, 72        | 0     |
| 3   | 2D    | 275/276 (99%)   | 0.05   | 6 (2%) 62 61   | 25, 43, 57, 71        | 0     |
| 4   | 1E    | 204/206 (99%)   | -0.41  | 0 100 100      | 14, 32, 53, 71        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.24   | 3 (1%) 71 71   | 28, 53, 65, 73        | 0     |
| 5   | 1F    | 203/210 (96%)   | -0.33  | 0 100 100      | 15, 35, 60, 77        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.31   | 4 (1%) 64 64   | 30, 61, 75, 83        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.23   | 6 (3%) 49 47   | 33, 50, 66, 81        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.38   | 28 (15%) 6 6   | 62, 73, 81, 89        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.01   | 3 (1%) 69 68   | 31, 45, 59, 63        | 0     |
| 7   | 2H    | 174/180 (96%)   | 1.40   | 33 (18%) 4 4   | 65, 78, 84, 88        | 0     |
| 8   | 1I    | 146/148 (98%)   | 0.62   | 1 (0%) 84 83   | 37, 66, 76, 80        | 0     |
| 8   | 2I    | 146/148 (98%)   | 0.73   | 6 (4%) 42 40   | 48, 65, 75, 81        | 0     |
| 9   | 1N    | 140/140 (100%)  | -0.34  | 1 (0%) 84 83   | 18, 31, 53, 63        | 0     |
| 9   | 2N    | 140/140 (100%)  | 0.55   | 2 (1%) 73 73   | 40, 57, 71, 79        | 0     |
| 10  | 1O    | 122/122 (100%)  | -0.37  | 0 100 100      | 21, 32, 48, 54        | 0     |
| 10  | 2O    | 122/122 (100%)  | 0.24   | 1 (0%) 82 82   | 41, 53, 63, 68        | 0     |
| 11  | 1P    | 149/150 (99%)   | -0.20  | 1 (0%) 84 83   | 14, 37, 63, 72        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.37   | 0 100 100      | 29, 61, 75, 82        | 0     |
| 12  | 1Q    | 141/141 (100%)  | -0.37  | 1 (0%) 84 83   | 21, 32, 50, 67        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 0.82   | 11 (7%) 20 19  | 40, 61, 72, 76        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | -0.52  | 0 100 100     | 18, 27, 41, 48        | 0     |
| 13  | 2R    | 118/118 (100%) | -0.01  | 1 (0%) 82 82  | 34, 45, 55, 65        | 0     |
| 14  | 1S    | 110/112 (98%)  | -0.11  | 0 100 100     | 30, 41, 54, 59        | 0     |
| 14  | 2S    | 110/112 (98%)  | 1.17   | 15 (13%) 8 7  | 56, 67, 75, 80        | 0     |
| 15  | 1T    | 131/146 (89%)  | -0.12  | 2 (1%) 71 71  | 24, 35, 61, 70        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.36   | 2 (1%) 71 71  | 44, 55, 73, 77        | 0     |
| 16  | 1U    | 116/118 (98%)  | -0.71  | 0 100 100     | 15, 23, 37, 54        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.34   | 0 100 100     | 38, 55, 69, 76        | 0     |
| 17  | 1V    | 101/101 (100%) | -0.51  | 0 100 100     | 15, 32, 47, 57        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.74   | 2 (1%) 64 64  | 35, 64, 70, 75        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.54  | 1 (0%) 81 80  | 17, 25, 44, 78        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.08   | 3 (2%) 56 54  | 31, 42, 59, 87        | 0     |
| 19  | 1X    | 95/96 (98%)    | -0.27  | 2 (2%) 63 63  | 17, 31, 52, 73        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.37   | 3 (3%) 50 48  | 38, 53, 65, 76        | 0     |
| 20  | 1Y    | 107/110 (97%)  | -0.02  | 3 (2%) 55 53  | 28, 42, 62, 77        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 0.87   | 7 (6%) 26 24  | 50, 65, 73, 80        | 0     |
| 21  | 1Z    | 154/206 (74%)  | 0.44   | 8 (5%) 34 31  | 33, 56, 77, 85        | 0     |
| 21  | 2Z    | 160/206 (77%)  | 1.50   | 39 (24%) 2 2  | 63, 76, 86, 89        | 0     |
| 22  | 10    | 83/85 (97%)    | -0.12  | 4 (4%) 36 35  | 22, 29, 51, 60        | 0     |
| 22  | 20    | 83/85 (97%)    | 0.99   | 9 (10%) 12 12 | 39, 58, 67, 74        | 0     |
| 23  | 11    | 97/98 (98%)    | -0.05  | 2 (2%) 63 63  | 20, 36, 62, 70        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.40   | 2 (2%) 63 63  | 33, 49, 69, 73        | 0     |
| 24  | 12    | 70/72 (97%)    | -0.05  | 1 (1%) 73 73  | 29, 41, 53, 67        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.39   | 1 (1%) 73 73  | 52, 63, 71, 76        | 0     |
| 25  | 13    | 59/60 (98%)    | -0.39  | 2 (3%) 48 46  | 17, 28, 50, 75        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.65   | 4 (6%) 25 23  | 46, 58, 75, 84        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.72   | 10 (14%) 7 6  | 41, 65, 81, 87        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.75   | 25 (36%) 1 1  | 71, 79, 87, 89        | 0     |
| 27  | 15    | 59/60 (98%)    | -0.58  | 1 (1%) 69 68  | 15, 24, 44, 53        | 0     |
| 27  | 25    | 59/60 (98%)    | -0.07  | 0 100 100     | 31, 46, 56, 72        | 0     |
| 28  | 16    | 53/54 (98%)    | -0.46  | 0 100 100     | 25, 34, 49, 56        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.42   | 0 100 100     | 42, 54, 63, 68        | 0     |
| 29  | 17    | 48/49 (97%)     | -0.50  | 1 (2%) 63 63  | 16, 22, 47, 54        | 0     |
| 29  | 27    | 48/49 (97%)     | -0.12  | 1 (2%) 63 63  | 27, 34, 57, 66        | 0     |
| 30  | 18    | 64/65 (98%)     | -0.53  | 0 100 100     | 21, 26, 36, 48        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.29   | 0 100 100     | 40, 49, 57, 60        | 0     |
| 31  | 19    | 37/37 (100%)    | -0.42  | 0 100 100     | 22, 31, 48, 53        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.08   | 3 (8%) 19 18  | 55, 63, 72, 73        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.17   | 48 (3%) 50 48 | 28, 57, 86, 101       | 0     |
| 33  | 1b    | 231/256 (90%)   | 1.08   | 35 (15%) 6 6  | 57, 72, 82, 90        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.49   | 57 (24%) 2 2  | 67, 80, 86, 91        | 0     |
| 34  | 1c    | 206/239 (86%)   | 0.70   | 5 (2%) 59 58  | 51, 64, 75, 82        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.64   | 66 (32%) 1 1  | 67, 78, 83, 88        | 0     |
| 35  | 1d    | 208/209 (99%)   | 0.82   | 14 (6%) 25 23 | 49, 61, 73, 81        | 0     |
| 35  | 2d    | 208/209 (99%)   | 1.03   | 19 (9%) 16 15 | 56, 66, 74, 81        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.44   | 2 (1%) 73 73  | 44, 55, 68, 72        | 0     |
| 36  | 2e    | 148/162 (91%)   | 1.39   | 28 (18%) 4 4  | 60, 72, 79, 84        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.49   | 0 100 100     | 44, 60, 69, 77        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.43   | 1 (1%) 79 79  | 50, 61, 69, 78        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.40   | 9 (5%) 30 28  | 46, 61, 74, 86        | 0     |
| 38  | 2g    | 155/156 (99%)   | 0.96   | 15 (9%) 15 14 | 62, 71, 80, 85        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.54   | 3 (2%) 62 61  | 48, 58, 65, 72        | 0     |
| 39  | 2h    | 137/138 (99%)   | 1.03   | 8 (5%) 30 28  | 60, 71, 76, 81        | 0     |
| 40  | 1i    | 127/128 (99%)   | 0.74   | 8 (6%) 27 25  | 47, 67, 76, 80        | 0     |
| 40  | 2i    | 127/128 (99%)   | 1.76   | 47 (37%) 1 1  | 66, 76, 82, 84        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.19   | 18 (18%) 4 4  | 48, 70, 80, 85        | 0     |
| 41  | 2j    | 96/105 (91%)    | 1.92   | 36 (37%) 1 1  | 70, 79, 87, 91        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.51   | 6 (5%) 33 31  | 36, 57, 68, 76        | 0     |
| 42  | 2k    | 114/129 (88%)   | 0.87   | 10 (8%) 17 16 | 48, 65, 74, 78        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.21   | 3 (2%) 58 57  | 36, 45, 57, 62        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.72   | 7 (5%) 30 28  | 48, 61, 71, 76        | 0     |
| 44  | 1m    | 123/126 (97%)   | 0.37   | 4 (3%) 49 47  | 46, 60, 69, 73        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 2m    | 122/126 (96%)     | 1.50   | 28 (22%) 2 3    | 65, 75, 80, 82        | 0     |
| 45  | 1n    | 60/61 (98%)       | 0.51   | 1 (1%) 69 68    | 50, 57, 66, 69        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.14   | 30 (50%) 0 1    | 70, 77, 81, 83        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.40   | 5 (5%) 30 28    | 42, 56, 67, 74        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.70   | 4 (4%) 39 37    | 53, 67, 75, 77        | 0     |
| 47  | 1p    | 82/88 (93%)       | 0.76   | 1 (1%) 76 76    | 48, 59, 69, 71        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.82   | 6 (7%) 22 20    | 55, 63, 70, 73        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.41   | 1 (1%) 79 79    | 47, 58, 70, 72        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.73   | 3 (3%) 52 50    | 56, 65, 74, 79        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.41   | 2 (2%) 54 52    | 49, 58, 70, 72        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.55   | 1 (1%) 71 71    | 53, 64, 74, 79        | 0     |
| 50  | 1s    | 83/93 (89%)       | 0.57   | 5 (6%) 29 27    | 52, 62, 70, 77        | 0     |
| 50  | 2s    | 83/93 (89%)       | 1.99   | 32 (38%) 1 1    | 71, 79, 85, 86        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.78   | 7 (7%) 22 20    | 49, 60, 71, 77        | 0     |
| 51  | 2t    | 96/106 (90%)      | 0.70   | 6 (6%) 27 25    | 54, 64, 75, 77        | 0     |
| 52  | 1u    | 23/27 (85%)       | 0.85   | 2 (8%) 17 16    | 53, 57, 63, 66        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.00   | 12 (52%) 0 1    | 68, 73, 77, 79        | 0     |
| 53  | 1v    | 13/24 (54%)       | 0.37   | 2 (15%) 6 6     | 41, 47, 71, 95        | 0     |
| 53  | 2v    | 13/24 (54%)       | 1.71   | 4 (30%) 1 2     | 59, 72, 89, 91        | 0     |
| 54  | 1w    | 67/76 (88%)       | 1.32   | 17 (25%) 2 2    | 34, 80, 94, 98        | 0     |
| 54  | 2w    | 65/76 (85%)       | 1.85   | 25 (38%) 1 1    | 52, 89, 95, 101       | 0     |
| 55  | 1x    | 72/77 (93%)       | 0.36   | 6 (8%) 19 17    | 28, 59, 75, 84        | 0     |
| 55  | 2x    | 72/77 (93%)       | 0.88   | 2 (2%) 55 53    | 43, 72, 83, 85        | 0     |
| 56  | 1y    | 68/76 (89%)       | 1.08   | 8 (11%) 10 10   | 28, 84, 91, 95        | 0     |
| 56  | 2y    | 67/76 (88%)       | 1.55   | 18 (26%) 2 2    | 46, 90, 94, 97        | 0     |
| 57  | 2a    | 1491/1521 (98%)   | 0.72   | 132 (8%) 17 16  | 42, 70, 89, 101       | 0     |
| 58  | A     | 13/18 (72%)       | 0.03   | 2 (15%) 6 6     | 17, 21, 65, 77        | 0     |
| 58  | B     | 13/18 (72%)       | 0.88   | 2 (15%) 6 6     | 32, 35, 69, 80        | 0     |
| All | All   | 20903/21784 (95%) | 0.28   | 1341 (6%) 27 24 | 13, 56, 83, 102       | 0     |

The worst 5 of 1341 RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 23  | 21    | 2       | SER  | 7.6  |
| 45  | 1n    | 2       | ALA  | 6.9  |
| 57  | 2a    | 1030(B) | C    | 6.2  |
| 1   | 2A    | 883     | G    | 6.1  |
| 38  | 1g    | 80      | VAL  | 6.1  |

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

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | PSU  | 2y    | 55   | 20/21 | 0.46 | 0.18 | 89,99,107,116              | 0     |
| 54  | G7M  | 2w    | 46   | 24/25 | 0.52 | 0.17 | 80,88,101,118              | 0     |
| 56  | 5MU  | 2y    | 54   | 21/22 | 0.54 | 0.16 | 86,91,105,122              | 0     |
| 56  | G7M  | 2y    | 46   | 24/25 | 0.54 | 0.18 | 82,90,99,118               | 0     |
| 56  | G7M  | 1y    | 46   | 24/25 | 0.55 | 0.18 | 80,88,98,108               | 0     |
| 54  | G7M  | 1w    | 46   | 24/25 | 0.58 | 0.18 | 70,80,100,123              | 0     |
| 56  | PSU  | 1y    | 55   | 20/21 | 0.62 | 0.14 | 84,90,100,105              | 0     |
| 56  | 5MU  | 1y    | 54   | 21/22 | 0.66 | 0.15 | 76,85,92,104               | 0     |
| 56  | 4SU  | 2y    | 8    | 20/21 | 0.67 | 0.14 | 85,90,98,107               | 0     |
| 56  | PSU  | 2y    | 32   | 20/21 | 0.74 | 0.14 | 74,82,94,96                | 0     |
| 54  | 4SU  | 2w    | 8    | 20/21 | 0.75 | 0.12 | 82,88,103,107              | 0     |
| 58  | BB9  | B     | 17   | 6/7   | 0.75 | 0.31 | 68,79,86,100               | 0     |
| 56  | 4SU  | 1y    | 8    | 20/21 | 0.77 | 0.14 | 83,88,102,104              | 0     |
| 54  | PSU  | 2w    | 55   | 20/21 | 0.78 | 0.12 | 73,83,90,98                | 0     |
| 56  | PSU  | 2y    | 39   | 20/21 | 0.79 | 0.14 | 72,80,86,98                | 0     |
| 54  | 4SU  | 1w    | 8    | 20/21 | 0.79 | 0.14 | 72,81,89,91                | 0     |
| 55  | 5MU  | 2x    | 54   | 21/22 | 0.82 | 0.14 | 70,77,80,92                | 0     |
| 55  | PSU  | 2x    | 55   | 20/21 | 0.83 | 0.13 | 69,73,79,80                | 0     |
| 57  | 2MG  | 2a    | 1207 | 24/25 | 0.84 | 0.14 | 72,80,87,88                | 0     |
| 56  | PSU  | 1y    | 32   | 20/21 | 0.84 | 0.13 | 70,78,86,87                | 0     |
| 54  | PSU  | 2w    | 32   | 20/21 | 0.85 | 0.12 | 70,77,85,91                | 0     |
| 54  | 5MU  | 2w    | 54   | 21/22 | 0.86 | 0.11 | 67,75,81,86                | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.86 | 0.16 | 41,42,49,76                | 0     |
| 58  | BB9  | A     | 17   | 6/7   | 0.86 | 0.19 | 54,69,80,92                | 0     |
| 55  | 4SU  | 2x    | 8    | 20/21 | 0.86 | 0.12 | 70,75,79,81                | 0     |
| 56  | PSU  | 1y    | 39   | 20/21 | 0.87 | 0.11 | 69,73,78,82                | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.87 | 0.16 | 58,62,66,84                | 0     |
| 57  | M2G  | 2a    | 966  | 25/26 | 0.87 | 0.15 | 56,62,75,78                | 0     |
| 54  | PSU  | 1w    | 55   | 20/21 | 0.89 | 0.10 | 53,69,78,80                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | 5MC  | 2a    | 967  | 21/22 | 0.91 | 0.12 | 60,65,76,77                 | 0     |
| 55  | 5MC  | 2x    | 32   | 21/22 | 0.91 | 0.13 | 62,66,70,75                 | 0     |
| 57  | PSU  | 2a    | 516  | 20/21 | 0.91 | 0.11 | 58,66,72,72                 | 0     |
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.91 | 0.10 | 58,65,68,73                 | 0     |
| 55  | 5MU  | 1x    | 54   | 21/22 | 0.92 | 0.10 | 54,61,65,73                 | 0     |
| 57  | 5MC  | 2a    | 1400 | 21/22 | 0.92 | 0.14 | 58,64,70,74                 | 0     |
| 57  | 4OC  | 2a    | 1402 | 22/23 | 0.92 | 0.12 | 48,57,64,65                 | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.92 | 0.10 | 50,55,60,77                 | 0     |
| 54  | PSU  | 1w    | 32   | 20/21 | 0.92 | 0.10 | 53,59,72,72                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.93 | 0.09 | 51,60,68,71                 | 0     |
| 54  | MIA  | 2w    | 37   | 25/30 | 0.93 | 0.10 | 63,70,76,77                 | 0     |
| 57  | G7M  | 2a    | 527  | 24/25 | 0.93 | 0.11 | 46,55,64,74                 | 0     |
| 57  | 5MC  | 2a    | 1404 | 21/22 | 0.93 | 0.10 | 46,51,59,64                 | 0     |
| 57  | 5MC  | 2a    | 1407 | 21/22 | 0.93 | 0.11 | 38,49,54,63                 | 0     |
| 54  | PSU  | 2w    | 39   | 20/21 | 0.93 | 0.10 | 65,72,79,80                 | 0     |
| 55  | PSU  | 1x    | 55   | 20/21 | 0.93 | 0.09 | 52,56,67,69                 | 0     |
| 1   | 4OC  | 2A    | 1920 | 21/23 | 0.94 | 0.09 | 50,55,58,59                 | 0     |
| 1   | 5MU  | 1A    | 1937 | 21/22 | 0.94 | 0.10 | 39,44,52,54                 | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.94 | 0.10 | 50,60,65,66                 | 0     |
| 55  | 4SU  | 1x    | 8    | 20/21 | 0.95 | 0.09 | 48,55,66,78                 | 0     |
| 57  | UR3  | 2a    | 1498 | 21/22 | 0.95 | 0.11 | 44,50,56,60                 | 0     |
| 57  | MA6  | 2a    | 1518 | 24/25 | 0.95 | 0.10 | 42,58,62,63                 | 0     |
| 57  | MA6  | 2a    | 1519 | 24/25 | 0.95 | 0.12 | 47,54,62,63                 | 0     |
| 54  | 5MU  | 1w    | 54   | 21/22 | 0.95 | 0.08 | 45,59,64,65                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.95 | 0.08 | 31,43,52,61                 | 0     |
| 55  | 5MC  | 1x    | 32   | 21/22 | 0.96 | 0.09 | 39,46,52,57                 | 0     |
| 1   | PSU  | 1A    | 1939 | 20/21 | 0.96 | 0.09 | 36,41,45,46                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.96 | 0.09 | 30,35,38,42                 | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.96 | 0.09 | 39,50,56,63                 | 0     |
| 54  | MIA  | 1w    | 37   | 29/30 | 0.96 | 0.09 | 36,44,57,62                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.96 | 0.07 | 45,49,50,51                 | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.96 | 0.08 | 31,38,45,46                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.96 | 0.10 | 39,44,51,60                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.97 | 0.07 | 33,37,41,47                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.09 | 26,30,33,36                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.08 | 24,33,36,37                 | 0     |
| 1   | 4OC  | 1A    | 1942 | 21/23 | 0.97 | 0.07 | 29,34,37,40                 | 0     |
| 1   | 5MC  | 1A    | 1964 | 21/22 | 0.97 | 0.07 | 24,31,36,43                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.97 | 0.08 | 42,45,51,54                 | 0     |
| 1   | PSU  | 1A    | 1933 | 20/21 | 0.97 | 0.08 | 31,38,41,42                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.97 | 0.07 | 30,41,43,48                 | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.97 | 0.07 | 33,38,43,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.08 | 30,33,39,42                 | 0     |
| 54  | PSU  | 1w    | 39   | 20/21 | 0.97 | 0.08 | 44,50,59,59                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.97 | 0.07 | 29,33,37,40                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.97 | 0.07 | 27,33,37,40                 | 0     |
| 1   | 5MC  | 1A    | 1984 | 21/22 | 0.98 | 0.05 | 18,26,30,37                 | 0     |
| 1   | 2MU  | 1A    | 2564 | 21/23 | 0.98 | 0.07 | 16,22,26,31                 | 0     |
| 1   | PSU  | 1A    | 2617 | 20/21 | 0.98 | 0.06 | 15,18,23,24                 | 0     |
| 1   | 5MU  | 1A    | 1961 | 21/22 | 0.98 | 0.07 | 15,20,24,26                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.98 | 0.06 | 27,33,37,39                 | 0     |
| 58  | BB9  | A     | 6    | 6/7   | 0.98 | 0.05 | 20,21,22,23                 | 0     |
| 58  | BB9  | B     | 9    | 6/7   | 0.98 | 0.07 | 32,35,36,37                 | 0     |
| 1   | 2MU  | 2A    | 2552 | 21/23 | 0.98 | 0.07 | 32,37,41,46                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.98 | 0.07 | 25,33,36,39                 | 0     |
| 58  | BB9  | A     | 9    | 6/7   | 0.99 | 0.05 | 14,16,16,19                 | 0     |
| 1   | OMG  | 1A    | 2263 | 24/25 | 0.99 | 0.04 | 15,19,22,25                 | 0     |
| 1   | 2MA  | 1A    | 2515 | 23/24 | 0.99 | 0.05 | 10,14,17,22                 | 0     |
| 58  | BB9  | B     | 6    | 6/7   | 0.99 | 0.05 | 23,30,33,35                 | 0     |

### 6.3 Carbohydrates

There are no monosaccharides 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2j    | 8002 | 1/1   | 0.36 | 0.17 | 85,85,85,85                 | 0     |
| 59  | MG   | 1A    | 3445 | 1/1   | 0.43 | 0.31 | 55,55,55,55                 | 0     |
| 59  | MG   | 2a    | 3113 | 1/1   | 0.44 | 0.31 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3528 | 1/1   | 0.45 | 0.32 | 81,81,81,81                 | 0     |
| 59  | MG   | 2A    | 3447 | 1/1   | 0.53 | 0.18 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 4115 | 1/1   | 0.55 | 0.23 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3259 | 1/1   | 0.56 | 0.19 | 82,82,82,82                 | 0     |
| 59  | MG   | 2A    | 3781 | 1/1   | 0.56 | 0.25 | 63,63,63,63                 | 0     |
| 59  | MG   | 2y    | 3005 | 1/1   | 0.56 | 0.19 | 98,98,98,98                 | 0     |
| 59  | MG   | 1w    | 111  | 1/1   | 0.58 | 0.30 | 80,80,80,80                 | 0     |
| 59  | MG   | 2A    | 3075 | 1/1   | 0.59 | 0.22 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3548 | 1/1   | 0.59 | 0.34 | 74,74,74,74                 | 0     |
| 59  | MG   | 2A    | 3520 | 1/1   | 0.61 | 0.18 | 79,79,79,79                 | 0     |
| 59  | MG   | 2v    | 103  | 1/1   | 0.61 | 0.32 | 70,70,70,70                 | 0     |
| 59  | MG   | 1y    | 104  | 1/1   | 0.61 | 0.40 | 80,80,80,80                 | 0     |
| 59  | MG   | 1A    | 3819 | 1/1   | 0.62 | 0.15 | 23,23,23,23                 | 0     |
| 59  | MG   | 1y    | 102  | 1/1   | 0.62 | 0.18 | 77,77,77,77                 | 0     |
| 59  | MG   | 2a    | 3221 | 1/1   | 0.62 | 0.30 | 76,76,76,76                 | 0     |
| 59  | MG   | 1y    | 105  | 1/1   | 0.63 | 0.17 | 80,80,80,80                 | 0     |
| 59  | MG   | 2A    | 3619 | 1/1   | 0.63 | 0.24 | 60,60,60,60                 | 0     |
| 59  | MG   | 1B    | 229  | 1/1   | 0.64 | 0.16 | 69,69,69,69                 | 0     |
| 59  | MG   | 2a    | 3211 | 1/1   | 0.64 | 0.28 | 65,65,65,65                 | 0     |
| 59  | MG   | 2U    | 202  | 1/1   | 0.65 | 0.25 | 69,69,69,69                 | 0     |
| 59  | MG   | 1B    | 225  | 1/1   | 0.65 | 0.17 | 59,59,59,59                 | 0     |
| 59  | MG   | 2a    | 3206 | 1/1   | 0.65 | 0.21 | 74,74,74,74                 | 0     |
| 59  | MG   | 1A    | 3420 | 1/1   | 0.65 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3482 | 1/1   | 0.67 | 0.28 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3191 | 1/1   | 0.68 | 0.20 | 59,59,59,59                 | 0     |
| 59  | MG   | 1a    | 3358 | 1/1   | 0.68 | 0.26 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 4118 | 1/1   | 0.68 | 0.18 | 69,69,69,69                 | 0     |
| 59  | MG   | 2j    | 8001 | 1/1   | 0.69 | 0.15 | 63,63,63,63                 | 0     |
| 59  | MG   | 1Z    | 303  | 1/1   | 0.69 | 0.10 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 3926 | 1/1   | 0.69 | 0.19 | 22,22,22,22                 | 0     |
| 59  | MG   | 2w    | 3004 | 1/1   | 0.69 | 0.17 | 75,75,75,75                 | 0     |
| 59  | MG   | 2a    | 3180 | 1/1   | 0.69 | 0.24 | 74,74,74,74                 | 0     |
| 59  | MG   | 1B    | 220  | 1/1   | 0.70 | 0.24 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3265 | 1/1   | 0.70 | 0.37 | 73,73,73,73                 | 0     |
| 59  | MG   | 2A    | 3733 | 1/1   | 0.70 | 0.23 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3146 | 1/1   | 0.70 | 0.21 | 78,78,78,78                 | 0     |
| 59  | MG   | 1y    | 103  | 1/1   | 0.70 | 0.21 | 88,88,88,88                 | 0     |
| 59  | MG   | 2A    | 3774 | 1/1   | 0.71 | 0.23 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3588 | 1/1   | 0.71 | 0.19 | 60,60,60,60                 | 0     |
| 59  | MG   | 2B    | 3003 | 1/1   | 0.71 | 0.28 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3611 | 1/1   | 0.71 | 0.14 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3307 | 1/1   | 0.71 | 0.29 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3622 | 1/1   | 0.71 | 0.25 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3421 | 1/1   | 0.71 | 0.20 | 64,64,64,64                 | 0     |
| 59  | MG   | 2y    | 3007 | 1/1   | 0.71 | 0.15 | 78,78,78,78                 | 0     |
| 59  | MG   | 1A    | 3405 | 1/1   | 0.72 | 0.12 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3265 | 1/1   | 0.72 | 0.16 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3212 | 1/1   | 0.72 | 0.26 | 73,73,73,73                 | 0     |
| 59  | MG   | 2A    | 3535 | 1/1   | 0.72 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3395 | 1/1   | 0.72 | 0.20 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2S    | 8001 | 1/1   | 0.72 | 0.19 | 73,73,73,73                 | 0     |
| 59  | MG   | 1Y    | 503  | 1/1   | 0.72 | 0.13 | 69,69,69,69                 | 0     |
| 59  | MG   | 2w    | 3003 | 1/1   | 0.72 | 0.16 | 74,74,74,74                 | 0     |
| 59  | MG   | 2a    | 3037 | 1/1   | 0.72 | 0.30 | 74,74,74,74                 | 0     |
| 59  | MG   | 2A    | 3018 | 1/1   | 0.72 | 0.23 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3722 | 1/1   | 0.72 | 0.28 | 72,72,72,72                 | 0     |
| 59  | MG   | 2a    | 3215 | 1/1   | 0.73 | 0.34 | 75,75,75,75                 | 0     |
| 59  | MG   | 2A    | 3689 | 1/1   | 0.73 | 0.14 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3725 | 1/1   | 0.73 | 0.17 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3702 | 1/1   | 0.73 | 0.14 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3347 | 1/1   | 0.73 | 0.20 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3182 | 1/1   | 0.73 | 0.20 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3253 | 1/1   | 0.73 | 0.20 | 61,61,61,61                 | 0     |
| 59  | MG   | 2x    | 103  | 1/1   | 0.73 | 0.30 | 74,74,74,74                 | 0     |
| 59  | MG   | 1A    | 4072 | 1/1   | 0.73 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3536 | 1/1   | 0.73 | 0.22 | 58,58,58,58                 | 0     |
| 59  | MG   | 2a    | 3235 | 1/1   | 0.74 | 0.24 | 80,80,80,80                 | 0     |
| 59  | MG   | 2a    | 3133 | 1/1   | 0.74 | 0.16 | 67,67,67,67                 | 0     |
| 59  | MG   | 1a    | 3557 | 1/1   | 0.74 | 0.27 | 63,63,63,63                 | 0     |
| 59  | MG   | 1s    | 3001 | 1/1   | 0.74 | 0.25 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 4011 | 1/1   | 0.74 | 0.20 | 59,59,59,59                 | 0     |
| 59  | MG   | 1x    | 116  | 1/1   | 0.74 | 0.12 | 70,70,70,70                 | 0     |
| 59  | MG   | 1A    | 3902 | 1/1   | 0.74 | 0.14 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3726 | 1/1   | 0.74 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3085 | 1/1   | 0.74 | 0.15 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3416 | 1/1   | 0.75 | 0.37 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3578 | 1/1   | 0.75 | 0.18 | 73,73,73,73                 | 0     |
| 59  | MG   | 1a    | 3426 | 1/1   | 0.75 | 0.37 | 55,55,55,55                 | 0     |
| 59  | MG   | 2g    | 8001 | 1/1   | 0.75 | 0.11 | 74,74,74,74                 | 0     |
| 59  | MG   | 2A    | 3539 | 1/1   | 0.75 | 0.16 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3118 | 1/1   | 0.75 | 0.50 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3555 | 1/1   | 0.75 | 0.23 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3765 | 1/1   | 0.75 | 0.18 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3769 | 1/1   | 0.75 | 0.21 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3247 | 1/1   | 0.75 | 0.30 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3454 | 1/1   | 0.75 | 0.13 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3494 | 1/1   | 0.75 | 0.15 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3396 | 1/1   | 0.76 | 0.20 | 62,62,62,62                 | 0     |
| 59  | MG   | 1w    | 112  | 1/1   | 0.76 | 0.11 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3531 | 1/1   | 0.76 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3492 | 1/1   | 0.76 | 0.12 | 75,75,75,75                 | 0     |
| 59  | MG   | 2A    | 3771 | 1/1   | 0.76 | 0.15 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3289 | 1/1   | 0.76 | 0.18 | 70,70,70,70                 | 0     |
| 59  | MG   | 2a    | 3220 | 1/1   | 0.76 | 0.31 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3166 | 1/1   | 0.76 | 0.24 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3789 | 1/1   | 0.76 | 0.23 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3795 | 1/1   | 0.76 | 0.23 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3836 | 1/1   | 0.76 | 0.28 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3209 | 1/1   | 0.76 | 0.20 | 60,60,60,60                 | 0     |
| 59  | MG   | 2q    | 205  | 1/1   | 0.76 | 0.26 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3596 | 1/1   | 0.76 | 0.19 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3376 | 1/1   | 0.76 | 0.16 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3402 | 1/1   | 0.76 | 0.27 | 57,57,57,57                 | 0     |
| 59  | MG   | 2w    | 3007 | 1/1   | 0.76 | 0.23 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3427 | 1/1   | 0.76 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3246 | 1/1   | 0.76 | 0.20 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3051 | 1/1   | 0.76 | 0.23 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3658 | 1/1   | 0.77 | 0.17 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 4174 | 1/1   | 0.77 | 0.25 | 52,52,52,52                 | 0     |
| 59  | MG   | 1a    | 3435 | 1/1   | 0.77 | 0.41 | 76,76,76,76                 | 0     |
| 59  | MG   | 2A    | 3516 | 1/1   | 0.77 | 0.31 | 64,64,64,64                 | 0     |
| 59  | MG   | 2a    | 3210 | 1/1   | 0.77 | 0.21 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3517 | 1/1   | 0.77 | 0.23 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3330 | 1/1   | 0.77 | 0.17 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3260 | 1/1   | 0.77 | 0.22 | 76,76,76,76                 | 0     |
| 59  | MG   | 1A    | 3798 | 1/1   | 0.77 | 0.31 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3273 | 1/1   | 0.77 | 0.23 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3100 | 1/1   | 0.77 | 0.22 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3290 | 1/1   | 0.77 | 0.12 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3558 | 1/1   | 0.77 | 0.14 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3126 | 1/1   | 0.77 | 0.23 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3449 | 1/1   | 0.77 | 0.13 | 54,54,54,54                 | 0     |
| 59  | MG   | 2v    | 102  | 1/1   | 0.77 | 0.29 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3597 | 1/1   | 0.77 | 0.19 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3292 | 1/1   | 0.77 | 0.20 | 71,71,71,71                 | 0     |
| 59  | MG   | 2a    | 3002 | 1/1   | 0.77 | 0.20 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 3515 | 1/1   | 0.77 | 0.48 | 71,71,71,71                 | 0     |
| 59  | MG   | 2a    | 3093 | 1/1   | 0.77 | 0.30 | 71,71,71,71                 | 0     |
| 59  | MG   | 1a    | 3572 | 1/1   | 0.77 | 0.15 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3626 | 1/1   | 0.77 | 0.15 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3731 | 1/1   | 0.78 | 0.18 | 72,72,72,72                 | 0     |
| 59  | MG   | 1A    | 3429 | 1/1   | 0.78 | 0.18 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3760 | 1/1   | 0.78 | 0.27 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3410 | 1/1   | 0.78 | 0.19 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2a    | 3205 | 1/1   | 0.78 | 0.19 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3073 | 1/1   | 0.78 | 0.23 | 63,63,63,63                 | 0     |
| 59  | MG   | 1a    | 3578 | 1/1   | 0.78 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3080 | 1/1   | 0.78 | 0.22 | 74,74,74,74                 | 0     |
| 59  | MG   | 1B    | 222  | 1/1   | 0.78 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | 1w    | 109  | 1/1   | 0.78 | 0.19 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3792 | 1/1   | 0.78 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3577 | 1/1   | 0.78 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3801 | 1/1   | 0.78 | 0.09 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 4106 | 1/1   | 0.78 | 0.18 | 58,58,58,58                 | 0     |
| 59  | MG   | 2B    | 3015 | 1/1   | 0.78 | 0.23 | 64,64,64,64                 | 0     |
| 59  | MG   | 2F    | 301  | 1/1   | 0.78 | 0.31 | 70,70,70,70                 | 0     |
| 59  | MG   | 2I    | 202  | 1/1   | 0.78 | 0.16 | 71,71,71,71                 | 0     |
| 59  | MG   | 2R    | 203  | 1/1   | 0.78 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 4111 | 1/1   | 0.78 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3243 | 1/1   | 0.78 | 0.20 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3806 | 1/1   | 0.78 | 0.25 | 47,47,47,47                 | 0     |
| 59  | MG   | 2a    | 3036 | 1/1   | 0.78 | 0.17 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3344 | 1/1   | 0.78 | 0.23 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3553 | 1/1   | 0.78 | 0.29 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3108 | 1/1   | 0.78 | 0.25 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3005 | 1/1   | 0.78 | 0.19 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3997 | 1/1   | 0.79 | 0.17 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3325 | 1/1   | 0.79 | 0.30 | 68,68,68,68                 | 0     |
| 59  | MG   | 18    | 101  | 1/1   | 0.79 | 0.24 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 4145 | 1/1   | 0.79 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3216 | 1/1   | 0.79 | 0.36 | 63,63,63,63                 | 0     |
| 59  | MG   | 1x    | 114  | 1/1   | 0.79 | 0.26 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3573 | 1/1   | 0.79 | 0.17 | 64,64,64,64                 | 0     |
| 59  | MG   | 2a    | 3005 | 1/1   | 0.79 | 0.33 | 74,74,74,74                 | 0     |
| 59  | MG   | 2A    | 3587 | 1/1   | 0.79 | 0.14 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3768 | 1/1   | 0.79 | 0.18 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3479 | 1/1   | 0.79 | 0.33 | 69,69,69,69                 | 0     |
| 59  | MG   | 2a    | 3101 | 1/1   | 0.79 | 0.29 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 4063 | 1/1   | 0.79 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3448 | 1/1   | 0.79 | 0.25 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3097 | 1/1   | 0.79 | 0.38 | 74,74,74,74                 | 0     |
| 59  | MG   | 1A    | 3892 | 1/1   | 0.79 | 0.15 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3645 | 1/1   | 0.79 | 0.30 | 63,63,63,63                 | 0     |
| 59  | MG   | 2w    | 3006 | 1/1   | 0.79 | 0.10 | 72,72,72,72                 | 0     |
| 59  | MG   | 1A    | 3911 | 1/1   | 0.79 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3199 | 1/1   | 0.79 | 0.16 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2y    | 3002 | 1/1   | 0.79 | 0.14 | 80,80,80,80                 | 0     |
| 59  | MG   | 2A    | 3636 | 1/1   | 0.79 | 0.19 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3740 | 1/1   | 0.79 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3029 | 1/1   | 0.80 | 0.29 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3105 | 1/1   | 0.80 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3183 | 1/1   | 0.80 | 0.18 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 4077 | 1/1   | 0.80 | 0.21 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3462 | 1/1   | 0.80 | 0.14 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3599 | 1/1   | 0.80 | 0.19 | 65,65,65,65                 | 0     |
| 59  | MG   | 1a    | 3543 | 1/1   | 0.80 | 0.17 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3813 | 1/1   | 0.80 | 0.18 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3161 | 1/1   | 0.80 | 0.19 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3275 | 1/1   | 0.80 | 0.25 | 66,66,66,66                 | 0     |
| 59  | MG   | 1a    | 3425 | 1/1   | 0.80 | 0.23 | 58,58,58,58                 | 0     |
| 59  | MG   | 2B    | 3020 | 1/1   | 0.80 | 0.10 | 80,80,80,80                 | 0     |
| 59  | MG   | 2A    | 3524 | 1/1   | 0.80 | 0.19 | 51,51,51,51                 | 0     |
| 59  | MG   | 1a    | 3550 | 1/1   | 0.80 | 0.24 | 78,78,78,78                 | 0     |
| 59  | MG   | 2A    | 3663 | 1/1   | 0.80 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3240 | 1/1   | 0.80 | 0.20 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3312 | 1/1   | 0.80 | 0.15 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3084 | 1/1   | 0.80 | 0.34 | 76,76,76,76                 | 0     |
| 59  | MG   | 2a    | 3017 | 1/1   | 0.80 | 0.25 | 76,76,76,76                 | 0     |
| 59  | MG   | 2A    | 3547 | 1/1   | 0.80 | 0.28 | 67,67,67,67                 | 0     |
| 59  | MG   | 1a    | 3393 | 1/1   | 0.80 | 0.15 | 70,70,70,70                 | 0     |
| 59  | MG   | 2a    | 3046 | 1/1   | 0.80 | 0.15 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3742 | 1/1   | 0.80 | 0.16 | 69,69,69,69                 | 0     |
| 59  | MG   | 2w    | 3005 | 1/1   | 0.80 | 0.12 | 73,73,73,73                 | 0     |
| 59  | MG   | 2A    | 3748 | 1/1   | 0.80 | 0.19 | 55,55,55,55                 | 0     |
| 59  | MG   | 2a    | 3106 | 1/1   | 0.80 | 0.35 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3022 | 1/1   | 0.80 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3564 | 1/1   | 0.80 | 0.20 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3249 | 1/1   | 0.80 | 0.15 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3583 | 1/1   | 0.80 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3907 | 1/1   | 0.81 | 0.18 | 74,74,74,74                 | 0     |
| 59  | MG   | 1a    | 3549 | 1/1   | 0.81 | 0.31 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3255 | 1/1   | 0.81 | 0.34 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3360 | 1/1   | 0.81 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3758 | 1/1   | 0.81 | 0.33 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3382 | 1/1   | 0.81 | 0.23 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3948 | 1/1   | 0.81 | 0.13 | 69,69,69,69                 | 0     |
| 59  | MG   | 2a    | 3146 | 1/1   | 0.81 | 0.20 | 79,79,79,79                 | 0     |
| 59  | MG   | 1a    | 3567 | 1/1   | 0.81 | 0.10 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3193 | 1/1   | 0.81 | 0.16 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3647 | 1/1   | 0.81 | 0.23 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3418 | 1/1   | 0.81 | 0.29 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3775 | 1/1   | 0.81 | 0.15 | 63,63,63,63                 | 0     |
| 59  | MG   | 1a    | 3420 | 1/1   | 0.81 | 0.21 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3503 | 1/1   | 0.81 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3869 | 1/1   | 0.81 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3793 | 1/1   | 0.81 | 0.20 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3346 | 1/1   | 0.81 | 0.22 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3143 | 1/1   | 0.81 | 0.21 | 77,77,77,77                 | 0     |
| 59  | MG   | 1A    | 3178 | 1/1   | 0.81 | 0.20 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3377 | 1/1   | 0.81 | 0.16 | 36,36,36,36                 | 0     |
| 59  | MG   | 2B    | 3008 | 1/1   | 0.81 | 0.22 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3605 | 1/1   | 0.81 | 0.22 | 55,55,55,55                 | 0     |
| 59  | MG   | 2B    | 3018 | 1/1   | 0.81 | 0.19 | 62,62,62,62                 | 0     |
| 59  | MG   | 1B    | 230  | 1/1   | 0.81 | 0.18 | 59,59,59,59                 | 0     |
| 59  | MG   | 2B    | 3022 | 1/1   | 0.81 | 0.26 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3413 | 1/1   | 0.81 | 0.12 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3188 | 1/1   | 0.81 | 0.20 | 53,53,53,53                 | 0     |
| 59  | MG   | 1a    | 3462 | 1/1   | 0.81 | 0.24 | 72,72,72,72                 | 0     |
| 59  | MG   | 1E    | 312  | 1/1   | 0.81 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3489 | 1/1   | 0.81 | 0.13 | 85,85,85,85                 | 0     |
| 59  | MG   | 2a    | 3003 | 1/1   | 0.81 | 0.25 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3480 | 1/1   | 0.81 | 0.13 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3687 | 1/1   | 0.81 | 0.12 | 39,39,39,39                 | 0     |
| 59  | MG   | 2a    | 3019 | 1/1   | 0.81 | 0.32 | 63,63,63,63                 | 0     |
| 59  | MG   | 1P    | 203  | 1/1   | 0.81 | 0.14 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4095 | 1/1   | 0.81 | 0.26 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3732 | 1/1   | 0.81 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3035 | 1/1   | 0.82 | 0.16 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3675 | 1/1   | 0.82 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3745 | 1/1   | 0.82 | 0.19 | 48,48,48,48                 | 0     |
| 59  | MG   | 2a    | 3044 | 1/1   | 0.82 | 0.22 | 66,66,66,66                 | 0     |
| 59  | MG   | 1a    | 3424 | 1/1   | 0.82 | 0.20 | 66,66,66,66                 | 0     |
| 59  | MG   | 2a    | 3066 | 1/1   | 0.82 | 0.22 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3081 | 1/1   | 0.82 | 0.19 | 67,67,67,67                 | 0     |
| 59  | MG   | 2a    | 3092 | 1/1   | 0.82 | 0.29 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3708 | 1/1   | 0.82 | 0.17 | 29,29,29,29                 | 0     |
| 59  | MG   | 2a    | 3098 | 1/1   | 0.82 | 0.26 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3193 | 1/1   | 0.82 | 0.23 | 40,40,40,40                 | 0     |
| 59  | MG   | 1a    | 3305 | 1/1   | 0.82 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3218 | 1/1   | 0.82 | 0.21 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3457 | 1/1   | 0.82 | 0.15 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3223 | 1/1   | 0.82 | 0.11 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3233 | 1/1   | 0.82 | 0.33 | 66,66,66,66                 | 0     |
| 59  | MG   | 2a    | 3134 | 1/1   | 0.82 | 0.13 | 80,80,80,80                 | 0     |
| 59  | MG   | 1B    | 231  | 1/1   | 0.82 | 0.23 | 63,63,63,63                 | 0     |
| 59  | MG   | 2a    | 3176 | 1/1   | 0.82 | 0.37 | 75,75,75,75                 | 0     |
| 59  | MG   | 2A    | 3044 | 1/1   | 0.82 | 0.15 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3181 | 1/1   | 0.82 | 0.18 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3336 | 1/1   | 0.82 | 0.28 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3067 | 1/1   | 0.82 | 0.19 | 55,55,55,55                 | 0     |
| 59  | MG   | 1b    | 3001 | 1/1   | 0.82 | 0.12 | 74,74,74,74                 | 0     |
| 59  | MG   | 1l    | 203  | 1/1   | 0.82 | 0.23 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3249 | 1/1   | 0.82 | 0.12 | 43,43,43,43                 | 0     |
| 59  | MG   | 2a    | 3209 | 1/1   | 0.82 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3258 | 1/1   | 0.82 | 0.25 | 68,68,68,68                 | 0     |
| 59  | MG   | 1a    | 3362 | 1/1   | 0.82 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 1a    | 3369 | 1/1   | 0.82 | 0.19 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3262 | 1/1   | 0.82 | 0.17 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3264 | 1/1   | 0.82 | 0.19 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3087 | 1/1   | 0.82 | 0.20 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3272 | 1/1   | 0.82 | 0.23 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3089 | 1/1   | 0.82 | 0.21 | 78,78,78,78                 | 0     |
| 59  | MG   | 2a    | 3238 | 1/1   | 0.82 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3370 | 1/1   | 0.82 | 0.30 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3287 | 1/1   | 0.82 | 0.33 | 65,65,65,65                 | 0     |
| 59  | MG   | 1a    | 3508 | 1/1   | 0.82 | 0.15 | 51,51,51,51                 | 0     |
| 59  | MG   | 2B    | 3016 | 1/1   | 0.82 | 0.24 | 77,77,77,77                 | 0     |
| 59  | MG   | 1F    | 310  | 1/1   | 0.82 | 0.23 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3295 | 1/1   | 0.82 | 0.18 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 4117 | 1/1   | 0.82 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | 1V    | 202  | 1/1   | 0.82 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 4019 | 1/1   | 0.82 | 0.36 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3154 | 1/1   | 0.82 | 0.32 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3340 | 1/1   | 0.82 | 0.35 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3162 | 1/1   | 0.82 | 0.14 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3651 | 1/1   | 0.82 | 0.13 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3169 | 1/1   | 0.82 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3399 | 1/1   | 0.82 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3669 | 1/1   | 0.82 | 0.12 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 4141 | 1/1   | 0.83 | 0.14 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3776 | 1/1   | 0.83 | 0.16 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3594 | 1/1   | 0.83 | 0.12 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1O    | 3006 | 1/1   | 0.83 | 0.12 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3904 | 1/1   | 0.83 | 0.13 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3402 | 1/1   | 0.83 | 0.24 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3415 | 1/1   | 0.83 | 0.34 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3508 | 1/1   | 0.83 | 0.14 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3163 | 1/1   | 0.83 | 0.11 | 91,91,91,91                 | 0     |
| 59  | MG   | 2A    | 3438 | 1/1   | 0.83 | 0.26 | 77,77,77,77                 | 0     |
| 59  | MG   | 2A    | 3845 | 1/1   | 0.83 | 0.52 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4178 | 1/1   | 0.83 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 4179 | 1/1   | 0.83 | 0.20 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3629 | 1/1   | 0.83 | 0.16 | 67,67,67,67                 | 0     |
| 59  | MG   | 2a    | 3193 | 1/1   | 0.83 | 0.18 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3634 | 1/1   | 0.83 | 0.17 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3656 | 1/1   | 0.83 | 0.20 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3170 | 1/1   | 0.83 | 0.20 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3208 | 1/1   | 0.83 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3474 | 1/1   | 0.83 | 0.22 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3378 | 1/1   | 0.83 | 0.29 | 62,62,62,62                 | 0     |
| 59  | MG   | 2R    | 202  | 1/1   | 0.83 | 0.24 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3521 | 1/1   | 0.83 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3285 | 1/1   | 0.83 | 0.12 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3286 | 1/1   | 0.83 | 0.34 | 58,58,58,58                 | 0     |
| 59  | MG   | 20    | 3001 | 1/1   | 0.83 | 0.26 | 66,66,66,66                 | 0     |
| 59  | MG   | 25    | 104  | 1/1   | 0.83 | 0.12 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3955 | 1/1   | 0.83 | 0.10 | 68,68,68,68                 | 0     |
| 59  | MG   | 1a    | 3345 | 1/1   | 0.83 | 0.35 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3350 | 1/1   | 0.83 | 0.23 | 61,61,61,61                 | 0     |
| 59  | MG   | 2a    | 3009 | 1/1   | 0.83 | 0.36 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 3223 | 1/1   | 0.83 | 0.19 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3489 | 1/1   | 0.83 | 0.12 | 33,33,33,33                 | 0     |
| 59  | MG   | 1x    | 112  | 1/1   | 0.83 | 0.15 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3088 | 1/1   | 0.83 | 0.17 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3329 | 1/1   | 0.83 | 0.12 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3557 | 1/1   | 0.83 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1a    | 3363 | 1/1   | 0.83 | 0.27 | 50,50,50,50                 | 0     |
| 59  | MG   | 2a    | 3064 | 1/1   | 0.83 | 0.29 | 70,70,70,70                 | 0     |
| 59  | MG   | 1A    | 3271 | 1/1   | 0.83 | 0.35 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3348 | 1/1   | 0.83 | 0.25 | 66,66,66,66                 | 0     |
| 59  | MG   | 2a    | 3082 | 1/1   | 0.83 | 0.24 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3354 | 1/1   | 0.83 | 0.21 | 61,61,61,61                 | 0     |
| 59  | MG   | 2y    | 3003 | 1/1   | 0.83 | 0.11 | 83,83,83,83                 | 0     |
| 59  | MG   | 2A    | 3584 | 1/1   | 0.83 | 0.18 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3366 | 1/1   | 0.83 | 0.35 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3309 | 1/1   | 0.84 | 0.15 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3958 | 1/1   | 0.84 | 0.15 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3559 | 1/1   | 0.84 | 0.16 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3313 | 1/1   | 0.84 | 0.25 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3338 | 1/1   | 0.84 | 0.17 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3673 | 1/1   | 0.84 | 0.16 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3110 | 1/1   | 0.84 | 0.16 | 71,71,71,71                 | 0     |
| 59  | MG   | 2a    | 3112 | 1/1   | 0.84 | 0.22 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3778 | 1/1   | 0.84 | 0.22 | 63,63,63,63                 | 0     |
| 59  | MG   | 2a    | 3116 | 1/1   | 0.84 | 0.26 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3338 | 1/1   | 0.84 | 0.47 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3828 | 1/1   | 0.84 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3518 | 1/1   | 0.84 | 0.39 | 63,63,63,63                 | 0     |
| 59  | MG   | 2a    | 3138 | 1/1   | 0.84 | 0.11 | 88,88,88,88                 | 0     |
| 59  | MG   | 1a    | 3544 | 1/1   | 0.84 | 0.24 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3113 | 1/1   | 0.84 | 0.20 | 37,37,37,37                 | 0     |
| 59  | MG   | 2a    | 3166 | 1/1   | 0.84 | 0.16 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 4074 | 1/1   | 0.84 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3284 | 1/1   | 0.84 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3391 | 1/1   | 0.84 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3606 | 1/1   | 0.84 | 0.13 | 73,73,73,73                 | 0     |
| 59  | MG   | 2B    | 3007 | 1/1   | 0.84 | 0.17 | 69,69,69,69                 | 0     |
| 59  | MG   | 2a    | 3187 | 1/1   | 0.84 | 0.14 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3390 | 1/1   | 0.84 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3198 | 1/1   | 0.84 | 0.20 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3138 | 1/1   | 0.84 | 0.23 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3641 | 1/1   | 0.84 | 0.17 | 40,40,40,40                 | 0     |
| 59  | MG   | 1D    | 313  | 1/1   | 0.84 | 0.30 | 34,34,34,34                 | 0     |
| 59  | MG   | 1a    | 3405 | 1/1   | 0.84 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4110 | 1/1   | 0.84 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 2D    | 304  | 1/1   | 0.84 | 0.60 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3910 | 1/1   | 0.84 | 0.16 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3637 | 1/1   | 0.84 | 0.11 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3095 | 1/1   | 0.84 | 0.22 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3746 | 1/1   | 0.84 | 0.18 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3662 | 1/1   | 0.84 | 0.20 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 3788 | 1/1   | 0.84 | 0.23 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3310 | 1/1   | 0.84 | 0.33 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3236 | 1/1   | 0.84 | 0.09 | 75,75,75,75                 | 0     |
| 59  | MG   | 28    | 102  | 1/1   | 0.84 | 0.29 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 4127 | 1/1   | 0.84 | 0.28 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3128 | 1/1   | 0.84 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | 1x    | 103  | 1/1   | 0.84 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 4131 | 1/1   | 0.84 | 0.18 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3013 | 1/1   | 0.84 | 0.24 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 4135 | 1/1   | 0.84 | 0.28 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3018 | 1/1   | 0.84 | 0.20 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 4138 | 1/1   | 0.84 | 0.14 | 76,76,76,76                 | 0     |
| 59  | MG   | 1a    | 3329 | 1/1   | 0.84 | 0.40 | 64,64,64,64                 | 0     |
| 59  | MG   | 1a    | 3478 | 1/1   | 0.84 | 0.12 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3292 | 1/1   | 0.84 | 0.20 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3328 | 1/1   | 0.84 | 0.28 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3749 | 1/1   | 0.84 | 0.18 | 55,55,55,55                 | 0     |
| 59  | MG   | 2x    | 104  | 1/1   | 0.84 | 0.21 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3306 | 1/1   | 0.84 | 0.30 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3551 | 1/1   | 0.84 | 0.15 | 60,60,60,60                 | 0     |
| 59  | MG   | 2y    | 3004 | 1/1   | 0.84 | 0.12 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3761 | 1/1   | 0.84 | 0.18 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3178 | 1/1   | 0.84 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3336 | 1/1   | 0.85 | 0.35 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3177 | 1/1   | 0.85 | 0.21 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3173 | 1/1   | 0.85 | 0.19 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3952 | 1/1   | 0.85 | 0.13 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 4124 | 1/1   | 0.85 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3189 | 1/1   | 0.85 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3365 | 1/1   | 0.85 | 0.15 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3809 | 1/1   | 0.85 | 0.12 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3654 | 1/1   | 0.85 | 0.14 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3252 | 1/1   | 0.85 | 0.10 | 28,28,28,28                 | 0     |
| 59  | MG   | 2a    | 3053 | 1/1   | 0.85 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 2a    | 3055 | 1/1   | 0.85 | 0.31 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3198 | 1/1   | 0.85 | 0.13 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3971 | 1/1   | 0.85 | 0.10 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3073 | 1/1   | 0.85 | 0.26 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3667 | 1/1   | 0.85 | 0.18 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3211 | 1/1   | 0.85 | 0.24 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 4137 | 1/1   | 0.85 | 0.22 | 64,64,64,64                 | 0     |
| 59  | MG   | 1a    | 3436 | 1/1   | 0.85 | 0.32 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3414 | 1/1   | 0.85 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3422 | 1/1   | 0.85 | 0.14 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3712 | 1/1   | 0.85 | 0.12 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3107 | 1/1   | 0.85 | 0.28 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3224 | 1/1   | 0.85 | 0.10 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3988 | 1/1   | 0.85 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3236 | 1/1   | 0.85 | 0.33 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3466 | 1/1   | 0.85 | 0.34 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3455 | 1/1   | 0.85 | 0.18 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3747 | 1/1   | 0.85 | 0.30 | 61,61,61,61                 | 0     |
| 59  | MG   | 2a    | 3122 | 1/1   | 0.85 | 0.24 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3242 | 1/1   | 0.85 | 0.20 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3472 | 1/1   | 0.85 | 0.28 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3471 | 1/1   | 0.85 | 0.30 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3990 | 1/1   | 0.85 | 0.21 | 46,46,46,46                 | 0     |
| 59  | MG   | 2a    | 3153 | 1/1   | 0.85 | 0.10 | 80,80,80,80                 | 0     |
| 59  | MG   | 2a    | 3158 | 1/1   | 0.85 | 0.13 | 71,71,71,71                 | 0     |
| 59  | MG   | 2a    | 3160 | 1/1   | 0.85 | 0.13 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 3995 | 1/1   | 0.85 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3764 | 1/1   | 0.85 | 0.16 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3486 | 1/1   | 0.85 | 0.23 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3491 | 1/1   | 0.85 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3629 | 1/1   | 0.85 | 0.10 | 17,17,17,17                 | 0     |
| 59  | MG   | 2A    | 3770 | 1/1   | 0.85 | 0.20 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3850 | 1/1   | 0.85 | 0.16 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3857 | 1/1   | 0.85 | 0.11 | 22,22,22,22                 | 0     |
| 59  | MG   | 1a    | 3511 | 1/1   | 0.85 | 0.15 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3254 | 1/1   | 0.85 | 0.24 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3526 | 1/1   | 0.85 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3204 | 1/1   | 0.85 | 0.30 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3126 | 1/1   | 0.85 | 0.27 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 4073 | 1/1   | 0.85 | 0.14 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3791 | 1/1   | 0.85 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3381 | 1/1   | 0.85 | 0.23 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3385 | 1/1   | 0.85 | 0.34 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3542 | 1/1   | 0.85 | 0.10 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3543 | 1/1   | 0.85 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3388 | 1/1   | 0.85 | 0.35 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3102 | 1/1   | 0.85 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | 2a    | 3217 | 1/1   | 0.85 | 0.20 | 58,58,58,58                 | 0     |
| 59  | MG   | 2a    | 3219 | 1/1   | 0.85 | 0.14 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 3758 | 1/1   | 0.85 | 0.11 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3394 | 1/1   | 0.85 | 0.25 | 61,61,61,61                 | 0     |
| 59  | MG   | 2a    | 3229 | 1/1   | 0.85 | 0.26 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3773 | 1/1   | 0.85 | 0.09 | 57,57,57,57                 | 0     |
| 59  | MG   | 2B    | 3010 | 1/1   | 0.85 | 0.24 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3110 | 1/1   | 0.85 | 0.19 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3119 | 1/1   | 0.85 | 0.21 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3566 | 1/1   | 0.85 | 0.12 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3909 | 1/1   | 0.85 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3291 | 1/1   | 0.85 | 0.31 | 74,74,74,74                 | 0     |
| 59  | MG   | 2p    | 3001 | 1/1   | 0.85 | 0.21 | 63,63,63,63                 | 0     |
| 59  | MG   | 2q    | 201  | 1/1   | 0.85 | 0.16 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3087 | 1/1   | 0.85 | 0.22 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3585 | 1/1   | 0.85 | 0.17 | 59,59,59,59                 | 0     |
| 59  | MG   | 2O    | 8001 | 1/1   | 0.85 | 0.15 | 53,53,53,53                 | 0     |
| 59  | MG   | 2Q    | 3004 | 1/1   | 0.85 | 0.16 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3409 | 1/1   | 0.85 | 0.15 | 74,74,74,74                 | 0     |
| 59  | MG   | 1a    | 3410 | 1/1   | 0.85 | 0.21 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3150 | 1/1   | 0.85 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1v    | 3001 | 1/1   | 0.85 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3414 | 1/1   | 0.85 | 0.32 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3526 | 1/1   | 0.85 | 0.23 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3315 | 1/1   | 0.85 | 0.34 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3168 | 1/1   | 0.85 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3678 | 1/1   | 0.85 | 0.22 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3614 | 1/1   | 0.85 | 0.15 | 63,63,63,63                 | 0     |
| 59  | MG   | 2a    | 3006 | 1/1   | 0.85 | 0.50 | 76,76,76,76                 | 0     |
| 59  | MG   | 1A    | 3132 | 1/1   | 0.86 | 0.16 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3234 | 1/1   | 0.86 | 0.32 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 4125 | 1/1   | 0.86 | 0.19 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3059 | 1/1   | 0.86 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3487 | 1/1   | 0.86 | 0.12 | 55,55,55,55                 | 0     |
| 59  | MG   | 2a    | 3065 | 1/1   | 0.86 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3458 | 1/1   | 0.86 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3652 | 1/1   | 0.86 | 0.13 | 35,35,35,35                 | 0     |
| 59  | MG   | 2a    | 3074 | 1/1   | 0.86 | 0.14 | 64,64,64,64                 | 0     |
| 59  | MG   | 2a    | 3080 | 1/1   | 0.86 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3289 | 1/1   | 0.86 | 0.35 | 29,29,29,29                 | 0     |
| 59  | MG   | 1a    | 3325 | 1/1   | 0.86 | 0.18 | 50,50,50,50                 | 0     |
| 59  | MG   | 2a    | 3087 | 1/1   | 0.86 | 0.29 | 65,65,65,65                 | 0     |
| 59  | MG   | 2a    | 3088 | 1/1   | 0.86 | 0.21 | 61,61,61,61                 | 0     |
| 59  | MG   | 2a    | 3089 | 1/1   | 0.86 | 0.25 | 67,67,67,67                 | 0     |
| 59  | MG   | 1a    | 3439 | 1/1   | 0.86 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | 1a    | 3453 | 1/1   | 0.86 | 0.13 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3250 | 1/1   | 0.86 | 0.13 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3755 | 1/1   | 0.86 | 0.25 | 64,64,64,64                 | 0     |
| 59  | MG   | 2a    | 3105 | 1/1   | 0.86 | 0.19 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3492 | 1/1   | 0.86 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3326 | 1/1   | 0.86 | 0.34 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3079 | 1/1   | 0.86 | 0.23 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3062 | 1/1   | 0.86 | 0.24 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3861 | 1/1   | 0.86 | 0.10 | 39,39,39,39                 | 0     |
| 59  | MG   | 1a    | 3335 | 1/1   | 0.86 | 0.18 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3413 | 1/1   | 0.86 | 0.25 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4036 | 1/1   | 0.86 | 0.10 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3103 | 1/1   | 0.86 | 0.13 | 34,34,34,34                 | 0     |
| 59  | MG   | 2a    | 3131 | 1/1   | 0.86 | 0.12 | 77,77,77,77                 | 0     |
| 59  | MG   | 2A    | 3271 | 1/1   | 0.86 | 0.16 | 71,71,71,71                 | 0     |
| 59  | MG   | 1a    | 3504 | 1/1   | 0.86 | 0.12 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3354 | 1/1   | 0.86 | 0.14 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3377 | 1/1   | 0.86 | 0.12 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3361 | 1/1   | 0.86 | 0.19 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3783 | 1/1   | 0.86 | 0.11 | 73,73,73,73                 | 0     |
| 59  | MG   | 2A    | 3788 | 1/1   | 0.86 | 0.15 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3440 | 1/1   | 0.86 | 0.18 | 70,70,70,70                 | 0     |
| 59  | MG   | 1A    | 4187 | 1/1   | 0.86 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3556 | 1/1   | 0.86 | 0.13 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3179 | 1/1   | 0.86 | 0.20 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3288 | 1/1   | 0.86 | 0.10 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3794 | 1/1   | 0.86 | 0.15 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 4188 | 1/1   | 0.86 | 0.27 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3798 | 1/1   | 0.86 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3186 | 1/1   | 0.86 | 0.41 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3806 | 1/1   | 0.86 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3809 | 1/1   | 0.86 | 0.12 | 55,55,55,55                 | 0     |
| 59  | MG   | 1B    | 204  | 1/1   | 0.86 | 0.28 | 48,48,48,48                 | 0     |
| 59  | MG   | 1a    | 3372 | 1/1   | 0.86 | 0.22 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3145 | 1/1   | 0.86 | 0.22 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3374 | 1/1   | 0.86 | 0.22 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3582 | 1/1   | 0.86 | 0.14 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3297 | 1/1   | 0.86 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | 1a    | 3380 | 1/1   | 0.86 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 2B    | 3011 | 1/1   | 0.86 | 0.21 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3151 | 1/1   | 0.86 | 0.19 | 74,74,74,74                 | 0     |
| 59  | MG   | 1B    | 217  | 1/1   | 0.86 | 0.12 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3159 | 1/1   | 0.86 | 0.27 | 62,62,62,62                 | 0     |
| 59  | MG   | 2B    | 3019 | 1/1   | 0.86 | 0.15 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3314 | 1/1   | 0.86 | 0.15 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3556 | 1/1   | 0.86 | 0.14 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3324 | 1/1   | 0.86 | 0.24 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3165 | 1/1   | 0.86 | 0.16 | 61,61,61,61                 | 0     |
| 59  | MG   | 2a    | 3223 | 1/1   | 0.86 | 0.22 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 4082 | 1/1   | 0.86 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3561 | 1/1   | 0.86 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3129 | 1/1   | 0.86 | 0.16 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3613 | 1/1   | 0.86 | 0.14 | 36,36,36,36                 | 0     |
| 59  | MG   | 2f    | 3002 | 1/1   | 0.86 | 0.21 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 3394 | 1/1   | 0.86 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3401 | 1/1   | 0.86 | 0.11 | 48,48,48,48                 | 0     |
| 59  | MG   | 2U    | 204  | 1/1   | 0.86 | 0.27 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3179 | 1/1   | 0.86 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3625 | 1/1   | 0.86 | 0.21 | 67,67,67,67                 | 0     |
| 59  | MG   | 1B    | 232  | 1/1   | 0.86 | 0.11 | 67,67,67,67                 | 0     |
| 59  | MG   | 1a    | 3404 | 1/1   | 0.86 | 0.43 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3617 | 1/1   | 0.86 | 0.11 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4112 | 1/1   | 0.86 | 0.14 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3461 | 1/1   | 0.86 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3638 | 1/1   | 0.86 | 0.11 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3468 | 1/1   | 0.86 | 0.34 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3216 | 1/1   | 0.86 | 0.16 | 47,47,47,47                 | 0     |
| 59  | MG   | 1P    | 204  | 1/1   | 0.86 | 0.21 | 41,41,41,41                 | 0     |
| 59  | MG   | 2x    | 102  | 1/1   | 0.86 | 0.18 | 64,64,64,64                 | 0     |
| 59  | MG   | 1R    | 203  | 1/1   | 0.86 | 0.16 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3027 | 1/1   | 0.86 | 0.35 | 63,63,63,63                 | 0     |
| 59  | MG   | 2y    | 3001 | 1/1   | 0.86 | 0.15 | 65,65,65,65                 | 0     |
| 59  | MG   | 1S    | 3001 | 1/1   | 0.86 | 0.30 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3225 | 1/1   | 0.86 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3428 | 1/1   | 0.86 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3231 | 1/1   | 0.86 | 0.11 | 75,75,75,75                 | 0     |
| 59  | MG   | 2a    | 3045 | 1/1   | 0.86 | 0.23 | 58,58,58,58                 | 0     |
| 59  | MG   | 16    | 104  | 1/1   | 0.87 | 0.23 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3745 | 1/1   | 0.87 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3303 | 1/1   | 0.87 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3060 | 1/1   | 0.87 | 0.23 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3473 | 1/1   | 0.87 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3573 | 1/1   | 0.87 | 0.10 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3757 | 1/1   | 0.87 | 0.18 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3427 | 1/1   | 0.87 | 0.15 | 64,64,64,64                 | 0     |
| 59  | MG   | 1a    | 3315 | 1/1   | 0.87 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | 2a    | 3091 | 1/1   | 0.87 | 0.17 | 77,77,77,77                 | 0     |
| 59  | MG   | 1a    | 3322 | 1/1   | 0.87 | 0.28 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3388 | 1/1   | 0.87 | 0.19 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3083 | 1/1   | 0.87 | 0.26 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3767 | 1/1   | 0.87 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3033 | 1/1   | 0.87 | 0.27 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3775 | 1/1   | 0.87 | 0.17 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3331 | 1/1   | 0.87 | 0.41 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3973 | 1/1   | 0.87 | 0.11 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3986 | 1/1   | 0.87 | 0.12 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3612 | 1/1   | 0.87 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3274 | 1/1   | 0.87 | 0.30 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3779 | 1/1   | 0.87 | 0.13 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3538 | 1/1   | 0.87 | 0.18 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3782 | 1/1   | 0.87 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3490 | 1/1   | 0.87 | 0.13 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3226 | 1/1   | 0.87 | 0.28 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3800 | 1/1   | 0.87 | 0.15 | 30,30,30,30                 | 0     |
| 59  | MG   | 1a    | 3505 | 1/1   | 0.87 | 0.11 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3628 | 1/1   | 0.87 | 0.08 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3553 | 1/1   | 0.87 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3485 | 1/1   | 0.87 | 0.26 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 4012 | 1/1   | 0.87 | 0.21 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 4205 | 1/1   | 0.87 | 0.16 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3801 | 1/1   | 0.87 | 0.13 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3364 | 1/1   | 0.87 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3269 | 1/1   | 0.87 | 0.33 | 27,27,27,27                 | 0     |
| 59  | MG   | 1B    | 212  | 1/1   | 0.87 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3565 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3837 | 1/1   | 0.87 | 0.16 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3298 | 1/1   | 0.87 | 0.25 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3300 | 1/1   | 0.87 | 0.26 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3574 | 1/1   | 0.87 | 0.20 | 56,56,56,56                 | 0     |
| 59  | MG   | 2a    | 3188 | 1/1   | 0.87 | 0.12 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3810 | 1/1   | 0.87 | 0.11 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4045 | 1/1   | 0.87 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 1B    | 221  | 1/1   | 0.87 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | 2a    | 3202 | 1/1   | 0.87 | 0.23 | 67,67,67,67                 | 0     |
| 59  | MG   | 1a    | 3562 | 1/1   | 0.87 | 0.22 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 4057 | 1/1   | 0.87 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3384 | 1/1   | 0.87 | 0.20 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3232 | 1/1   | 0.87 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3644 | 1/1   | 0.87 | 0.09 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3327 | 1/1   | 0.87 | 0.26 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3172 | 1/1   | 0.87 | 0.17 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2E    | 303  | 1/1   | 0.87 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3835 | 1/1   | 0.87 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 2F    | 303  | 1/1   | 0.87 | 0.47 | 54,54,54,54                 | 0     |
| 59  | MG   | 2G    | 3001 | 1/1   | 0.87 | 0.25 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3277 | 1/1   | 0.87 | 0.13 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3344 | 1/1   | 0.87 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 4076 | 1/1   | 0.87 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1w    | 104  | 1/1   | 0.87 | 0.14 | 66,66,66,66                 | 0     |
| 59  | MG   | 1w    | 108  | 1/1   | 0.87 | 0.19 | 59,59,59,59                 | 0     |
| 59  | MG   | 1B    | 233  | 1/1   | 0.87 | 0.16 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3237 | 1/1   | 0.87 | 0.16 | 52,52,52,52                 | 0     |
| 59  | MG   | 2Z    | 8001 | 1/1   | 0.87 | 0.22 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 3350 | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3628 | 1/1   | 0.87 | 0.13 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3367 | 1/1   | 0.87 | 0.17 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3368 | 1/1   | 0.87 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 4085 | 1/1   | 0.87 | 0.16 | 64,64,64,64                 | 0     |
| 59  | MG   | 1x    | 111  | 1/1   | 0.87 | 0.20 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3639 | 1/1   | 0.87 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3380 | 1/1   | 0.87 | 0.12 | 41,41,41,41                 | 0     |
| 59  | MG   | 2t    | 3001 | 1/1   | 0.87 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3652 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3215 | 1/1   | 0.87 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | 2w    | 3002 | 1/1   | 0.87 | 0.19 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 3516 | 1/1   | 0.87 | 0.20 | 49,49,49,49                 | 0     |
| 59  | MG   | 1a    | 3406 | 1/1   | 0.87 | 0.22 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3671 | 1/1   | 0.87 | 0.14 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3045 | 1/1   | 0.87 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1a    | 3412 | 1/1   | 0.87 | 0.22 | 51,51,51,51                 | 0     |
| 59  | MG   | 2x    | 101  | 1/1   | 0.87 | 0.18 | 72,72,72,72                 | 0     |
| 59  | MG   | 1A    | 3441 | 1/1   | 0.87 | 0.10 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3001 | 1/1   | 0.87 | 0.11 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3533 | 1/1   | 0.87 | 0.13 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3441 | 1/1   | 0.87 | 0.11 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3300 | 1/1   | 0.87 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3239 | 1/1   | 0.87 | 0.21 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3452 | 1/1   | 0.87 | 0.23 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3560 | 1/1   | 0.87 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 1l    | 101  | 1/1   | 0.87 | 0.16 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3487 | 1/1   | 0.88 | 0.21 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3099 | 1/1   | 0.88 | 0.15 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3201 | 1/1   | 0.88 | 0.17 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3824 | 1/1   | 0.88 | 0.08 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 4003 | 1/1   | 0.88 | 0.13 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3600 | 1/1   | 0.88 | 0.15 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3601 | 1/1   | 0.88 | 0.15 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3602 | 1/1   | 0.88 | 0.12 | 51,51,51,51                 | 0     |
| 59  | MG   | 1a    | 3493 | 1/1   | 0.88 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3014 | 1/1   | 0.88 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3122 | 1/1   | 0.88 | 0.38 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 4005 | 1/1   | 0.88 | 0.18 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3127 | 1/1   | 0.88 | 0.37 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3359 | 1/1   | 0.88 | 0.21 | 66,66,66,66                 | 0     |
| 59  | MG   | 2a    | 3030 | 1/1   | 0.88 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3031 | 1/1   | 0.88 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3034 | 1/1   | 0.88 | 0.21 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3318 | 1/1   | 0.88 | 0.27 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3320 | 1/1   | 0.88 | 0.25 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3699 | 1/1   | 0.88 | 0.11 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 4190 | 1/1   | 0.88 | 0.30 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3535 | 1/1   | 0.88 | 0.16 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3833 | 1/1   | 0.88 | 0.08 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3332 | 1/1   | 0.88 | 0.43 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3081 | 1/1   | 0.88 | 0.23 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3153 | 1/1   | 0.88 | 0.15 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3340 | 1/1   | 0.88 | 0.28 | 59,59,59,59                 | 0     |
| 59  | MG   | 1a    | 3366 | 1/1   | 0.88 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3367 | 1/1   | 0.88 | 0.25 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3843 | 1/1   | 0.88 | 0.14 | 19,19,19,19                 | 0     |
| 59  | MG   | 1B    | 214  | 1/1   | 0.88 | 0.09 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3350 | 1/1   | 0.88 | 0.30 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3352 | 1/1   | 0.88 | 0.09 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3844 | 1/1   | 0.88 | 0.17 | 35,35,35,35                 | 0     |
| 59  | MG   | 2a    | 3085 | 1/1   | 0.88 | 0.24 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3361 | 1/1   | 0.88 | 0.10 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3671 | 1/1   | 0.88 | 0.18 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3362 | 1/1   | 0.88 | 0.09 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3686 | 1/1   | 0.88 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 4048 | 1/1   | 0.88 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | 1a    | 3559 | 1/1   | 0.88 | 0.19 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3690 | 1/1   | 0.88 | 0.15 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3561 | 1/1   | 0.88 | 0.14 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3102 | 1/1   | 0.88 | 0.16 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3171 | 1/1   | 0.88 | 0.10 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3718 | 1/1   | 0.88 | 0.11 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3722 | 1/1   | 0.88 | 0.12 | 72,72,72,72                 | 0     |
| 59  | MG   | 1A    | 4052 | 1/1   | 0.88 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3565 | 1/1   | 0.88 | 0.16 | 35,35,35,35                 | 0     |
| 59  | MG   | 2a    | 3111 | 1/1   | 0.88 | 0.26 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3174 | 1/1   | 0.88 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3846 | 1/1   | 0.88 | 0.14 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3114 | 1/1   | 0.88 | 0.37 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3739 | 1/1   | 0.88 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3849 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3183 | 1/1   | 0.88 | 0.26 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3185 | 1/1   | 0.88 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3424 | 1/1   | 0.88 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3730 | 1/1   | 0.88 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3135 | 1/1   | 0.88 | 0.16 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3751 | 1/1   | 0.88 | 0.19 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3752 | 1/1   | 0.88 | 0.10 | 61,61,61,61                 | 0     |
| 59  | MG   | 1f    | 3003 | 1/1   | 0.88 | 0.30 | 57,57,57,57                 | 0     |
| 59  | MG   | 1l    | 202  | 1/1   | 0.88 | 0.11 | 82,82,82,82                 | 0     |
| 59  | MG   | 1A    | 3321 | 1/1   | 0.88 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3205 | 1/1   | 0.88 | 0.37 | 73,73,73,73                 | 0     |
| 59  | MG   | 2A    | 3207 | 1/1   | 0.88 | 0.09 | 56,56,56,56                 | 0     |
| 59  | MG   | 2a    | 3174 | 1/1   | 0.88 | 0.15 | 74,74,74,74                 | 0     |
| 59  | MG   | 2A    | 3208 | 1/1   | 0.88 | 0.13 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 4075 | 1/1   | 0.88 | 0.14 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3210 | 1/1   | 0.88 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3504 | 1/1   | 0.88 | 0.22 | 53,53,53,53                 | 0     |
| 59  | MG   | 1B    | 236  | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3399 | 1/1   | 0.88 | 0.17 | 42,42,42,42                 | 0     |
| 59  | MG   | 1D    | 310  | 1/1   | 0.88 | 0.16 | 43,43,43,43                 | 0     |
| 59  | MG   | 1w    | 110  | 1/1   | 0.88 | 0.13 | 81,81,81,81                 | 0     |
| 59  | MG   | 1D    | 312  | 1/1   | 0.88 | 0.10 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3477 | 1/1   | 0.88 | 0.21 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3196 | 1/1   | 0.88 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3889 | 1/1   | 0.88 | 0.07 | 22,22,22,22                 | 0     |
| 59  | MG   | 2A    | 3481 | 1/1   | 0.88 | 0.11 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3436 | 1/1   | 0.88 | 0.35 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3487 | 1/1   | 0.88 | 0.13 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3786 | 1/1   | 0.88 | 0.21 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3896 | 1/1   | 0.88 | 0.15 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 4091 | 1/1   | 0.88 | 0.16 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3021 | 1/1   | 0.88 | 0.24 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3507 | 1/1   | 0.88 | 0.13 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3510 | 1/1   | 0.88 | 0.10 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3291 | 1/1   | 0.88 | 0.11 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 4109 | 1/1   | 0.88 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3796 | 1/1   | 0.88 | 0.15 | 70,70,70,70                 | 0     |
| 59  | MG   | 1A    | 3392 | 1/1   | 0.88 | 0.11 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3799 | 1/1   | 0.88 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3642 | 1/1   | 0.88 | 0.13 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3774 | 1/1   | 0.88 | 0.10 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3227 | 1/1   | 0.88 | 0.18 | 50,50,50,50                 | 0     |
| 59  | MG   | 2a    | 3226 | 1/1   | 0.88 | 0.23 | 59,59,59,59                 | 0     |
| 59  | MG   | 10    | 106  | 1/1   | 0.88 | 0.24 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3828 | 1/1   | 0.88 | 0.12 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3778 | 1/1   | 0.88 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3783 | 1/1   | 0.88 | 0.12 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3032 | 1/1   | 0.88 | 0.28 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3033 | 1/1   | 0.88 | 0.17 | 58,58,58,58                 | 0     |
| 59  | MG   | 2B    | 3006 | 1/1   | 0.88 | 0.27 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3041 | 1/1   | 0.88 | 0.29 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3545 | 1/1   | 0.88 | 0.13 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 4122 | 1/1   | 0.88 | 0.12 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3550 | 1/1   | 0.88 | 0.10 | 56,56,56,56                 | 0     |
| 59  | MG   | 2q    | 203  | 1/1   | 0.88 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3949 | 1/1   | 0.88 | 0.12 | 52,52,52,52                 | 0     |
| 59  | MG   | 1a    | 3429 | 1/1   | 0.88 | 0.24 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3074 | 1/1   | 0.88 | 0.40 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3068 | 1/1   | 0.88 | 0.16 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3069 | 1/1   | 0.88 | 0.27 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3794 | 1/1   | 0.88 | 0.10 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3399 | 1/1   | 0.88 | 0.30 | 67,67,67,67                 | 0     |
| 59  | MG   | 2E    | 301  | 1/1   | 0.88 | 0.15 | 66,66,66,66                 | 0     |
| 59  | MG   | 1a    | 3441 | 1/1   | 0.88 | 0.11 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3462 | 1/1   | 0.88 | 0.10 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3459 | 1/1   | 0.88 | 0.11 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3568 | 1/1   | 0.88 | 0.13 | 74,74,74,74                 | 0     |
| 59  | MG   | 2A    | 3571 | 1/1   | 0.88 | 0.13 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 3349 | 1/1   | 0.88 | 0.09 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3155 | 1/1   | 0.88 | 0.16 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3569 | 1/1   | 0.88 | 0.13 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3476 | 1/1   | 0.88 | 0.09 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3677 | 1/1   | 0.88 | 0.10 | 10,10,10,10                 | 0     |
| 59  | MG   | 1A    | 4162 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3293 | 1/1   | 0.88 | 0.20 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3640 | 1/1   | 0.89 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | 2a    | 3015 | 1/1   | 0.89 | 0.12 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3641 | 1/1   | 0.89 | 0.16 | 75,75,75,75                 | 0     |
| 59  | MG   | 1A    | 3426 | 1/1   | 0.89 | 0.15 | 46,46,46,46                 | 0     |
| 59  | MG   | 1w    | 102  | 1/1   | 0.89 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | 2a    | 3025 | 1/1   | 0.89 | 0.28 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 4086 | 1/1   | 0.89 | 0.10 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3028 | 1/1   | 0.89 | 0.22 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3769 | 1/1   | 0.89 | 0.18 | 48,48,48,48                 | 0     |
| 59  | MG   | 1F    | 302  | 1/1   | 0.89 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3199 | 1/1   | 0.89 | 0.13 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3204 | 1/1   | 0.89 | 0.24 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3410 | 1/1   | 0.89 | 0.10 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3367 | 1/1   | 0.89 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 2a    | 3038 | 1/1   | 0.89 | 0.19 | 78,78,78,78                 | 0     |
| 59  | MG   | 2a    | 3042 | 1/1   | 0.89 | 0.08 | 70,70,70,70                 | 0     |
| 59  | MG   | 2a    | 3043 | 1/1   | 0.89 | 0.26 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3674 | 1/1   | 0.89 | 0.30 | 61,61,61,61                 | 0     |
| 59  | MG   | 1a    | 3407 | 1/1   | 0.89 | 0.12 | 36,36,36,36                 | 0     |
| 59  | MG   | 1O    | 3003 | 1/1   | 0.89 | 0.15 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3433 | 1/1   | 0.89 | 0.15 | 56,56,56,56                 | 0     |
| 59  | MG   | 1x    | 109  | 1/1   | 0.89 | 0.15 | 68,68,68,68                 | 0     |
| 59  | MG   | 2a    | 3058 | 1/1   | 0.89 | 0.24 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3434 | 1/1   | 0.89 | 0.09 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3702 | 1/1   | 0.89 | 0.10 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3706 | 1/1   | 0.89 | 0.09 | 70,70,70,70                 | 0     |
| 59  | MG   | 2A    | 3436 | 1/1   | 0.89 | 0.09 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3375 | 1/1   | 0.89 | 0.13 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3308 | 1/1   | 0.89 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3079 | 1/1   | 0.89 | 0.29 | 67,67,67,67                 | 0     |
| 59  | MG   | 1Q    | 203  | 1/1   | 0.89 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | 1Q    | 204  | 1/1   | 0.89 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3918 | 1/1   | 0.89 | 0.09 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3921 | 1/1   | 0.89 | 0.11 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3924 | 1/1   | 0.89 | 0.14 | 22,22,22,22                 | 0     |
| 59  | MG   | 2A    | 3737 | 1/1   | 0.89 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3188 | 1/1   | 0.89 | 0.23 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3930 | 1/1   | 0.89 | 0.14 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3468 | 1/1   | 0.89 | 0.10 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3470 | 1/1   | 0.89 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3095 | 1/1   | 0.89 | 0.10 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2a    | 3097 | 1/1   | 0.89 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3787 | 1/1   | 0.89 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3276 | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3023 | 1/1   | 0.89 | 0.08 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3428 | 1/1   | 0.89 | 0.24 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3106 | 1/1   | 0.89 | 0.23 | 33,33,33,33                 | 0     |
| 59  | MG   | 17    | 101  | 1/1   | 0.89 | 0.14 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4126 | 1/1   | 0.89 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3109 | 1/1   | 0.89 | 0.25 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3649 | 1/1   | 0.89 | 0.10 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3314 | 1/1   | 0.89 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3544 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 4134 | 1/1   | 0.89 | 0.14 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3654 | 1/1   | 0.89 | 0.13 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3655 | 1/1   | 0.89 | 0.15 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3327 | 1/1   | 0.89 | 0.22 | 60,60,60,60                 | 0     |
| 59  | MG   | 2a    | 3119 | 1/1   | 0.89 | 0.22 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 3982 | 1/1   | 0.89 | 0.12 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3773 | 1/1   | 0.89 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 1a    | 3477 | 1/1   | 0.89 | 0.16 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 3545 | 1/1   | 0.89 | 0.12 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3082 | 1/1   | 0.89 | 0.14 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3527 | 1/1   | 0.89 | 0.15 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3657 | 1/1   | 0.89 | 0.17 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 4155 | 1/1   | 0.89 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3533 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3812 | 1/1   | 0.89 | 0.16 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3109 | 1/1   | 0.89 | 0.19 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3346 | 1/1   | 0.89 | 0.29 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3170 | 1/1   | 0.89 | 0.18 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3331 | 1/1   | 0.89 | 0.11 | 41,41,41,41                 | 0     |
| 59  | MG   | 1a    | 3495 | 1/1   | 0.89 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3286 | 1/1   | 0.89 | 0.17 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3546 | 1/1   | 0.89 | 0.16 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3110 | 1/1   | 0.89 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3690 | 1/1   | 0.89 | 0.13 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3044 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3185 | 1/1   | 0.89 | 0.09 | 64,64,64,64                 | 0     |
| 59  | MG   | 1a    | 3525 | 1/1   | 0.89 | 0.11 | 76,76,76,76                 | 0     |
| 59  | MG   | 1A    | 3255 | 1/1   | 0.89 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3711 | 1/1   | 0.89 | 0.11 | 34,34,34,34                 | 0     |
| 59  | MG   | 1a    | 3542 | 1/1   | 0.89 | 0.12 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2a    | 3195 | 1/1   | 0.89 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3808 | 1/1   | 0.89 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 4037 | 1/1   | 0.89 | 0.11 | 40,40,40,40                 | 0     |
| 59  | MG   | 1a    | 3365 | 1/1   | 0.89 | 0.14 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3814 | 1/1   | 0.89 | 0.10 | 44,44,44,44                 | 0     |
| 59  | MG   | 2a    | 3203 | 1/1   | 0.89 | 0.18 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3816 | 1/1   | 0.89 | 0.13 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3299 | 1/1   | 0.89 | 0.24 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3829 | 1/1   | 0.89 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3831 | 1/1   | 0.89 | 0.34 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3140 | 1/1   | 0.89 | 0.35 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3303 | 1/1   | 0.89 | 0.13 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3844 | 1/1   | 0.89 | 0.27 | 48,48,48,48                 | 0     |
| 59  | MG   | 1B    | 213  | 1/1   | 0.89 | 0.16 | 43,43,43,43                 | 0     |
| 59  | MG   | 2a    | 3214 | 1/1   | 0.89 | 0.26 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3569 | 1/1   | 0.89 | 0.20 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3187 | 1/1   | 0.89 | 0.09 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3584 | 1/1   | 0.89 | 0.11 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3310 | 1/1   | 0.89 | 0.20 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3147 | 1/1   | 0.89 | 0.22 | 53,53,53,53                 | 0     |
| 59  | MG   | 1B    | 218  | 1/1   | 0.89 | 0.14 | 36,36,36,36                 | 0     |
| 59  | MG   | 2B    | 3012 | 1/1   | 0.89 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | 2B    | 3014 | 1/1   | 0.89 | 0.18 | 67,67,67,67                 | 0     |
| 59  | MG   | 2a    | 3228 | 1/1   | 0.89 | 0.20 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3594 | 1/1   | 0.89 | 0.08 | 15,15,15,15                 | 0     |
| 59  | MG   | 2a    | 3234 | 1/1   | 0.89 | 0.21 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3373 | 1/1   | 0.89 | 0.24 | 59,59,59,59                 | 0     |
| 59  | MG   | 2B    | 3017 | 1/1   | 0.89 | 0.15 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3603 | 1/1   | 0.89 | 0.10 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3741 | 1/1   | 0.89 | 0.15 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3876 | 1/1   | 0.89 | 0.15 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3883 | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3164 | 1/1   | 0.89 | 0.23 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3571 | 1/1   | 0.89 | 0.12 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3353 | 1/1   | 0.89 | 0.20 | 51,51,51,51                 | 0     |
| 59  | MG   | 1a    | 3575 | 1/1   | 0.89 | 0.23 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3228 | 1/1   | 0.89 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3343 | 1/1   | 0.89 | 0.25 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3893 | 1/1   | 0.89 | 0.20 | 39,39,39,39                 | 0     |
| 59  | MG   | 2O    | 8002 | 1/1   | 0.89 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 1d    | 502  | 1/1   | 0.89 | 0.27 | 52,52,52,52                 | 0     |
| 59  | MG   | 2w    | 3001 | 1/1   | 0.89 | 0.21 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3895 | 1/1   | 0.89 | 0.10 | 39,39,39,39                 | 0     |
| 59  | MG   | 1B    | 235  | 1/1   | 0.89 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3618 | 1/1   | 0.89 | 0.33 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3176 | 1/1   | 0.89 | 0.13 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3177 | 1/1   | 0.89 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3623 | 1/1   | 0.89 | 0.11 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4078 | 1/1   | 0.89 | 0.09 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3357 | 1/1   | 0.89 | 0.14 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3627 | 1/1   | 0.89 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3359 | 1/1   | 0.89 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | 1n    | 503  | 1/1   | 0.89 | 0.15 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3180 | 1/1   | 0.89 | 0.15 | 53,53,53,53                 | 0     |
| 59  | MG   | 1p    | 101  | 1/1   | 0.89 | 0.18 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3622 | 1/1   | 0.89 | 0.13 | 17,17,17,17                 | 0     |
| 59  | MG   | 2a    | 3012 | 1/1   | 0.89 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3186 | 1/1   | 0.89 | 0.26 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 4098 | 1/1   | 0.90 | 0.14 | 37,37,37,37                 | 0     |
| 59  | MG   | 2a    | 3052 | 1/1   | 0.90 | 0.18 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 4102 | 1/1   | 0.90 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 4104 | 1/1   | 0.90 | 0.14 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3057 | 1/1   | 0.90 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3977 | 1/1   | 0.90 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3078 | 1/1   | 0.90 | 0.21 | 48,48,48,48                 | 0     |
| 59  | MG   | 2a    | 3062 | 1/1   | 0.90 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3063 | 1/1   | 0.90 | 0.20 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3530 | 1/1   | 0.90 | 0.11 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3344 | 1/1   | 0.90 | 0.21 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3143 | 1/1   | 0.90 | 0.26 | 56,56,56,56                 | 0     |
| 59  | MG   | 2a    | 3067 | 1/1   | 0.90 | 0.15 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3326 | 1/1   | 0.90 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3301 | 1/1   | 0.90 | 0.27 | 41,41,41,41                 | 0     |
| 59  | MG   | 2a    | 3078 | 1/1   | 0.90 | 0.21 | 70,70,70,70                 | 0     |
| 59  | MG   | 1a    | 3430 | 1/1   | 0.90 | 0.16 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3766 | 1/1   | 0.90 | 0.09 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3376 | 1/1   | 0.90 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 1a    | 3353 | 1/1   | 0.90 | 0.25 | 58,58,58,58                 | 0     |
| 59  | MG   | 2a    | 3084 | 1/1   | 0.90 | 0.11 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3071 | 1/1   | 0.90 | 0.38 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3586 | 1/1   | 0.90 | 0.14 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3311 | 1/1   | 0.90 | 0.19 | 44,44,44,44                 | 0     |
| 59  | MG   | 1x    | 102  | 1/1   | 0.90 | 0.31 | 59,59,59,59                 | 0     |
| 59  | MG   | 2a    | 3090 | 1/1   | 0.90 | 0.11 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3443 | 1/1   | 0.90 | 0.28 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3314 | 1/1   | 0.90 | 0.32 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3589 | 1/1   | 0.90 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3317 | 1/1   | 0.90 | 0.18 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3330 | 1/1   | 0.90 | 0.34 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3460 | 1/1   | 0.90 | 0.18 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 4009 | 1/1   | 0.90 | 0.09 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3674 | 1/1   | 0.90 | 0.08 | 14,14,14,14                 | 0     |
| 59  | MG   | 2A    | 3181 | 1/1   | 0.90 | 0.23 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3595 | 1/1   | 0.90 | 0.08 | 18,18,18,18                 | 0     |
| 59  | MG   | 2A    | 3567 | 1/1   | 0.90 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | 1E    | 305  | 1/1   | 0.90 | 0.18 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3335 | 1/1   | 0.90 | 0.10 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3510 | 1/1   | 0.90 | 0.16 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3380 | 1/1   | 0.90 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 1F    | 309  | 1/1   | 0.90 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3579 | 1/1   | 0.90 | 0.15 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3341 | 1/1   | 0.90 | 0.29 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3693 | 1/1   | 0.90 | 0.12 | 13,13,13,13                 | 0     |
| 59  | MG   | 2A    | 3192 | 1/1   | 0.90 | 0.16 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3021 | 1/1   | 0.90 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3371 | 1/1   | 0.90 | 0.15 | 55,55,55,55                 | 0     |
| 59  | MG   | 2a    | 3124 | 1/1   | 0.90 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3126 | 1/1   | 0.90 | 0.08 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3810 | 1/1   | 0.90 | 0.11 | 59,59,59,59                 | 0     |
| 59  | MG   | 1G    | 3004 | 1/1   | 0.90 | 0.08 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3591 | 1/1   | 0.90 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3201 | 1/1   | 0.90 | 0.23 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3202 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3141 | 1/1   | 0.90 | 0.16 | 56,56,56,56                 | 0     |
| 59  | MG   | 1O    | 3001 | 1/1   | 0.90 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3150 | 1/1   | 0.90 | 0.10 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3151 | 1/1   | 0.90 | 0.10 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 3274 | 1/1   | 0.90 | 0.22 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3157 | 1/1   | 0.90 | 0.11 | 77,77,77,77                 | 0     |
| 59  | MG   | 1A    | 3332 | 1/1   | 0.90 | 0.21 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3035 | 1/1   | 0.90 | 0.26 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3843 | 1/1   | 0.90 | 0.09 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3037 | 1/1   | 0.90 | 0.21 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3038 | 1/1   | 0.90 | 0.21 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3846 | 1/1   | 0.90 | 0.13 | 38,38,38,38                 | 0     |
| 59  | MG   | 1a    | 3499 | 1/1   | 0.90 | 0.12 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2a    | 3177 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3607 | 1/1   | 0.90 | 0.10 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3623 | 1/1   | 0.90 | 0.10 | 15,15,15,15                 | 0     |
| 59  | MG   | 1a    | 3382 | 1/1   | 0.90 | 0.09 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3375 | 1/1   | 0.90 | 0.10 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3053 | 1/1   | 0.90 | 0.28 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3219 | 1/1   | 0.90 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 4053 | 1/1   | 0.90 | 0.25 | 69,69,69,69                 | 0     |
| 59  | MG   | 1a    | 3510 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3296 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3514 | 1/1   | 0.90 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3405 | 1/1   | 0.90 | 0.10 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3232 | 1/1   | 0.90 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | 1a    | 3386 | 1/1   | 0.90 | 0.25 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3630 | 1/1   | 0.90 | 0.19 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 4148 | 1/1   | 0.90 | 0.28 | 60,60,60,60                 | 0     |
| 59  | MG   | 2D    | 305  | 1/1   | 0.90 | 0.32 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3235 | 1/1   | 0.90 | 0.31 | 62,62,62,62                 | 0     |
| 59  | MG   | 2E    | 302  | 1/1   | 0.90 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | 1a    | 3389 | 1/1   | 0.90 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 2E    | 306  | 1/1   | 0.90 | 0.11 | 29,29,29,29                 | 0     |
| 59  | MG   | 1a    | 3537 | 1/1   | 0.90 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3539 | 1/1   | 0.90 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 4060 | 1/1   | 0.90 | 0.15 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3022 | 1/1   | 0.90 | 0.14 | 39,39,39,39                 | 0     |
| 59  | MG   | 1T    | 8001 | 1/1   | 0.90 | 0.13 | 43,43,43,43                 | 0     |
| 59  | MG   | 2Q    | 3002 | 1/1   | 0.90 | 0.25 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3653 | 1/1   | 0.90 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3445 | 1/1   | 0.90 | 0.13 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3261 | 1/1   | 0.90 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 4176 | 1/1   | 0.90 | 0.14 | 15,15,15,15                 | 0     |
| 59  | MG   | 2T    | 201  | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3451 | 1/1   | 0.90 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3455 | 1/1   | 0.90 | 0.18 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3306 | 1/1   | 0.90 | 0.23 | 47,47,47,47                 | 0     |
| 59  | MG   | 1a    | 3556 | 1/1   | 0.90 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3256 | 1/1   | 0.90 | 0.23 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3837 | 1/1   | 0.90 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3682 | 1/1   | 0.90 | 0.10 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3685 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 59  | MG   | 2d    | 502  | 1/1   | 0.90 | 0.17 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3466 | 1/1   | 0.90 | 0.20 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3558 | 1/1   | 0.90 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | 2a    | 3007 | 1/1   | 0.90 | 0.22 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3839 | 1/1   | 0.90 | 0.26 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3643 | 1/1   | 0.90 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3111 | 1/1   | 0.90 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3400 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 59  | MG   | 2q    | 202  | 1/1   | 0.90 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3266 | 1/1   | 0.90 | 0.09 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3408 | 1/1   | 0.90 | 0.50 | 60,60,60,60                 | 0     |
| 59  | MG   | 2r    | 3001 | 1/1   | 0.90 | 0.20 | 77,77,77,77                 | 0     |
| 59  | MG   | 2A    | 3717 | 1/1   | 0.90 | 0.09 | 63,63,63,63                 | 0     |
| 59  | MG   | 2v    | 101  | 1/1   | 0.90 | 0.25 | 49,49,49,49                 | 0     |
| 59  | MG   | 1B    | 201  | 1/1   | 0.90 | 0.17 | 44,44,44,44                 | 0     |
| 59  | MG   | 2a    | 3023 | 1/1   | 0.90 | 0.37 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3752 | 1/1   | 0.90 | 0.09 | 27,27,27,27                 | 0     |
| 59  | MG   | 1B    | 208  | 1/1   | 0.90 | 0.24 | 63,63,63,63                 | 0     |
| 59  | MG   | 1a    | 3413 | 1/1   | 0.90 | 0.23 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3728 | 1/1   | 0.90 | 0.08 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3141 | 1/1   | 0.90 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | 2a    | 3033 | 1/1   | 0.90 | 0.17 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3959 | 1/1   | 0.90 | 0.12 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3735 | 1/1   | 0.90 | 0.22 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3736 | 1/1   | 0.90 | 0.17 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3970 | 1/1   | 0.90 | 0.08 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3283 | 1/1   | 0.90 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3040 | 1/1   | 0.90 | 0.24 | 47,47,47,47                 | 0     |
| 59  | MG   | 2a    | 3041 | 1/1   | 0.90 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3740 | 1/1   | 0.90 | 0.10 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3511 | 1/1   | 0.90 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | 1e    | 3001 | 1/1   | 0.90 | 0.12 | 67,67,67,67                 | 0     |
| 59  | MG   | 2y    | 3006 | 1/1   | 0.90 | 0.08 | 89,89,89,89                 | 0     |
| 59  | MG   | 1A    | 3263 | 1/1   | 0.90 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 1E    | 314  | 1/1   | 0.91 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3124 | 1/1   | 0.91 | 0.10 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3378 | 1/1   | 0.91 | 0.26 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3194 | 1/1   | 0.91 | 0.34 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3388 | 1/1   | 0.91 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3077 | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3724 | 1/1   | 0.91 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3684 | 1/1   | 0.91 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | 1G    | 3003 | 1/1   | 0.91 | 0.07 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3404 | 1/1   | 0.91 | 0.13 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3381 | 1/1   | 0.91 | 0.15 | 41,41,41,41                 | 0     |
| 59  | MG   | 1I    | 3001 | 1/1   | 0.91 | 0.12 | 62,62,62,62                 | 0     |
| 59  | MG   | 1N    | 3004 | 1/1   | 0.91 | 0.11 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3175 | 1/1   | 0.91 | 0.14 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 4090 | 1/1   | 0.91 | 0.14 | 34,34,34,34                 | 0     |
| 59  | MG   | 2a    | 3047 | 1/1   | 0.91 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3898 | 1/1   | 0.91 | 0.14 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3585 | 1/1   | 0.91 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 1x    | 117  | 1/1   | 0.91 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3213 | 1/1   | 0.91 | 0.31 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3214 | 1/1   | 0.91 | 0.13 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3387 | 1/1   | 0.91 | 0.19 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3905 | 1/1   | 0.91 | 0.07 | 71,71,71,71                 | 0     |
| 59  | MG   | 2A    | 3446 | 1/1   | 0.91 | 0.12 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3020 | 1/1   | 0.91 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3341 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3221 | 1/1   | 0.91 | 0.18 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3343 | 1/1   | 0.91 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3017 | 1/1   | 0.91 | 0.20 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3470 | 1/1   | 0.91 | 0.26 | 47,47,47,47                 | 0     |
| 59  | MG   | 2a    | 3076 | 1/1   | 0.91 | 0.32 | 56,56,56,56                 | 0     |
| 59  | MG   | 2a    | 3077 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 59  | MG   | 1T    | 8002 | 1/1   | 0.91 | 0.15 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3741 | 1/1   | 0.91 | 0.15 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3051 | 1/1   | 0.91 | 0.21 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3481 | 1/1   | 0.91 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3024 | 1/1   | 0.91 | 0.12 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3469 | 1/1   | 0.91 | 0.22 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3025 | 1/1   | 0.91 | 0.09 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3026 | 1/1   | 0.91 | 0.15 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3472 | 1/1   | 0.91 | 0.21 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3754 | 1/1   | 0.91 | 0.21 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3237 | 1/1   | 0.91 | 0.12 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3482 | 1/1   | 0.91 | 0.13 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3438 | 1/1   | 0.91 | 0.21 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3478 | 1/1   | 0.91 | 0.17 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3241 | 1/1   | 0.91 | 0.21 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3053 | 1/1   | 0.91 | 0.18 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3483 | 1/1   | 0.91 | 0.16 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3485 | 1/1   | 0.91 | 0.11 | 36,36,36,36                 | 0     |
| 59  | MG   | 10    | 107  | 1/1   | 0.91 | 0.13 | 38,38,38,38                 | 0     |
| 59  | MG   | 2a    | 3103 | 1/1   | 0.91 | 0.17 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2a    | 3104 | 1/1   | 0.91 | 0.27 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3626 | 1/1   | 0.91 | 0.10 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3942 | 1/1   | 0.91 | 0.18 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3076 | 1/1   | 0.91 | 0.17 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3782 | 1/1   | 0.91 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3497 | 1/1   | 0.91 | 0.11 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3498 | 1/1   | 0.91 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3501 | 1/1   | 0.91 | 0.16 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3777 | 1/1   | 0.91 | 0.10 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3252 | 1/1   | 0.91 | 0.15 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3302 | 1/1   | 0.91 | 0.23 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3780 | 1/1   | 0.91 | 0.21 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3404 | 1/1   | 0.91 | 0.17 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3513 | 1/1   | 0.91 | 0.14 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3057 | 1/1   | 0.91 | 0.22 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3785 | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3125 | 1/1   | 0.91 | 0.15 | 79,79,79,79                 | 0     |
| 59  | MG   | 2A    | 3058 | 1/1   | 0.91 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3127 | 1/1   | 0.91 | 0.09 | 74,74,74,74                 | 0     |
| 59  | MG   | 1A    | 3490 | 1/1   | 0.91 | 0.24 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3522 | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3062 | 1/1   | 0.91 | 0.27 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3261 | 1/1   | 0.91 | 0.06 | 59,59,59,59                 | 0     |
| 59  | MG   | 1a    | 3475 | 1/1   | 0.91 | 0.16 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3493 | 1/1   | 0.91 | 0.34 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3321 | 1/1   | 0.91 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3351 | 1/1   | 0.91 | 0.11 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3270 | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3966 | 1/1   | 0.91 | 0.12 | 44,44,44,44                 | 0     |
| 59  | MG   | 2a    | 3156 | 1/1   | 0.91 | 0.10 | 77,77,77,77                 | 0     |
| 59  | MG   | 2A    | 3077 | 1/1   | 0.91 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3484 | 1/1   | 0.91 | 0.12 | 41,41,41,41                 | 0     |
| 59  | MG   | 2a    | 3159 | 1/1   | 0.91 | 0.18 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3968 | 1/1   | 0.91 | 0.08 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3796 | 1/1   | 0.91 | 0.15 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3281 | 1/1   | 0.91 | 0.23 | 67,67,67,67                 | 0     |
| 59  | MG   | 2A    | 3284 | 1/1   | 0.91 | 0.12 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3406 | 1/1   | 0.91 | 0.12 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3506 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3822 | 1/1   | 0.91 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3409 | 1/1   | 0.91 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3153 | 1/1   | 0.91 | 0.27 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3984 | 1/1   | 0.91 | 0.09 | 10,10,10,10                 | 0     |
| 59  | MG   | 1a    | 3341 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3358 | 1/1   | 0.91 | 0.25 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3840 | 1/1   | 0.91 | 0.10 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3650 | 1/1   | 0.91 | 0.13 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3989 | 1/1   | 0.91 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3560 | 1/1   | 0.91 | 0.07 | 61,61,61,61                 | 0     |
| 59  | MG   | 2a    | 3192 | 1/1   | 0.91 | 0.15 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3294 | 1/1   | 0.91 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 2B    | 3001 | 1/1   | 0.91 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3651 | 1/1   | 0.91 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | 2B    | 3004 | 1/1   | 0.91 | 0.07 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3104 | 1/1   | 0.91 | 0.16 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 4184 | 1/1   | 0.91 | 0.14 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3415 | 1/1   | 0.91 | 0.17 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3821 | 1/1   | 0.91 | 0.07 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3823 | 1/1   | 0.91 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3319 | 1/1   | 0.91 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3305 | 1/1   | 0.91 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 4210 | 1/1   | 0.91 | 0.18 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3581 | 1/1   | 0.91 | 0.07 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4221 | 1/1   | 0.91 | 0.28 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3308 | 1/1   | 0.91 | 0.19 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3825 | 1/1   | 0.91 | 0.19 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3137 | 1/1   | 0.91 | 0.29 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3197 | 1/1   | 0.91 | 0.23 | 32,32,32,32                 | 0     |
| 59  | MG   | 1a    | 3546 | 1/1   | 0.91 | 0.16 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3590 | 1/1   | 0.91 | 0.10 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3830 | 1/1   | 0.91 | 0.11 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3593 | 1/1   | 0.91 | 0.09 | 37,37,37,37                 | 0     |
| 59  | MG   | 1B    | 209  | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3368 | 1/1   | 0.91 | 0.35 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 4013 | 1/1   | 0.91 | 0.09 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3598 | 1/1   | 0.91 | 0.11 | 63,63,63,63                 | 0     |
| 59  | MG   | 2F    | 304  | 1/1   | 0.91 | 0.11 | 74,74,74,74                 | 0     |
| 59  | MG   | 1A    | 4014 | 1/1   | 0.91 | 0.08 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3368 | 1/1   | 0.91 | 0.13 | 39,39,39,39                 | 0     |
| 59  | MG   | 2a    | 3237 | 1/1   | 0.91 | 0.21 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3427 | 1/1   | 0.91 | 0.19 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3666 | 1/1   | 0.91 | 0.11 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3326 | 1/1   | 0.91 | 0.18 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3560 | 1/1   | 0.91 | 0.10 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 4039 | 1/1   | 0.91 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3377 | 1/1   | 0.91 | 0.27 | 61,61,61,61                 | 0     |
| 59  | MG   | 2k    | 3001 | 1/1   | 0.91 | 0.26 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3536 | 1/1   | 0.91 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3842 | 1/1   | 0.91 | 0.10 | 15,15,15,15                 | 0     |
| 59  | MG   | 1A    | 3537 | 1/1   | 0.91 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | 1B    | 226  | 1/1   | 0.91 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3370 | 1/1   | 0.91 | 0.23 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4056 | 1/1   | 0.91 | 0.10 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3431 | 1/1   | 0.91 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | 1b    | 3002 | 1/1   | 0.91 | 0.18 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 4059 | 1/1   | 0.91 | 0.18 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3004 | 1/1   | 0.91 | 0.24 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3154 | 1/1   | 0.91 | 0.17 | 42,42,42,42                 | 0     |
| 59  | MG   | 1f    | 3001 | 1/1   | 0.91 | 0.18 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 4061 | 1/1   | 0.91 | 0.13 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3008 | 1/1   | 0.91 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3680 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3011 | 1/1   | 0.91 | 0.23 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3209 | 1/1   | 0.91 | 0.15 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3358 | 1/1   | 0.91 | 0.25 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3398 | 1/1   | 0.91 | 0.27 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3438 | 1/1   | 0.91 | 0.14 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3697 | 1/1   | 0.91 | 0.10 | 18,18,18,18                 | 0     |
| 59  | MG   | 2A    | 3364 | 1/1   | 0.91 | 0.15 | 63,63,63,63                 | 0     |
| 59  | MG   | 1t    | 3001 | 1/1   | 0.91 | 0.13 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3262 | 1/1   | 0.91 | 0.22 | 41,41,41,41                 | 0     |
| 59  | MG   | 2a    | 3024 | 1/1   | 0.91 | 0.26 | 59,59,59,59                 | 0     |
| 59  | MG   | 1E    | 308  | 1/1   | 0.91 | 0.25 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3190 | 1/1   | 0.91 | 0.14 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3572 | 1/1   | 0.91 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 2a    | 3029 | 1/1   | 0.91 | 0.26 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3173 | 1/1   | 0.92 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3442 | 1/1   | 0.92 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3305 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3397 | 1/1   | 0.92 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3003 | 1/1   | 0.92 | 0.34 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3574 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 59  | MG   | 2Q    | 3003 | 1/1   | 0.92 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3091 | 1/1   | 0.92 | 0.06 | 17,17,17,17                 | 0     |
| 59  | MG   | 2R    | 201  | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | 1a    | 3400 | 1/1   | 0.92 | 0.19 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3307 | 1/1   | 0.92 | 0.12 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3267 | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 59  | MG   | 1B    | 234  | 1/1   | 0.92 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 2T    | 202  | 1/1   | 0.92 | 0.18 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3125 | 1/1   | 0.92 | 0.26 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4065 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | 1D    | 302  | 1/1   | 0.92 | 0.15 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 4066 | 1/1   | 0.92 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 23    | 102  | 1/1   | 0.92 | 0.11 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3028 | 1/1   | 0.92 | 0.13 | 25,25,25,25                 | 0     |
| 59  | MG   | 28    | 101  | 1/1   | 0.92 | 0.34 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 4067 | 1/1   | 0.92 | 0.14 | 36,36,36,36                 | 0     |
| 59  | MG   | 2a    | 3001 | 1/1   | 0.92 | 0.08 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3283 | 1/1   | 0.92 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 4070 | 1/1   | 0.92 | 0.08 | 33,33,33,33                 | 0     |
| 59  | MG   | 1E    | 301  | 1/1   | 0.92 | 0.12 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3728 | 1/1   | 0.92 | 0.13 | 16,16,16,16                 | 0     |
| 59  | MG   | 1E    | 307  | 1/1   | 0.92 | 0.15 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3729 | 1/1   | 0.92 | 0.12 | 11,11,11,11                 | 0     |
| 59  | MG   | 1A    | 3891 | 1/1   | 0.92 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3042 | 1/1   | 0.92 | 0.11 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3100 | 1/1   | 0.92 | 0.22 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3186 | 1/1   | 0.92 | 0.26 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3052 | 1/1   | 0.92 | 0.16 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3386 | 1/1   | 0.92 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3055 | 1/1   | 0.92 | 0.07 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3591 | 1/1   | 0.92 | 0.09 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3742 | 1/1   | 0.92 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 4083 | 1/1   | 0.92 | 0.11 | 68,68,68,68                 | 0     |
| 59  | MG   | 2a    | 3021 | 1/1   | 0.92 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3022 | 1/1   | 0.92 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3899 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3603 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3065 | 1/1   | 0.92 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3066 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3304 | 1/1   | 0.92 | 0.35 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3128 | 1/1   | 0.92 | 0.20 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3612 | 1/1   | 0.92 | 0.12 | 44,44,44,44                 | 0     |
| 59  | MG   | 1N    | 3009 | 1/1   | 0.92 | 0.16 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 4088 | 1/1   | 0.92 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3617 | 1/1   | 0.92 | 0.11 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3072 | 1/1   | 0.92 | 0.12 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3474 | 1/1   | 0.92 | 0.20 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3621 | 1/1   | 0.92 | 0.11 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3434 | 1/1   | 0.92 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3076 | 1/1   | 0.92 | 0.13 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3596 | 1/1   | 0.92 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 4093 | 1/1   | 0.92 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3753 | 1/1   | 0.92 | 0.09 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 4096 | 1/1   | 0.92 | 0.32 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3316 | 1/1   | 0.92 | 0.26 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3754 | 1/1   | 0.92 | 0.19 | 32,32,32,32                 | 0     |
| 59  | MG   | 1R    | 201  | 1/1   | 0.92 | 0.10 | 28,28,28,28                 | 0     |
| 59  | MG   | 2a    | 3049 | 1/1   | 0.92 | 0.14 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3448 | 1/1   | 0.92 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3597 | 1/1   | 0.92 | 0.10 | 34,34,34,34                 | 0     |
| 59  | MG   | 1a    | 3454 | 1/1   | 0.92 | 0.10 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3458 | 1/1   | 0.92 | 0.13 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3762 | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3096 | 1/1   | 0.92 | 0.18 | 55,55,55,55                 | 0     |
| 59  | MG   | 2a    | 3061 | 1/1   | 0.92 | 0.16 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3330 | 1/1   | 0.92 | 0.14 | 53,53,53,53                 | 0     |
| 59  | MG   | 1S    | 3002 | 1/1   | 0.92 | 0.18 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3915 | 1/1   | 0.92 | 0.08 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3655 | 1/1   | 0.92 | 0.08 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3036 | 1/1   | 0.92 | 0.17 | 23,23,23,23                 | 0     |
| 59  | MG   | 2A    | 3337 | 1/1   | 0.92 | 0.17 | 44,44,44,44                 | 0     |
| 59  | MG   | 2a    | 3068 | 1/1   | 0.92 | 0.17 | 52,52,52,52                 | 0     |
| 59  | MG   | 2a    | 3069 | 1/1   | 0.92 | 0.35 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3102 | 1/1   | 0.92 | 0.17 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3664 | 1/1   | 0.92 | 0.12 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3666 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3467 | 1/1   | 0.92 | 0.14 | 53,53,53,53                 | 0     |
| 59  | MG   | 1U    | 202  | 1/1   | 0.92 | 0.18 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3109 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3480 | 1/1   | 0.92 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3345 | 1/1   | 0.92 | 0.17 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3677 | 1/1   | 0.92 | 0.10 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3678 | 1/1   | 0.92 | 0.15 | 64,64,64,64                 | 0     |
| 59  | MG   | 1Y    | 502  | 1/1   | 0.92 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 2a    | 3086 | 1/1   | 0.92 | 0.25 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3770 | 1/1   | 0.92 | 0.11 | 40,40,40,40                 | 0     |
| 59  | MG   | 1Z    | 302  | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3349 | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3124 | 1/1   | 0.92 | 0.18 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3771 | 1/1   | 0.92 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3353 | 1/1   | 0.92 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3692 | 1/1   | 0.92 | 0.09 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3695 | 1/1   | 0.92 | 0.11 | 53,53,53,53                 | 0     |
| 59  | MG   | 1a    | 3483 | 1/1   | 0.92 | 0.14 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3325 | 1/1   | 0.92 | 0.25 | 31,31,31,31                 | 0     |
| 59  | MG   | 2a    | 3099 | 1/1   | 0.92 | 0.25 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3707 | 1/1   | 0.92 | 0.15 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 4116 | 1/1   | 0.92 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3936 | 1/1   | 0.92 | 0.09 | 19,19,19,19                 | 0     |
| 59  | MG   | 12    | 3001 | 1/1   | 0.92 | 0.09 | 40,40,40,40                 | 0     |
| 59  | MG   | 13    | 3001 | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3057 | 1/1   | 0.92 | 0.06 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3724 | 1/1   | 0.92 | 0.16 | 34,34,34,34                 | 0     |
| 59  | MG   | 1a    | 3494 | 1/1   | 0.92 | 0.10 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 4121 | 1/1   | 0.92 | 0.11 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3264 | 1/1   | 0.92 | 0.10 | 56,56,56,56                 | 0     |
| 59  | MG   | 19    | 101  | 1/1   | 0.92 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3732 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3396 | 1/1   | 0.92 | 0.10 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3734 | 1/1   | 0.92 | 0.10 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3506 | 1/1   | 0.92 | 0.11 | 59,59,59,59                 | 0     |
| 59  | MG   | 2a    | 3117 | 1/1   | 0.92 | 0.27 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3155 | 1/1   | 0.92 | 0.16 | 44,44,44,44                 | 0     |
| 59  | MG   | 1a    | 3507 | 1/1   | 0.92 | 0.09 | 64,64,64,64                 | 0     |
| 59  | MG   | 2a    | 3120 | 1/1   | 0.92 | 0.10 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3738 | 1/1   | 0.92 | 0.20 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3303 | 1/1   | 0.92 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3381 | 1/1   | 0.92 | 0.16 | 17,17,17,17                 | 0     |
| 59  | MG   | 2A    | 3385 | 1/1   | 0.92 | 0.13 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3386 | 1/1   | 0.92 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3304 | 1/1   | 0.92 | 0.20 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3781 | 1/1   | 0.92 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3391 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3195 | 1/1   | 0.92 | 0.12 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3166 | 1/1   | 0.92 | 0.27 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3105 | 1/1   | 0.92 | 0.12 | 30,30,30,30                 | 0     |
| 59  | MG   | 1a    | 3531 | 1/1   | 0.92 | 0.07 | 49,49,49,49                 | 0     |
| 59  | MG   | 2a    | 3148 | 1/1   | 0.92 | 0.12 | 73,73,73,73                 | 0     |
| 59  | MG   | 1A    | 4130 | 1/1   | 0.92 | 0.10 | 65,65,65,65                 | 0     |
| 59  | MG   | 2A    | 3412 | 1/1   | 0.92 | 0.09 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3786 | 1/1   | 0.92 | 0.08 | 26,26,26,26                 | 0     |
| 59  | MG   | 2a    | 3154 | 1/1   | 0.92 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3324 | 1/1   | 0.92 | 0.20 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3415 | 1/1   | 0.92 | 0.10 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3763 | 1/1   | 0.92 | 0.14 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3416 | 1/1   | 0.92 | 0.09 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3015 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3494 | 1/1   | 0.92 | 0.21 | 49,49,49,49                 | 0     |
| 59  | MG   | 2a    | 3164 | 1/1   | 0.92 | 0.08 | 75,75,75,75                 | 0     |
| 59  | MG   | 1A    | 3789 | 1/1   | 0.92 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3019 | 1/1   | 0.92 | 0.17 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3173 | 1/1   | 0.92 | 0.18 | 61,61,61,61                 | 0     |
| 59  | MG   | 1a    | 3545 | 1/1   | 0.92 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3339 | 1/1   | 0.92 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3505 | 1/1   | 0.92 | 0.10 | 51,51,51,51                 | 0     |
| 59  | MG   | 1a    | 3334 | 1/1   | 0.92 | 0.20 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3182 | 1/1   | 0.92 | 0.19 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 4147 | 1/1   | 0.92 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3184 | 1/1   | 0.92 | 0.20 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3551 | 1/1   | 0.92 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3275 | 1/1   | 0.92 | 0.11 | 38,38,38,38                 | 0     |
| 59  | MG   | 1a    | 3555 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1a    | 3337 | 1/1   | 0.92 | 0.30 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 4151 | 1/1   | 0.92 | 0.10 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3189 | 1/1   | 0.92 | 0.20 | 57,57,57,57                 | 0     |
| 59  | MG   | 2a    | 3191 | 1/1   | 0.92 | 0.15 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3343 | 1/1   | 0.92 | 0.15 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3211 | 1/1   | 0.92 | 0.22 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4156 | 1/1   | 0.92 | 0.17 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3787 | 1/1   | 0.92 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3212 | 1/1   | 0.92 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3808 | 1/1   | 0.92 | 0.22 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3200 | 1/1   | 0.92 | 0.12 | 65,65,65,65                 | 0     |
| 59  | MG   | 2a    | 3201 | 1/1   | 0.92 | 0.21 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3351 | 1/1   | 0.92 | 0.15 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3200 | 1/1   | 0.92 | 0.22 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3566 | 1/1   | 0.92 | 0.11 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3511 | 1/1   | 0.92 | 0.23 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3203 | 1/1   | 0.92 | 0.30 | 61,61,61,61                 | 0     |
| 59  | MG   | 1a    | 3569 | 1/1   | 0.92 | 0.16 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3797 | 1/1   | 0.92 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3214 | 1/1   | 0.92 | 0.15 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3355 | 1/1   | 0.92 | 0.22 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3218 | 1/1   | 0.92 | 0.20 | 38,38,38,38                 | 0     |
| 59  | MG   | 2a    | 3213 | 1/1   | 0.92 | 0.13 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 3222 | 1/1   | 0.92 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1a    | 3360 | 1/1   | 0.92 | 0.11 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3425 | 1/1   | 0.92 | 0.08 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3523 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3812 | 1/1   | 0.92 | 0.09 | 72,72,72,72                 | 0     |
| 59  | MG   | 1A    | 4007 | 1/1   | 0.92 | 0.16 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3493 | 1/1   | 0.92 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 2a    | 3222 | 1/1   | 0.92 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 4194 | 1/1   | 0.92 | 0.24 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 4197 | 1/1   | 0.92 | 0.25 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3827 | 1/1   | 0.92 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3217 | 1/1   | 0.92 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | 2a    | 3232 | 1/1   | 0.92 | 0.20 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3082 | 1/1   | 0.92 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 4010 | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3835 | 1/1   | 0.92 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | 1n    | 502  | 1/1   | 0.92 | 0.29 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3665 | 1/1   | 0.92 | 0.21 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3838 | 1/1   | 0.92 | 0.18 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4229 | 1/1   | 0.92 | 0.10 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3842 | 1/1   | 0.92 | 0.32 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3514 | 1/1   | 0.92 | 0.20 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3290 | 1/1   | 0.92 | 0.19 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3226 | 1/1   | 0.92 | 0.09 | 53,53,53,53                 | 0     |
| 59  | MG   | 2l    | 201  | 1/1   | 0.92 | 0.10 | 65,65,65,65                 | 0     |
| 59  | MG   | 1B    | 203  | 1/1   | 0.92 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3521 | 1/1   | 0.92 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3670 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3832 | 1/1   | 0.92 | 0.16 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3525 | 1/1   | 0.92 | 0.16 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3111 | 1/1   | 0.92 | 0.13 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 4021 | 1/1   | 0.92 | 0.08 | 27,27,27,27                 | 0     |
| 59  | MG   | 1a    | 3378 | 1/1   | 0.92 | 0.21 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 4025 | 1/1   | 0.92 | 0.09 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3238 | 1/1   | 0.92 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | 2B    | 3013 | 1/1   | 0.92 | 0.24 | 63,63,63,63                 | 0     |
| 59  | MG   | 2v    | 104  | 1/1   | 0.92 | 0.17 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3532 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3359 | 1/1   | 0.92 | 0.17 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3163 | 1/1   | 0.92 | 0.10 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3002 | 1/1   | 0.92 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 4043 | 1/1   | 0.92 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3540 | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 1x    | 104  | 1/1   | 0.92 | 0.14 | 61,61,61,61                 | 0     |
| 59  | MG   | 2B    | 3021 | 1/1   | 0.92 | 0.25 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 3167 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 59  | MG   | 2D    | 302  | 1/1   | 0.92 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | 1x    | 110  | 1/1   | 0.92 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 1a    | 3387 | 1/1   | 0.92 | 0.24 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3439 | 1/1   | 0.92 | 0.14 | 39,39,39,39                 | 0     |
| 59  | MG   | 1B    | 223  | 1/1   | 0.92 | 0.16 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3390 | 1/1   | 0.92 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3302 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2E    | 307  | 1/1   | 0.92 | 0.11 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3554 | 1/1   | 0.92 | 0.19 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3010 | 1/1   | 0.93 | 0.24 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3139 | 1/1   | 0.93 | 0.14 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3951 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3446 | 1/1   | 0.93 | 0.16 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3447 | 1/1   | 0.93 | 0.29 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3144 | 1/1   | 0.93 | 0.15 | 65,65,65,65                 | 0     |
| 59  | MG   | 2a    | 3016 | 1/1   | 0.93 | 0.08 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3541 | 1/1   | 0.93 | 0.19 | 61,61,61,61                 | 0     |
| 59  | MG   | 1a    | 3333 | 1/1   | 0.93 | 0.23 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3575 | 1/1   | 0.93 | 0.07 | 13,13,13,13                 | 0     |
| 59  | MG   | 2a    | 3020 | 1/1   | 0.93 | 0.20 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3760 | 1/1   | 0.93 | 0.17 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4153 | 1/1   | 0.93 | 0.09 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3648 | 1/1   | 0.93 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 2A    | 3152 | 1/1   | 0.93 | 0.20 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3962 | 1/1   | 0.93 | 0.18 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3174 | 1/1   | 0.93 | 0.08 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3967 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3156 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3157 | 1/1   | 0.93 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3158 | 1/1   | 0.93 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3360 | 1/1   | 0.93 | 0.13 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 4168 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3452 | 1/1   | 0.93 | 0.17 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4175 | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3554 | 1/1   | 0.93 | 0.13 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3768 | 1/1   | 0.93 | 0.14 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3133 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3097 | 1/1   | 0.93 | 0.08 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3370 | 1/1   | 0.93 | 0.07 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3372 | 1/1   | 0.93 | 0.23 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3680 | 1/1   | 0.93 | 0.15 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3457 | 1/1   | 0.93 | 0.30 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 4185 | 1/1   | 0.93 | 0.17 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3356 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3459 | 1/1   | 0.93 | 0.09 | 58,58,58,58                 | 0     |
| 59  | MG   | 2a    | 3051 | 1/1   | 0.93 | 0.21 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3317 | 1/1   | 0.93 | 0.27 | 32,32,32,32                 | 0     |
| 59  | MG   | 1a    | 3564 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3175 | 1/1   | 0.93 | 0.10 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3593 | 1/1   | 0.93 | 0.09 | 18,18,18,18                 | 0     |
| 59  | MG   | 2A    | 3387 | 1/1   | 0.93 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3696 | 1/1   | 0.93 | 0.08 | 73,73,73,73                 | 0     |
| 59  | MG   | 2A    | 3699 | 1/1   | 0.93 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4191 | 1/1   | 0.93 | 0.10 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 4193 | 1/1   | 0.93 | 0.08 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3777 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3397 | 1/1   | 0.93 | 0.07 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3318 | 1/1   | 0.93 | 0.10 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3464 | 1/1   | 0.93 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3216 | 1/1   | 0.93 | 0.13 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3576 | 1/1   | 0.93 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3407 | 1/1   | 0.93 | 0.09 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3469 | 1/1   | 0.93 | 0.21 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 4223 | 1/1   | 0.93 | 0.13 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 4228 | 1/1   | 0.93 | 0.28 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3729 | 1/1   | 0.93 | 0.09 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3730 | 1/1   | 0.93 | 0.07 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3599 | 1/1   | 0.93 | 0.12 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3600 | 1/1   | 0.93 | 0.08 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3266 | 1/1   | 0.93 | 0.17 | 45,45,45,45                 | 0     |
| 59  | MG   | 2a    | 3083 | 1/1   | 0.93 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3322 | 1/1   | 0.93 | 0.21 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3423 | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3792 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3476 | 1/1   | 0.93 | 0.31 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3431 | 1/1   | 0.93 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3795 | 1/1   | 0.93 | 0.10 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3323 | 1/1   | 0.93 | 0.45 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3389 | 1/1   | 0.93 | 0.27 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3440 | 1/1   | 0.93 | 0.16 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3744 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4015 | 1/1   | 0.93 | 0.14 | 52,52,52,52                 | 0     |
| 59  | MG   | 2a    | 3096 | 1/1   | 0.93 | 0.47 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 4018 | 1/1   | 0.93 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3799 | 1/1   | 0.93 | 0.15 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3217 | 1/1   | 0.93 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3270 | 1/1   | 0.93 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3450 | 1/1   | 0.93 | 0.09 | 53,53,53,53                 | 0     |
| 59  | MG   | 1w    | 107  | 1/1   | 0.93 | 0.10 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3206 | 1/1   | 0.93 | 0.24 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 4030 | 1/1   | 0.93 | 0.20 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3802 | 1/1   | 0.93 | 0.23 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3005 | 1/1   | 0.93 | 0.14 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3459 | 1/1   | 0.93 | 0.19 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3632 | 1/1   | 0.93 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 4041 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3467 | 1/1   | 0.93 | 0.16 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3212 | 1/1   | 0.93 | 0.11 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3636 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 4044 | 1/1   | 0.93 | 0.10 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3182 | 1/1   | 0.93 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1x    | 107  | 1/1   | 0.93 | 0.13 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3639 | 1/1   | 0.93 | 0.08 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3116 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3225 | 1/1   | 0.93 | 0.27 | 64,64,64,64                 | 0     |
| 59  | MG   | 2a    | 3121 | 1/1   | 0.93 | 0.26 | 61,61,61,61                 | 0     |
| 59  | MG   | 1B    | 238  | 1/1   | 0.93 | 0.09 | 30,30,30,30                 | 0     |
| 59  | MG   | 1x    | 113  | 1/1   | 0.93 | 0.15 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3822 | 1/1   | 0.93 | 0.06 | 11,11,11,11                 | 0     |
| 59  | MG   | 1A    | 3491 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3039 | 1/1   | 0.93 | 0.05 | 22,22,22,22                 | 0     |
| 59  | MG   | 2A    | 3229 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3132 | 1/1   | 0.93 | 0.09 | 68,68,68,68                 | 0     |
| 59  | MG   | 1A    | 3278 | 1/1   | 0.93 | 0.34 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3490 | 1/1   | 0.93 | 0.09 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3498 | 1/1   | 0.93 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3136 | 1/1   | 0.93 | 0.08 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3648 | 1/1   | 0.93 | 0.12 | 31,31,31,31                 | 0     |
| 59  | MG   | 2a    | 3140 | 1/1   | 0.93 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3502 | 1/1   | 0.93 | 0.14 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3049 | 1/1   | 0.93 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3004 | 1/1   | 0.93 | 0.17 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3161 | 1/1   | 0.93 | 0.15 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3008 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3505 | 1/1   | 0.93 | 0.12 | 35,35,35,35                 | 0     |
| 59  | MG   | 1E    | 313  | 1/1   | 0.93 | 0.22 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3088 | 1/1   | 0.93 | 0.15 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3019 | 1/1   | 0.93 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3411 | 1/1   | 0.93 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 1F    | 307  | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3507 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3800 | 1/1   | 0.93 | 0.09 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3419 | 1/1   | 0.93 | 0.22 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3233 | 1/1   | 0.93 | 0.16 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3167 | 1/1   | 0.93 | 0.08 | 74,74,74,74                 | 0     |
| 59  | MG   | 2a    | 3169 | 1/1   | 0.93 | 0.15 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3345 | 1/1   | 0.93 | 0.21 | 37,37,37,37                 | 0     |
| 59  | MG   | 2a    | 3171 | 1/1   | 0.93 | 0.09 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3661 | 1/1   | 0.93 | 0.08 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3523 | 1/1   | 0.93 | 0.13 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3848 | 1/1   | 0.93 | 0.07 | 72,72,72,72                 | 0     |
| 59  | MG   | 1A    | 3089 | 1/1   | 0.93 | 0.07 | 28,28,28,28                 | 0     |
| 59  | MG   | 2a    | 3178 | 1/1   | 0.93 | 0.21 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3513 | 1/1   | 0.93 | 0.12 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3257 | 1/1   | 0.93 | 0.10 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3819 | 1/1   | 0.93 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3239 | 1/1   | 0.93 | 0.27 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3242 | 1/1   | 0.93 | 0.24 | 24,24,24,24                 | 0     |
| 59  | MG   | 2a    | 3184 | 1/1   | 0.93 | 0.26 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3517 | 1/1   | 0.93 | 0.19 | 41,41,41,41                 | 0     |
| 59  | MG   | 1a    | 3432 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 59  | MG   | 1a    | 3433 | 1/1   | 0.93 | 0.43 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 4087 | 1/1   | 0.93 | 0.11 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3045 | 1/1   | 0.93 | 0.09 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3047 | 1/1   | 0.93 | 0.13 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3048 | 1/1   | 0.93 | 0.20 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3839 | 1/1   | 0.93 | 0.23 | 39,39,39,39                 | 0     |
| 59  | MG   | 2a    | 3194 | 1/1   | 0.93 | 0.15 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3268 | 1/1   | 0.93 | 0.23 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3049 | 1/1   | 0.93 | 0.09 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3544 | 1/1   | 0.93 | 0.11 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3246 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4089 | 1/1   | 0.93 | 0.16 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3675 | 1/1   | 0.93 | 0.17 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3549 | 1/1   | 0.93 | 0.16 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3356 | 1/1   | 0.93 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3522 | 1/1   | 0.93 | 0.23 | 28,28,28,28                 | 0     |
| 59  | MG   | 2B    | 3005 | 1/1   | 0.93 | 0.29 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3277 | 1/1   | 0.93 | 0.30 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3207 | 1/1   | 0.93 | 0.22 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3279 | 1/1   | 0.93 | 0.26 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3428 | 1/1   | 0.93 | 0.22 | 56,56,56,56                 | 0     |
| 59  | MG   | 2B    | 3009 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3688 | 1/1   | 0.93 | 0.13 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3042 | 1/1   | 0.93 | 0.07 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 4099 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3529 | 1/1   | 0.93 | 0.41 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 4103 | 1/1   | 0.93 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3561 | 1/1   | 0.93 | 0.10 | 31,31,31,31                 | 0     |
| 59  | MG   | 1W    | 201  | 1/1   | 0.93 | 0.20 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3530 | 1/1   | 0.93 | 0.08 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3071 | 1/1   | 0.93 | 0.12 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3430 | 1/1   | 0.93 | 0.23 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3535 | 1/1   | 0.93 | 0.14 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3074 | 1/1   | 0.93 | 0.07 | 49,49,49,49                 | 0     |
| 59  | MG   | 2a    | 3225 | 1/1   | 0.93 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3570 | 1/1   | 0.93 | 0.09 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3202 | 1/1   | 0.93 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1Z    | 304  | 1/1   | 0.93 | 0.21 | 50,50,50,50                 | 0     |
| 59  | MG   | 2a    | 3231 | 1/1   | 0.93 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | 10    | 105  | 1/1   | 0.93 | 0.14 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3576 | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3714 | 1/1   | 0.93 | 0.07 | 10,10,10,10                 | 0     |
| 59  | MG   | 1A    | 3203 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 59  | MG   | 2E    | 304  | 1/1   | 0.93 | 0.20 | 59,59,59,59                 | 0     |
| 59  | MG   | 2E    | 305  | 1/1   | 0.93 | 0.12 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3081 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | 2e    | 3001 | 1/1   | 0.93 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 4113 | 1/1   | 0.93 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3302 | 1/1   | 0.93 | 0.37 | 57,57,57,57                 | 0     |
| 59  | MG   | 11    | 103  | 1/1   | 0.93 | 0.16 | 70,70,70,70                 | 0     |
| 59  | MG   | 1A    | 3543 | 1/1   | 0.93 | 0.09 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 3362 | 1/1   | 0.93 | 0.11 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 15    | 103  | 1/1   | 0.93 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3366 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3547 | 1/1   | 0.93 | 0.10 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3094 | 1/1   | 0.93 | 0.14 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3551 | 1/1   | 0.93 | 0.10 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3734 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3304 | 1/1   | 0.93 | 0.15 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3206 | 1/1   | 0.93 | 0.12 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3503 | 1/1   | 0.93 | 0.10 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 3258 | 1/1   | 0.93 | 0.15 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3567 | 1/1   | 0.93 | 0.07 | 27,27,27,27                 | 0     |
| 59  | MG   | 2T    | 203  | 1/1   | 0.93 | 0.23 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 4128 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 2U    | 203  | 1/1   | 0.93 | 0.24 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 4129 | 1/1   | 0.93 | 0.10 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3317 | 1/1   | 0.93 | 0.07 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3321 | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3608 | 1/1   | 0.93 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 25    | 103  | 1/1   | 0.93 | 0.15 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3372 | 1/1   | 0.93 | 0.20 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3945 | 1/1   | 0.93 | 0.08 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3947 | 1/1   | 0.93 | 0.13 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3519 | 1/1   | 0.93 | 0.19 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3748 | 1/1   | 0.93 | 0.29 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3092 | 1/1   | 0.93 | 0.23 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3331 | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3532 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3334 | 1/1   | 0.93 | 0.18 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3131 | 1/1   | 0.93 | 0.23 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3950 | 1/1   | 0.93 | 0.14 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3138 | 1/1   | 0.93 | 0.20 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3897 | 1/1   | 0.94 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3631 | 1/1   | 0.94 | 0.18 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3285 | 1/1   | 0.94 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3900 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3763 | 1/1   | 0.94 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3903 | 1/1   | 0.94 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3765 | 1/1   | 0.94 | 0.15 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3327 | 1/1   | 0.94 | 0.39 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3443 | 1/1   | 0.94 | 0.23 | 49,49,49,49                 | 0     |
| 59  | MG   | 1D    | 301  | 1/1   | 0.94 | 0.22 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3114 | 1/1   | 0.94 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1D    | 308  | 1/1   | 0.94 | 0.18 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3288 | 1/1   | 0.94 | 0.22 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3670 | 1/1   | 0.94 | 0.10 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3149 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3672 | 1/1   | 0.94 | 0.08 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3913 | 1/1   | 0.94 | 0.11 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3253 | 1/1   | 0.94 | 0.16 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3676 | 1/1   | 0.94 | 0.08 | 60,60,60,60                 | 0     |
| 59  | MG   | 1E    | 302  | 1/1   | 0.94 | 0.11 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3395 | 1/1   | 0.94 | 0.07 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3187 | 1/1   | 0.94 | 0.45 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3916 | 1/1   | 0.94 | 0.08 | 12,12,12,12                 | 0     |
| 59  | MG   | 2A    | 3400 | 1/1   | 0.94 | 0.08 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3401 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 59  | MG   | 1a    | 3392 | 1/1   | 0.94 | 0.21 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3451 | 1/1   | 0.94 | 0.17 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4092 | 1/1   | 0.94 | 0.13 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3919 | 1/1   | 0.94 | 0.05 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 3527 | 1/1   | 0.94 | 0.16 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3923 | 1/1   | 0.94 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3197 | 1/1   | 0.94 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | 1F    | 301  | 1/1   | 0.94 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3184 | 1/1   | 0.94 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3079 | 1/1   | 0.94 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3418 | 1/1   | 0.94 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1x    | 101  | 1/1   | 0.94 | 0.10 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3780 | 1/1   | 0.94 | 0.07 | 10,10,10,10                 | 0     |
| 59  | MG   | 1A    | 3121 | 1/1   | 0.94 | 0.09 | 37,37,37,37                 | 0     |
| 59  | MG   | 1G    | 3002 | 1/1   | 0.94 | 0.16 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3430 | 1/1   | 0.94 | 0.07 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3534 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 1x    | 108  | 1/1   | 0.94 | 0.23 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3435 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3456 | 1/1   | 0.94 | 0.09 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3784 | 1/1   | 0.94 | 0.09 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3391 | 1/1   | 0.94 | 0.14 | 41,41,41,41                 | 0     |
| 59  | MG   | 2a    | 3072 | 1/1   | 0.94 | 0.32 | 50,50,50,50                 | 0     |
| 59  | MG   | 1N    | 3005 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 0     |
| 59  | MG   | 1N    | 3006 | 1/1   | 0.94 | 0.19 | 41,41,41,41                 | 0     |
| 59  | MG   | 1N    | 3007 | 1/1   | 0.94 | 0.27 | 49,49,49,49                 | 0     |
| 59  | MG   | 1x    | 115  | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3299 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3393 | 1/1   | 0.94 | 0.16 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3342 | 1/1   | 0.94 | 0.09 | 42,42,42,42                 | 0     |
| 59  | MG   | 1O    | 3005 | 1/1   | 0.94 | 0.13 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3453 | 1/1   | 0.94 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 4114 | 1/1   | 0.94 | 0.14 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3220 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3220 | 1/1   | 0.94 | 0.18 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3002 | 1/1   | 0.94 | 0.28 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3221 | 1/1   | 0.94 | 0.15 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3464 | 1/1   | 0.94 | 0.15 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3465 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3423 | 1/1   | 0.94 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3043 | 1/1   | 0.94 | 0.12 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3347 | 1/1   | 0.94 | 0.18 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3227 | 1/1   | 0.94 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3015 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3756 | 1/1   | 0.94 | 0.11 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3473 | 1/1   | 0.94 | 0.32 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3965 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3403 | 1/1   | 0.94 | 0.22 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3100 | 1/1   | 0.94 | 0.26 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3348 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3157 | 1/1   | 0.94 | 0.11 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3431 | 1/1   | 0.94 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3479 | 1/1   | 0.94 | 0.09 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3969 | 1/1   | 0.94 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3068 | 1/1   | 0.94 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 1U    | 204  | 1/1   | 0.94 | 0.06 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3484 | 1/1   | 0.94 | 0.10 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3803 | 1/1   | 0.94 | 0.18 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3804 | 1/1   | 0.94 | 0.22 | 27,27,27,27                 | 0     |
| 59  | MG   | 1a    | 3437 | 1/1   | 0.94 | 0.34 | 58,58,58,58                 | 0     |
| 59  | MG   | 1X    | 3004 | 1/1   | 0.94 | 0.07 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3245 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3023 | 1/1   | 0.94 | 0.37 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3036 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 59  | MG   | 1a    | 3440 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3496 | 1/1   | 0.94 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3981 | 1/1   | 0.94 | 0.07 | 13,13,13,13                 | 0     |
| 59  | MG   | 2A    | 3251 | 1/1   | 0.94 | 0.08 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3499 | 1/1   | 0.94 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 1Y    | 504  | 1/1   | 0.94 | 0.24 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3447 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3254 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3509 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3352 | 1/1   | 0.94 | 0.08 | 43,43,43,43                 | 0     |
| 59  | MG   | 2a    | 3128 | 1/1   | 0.94 | 0.07 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3483 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3046 | 1/1   | 0.94 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3985 | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3515 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 10    | 101  | 1/1   | 0.94 | 0.17 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3686 | 1/1   | 0.94 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3518 | 1/1   | 0.94 | 0.19 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3519 | 1/1   | 0.94 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3050 | 1/1   | 0.94 | 0.13 | 48,48,48,48                 | 0     |
| 59  | MG   | 2a    | 3143 | 1/1   | 0.94 | 0.08 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 4142 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3263 | 1/1   | 0.94 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 2a    | 3149 | 1/1   | 0.94 | 0.08 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3803 | 1/1   | 0.94 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3804 | 1/1   | 0.94 | 0.11 | 59,59,59,59                 | 0     |
| 59  | MG   | 2a    | 3152 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 59  | MG   | 1a    | 3461 | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3052 | 1/1   | 0.94 | 0.25 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3813 | 1/1   | 0.94 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3056 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3354 | 1/1   | 0.94 | 0.21 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3269 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3470 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 59  | MG   | 2a    | 3162 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 59  | MG   | 1a    | 3471 | 1/1   | 0.94 | 0.11 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4149 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 2a    | 3165 | 1/1   | 0.94 | 0.08 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3820 | 1/1   | 0.94 | 0.17 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3473 | 1/1   | 0.94 | 0.16 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3823 | 1/1   | 0.94 | 0.18 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3824 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3991 | 1/1   | 0.94 | 0.12 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3172 | 1/1   | 0.94 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 13    | 3002 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3579 | 1/1   | 0.94 | 0.08 | 30,30,30,30                 | 0     |
| 59  | MG   | 2a    | 3175 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 4154 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3832 | 1/1   | 0.94 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3834 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3695 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 59  | MG   | 1A    | 3488 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | 18    | 103  | 1/1   | 0.94 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | 1a    | 3486 | 1/1   | 0.94 | 0.13 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3698 | 1/1   | 0.94 | 0.10 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 4164 | 1/1   | 0.94 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3841 | 1/1   | 0.94 | 0.08 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3548 | 1/1   | 0.94 | 0.08 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3075 | 1/1   | 0.94 | 0.28 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3078 | 1/1   | 0.94 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 4172 | 1/1   | 0.94 | 0.30 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3700 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3847 | 1/1   | 0.94 | 0.31 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3309 | 1/1   | 0.94 | 0.24 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3416 | 1/1   | 0.94 | 0.14 | 52,52,52,52                 | 0     |
| 59  | MG   | 1a    | 3497 | 1/1   | 0.94 | 0.11 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3709 | 1/1   | 0.94 | 0.07 | 20,20,20,20                 | 0     |
| 59  | MG   | 2a    | 3197 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3501 | 1/1   | 0.94 | 0.07 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3357 | 1/1   | 0.94 | 0.24 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3713 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3492 | 1/1   | 0.94 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3562 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3091 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3093 | 1/1   | 0.94 | 0.27 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3720 | 1/1   | 0.94 | 0.07 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3037 | 1/1   | 0.94 | 0.18 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3311 | 1/1   | 0.94 | 0.12 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 4189 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3313 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4024 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 4192 | 1/1   | 0.94 | 0.31 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3103 | 1/1   | 0.94 | 0.25 | 62,62,62,62                 | 0     |
| 59  | MG   | 2A    | 3575 | 1/1   | 0.94 | 0.13 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3500 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 2D    | 301  | 1/1   | 0.94 | 0.21 | 47,47,47,47                 | 0     |
| 59  | MG   | 1a    | 3526 | 1/1   | 0.94 | 0.18 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3527 | 1/1   | 0.94 | 0.07 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3528 | 1/1   | 0.94 | 0.07 | 59,59,59,59                 | 0     |
| 59  | MG   | 1a    | 3530 | 1/1   | 0.94 | 0.08 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3114 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3117 | 1/1   | 0.94 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 4027 | 1/1   | 0.94 | 0.05 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3847 | 1/1   | 0.94 | 0.06 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3589 | 1/1   | 0.94 | 0.08 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 4203 | 1/1   | 0.94 | 0.20 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3323 | 1/1   | 0.94 | 0.27 | 47,47,47,47                 | 0     |
| 59  | MG   | 2F    | 302  | 1/1   | 0.94 | 0.13 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3204 | 1/1   | 0.94 | 0.20 | 23,23,23,23                 | 0     |
| 59  | MG   | 1a    | 3338 | 1/1   | 0.94 | 0.20 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3363 | 1/1   | 0.94 | 0.13 | 30,30,30,30                 | 0     |
| 59  | MG   | 1a    | 3540 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3328 | 1/1   | 0.94 | 0.28 | 51,51,51,51                 | 0     |
| 59  | MG   | 2P    | 201  | 1/1   | 0.94 | 0.25 | 51,51,51,51                 | 0     |
| 59  | MG   | 2Q    | 3001 | 1/1   | 0.94 | 0.07 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 4212 | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3234 | 1/1   | 0.94 | 0.10 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3048 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 4225 | 1/1   | 0.94 | 0.19 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3333 | 1/1   | 0.94 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3348 | 1/1   | 0.94 | 0.20 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3142 | 1/1   | 0.94 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3349 | 1/1   | 0.94 | 0.11 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3547 | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3859 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 59  | MG   | 2U    | 201  | 1/1   | 0.94 | 0.15 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3860 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 59  | MG   | 2q    | 204  | 1/1   | 0.94 | 0.10 | 70,70,70,70                 | 0     |
| 59  | MG   | 1A    | 3608 | 1/1   | 0.94 | 0.10 | 16,16,16,16                 | 0     |
| 59  | MG   | 2A    | 3148 | 1/1   | 0.94 | 0.13 | 65,65,65,65                 | 0     |
| 59  | MG   | 2V    | 201  | 1/1   | 0.94 | 0.18 | 60,60,60,60                 | 0     |
| 59  | MG   | 2X    | 3001 | 1/1   | 0.94 | 0.16 | 59,59,59,59                 | 0     |
| 59  | MG   | 2A    | 3615 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3058 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3874 | 1/1   | 0.94 | 0.10 | 13,13,13,13                 | 0     |
| 59  | MG   | 1A    | 3744 | 1/1   | 0.94 | 0.08 | 44,44,44,44                 | 0     |
| 59  | MG   | 1a    | 3357 | 1/1   | 0.94 | 0.13 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3880 | 1/1   | 0.94 | 0.10 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3881 | 1/1   | 0.94 | 0.15 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4058 | 1/1   | 0.94 | 0.13 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3210 | 1/1   | 0.94 | 0.08 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3884 | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3371 | 1/1   | 0.94 | 0.22 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3509 | 1/1   | 0.94 | 0.17 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 4064 | 1/1   | 0.94 | 0.11 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3631 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3632 | 1/1   | 0.94 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3625 | 1/1   | 0.94 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3281 | 1/1   | 0.94 | 0.22 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3139 | 1/1   | 0.94 | 0.09 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3167 | 1/1   | 0.94 | 0.34 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3247 | 1/1   | 0.94 | 0.18 | 47,47,47,47                 | 0     |
| 59  | MG   | 1a    | 3570 | 1/1   | 0.94 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | A     | 8001 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3134 | 1/1   | 0.95 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 1a    | 3307 | 1/1   | 0.95 | 0.27 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3351 | 1/1   | 0.95 | 0.07 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3308 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3980 | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 4152 | 1/1   | 0.95 | 0.08 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3633 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3355 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3453 | 1/1   | 0.95 | 0.10 | 18,18,18,18                 | 0     |
| 59  | MG   | 1A    | 3194 | 1/1   | 0.95 | 0.20 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3320 | 1/1   | 0.95 | 0.18 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3983 | 1/1   | 0.95 | 0.11 | 63,63,63,63                 | 0     |
| 59  | MG   | 1A    | 3538 | 1/1   | 0.95 | 0.10 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3643 | 1/1   | 0.95 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | 1a    | 3323 | 1/1   | 0.95 | 0.14 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3363 | 1/1   | 0.95 | 0.14 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4160 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 4161 | 1/1   | 0.95 | 0.06 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3539 | 1/1   | 0.95 | 0.08 | 26,26,26,26                 | 0     |
| 59  | MG   | 2a    | 3026 | 1/1   | 0.95 | 0.27 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3542 | 1/1   | 0.95 | 0.09 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3656 | 1/1   | 0.95 | 0.06 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3657 | 1/1   | 0.95 | 0.08 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 4167 | 1/1   | 0.95 | 0.05 | 19,19,19,19                 | 0     |
| 59  | MG   | 2A    | 3661 | 1/1   | 0.95 | 0.11 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3032 | 1/1   | 0.95 | 0.08 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3987 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3807 | 1/1   | 0.95 | 0.13 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3373 | 1/1   | 0.95 | 0.07 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3665 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3332 | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3384 | 1/1   | 0.95 | 0.08 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3039 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3385 | 1/1   | 0.95 | 0.17 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3329 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4177 | 1/1   | 0.95 | 0.19 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3229 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3673 | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3996 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3339 | 1/1   | 0.95 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3340 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3679 | 1/1   | 0.95 | 0.07 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3342 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3679 | 1/1   | 0.95 | 0.11 | 79,79,79,79                 | 0     |
| 59  | MG   | 1A    | 4000 | 1/1   | 0.95 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3392 | 1/1   | 0.95 | 0.07 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 4002 | 1/1   | 0.95 | 0.06 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3815 | 1/1   | 0.95 | 0.10 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3818 | 1/1   | 0.95 | 0.09 | 14,14,14,14                 | 0     |
| 59  | MG   | 2a    | 3060 | 1/1   | 0.95 | 0.20 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4006 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3230 | 1/1   | 0.95 | 0.23 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3682 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3403 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3552 | 1/1   | 0.95 | 0.10 | 7,7,7,7                     | 0     |
| 59  | MG   | 1a    | 3568 | 1/1   | 0.95 | 0.06 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3697 | 1/1   | 0.95 | 0.07 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3687 | 1/1   | 0.95 | 0.16 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3408 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 2a    | 3071 | 1/1   | 0.95 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4195 | 1/1   | 0.95 | 0.17 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3231 | 1/1   | 0.95 | 0.17 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3689 | 1/1   | 0.95 | 0.08 | 41,41,41,41                 | 0     |
| 59  | MG   | 1a    | 3573 | 1/1   | 0.95 | 0.20 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3463 | 1/1   | 0.95 | 0.20 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3691 | 1/1   | 0.95 | 0.13 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3417 | 1/1   | 0.95 | 0.10 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 4016 | 1/1   | 0.95 | 0.11 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 4213 | 1/1   | 0.95 | 0.14 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 4017 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3333 | 1/1   | 0.95 | 0.16 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3564 | 1/1   | 0.95 | 0.05 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3334 | 1/1   | 0.95 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3335 | 1/1   | 0.95 | 0.11 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3433 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3336 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | 1B    | 202  | 1/1   | 0.95 | 0.23 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 4026 | 1/1   | 0.95 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3437 | 1/1   | 0.95 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3156 | 1/1   | 0.95 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3196 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3094 | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | 1B    | 205  | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3443 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3034 | 1/1   | 0.95 | 0.07 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 4031 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1B    | 210  | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 59  | MG   | 1w    | 101  | 1/1   | 0.95 | 0.11 | 56,56,56,56                 | 0     |
| 59  | MG   | 1B    | 211  | 1/1   | 0.95 | 0.30 | 52,52,52,52                 | 0     |
| 59  | MG   | 1w    | 103  | 1/1   | 0.95 | 0.14 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3375 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | 1w    | 105  | 1/1   | 0.95 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | 1w    | 106  | 1/1   | 0.95 | 0.15 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3753 | 1/1   | 0.95 | 0.13 | 52,52,52,52                 | 0     |
| 59  | MG   | 1a    | 3376 | 1/1   | 0.95 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 4033 | 1/1   | 0.95 | 0.06 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3705 | 1/1   | 0.95 | 0.07 | 17,17,17,17                 | 0     |
| 59  | MG   | 1a    | 3379 | 1/1   | 0.95 | 0.08 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3708 | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 59  | MG   | 1B    | 215  | 1/1   | 0.95 | 0.06 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3398 | 1/1   | 0.95 | 0.11 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3198 | 1/1   | 0.95 | 0.21 | 27,27,27,27                 | 0     |
| 59  | MG   | 2a    | 3115 | 1/1   | 0.95 | 0.27 | 59,59,59,59                 | 0     |
| 59  | MG   | 1B    | 219  | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 4042 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 59  | MG   | 1x    | 105  | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3767 | 1/1   | 0.95 | 0.13 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3236 | 1/1   | 0.95 | 0.18 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3402 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3717 | 1/1   | 0.95 | 0.06 | 21,21,21,21                 | 0     |
| 59  | MG   | 2a    | 3123 | 1/1   | 0.95 | 0.16 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3199 | 1/1   | 0.95 | 0.07 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3772 | 1/1   | 0.95 | 0.11 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 4049 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3721 | 1/1   | 0.95 | 0.08 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3159 | 1/1   | 0.95 | 0.18 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4054 | 1/1   | 0.95 | 0.20 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3395 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3482 | 1/1   | 0.95 | 0.08 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3723 | 1/1   | 0.95 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3230 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3127 | 1/1   | 0.95 | 0.19 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3875 | 1/1   | 0.95 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3139 | 1/1   | 0.95 | 0.08 | 65,65,65,65                 | 0     |
| 59  | MG   | 1A    | 3107 | 1/1   | 0.95 | 0.27 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3784 | 1/1   | 0.95 | 0.09 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3488 | 1/1   | 0.95 | 0.23 | 54,54,54,54                 | 0     |
| 59  | MG   | 2a    | 3144 | 1/1   | 0.95 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3877 | 1/1   | 0.95 | 0.06 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3879 | 1/1   | 0.95 | 0.08 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3001 | 1/1   | 0.95 | 0.32 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3407 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3294 | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 59  | MG   | 1D    | 305  | 1/1   | 0.95 | 0.11 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3295 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3164 | 1/1   | 0.95 | 0.26 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3013 | 1/1   | 0.95 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3500 | 1/1   | 0.95 | 0.11 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3886 | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3503 | 1/1   | 0.95 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3504 | 1/1   | 0.95 | 0.10 | 27,27,27,27                 | 0     |
| 59  | MG   | 2a    | 3161 | 1/1   | 0.95 | 0.10 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3244 | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4068 | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3508 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3888 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3805 | 1/1   | 0.95 | 0.11 | 53,53,53,53                 | 0     |
| 59  | MG   | 1a    | 3411 | 1/1   | 0.95 | 0.28 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3735 | 1/1   | 0.95 | 0.06 | 20,20,20,20                 | 0     |
| 59  | MG   | 1A    | 3298 | 1/1   | 0.95 | 0.16 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3165 | 1/1   | 0.95 | 0.29 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3250 | 1/1   | 0.95 | 0.11 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3894 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3743 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3495 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 4079 | 1/1   | 0.95 | 0.15 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3031 | 1/1   | 0.95 | 0.22 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3496 | 1/1   | 0.95 | 0.18 | 50,50,50,50                 | 0     |
| 59  | MG   | 1F    | 306  | 1/1   | 0.95 | 0.09 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3013 | 1/1   | 0.95 | 0.23 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 4084 | 1/1   | 0.95 | 0.11 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3499 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3751 | 1/1   | 0.95 | 0.07 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3614 | 1/1   | 0.95 | 0.06 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3615 | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | 2A    | 3529 | 1/1   | 0.95 | 0.11 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3043 | 1/1   | 0.95 | 0.12 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 3422 | 1/1   | 0.95 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | 1N    | 3001 | 1/1   | 0.95 | 0.28 | 52,52,52,52                 | 0     |
| 59  | MG   | 2a    | 3190 | 1/1   | 0.95 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3756 | 1/1   | 0.95 | 0.07 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3619 | 1/1   | 0.95 | 0.07 | 19,19,19,19                 | 0     |
| 59  | MG   | 1A    | 3908 | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3759 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3423 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3541 | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3761 | 1/1   | 0.95 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4097 | 1/1   | 0.95 | 0.11 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3014 | 1/1   | 0.95 | 0.14 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3054 | 1/1   | 0.95 | 0.08 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3280 | 1/1   | 0.95 | 0.08 | 49,49,49,49                 | 0     |
| 59  | MG   | 2B    | 3002 | 1/1   | 0.95 | 0.33 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3028 | 1/1   | 0.95 | 0.05 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3137 | 1/1   | 0.95 | 0.20 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3766 | 1/1   | 0.95 | 0.06 | 21,21,21,21                 | 0     |
| 59  | MG   | 1a    | 3444 | 1/1   | 0.95 | 0.14 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3059 | 1/1   | 0.95 | 0.06 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3552 | 1/1   | 0.95 | 0.06 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3446 | 1/1   | 0.95 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3040 | 1/1   | 0.95 | 0.12 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3259 | 1/1   | 0.95 | 0.21 | 41,41,41,41                 | 0     |
| 59  | MG   | 1a    | 3449 | 1/1   | 0.95 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 4107 | 1/1   | 0.95 | 0.11 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 3630 | 1/1   | 0.95 | 0.08 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3215 | 1/1   | 0.95 | 0.28 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3925 | 1/1   | 0.95 | 0.07 | 10,10,10,10                 | 0     |
| 59  | MG   | 1S    | 3003 | 1/1   | 0.95 | 0.06 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 3065 | 1/1   | 0.95 | 0.30 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3772 | 1/1   | 0.95 | 0.20 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3140 | 1/1   | 0.95 | 0.25 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3432 | 1/1   | 0.95 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 1a    | 3468 | 1/1   | 0.95 | 0.13 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3224 | 1/1   | 0.95 | 0.19 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3943 | 1/1   | 0.95 | 0.08 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3364 | 1/1   | 0.95 | 0.28 | 34,34,34,34                 | 0     |
| 59  | MG   | 1W    | 202  | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3640 | 1/1   | 0.95 | 0.11 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3572 | 1/1   | 0.95 | 0.08 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 4119 | 1/1   | 0.95 | 0.08 | 22,22,22,22                 | 0     |
| 59  | MG   | 2a    | 3233 | 1/1   | 0.95 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3365 | 1/1   | 0.95 | 0.22 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3779 | 1/1   | 0.95 | 0.17 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3180 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3086 | 1/1   | 0.95 | 0.18 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3580 | 1/1   | 0.95 | 0.09 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3115 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3145 | 1/1   | 0.95 | 0.10 | 44,44,44,44                 | 0     |
| 59  | MG   | 2f    | 3001 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3519 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3090 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | 10    | 103  | 1/1   | 0.95 | 0.11 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3050 | 1/1   | 0.95 | 0.15 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3004 | 1/1   | 0.95 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3224 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3319 | 1/1   | 0.95 | 0.24 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3491 | 1/1   | 0.95 | 0.08 | 75,75,75,75                 | 0     |
| 59  | MG   | 1A    | 3964 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3322 | 1/1   | 0.95 | 0.34 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3525 | 1/1   | 0.95 | 0.21 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3444 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 4136 | 1/1   | 0.95 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3272 | 1/1   | 0.95 | 0.12 | 36,36,36,36                 | 0     |
| 59  | MG   | 13    | 3003 | 1/1   | 0.95 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3273 | 1/1   | 0.95 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3106 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3107 | 1/1   | 0.95 | 0.23 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3604 | 1/1   | 0.95 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 4139 | 1/1   | 0.95 | 0.06 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 4140 | 1/1   | 0.95 | 0.05 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3324 | 1/1   | 0.95 | 0.19 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 18    | 102  | 1/1   | 0.95 | 0.22 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3084 | 1/1   | 0.95 | 0.09 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3192 | 1/1   | 0.95 | 0.21 | 27,27,27,27                 | 0     |
| 59  | MG   | 23    | 101  | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3121 | 1/1   | 0.95 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | 1a    | 3301 | 1/1   | 0.95 | 0.24 | 49,49,49,49                 | 0     |
| 59  | MG   | 2A    | 3339 | 1/1   | 0.95 | 0.33 | 50,50,50,50                 | 0     |
| 59  | MG   | 27    | 3001 | 1/1   | 0.95 | 0.28 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3972 | 1/1   | 0.95 | 0.11 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3125 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3086 | 1/1   | 0.95 | 0.07 | 31,31,31,31                 | 0     |
| 59  | MG   | 1a    | 3517 | 1/1   | 0.95 | 0.07 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3664 | 1/1   | 0.95 | 0.06 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3130 | 1/1   | 0.95 | 0.24 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 4150 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3133 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 59  | MG   | B     | 3001 | 1/1   | 0.95 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3389 | 1/1   | 0.96 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | 1a    | 3577 | 1/1   | 0.96 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3621 | 1/1   | 0.96 | 0.11 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3267 | 1/1   | 0.96 | 0.13 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3747 | 1/1   | 0.96 | 0.15 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3396 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3660 | 1/1   | 0.96 | 0.07 | 76,76,76,76                 | 0     |
| 59  | MG   | 1A    | 3369 | 1/1   | 0.96 | 0.28 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3398 | 1/1   | 0.96 | 0.16 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3750 | 1/1   | 0.96 | 0.09 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3624 | 1/1   | 0.96 | 0.05 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3032 | 1/1   | 0.96 | 0.20 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3141 | 1/1   | 0.96 | 0.10 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3320 | 1/1   | 0.96 | 0.09 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3755 | 1/1   | 0.96 | 0.07 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3901 | 1/1   | 0.96 | 0.06 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3142 | 1/1   | 0.96 | 0.17 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 4069 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3409 | 1/1   | 0.96 | 0.10 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3183 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3056 | 1/1   | 0.96 | 0.11 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3144 | 1/1   | 0.96 | 0.41 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3633 | 1/1   | 0.96 | 0.08 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3634 | 1/1   | 0.96 | 0.06 | 12,12,12,12                 | 0     |
| 59  | MG   | 1A    | 3635 | 1/1   | 0.96 | 0.07 | 8,8,8,8                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3764 | 1/1   | 0.96 | 0.06 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3520 | 1/1   | 0.96 | 0.13 | 16,16,16,16                 | 0     |
| 59  | MG   | 2A    | 3420 | 1/1   | 0.96 | 0.09 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3421 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3379 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3914 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3424 | 1/1   | 0.96 | 0.08 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3195 | 1/1   | 0.96 | 0.21 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3094 | 1/1   | 0.96 | 0.25 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3429 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 59  | MG   | 1D    | 306  | 1/1   | 0.96 | 0.15 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3448 | 1/1   | 0.96 | 0.28 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3917 | 1/1   | 0.96 | 0.09 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3700 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3524 | 1/1   | 0.96 | 0.14 | 31,31,31,31                 | 0     |
| 59  | MG   | 2a    | 3056 | 1/1   | 0.96 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | 2A    | 3704 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3146 | 1/1   | 0.96 | 0.13 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3190 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3191 | 1/1   | 0.96 | 0.15 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3709 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3279 | 1/1   | 0.96 | 0.14 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3715 | 1/1   | 0.96 | 0.09 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3439 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | 1x    | 106  | 1/1   | 0.96 | 0.20 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3719 | 1/1   | 0.96 | 0.06 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3720 | 1/1   | 0.96 | 0.06 | 42,42,42,42                 | 0     |
| 59  | MG   | 1E    | 306  | 1/1   | 0.96 | 0.13 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3646 | 1/1   | 0.96 | 0.06 | 8,8,8,8                     | 0     |
| 59  | MG   | 2A    | 3444 | 1/1   | 0.96 | 0.10 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3280 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 1E    | 309  | 1/1   | 0.96 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1E    | 310  | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 59  | MG   | 1E    | 311  | 1/1   | 0.96 | 0.10 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3449 | 1/1   | 0.96 | 0.11 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 3776 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3931 | 1/1   | 0.96 | 0.06 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3932 | 1/1   | 0.96 | 0.05 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3933 | 1/1   | 0.96 | 0.08 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3934 | 1/1   | 0.96 | 0.07 | 16,16,16,16                 | 0     |
| 59  | MG   | 1F    | 304  | 1/1   | 0.96 | 0.12 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3531 | 1/1   | 0.96 | 0.24 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 4100 | 1/1   | 0.96 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 1F    | 308  | 1/1   | 0.96 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3463 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3940 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3095 | 1/1   | 0.96 | 0.09 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3282 | 1/1   | 0.96 | 0.19 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3746 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3944 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3151 | 1/1   | 0.96 | 0.06 | 15,15,15,15                 | 0     |
| 59  | MG   | 1G    | 3005 | 1/1   | 0.96 | 0.09 | 51,51,51,51                 | 0     |
| 59  | MG   | 2A    | 3009 | 1/1   | 0.96 | 0.05 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3010 | 1/1   | 0.96 | 0.06 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 4108 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3458 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 1a    | 3417 | 1/1   | 0.96 | 0.33 | 50,50,50,50                 | 0     |
| 59  | MG   | 1N    | 3002 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 59  | MG   | 1N    | 3003 | 1/1   | 0.96 | 0.25 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3096 | 1/1   | 0.96 | 0.14 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3759 | 1/1   | 0.96 | 0.08 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3460 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3119 | 1/1   | 0.96 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3762 | 1/1   | 0.96 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3540 | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3659 | 1/1   | 0.96 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3953 | 1/1   | 0.96 | 0.06 | 64,64,64,64                 | 0     |
| 59  | MG   | 2A    | 3027 | 1/1   | 0.96 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | 1O    | 3002 | 1/1   | 0.96 | 0.30 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3541 | 1/1   | 0.96 | 0.09 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3030 | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3235 | 1/1   | 0.96 | 0.18 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3337 | 1/1   | 0.96 | 0.18 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3248 | 1/1   | 0.96 | 0.14 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3287 | 1/1   | 0.96 | 0.20 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4120 | 1/1   | 0.96 | 0.06 | 33,33,33,33                 | 0     |
| 59  | MG   | 2A    | 3495 | 1/1   | 0.96 | 0.13 | 37,37,37,37                 | 0     |
| 59  | MG   | 1Q    | 201  | 1/1   | 0.96 | 0.07 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3070 | 1/1   | 0.96 | 0.12 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3397 | 1/1   | 0.96 | 0.18 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3040 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 59  | MG   | 1Q    | 205  | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 59  | MG   | 1Q    | 206  | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3502 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 4123 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3549 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 59  | MG   | 2a    | 3129 | 1/1   | 0.96 | 0.09 | 75,75,75,75                 | 0     |
| 59  | MG   | 1A    | 3123 | 1/1   | 0.96 | 0.23 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3472 | 1/1   | 0.96 | 0.10 | 26,26,26,26                 | 0     |
| 59  | MG   | 1a    | 3442 | 1/1   | 0.96 | 0.13 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3676 | 1/1   | 0.96 | 0.06 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3554 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3790 | 1/1   | 0.96 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3555 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3238 | 1/1   | 0.96 | 0.23 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3805 | 1/1   | 0.96 | 0.26 | 30,30,30,30                 | 0     |
| 59  | MG   | 1U    | 205  | 1/1   | 0.96 | 0.22 | 29,29,29,29                 | 0     |
| 59  | MG   | 2a    | 3142 | 1/1   | 0.96 | 0.06 | 67,67,67,67                 | 0     |
| 59  | MG   | 1a    | 3450 | 1/1   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | 1a    | 3452 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3974 | 1/1   | 0.96 | 0.07 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 3975 | 1/1   | 0.96 | 0.15 | 23,23,23,23                 | 0     |
| 59  | MG   | 1a    | 3455 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 59  | MG   | 1a    | 3456 | 1/1   | 0.96 | 0.14 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3098 | 1/1   | 0.96 | 0.20 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3802 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | 1W    | 203  | 1/1   | 0.96 | 0.19 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3276 | 1/1   | 0.96 | 0.12 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3063 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 59  | MG   | 1X    | 3001 | 1/1   | 0.96 | 0.13 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3807 | 1/1   | 0.96 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3979 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3681 | 1/1   | 0.96 | 0.05 | 23,23,23,23                 | 0     |
| 59  | MG   | 2A    | 3282 | 1/1   | 0.96 | 0.30 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3240 | 1/1   | 0.96 | 0.17 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3478 | 1/1   | 0.96 | 0.27 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3070 | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 59  | MG   | 1Z    | 301  | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3817 | 1/1   | 0.96 | 0.12 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3818 | 1/1   | 0.96 | 0.07 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3534 | 1/1   | 0.96 | 0.13 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3565 | 1/1   | 0.96 | 0.06 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3536 | 1/1   | 0.96 | 0.10 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3158 | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 4144 | 1/1   | 0.96 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3825 | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3826 | 1/1   | 0.96 | 0.07 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3568 | 1/1   | 0.96 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | 10    | 102  | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3099 | 1/1   | 0.96 | 0.19 | 31,31,31,31                 | 0     |
| 59  | MG   | 2A    | 3830 | 1/1   | 0.96 | 0.23 | 32,32,32,32                 | 0     |
| 59  | MG   | 10    | 104  | 1/1   | 0.96 | 0.05 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3817 | 1/1   | 0.96 | 0.06 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3570 | 1/1   | 0.96 | 0.11 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3296 | 1/1   | 0.96 | 0.15 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3346 | 1/1   | 0.96 | 0.20 | 52,52,52,52                 | 0     |
| 59  | MG   | 10    | 108  | 1/1   | 0.96 | 0.04 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3820 | 1/1   | 0.96 | 0.08 | 13,13,13,13                 | 0     |
| 59  | MG   | 11    | 102  | 1/1   | 0.96 | 0.07 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3017 | 1/1   | 0.96 | 0.05 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3992 | 1/1   | 0.96 | 0.05 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3994 | 1/1   | 0.96 | 0.06 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3696 | 1/1   | 0.96 | 0.09 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3297 | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3484 | 1/1   | 0.96 | 0.19 | 27,27,27,27                 | 0     |
| 59  | MG   | 16    | 101  | 1/1   | 0.96 | 0.10 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3083 | 1/1   | 0.96 | 0.16 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3848 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 4001 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 4163 | 1/1   | 0.96 | 0.16 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3205 | 1/1   | 0.96 | 0.20 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3072 | 1/1   | 0.96 | 0.13 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3098 | 1/1   | 0.96 | 0.20 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3831 | 1/1   | 0.96 | 0.24 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 4171 | 1/1   | 0.96 | 0.24 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3101 | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3704 | 1/1   | 0.96 | 0.08 | 13,13,13,13                 | 0     |
| 59  | MG   | 1A    | 4173 | 1/1   | 0.96 | 0.35 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3581 | 1/1   | 0.96 | 0.06 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3707 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 59  | MG   | 1a    | 3512 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 59  | MG   | 1a    | 3306 | 1/1   | 0.96 | 0.16 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3836 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3518 | 1/1   | 0.96 | 0.07 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3583 | 1/1   | 0.96 | 0.07 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3301 | 1/1   | 0.96 | 0.27 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3115 | 1/1   | 0.96 | 0.30 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3313 | 1/1   | 0.96 | 0.23 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3208 | 1/1   | 0.96 | 0.19 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3218 | 1/1   | 0.96 | 0.07 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3120 | 1/1   | 0.96 | 0.13 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 4183 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3104 | 1/1   | 0.96 | 0.26 | 32,32,32,32                 | 0     |
| 59  | MG   | 2D    | 303  | 1/1   | 0.96 | 0.04 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3123 | 1/1   | 0.96 | 0.21 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3319 | 1/1   | 0.96 | 0.05 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3417 | 1/1   | 0.96 | 0.18 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3715 | 1/1   | 0.96 | 0.06 | 62,62,62,62                 | 0     |
| 59  | MG   | 2a    | 3227 | 1/1   | 0.96 | 0.18 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3590 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3719 | 1/1   | 0.96 | 0.05 | 44,44,44,44                 | 0     |
| 59  | MG   | 2a    | 3230 | 1/1   | 0.96 | 0.07 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3129 | 1/1   | 0.96 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3418 | 1/1   | 0.96 | 0.17 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3355 | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3342 | 1/1   | 0.96 | 0.06 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 4022 | 1/1   | 0.96 | 0.08 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3026 | 1/1   | 0.96 | 0.37 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3135 | 1/1   | 0.96 | 0.16 | 58,58,58,58                 | 0     |
| 59  | MG   | 2A    | 3136 | 1/1   | 0.96 | 0.20 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3060 | 1/1   | 0.96 | 0.31 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3168 | 1/1   | 0.96 | 0.37 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3726 | 1/1   | 0.96 | 0.06 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 4198 | 1/1   | 0.96 | 0.12 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3864 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3868 | 1/1   | 0.96 | 0.06 | 30,30,30,30                 | 0     |
| 59  | MG   | 2A    | 3610 | 1/1   | 0.96 | 0.19 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 4207 | 1/1   | 0.96 | 0.15 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 4032 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3169 | 1/1   | 0.96 | 0.08 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 4034 | 1/1   | 0.96 | 0.07 | 61,61,61,61                 | 0     |
| 59  | MG   | 1A    | 4215 | 1/1   | 0.96 | 0.36 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 4218 | 1/1   | 0.96 | 0.17 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3149 | 1/1   | 0.96 | 0.14 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3871 | 1/1   | 0.96 | 0.05 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3620 | 1/1   | 0.96 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 4222 | 1/1   | 0.96 | 0.25 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3135 | 1/1   | 0.96 | 0.19 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 4038 | 1/1   | 0.96 | 0.10 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3501 | 1/1   | 0.96 | 0.16 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3361 | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3347 | 1/1   | 0.96 | 0.13 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3733 | 1/1   | 0.96 | 0.04 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3607 | 1/1   | 0.96 | 0.04 | 17,17,17,17                 | 0     |
| 59  | MG   | 25    | 102  | 1/1   | 0.96 | 0.18 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3309 | 1/1   | 0.96 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | 2A    | 3160 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3736 | 1/1   | 0.96 | 0.11 | 15,15,15,15                 | 0     |
| 59  | MG   | 1a    | 3352 | 1/1   | 0.96 | 0.17 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3163 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 59  | MG   | 1A    | 4046 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3379 | 1/1   | 0.96 | 0.07 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3638 | 1/1   | 0.96 | 0.11 | 55,55,55,55                 | 0     |
| 59  | MG   | 1B    | 206  | 1/1   | 0.96 | 0.26 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3018 | 1/1   | 0.96 | 0.05 | 8,8,8,8                     | 0     |
| 59  | MG   | 2A    | 3383 | 1/1   | 0.96 | 0.14 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3064 | 1/1   | 0.96 | 0.12 | 19,19,19,19                 | 0     |
| 59  | MG   | 2A    | 3645 | 1/1   | 0.96 | 0.06 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3176 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3649 | 1/1   | 0.96 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3090 | 1/1   | 0.96 | 0.11 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3316 | 1/1   | 0.96 | 0.11 | 15,15,15,15                 | 0     |
| 60  | ZN   | 24    | 501  | 1/1   | 0.96 | 0.10 | 111,111,111,111             | 0     |
| 60  | ZN   | 2n    | 501  | 1/1   | 0.96 | 0.06 | 90,90,90,90                 | 0     |
| 59  | MG   | 1A    | 3475 | 1/1   | 0.97 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3007 | 1/1   | 0.97 | 0.13 | 40,40,40,40                 | 0     |
| 59  | MG   | 2A    | 3371 | 1/1   | 0.97 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | 1a    | 3451 | 1/1   | 0.97 | 0.10 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3038 | 1/1   | 0.97 | 0.10 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3978 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4094 | 1/1   | 0.97 | 0.10 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3014 | 1/1   | 0.97 | 0.06 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3477 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3251 | 1/1   | 0.97 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3867 | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3108 | 1/1   | 0.97 | 0.27 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3598 | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3080 | 1/1   | 0.97 | 0.12 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3873 | 1/1   | 0.97 | 0.04 | 30,30,30,30                 | 0     |
| 59  | MG   | 1a    | 3463 | 1/1   | 0.97 | 0.16 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3196 | 1/1   | 0.97 | 0.17 | 26,26,26,26                 | 0     |
| 59  | MG   | 1a    | 3310 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1a    | 3312 | 1/1   | 0.97 | 0.11 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3602 | 1/1   | 0.97 | 0.06 | 19,19,19,19                 | 0     |
| 59  | MG   | 1A    | 3390 | 1/1   | 0.97 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3054 | 1/1   | 0.97 | 0.11 | 24,24,24,24                 | 0     |
| 59  | MG   | 1a    | 3316 | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 1a    | 3474 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3257 | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3034 | 1/1   | 0.97 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 1B    | 224  | 1/1   | 0.97 | 0.17 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3610 | 1/1   | 0.97 | 0.06 | 19,19,19,19                 | 0     |
| 59  | MG   | 1A    | 3055 | 1/1   | 0.97 | 0.15 | 50,50,50,50                 | 0     |
| 59  | MG   | 1a    | 3481 | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3039 | 1/1   | 0.97 | 0.14 | 23,23,23,23                 | 0     |
| 59  | MG   | 1B    | 228  | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3993 | 1/1   | 0.97 | 0.05 | 20,20,20,20                 | 0     |
| 59  | MG   | 1A    | 3613 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | 1a    | 3485 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3694 | 1/1   | 0.97 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3885 | 1/1   | 0.97 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3486 | 1/1   | 0.97 | 0.21 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3998 | 1/1   | 0.97 | 0.06 | 13,13,13,13                 | 0     |
| 59  | MG   | 2A    | 3228 | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3833 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3887 | 1/1   | 0.97 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3616 | 1/1   | 0.97 | 0.08 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3147 | 1/1   | 0.97 | 0.36 | 26,26,26,26                 | 0     |
| 59  | MG   | 1B    | 237  | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3260 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3200 | 1/1   | 0.97 | 0.16 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3496 | 1/1   | 0.97 | 0.12 | 66,66,66,66                 | 0     |
| 59  | MG   | 1A    | 4004 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 59  | MG   | 1a    | 3498 | 1/1   | 0.97 | 0.07 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3624 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 59  | MG   | 2A    | 3426 | 1/1   | 0.97 | 0.06 | 23,23,23,23                 | 0     |
| 59  | MG   | 1D    | 303  | 1/1   | 0.97 | 0.19 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3500 | 1/1   | 0.97 | 0.07 | 64,64,64,64                 | 0     |
| 59  | MG   | 1D    | 304  | 1/1   | 0.97 | 0.14 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3293 | 1/1   | 0.97 | 0.10 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3148 | 1/1   | 0.97 | 0.20 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3432 | 1/1   | 0.97 | 0.08 | 26,26,26,26                 | 0     |
| 59  | MG   | 2A    | 3061 | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3112 | 1/1   | 0.97 | 0.15 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 4008 | 1/1   | 0.97 | 0.10 | 54,54,54,54                 | 0     |
| 59  | MG   | 2A    | 3635 | 1/1   | 0.97 | 0.08 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3785 | 1/1   | 0.97 | 0.10 | 18,18,18,18                 | 0     |
| 59  | MG   | 1A    | 3150 | 1/1   | 0.97 | 0.14 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3401 | 1/1   | 0.97 | 0.07 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3706 | 1/1   | 0.97 | 0.04 | 28,28,28,28                 | 0     |
| 59  | MG   | 1E    | 303  | 1/1   | 0.97 | 0.22 | 33,33,33,33                 | 0     |
| 59  | MG   | 1E    | 304  | 1/1   | 0.97 | 0.13 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3642 | 1/1   | 0.97 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | 2A    | 3442 | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3548 | 1/1   | 0.97 | 0.07 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3101 | 1/1   | 0.97 | 0.19 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 4132 | 1/1   | 0.97 | 0.13 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3520 | 1/1   | 0.97 | 0.06 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3522 | 1/1   | 0.97 | 0.07 | 66,66,66,66                 | 0     |
| 59  | MG   | 1a    | 3524 | 1/1   | 0.97 | 0.05 | 71,71,71,71                 | 0     |
| 59  | MG   | 1A    | 4133 | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3030 | 1/1   | 0.97 | 0.16 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3710 | 1/1   | 0.97 | 0.06 | 18,18,18,18                 | 0     |
| 59  | MG   | 1A    | 3093 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3797 | 1/1   | 0.97 | 0.15 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3659 | 1/1   | 0.97 | 0.06 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3454 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3268 | 1/1   | 0.97 | 0.13 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3134 | 1/1   | 0.97 | 0.16 | 24,24,24,24                 | 0     |
| 59  | MG   | 1a    | 3533 | 1/1   | 0.97 | 0.06 | 59,59,59,59                 | 0     |
| 59  | MG   | 2a    | 3168 | 1/1   | 0.97 | 0.19 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3534 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3066 | 1/1   | 0.97 | 0.16 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 4023 | 1/1   | 0.97 | 0.04 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3557 | 1/1   | 0.97 | 0.04 | 23,23,23,23                 | 0     |
| 59  | MG   | 1F    | 305  | 1/1   | 0.97 | 0.18 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 4143 | 1/1   | 0.97 | 0.12 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3558 | 1/1   | 0.97 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3092 | 1/1   | 0.97 | 0.13 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3559 | 1/1   | 0.97 | 0.10 | 28,28,28,28                 | 0     |
| 59  | MG   | 2N    | 8001 | 1/1   | 0.97 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 4146 | 1/1   | 0.97 | 0.07 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3637 | 1/1   | 0.97 | 0.06 | 18,18,18,18                 | 0     |
| 59  | MG   | 1G    | 3001 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4029 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3408 | 1/1   | 0.97 | 0.20 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3476 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3136 | 1/1   | 0.97 | 0.24 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3185 | 1/1   | 0.97 | 0.22 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3683 | 1/1   | 0.97 | 0.08 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3725 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3117 | 1/1   | 0.97 | 0.21 | 25,25,25,25                 | 0     |
| 59  | MG   | 1a    | 3552 | 1/1   | 0.97 | 0.13 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 4035 | 1/1   | 0.97 | 0.10 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3566 | 1/1   | 0.97 | 0.06 | 13,13,13,13                 | 0     |
| 59  | MG   | 1A    | 3412 | 1/1   | 0.97 | 0.09 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 4159 | 1/1   | 0.97 | 0.09 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3694 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3922 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 59  | MG   | 1A    | 3118 | 1/1   | 0.97 | 0.23 | 33,33,33,33                 | 0     |
| 59  | MG   | 1N    | 3008 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3489 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3112 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 59  | MG   | 20    | 3003 | 1/1   | 0.97 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3113 | 1/1   | 0.97 | 0.11 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4040 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3705 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3731 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | 1a    | 3383 | 1/1   | 0.97 | 0.22 | 43,43,43,43                 | 0     |
| 59  | MG   | 1a    | 3563 | 1/1   | 0.97 | 0.11 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3414 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 59  | MG   | 2A    | 3710 | 1/1   | 0.97 | 0.08 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3711 | 1/1   | 0.97 | 0.06 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3008 | 1/1   | 0.97 | 0.04 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3929 | 1/1   | 0.97 | 0.10 | 52,52,52,52                 | 0     |
| 59  | MG   | 1A    | 3162 | 1/1   | 0.97 | 0.30 | 30,30,30,30                 | 0     |
| 59  | MG   | 1P    | 201  | 1/1   | 0.97 | 0.21 | 23,23,23,23                 | 0     |
| 59  | MG   | 1P    | 202  | 1/1   | 0.97 | 0.33 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3243 | 1/1   | 0.97 | 0.35 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 4047 | 1/1   | 0.97 | 0.13 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3512 | 1/1   | 0.97 | 0.10 | 40,40,40,40                 | 0     |
| 59  | MG   | 1Q    | 202  | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3506 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3739 | 1/1   | 0.97 | 0.32 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3009 | 1/1   | 0.97 | 0.09 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3132 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3514 | 1/1   | 0.97 | 0.30 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3939 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3419 | 1/1   | 0.97 | 0.24 | 30,30,30,30                 | 0     |
| 59  | MG   | 1R    | 202  | 1/1   | 0.97 | 0.43 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 4181 | 1/1   | 0.97 | 0.27 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 4182 | 1/1   | 0.97 | 0.21 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3941 | 1/1   | 0.97 | 0.08 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3466 | 1/1   | 0.97 | 0.22 | 24,24,24,24                 | 0     |
| 59  | MG   | 1k    | 201  | 1/1   | 0.97 | 0.12 | 39,39,39,39                 | 0     |
| 59  | MG   | 1l    | 201  | 1/1   | 0.97 | 0.13 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3829 | 1/1   | 0.97 | 0.08 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3580 | 1/1   | 0.97 | 0.05 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3467 | 1/1   | 0.97 | 0.09 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 4062 | 1/1   | 0.97 | 0.06 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3122 | 1/1   | 0.97 | 0.23 | 28,28,28,28                 | 0     |
| 59  | MG   | 2a    | 3239 | 1/1   | 0.97 | 0.13 | 42,42,42,42                 | 0     |
| 59  | MG   | 1V    | 201  | 1/1   | 0.97 | 0.14 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3658 | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3421 | 1/1   | 0.97 | 0.13 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3660 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3248 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 59  | MG   | 1W    | 205  | 1/1   | 0.97 | 0.17 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3838 | 1/1   | 0.97 | 0.13 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3471 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3954 | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 4201 | 1/1   | 0.97 | 0.08 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4071 | 1/1   | 0.97 | 0.08 | 50,50,50,50                 | 0     |
| 59  | MG   | 2A    | 3537 | 1/1   | 0.97 | 0.18 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 4204 | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 59  | MG   | 1a    | 3422 | 1/1   | 0.97 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3587 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3588 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 4208 | 1/1   | 0.97 | 0.31 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3667 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | 2a    | 3048 | 1/1   | 0.97 | 0.16 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 4211 | 1/1   | 0.97 | 0.14 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3960 | 1/1   | 0.97 | 0.07 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3845 | 1/1   | 0.97 | 0.20 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3963 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3669 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4219 | 1/1   | 0.97 | 0.18 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4220 | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3757 | 1/1   | 0.97 | 0.04 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 4081 | 1/1   | 0.97 | 0.04 | 14,14,14,14                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3219 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 3383 | 1/1   | 0.97 | 0.11 | 38,38,38,38                 | 0     |
| 59  | MG   | 12    | 3002 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 4227 | 1/1   | 0.97 | 0.17 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3315 | 1/1   | 0.97 | 0.20 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3851 | 1/1   | 0.97 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1y    | 101  | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 59  | MG   | 15    | 102  | 1/1   | 0.97 | 0.12 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3852 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3853 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 59  | MG   | 2a    | 3070 | 1/1   | 0.97 | 0.16 | 60,60,60,60                 | 0     |
| 59  | MG   | 1a    | 3445 | 1/1   | 0.97 | 0.09 | 32,32,32,32                 | 0     |
| 59  | MG   | 16    | 103  | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3856 | 1/1   | 0.97 | 0.06 | 39,39,39,39                 | 0     |
| 60  | ZN   | 14    | 501  | 1/1   | 0.97 | 0.06 | 87,87,87,87                 | 0     |
| 59  | MG   | 1A    | 3592 | 1/1   | 0.97 | 0.04 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 3858 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 62  | K    | 2A    | 3849 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 59  | MG   | 17    | 102  | 1/1   | 0.98 | 0.07 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3668 | 1/1   | 0.98 | 0.05 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3890 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 59  | MG   | 1D    | 307  | 1/1   | 0.98 | 0.19 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3668 | 1/1   | 0.98 | 0.09 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3609 | 1/1   | 0.98 | 0.04 | 17,17,17,17                 | 0     |
| 59  | MG   | 1D    | 309  | 1/1   | 0.98 | 0.10 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 4165 | 1/1   | 0.98 | 0.09 | 9,9,9,9                     | 0     |
| 59  | MG   | 1D    | 311  | 1/1   | 0.98 | 0.21 | 19,19,19,19                 | 0     |
| 59  | MG   | 1A    | 4166 | 1/1   | 0.98 | 0.08 | 11,11,11,11                 | 0     |
| 59  | MG   | 1A    | 3085 | 1/1   | 0.98 | 0.17 | 15,15,15,15                 | 0     |
| 59  | MG   | 1A    | 3738 | 1/1   | 0.98 | 0.03 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 4169 | 1/1   | 0.98 | 0.10 | 22,22,22,22                 | 0     |
| 59  | MG   | 2A    | 3356 | 1/1   | 0.98 | 0.11 | 18,18,18,18                 | 0     |
| 59  | MG   | 2A    | 3512 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 4170 | 1/1   | 0.98 | 0.11 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3611 | 1/1   | 0.98 | 0.06 | 17,17,17,17                 | 0     |
| 59  | MG   | 2A    | 3681 | 1/1   | 0.98 | 0.06 | 62,62,62,62                 | 0     |
| 59  | MG   | 1A    | 3672 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 59  | MG   | 1a    | 3311 | 1/1   | 0.98 | 0.04 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3035 | 1/1   | 0.98 | 0.27 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3181 | 1/1   | 0.98 | 0.23 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3222 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3562 | 1/1   | 0.98 | 0.08 | 18,18,18,18                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3688 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 4080 | 1/1   | 0.98 | 0.10 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3563 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3691 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 59  | MG   | 2a    | 3130 | 1/1   | 0.98 | 0.06 | 79,79,79,79                 | 0     |
| 59  | MG   | 1A    | 3814 | 1/1   | 0.98 | 0.04 | 22,22,22,22                 | 0     |
| 59  | MG   | 2A    | 3693 | 1/1   | 0.98 | 0.10 | 32,32,32,32                 | 0     |
| 59  | MG   | 1a    | 3318 | 1/1   | 0.98 | 0.04 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3369 | 1/1   | 0.98 | 0.04 | 67,67,67,67                 | 0     |
| 59  | MG   | 1A    | 3027 | 1/1   | 0.98 | 0.21 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 4180 | 1/1   | 0.98 | 0.20 | 28,28,28,28                 | 0     |
| 59  | MG   | 2a    | 3137 | 1/1   | 0.98 | 0.07 | 68,68,68,68                 | 0     |
| 59  | MG   | 2A    | 3698 | 1/1   | 0.98 | 0.05 | 49,49,49,49                 | 0     |
| 59  | MG   | 1A    | 3207 | 1/1   | 0.98 | 0.20 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3620 | 1/1   | 0.98 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3374 | 1/1   | 0.98 | 0.07 | 49,49,49,49                 | 0     |
| 59  | MG   | 1f    | 3002 | 1/1   | 0.98 | 0.09 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3120 | 1/1   | 0.98 | 0.11 | 10,10,10,10                 | 0     |
| 59  | MG   | 1A    | 3749 | 1/1   | 0.98 | 0.03 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3450 | 1/1   | 0.98 | 0.21 | 31,31,31,31                 | 0     |
| 59  | MG   | 2a    | 3147 | 1/1   | 0.98 | 0.04 | 59,59,59,59                 | 0     |
| 59  | MG   | 1A    | 3047 | 1/1   | 0.98 | 0.05 | 19,19,19,19                 | 0     |
| 59  | MG   | 1A    | 3683 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 59  | MG   | 1a    | 3328 | 1/1   | 0.98 | 0.12 | 17,17,17,17                 | 0     |
| 59  | MG   | 2A    | 3382 | 1/1   | 0.98 | 0.04 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 3160 | 1/1   | 0.98 | 0.30 | 36,36,36,36                 | 0     |
| 59  | MG   | 2A    | 3714 | 1/1   | 0.98 | 0.06 | 66,66,66,66                 | 0     |
| 59  | MG   | 2A    | 3384 | 1/1   | 0.98 | 0.07 | 28,28,28,28                 | 0     |
| 59  | MG   | 2a    | 3155 | 1/1   | 0.98 | 0.05 | 72,72,72,72                 | 0     |
| 59  | MG   | 2A    | 3716 | 1/1   | 0.98 | 0.07 | 56,56,56,56                 | 0     |
| 59  | MG   | 1A    | 3073 | 1/1   | 0.98 | 0.17 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3912 | 1/1   | 0.98 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3826 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3571 | 1/1   | 0.98 | 0.10 | 13,13,13,13                 | 0     |
| 59  | MG   | 2A    | 3721 | 1/1   | 0.98 | 0.03 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 3627 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3003 | 1/1   | 0.98 | 0.07 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 4196 | 1/1   | 0.98 | 0.22 | 29,29,29,29                 | 0     |
| 59  | MG   | 2A    | 3108 | 1/1   | 0.98 | 0.08 | 43,43,43,43                 | 0     |
| 59  | MG   | 2A    | 3393 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3394 | 1/1   | 0.98 | 0.04 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3528 | 1/1   | 0.98 | 0.12 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3007 | 1/1   | 0.98 | 0.12 | 17,17,17,17                 | 0     |
| 59  | MG   | 1A    | 4199 | 1/1   | 0.98 | 0.19 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 4200 | 1/1   | 0.98 | 0.25 | 27,27,27,27                 | 0     |
| 59  | MG   | 2X    | 3002 | 1/1   | 0.98 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | 1a    | 3464 | 1/1   | 0.98 | 0.03 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3189 | 1/1   | 0.98 | 0.27 | 43,43,43,43                 | 0     |
| 59  | MG   | 20    | 3002 | 1/1   | 0.98 | 0.09 | 51,51,51,51                 | 0     |
| 59  | MG   | 1A    | 4202 | 1/1   | 0.98 | 0.19 | 27,27,27,27                 | 0     |
| 59  | MG   | 2A    | 3116 | 1/1   | 0.98 | 0.25 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 4101 | 1/1   | 0.98 | 0.08 | 41,41,41,41                 | 0     |
| 59  | MG   | 2A    | 3118 | 1/1   | 0.98 | 0.18 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3920 | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |
| 59  | MG   | 2A    | 3406 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | 2A    | 3563 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 59  | MG   | 2A    | 3743 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3576 | 1/1   | 0.98 | 0.12 | 9,9,9,9                     | 0     |
| 59  | MG   | 1A    | 4206 | 1/1   | 0.98 | 0.17 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3241 | 1/1   | 0.98 | 0.16 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 4105 | 1/1   | 0.98 | 0.09 | 53,53,53,53                 | 0     |
| 59  | MG   | 2A    | 3411 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 4209 | 1/1   | 0.98 | 0.13 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3750 | 1/1   | 0.98 | 0.06 | 51,51,51,51                 | 0     |
| 59  | MG   | 1O    | 3004 | 1/1   | 0.98 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3061 | 1/1   | 0.98 | 0.09 | 8,8,8,8                     | 0     |
| 59  | MG   | 1A    | 3031 | 1/1   | 0.98 | 0.27 | 24,24,24,24                 | 0     |
| 59  | MG   | 1a    | 3479 | 1/1   | 0.98 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | 1a    | 3480 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 59  | MG   | 1A    | 3244 | 1/1   | 0.98 | 0.18 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3419 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3577 | 1/1   | 0.98 | 0.06 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3841 | 1/1   | 0.98 | 0.04 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 4214 | 1/1   | 0.98 | 0.30 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3927 | 1/1   | 0.98 | 0.09 | 12,12,12,12                 | 0     |
| 59  | MG   | 1A    | 4216 | 1/1   | 0.98 | 0.08 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 4217 | 1/1   | 0.98 | 0.14 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3425 | 1/1   | 0.98 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3497 | 1/1   | 0.98 | 0.19 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3586 | 1/1   | 0.98 | 0.04 | 46,46,46,46                 | 0     |
| 59  | MG   | 1a    | 3488 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 4020 | 1/1   | 0.98 | 0.15 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3278 | 1/1   | 0.98 | 0.17 | 40,40,40,40                 | 0     |
| 59  | MG   | 1A    | 3701 | 1/1   | 0.98 | 0.04 | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3582 | 1/1   | 0.98 | 0.03 | 24,24,24,24                 | 0     |
| 59  | MG   | 2A    | 3592 | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3703 | 1/1   | 0.98 | 0.07 | 55,55,55,55                 | 0     |
| 59  | MG   | 1A    | 3245 | 1/1   | 0.98 | 0.24 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 4224 | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3063 | 1/1   | 0.98 | 0.06 | 15,15,15,15                 | 0     |
| 59  | MG   | 1A    | 4226 | 1/1   | 0.98 | 0.08 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3935 | 1/1   | 0.98 | 0.04 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3012 | 1/1   | 0.98 | 0.09 | 18,18,18,18                 | 0     |
| 59  | MG   | 1A    | 4028 | 1/1   | 0.98 | 0.10 | 50,50,50,50                 | 0     |
| 59  | MG   | 1U    | 201  | 1/1   | 0.98 | 0.20 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3937 | 1/1   | 0.98 | 0.06 | 22,22,22,22                 | 0     |
| 59  | MG   | 2A    | 3011 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 59  | MG   | 2A    | 3012 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 59  | MG   | 1a    | 3502 | 1/1   | 0.98 | 0.06 | 67,67,67,67                 | 0     |
| 59  | MG   | 1U    | 203  | 1/1   | 0.98 | 0.22 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3041 | 1/1   | 0.98 | 0.08 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3609 | 1/1   | 0.98 | 0.03 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3465 | 1/1   | 0.98 | 0.18 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3131 | 1/1   | 0.98 | 0.30 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3171 | 1/1   | 0.98 | 0.06 | 25,25,25,25                 | 0     |
| 59  | MG   | 2A    | 3020 | 1/1   | 0.98 | 0.05 | 24,24,24,24                 | 0     |
| 59  | MG   | 1A    | 3172 | 1/1   | 0.98 | 0.04 | 25,25,25,25                 | 0     |
| 59  | MG   | 2a    | 3050 | 1/1   | 0.98 | 0.04 | 54,54,54,54                 | 0     |
| 59  | MG   | 1a    | 3509 | 1/1   | 0.98 | 0.05 | 61,61,61,61                 | 0     |
| 59  | MG   | 1B    | 207  | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3855 | 1/1   | 0.98 | 0.07 | 51,51,51,51                 | 0     |
| 59  | MG   | 2a    | 3054 | 1/1   | 0.98 | 0.17 | 41,41,41,41                 | 0     |
| 59  | MG   | 1W    | 204  | 1/1   | 0.98 | 0.13 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3456 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 59  | MG   | 1A    | 3712 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 59  | MG   | 1a    | 3516 | 1/1   | 0.98 | 0.10 | 64,64,64,64                 | 0     |
| 59  | MG   | 1A    | 3024 | 1/1   | 0.98 | 0.25 | 19,19,19,19                 | 0     |
| 59  | MG   | 1X    | 3002 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |
| 59  | MG   | 1X    | 3003 | 1/1   | 0.98 | 0.14 | 32,32,32,32                 | 0     |
| 59  | MG   | 1A    | 3546 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 59  | MG   | 1X    | 3005 | 1/1   | 0.98 | 0.06 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3434 | 1/1   | 0.98 | 0.14 | 21,21,21,21                 | 0     |
| 59  | MG   | 1A    | 3716 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3435 | 1/1   | 0.98 | 0.22 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3862 | 1/1   | 0.98 | 0.05 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3863 | 1/1   | 0.98 | 0.04 | 9,9,9,9                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 2A    | 3811 | 1/1   | 0.98 | 0.09 | 62,62,62,62                 | 0     |
| 59  | MG   | 1a    | 3529 | 1/1   | 0.98 | 0.05 | 53,53,53,53                 | 0     |
| 59  | MG   | 1A    | 3718 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 59  | MG   | 1A    | 3865 | 1/1   | 0.98 | 0.04 | 42,42,42,42                 | 0     |
| 59  | MG   | 1A    | 3067 | 1/1   | 0.98 | 0.11 | 19,19,19,19                 | 0     |
| 59  | MG   | 2A    | 3475 | 1/1   | 0.98 | 0.04 | 48,48,48,48                 | 0     |
| 59  | MG   | 2a    | 3075 | 1/1   | 0.98 | 0.17 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3550 | 1/1   | 0.98 | 0.06 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3437 | 1/1   | 0.98 | 0.13 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3961 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 59  | MG   | 2A    | 3821 | 1/1   | 0.98 | 0.06 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 4050 | 1/1   | 0.98 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3870 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 59  | MG   | 1a    | 3538 | 1/1   | 0.98 | 0.09 | 44,44,44,44                 | 0     |
| 59  | MG   | 1A    | 3312 | 1/1   | 0.98 | 0.23 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3872 | 1/1   | 0.98 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | 2A    | 3647 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | 1a    | 3403 | 1/1   | 0.98 | 0.10 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3553 | 1/1   | 0.98 | 0.05 | 20,20,20,20                 | 0     |
| 59  | MG   | 2A    | 3650 | 1/1   | 0.98 | 0.14 | 60,60,60,60                 | 0     |
| 59  | MG   | 1A    | 3790 | 1/1   | 0.98 | 0.13 | 35,35,35,35                 | 0     |
| 59  | MG   | 1A    | 3791 | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3373 | 1/1   | 0.98 | 0.12 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3793 | 1/1   | 0.98 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3601 | 1/1   | 0.98 | 0.05 | 12,12,12,12                 | 0     |
| 59  | MG   | 1A    | 3152 | 1/1   | 0.98 | 0.07 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3727 | 1/1   | 0.98 | 0.08 | 15,15,15,15                 | 0     |
| 59  | MG   | 1A    | 3016 | 1/1   | 0.98 | 0.03 | 20,20,20,20                 | 0     |
| 59  | MG   | 1A    | 3604 | 1/1   | 0.98 | 0.05 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3605 | 1/1   | 0.98 | 0.05 | 14,14,14,14                 | 0     |
| 60  | ZN   | 2Y    | 501  | 1/1   | 0.98 | 0.04 | 86,86,86,86                 | 0     |
| 59  | MG   | 1A    | 3606 | 1/1   | 0.98 | 0.07 | 17,17,17,17                 | 0     |
| 60  | ZN   | 29    | 501  | 1/1   | 0.98 | 0.04 | 69,69,69,69                 | 0     |
| 59  | MG   | 1A    | 3256 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 61  | SF4  | 2d    | 501  | 8/8   | 0.98 | 0.05 | 56,66,80,82                 | 0     |
| 59  | MG   | 1A    | 3069 | 1/1   | 0.98 | 0.12 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 4051 | 1/1   | 0.99 | 0.04 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3046 | 1/1   | 0.99 | 0.08 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3816 | 1/1   | 0.99 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | 2A    | 3006 | 1/1   | 0.99 | 0.06 | 30,30,30,30                 | 0     |
| 59  | MG   | 1A    | 3840 | 1/1   | 0.99 | 0.04 | 16,16,16,16                 | 0     |
| 59  | MG   | 2A    | 3595 | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 4055 | 1/1   | 0.99 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3713 | 1/1   | 0.99 | 0.04 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3011 | 1/1   | 0.99 | 0.21 | 16,16,16,16                 | 0     |
| 59  | MG   | 1B    | 216  | 1/1   | 0.99 | 0.09 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3130 | 1/1   | 0.99 | 0.16 | 32,32,32,32                 | 0     |
| 59  | MG   | 2A    | 3064 | 1/1   | 0.99 | 0.11 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3006 | 1/1   | 0.99 | 0.04 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3956 | 1/1   | 0.99 | 0.06 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3957 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 59  | MG   | 1A    | 3684 | 1/1   | 0.99 | 0.04 | 28,28,28,28                 | 0     |
| 59  | MG   | 2A    | 3016 | 1/1   | 0.99 | 0.07 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3723 | 1/1   | 0.99 | 0.03 | 47,47,47,47                 | 0     |
| 59  | MG   | 1A    | 3685 | 1/1   | 0.99 | 0.04 | 14,14,14,14                 | 0     |
| 59  | MG   | 1A    | 3059 | 1/1   | 0.99 | 0.15 | 10,10,10,10                 | 0     |
| 59  | MG   | 1A    | 3025 | 1/1   | 0.99 | 0.12 | 21,21,21,21                 | 0     |
| 59  | MG   | 2A    | 3727 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 59  | MG   | 1A    | 3213 | 1/1   | 0.99 | 0.20 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 3374 | 1/1   | 0.99 | 0.16 | 27,27,27,27                 | 0     |
| 59  | MG   | 1F    | 303  | 1/1   | 0.99 | 0.03 | 24,24,24,24                 | 0     |
| 59  | MG   | 1B    | 227  | 1/1   | 0.99 | 0.05 | 31,31,31,31                 | 0     |
| 59  | MG   | 1a    | 3457 | 1/1   | 0.99 | 0.07 | 28,28,28,28                 | 0     |
| 59  | MG   | 1A    | 3029 | 1/1   | 0.99 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | 1A    | 3827 | 1/1   | 0.99 | 0.05 | 23,23,23,23                 | 0     |
| 59  | MG   | 1A    | 3999 | 1/1   | 0.99 | 0.03 | 20,20,20,20                 | 0     |
| 59  | MG   | 1A    | 3878 | 1/1   | 0.99 | 0.02 | 38,38,38,38                 | 0     |
| 59  | MG   | 1A    | 3906 | 1/1   | 0.99 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3170 | 1/1   | 0.99 | 0.15 | 10,10,10,10                 | 0     |
| 59  | MG   | 1A    | 3692 | 1/1   | 0.99 | 0.07 | 37,37,37,37                 | 0     |
| 59  | MG   | 1a    | 3465 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 59  | MG   | 1A    | 3938 | 1/1   | 0.99 | 0.02 | 22,22,22,22                 | 0     |
| 59  | MG   | 1A    | 3854 | 1/1   | 0.99 | 0.04 | 52,52,52,52                 | 0     |
| 59  | MG   | 1a    | 3513 | 1/1   | 0.99 | 0.03 | 61,61,61,61                 | 0     |
| 59  | MG   | 2A    | 3461 | 1/1   | 0.99 | 0.03 | 27,27,27,27                 | 0     |
| 59  | MG   | 1A    | 4186 | 1/1   | 0.99 | 0.09 | 27,27,27,27                 | 0     |
| 59  | MG   | 1a    | 3515 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 59  | MG   | 1a    | 3469 | 1/1   | 0.99 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | 1A    | 3882 | 1/1   | 0.99 | 0.07 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3179 | 1/1   | 0.99 | 0.05 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3616 | 1/1   | 0.99 | 0.09 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 3532 | 1/1   | 0.99 | 0.22 | 25,25,25,25                 | 0     |
| 59  | MG   | 1a    | 3521 | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 59  | MG   | 2A    | 3815 | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | 1A    | 3976 | 1/1   | 0.99 | 0.10 | 56,56,56,56                 | 0     |
| 59  | MG   | 1a    | 3523 | 1/1   | 0.99 | 0.02 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3811 | 1/1   | 0.99 | 0.04 | 30,30,30,30                 | 0     |
| 59  | MG   | 1a    | 3574 | 1/1   | 0.99 | 0.05 | 43,43,43,43                 | 0     |
| 59  | MG   | 1A    | 3834 | 1/1   | 0.99 | 0.06 | 34,34,34,34                 | 0     |
| 59  | MG   | 1A    | 3946 | 1/1   | 0.99 | 0.03 | 46,46,46,46                 | 0     |
| 59  | MG   | 1A    | 3618 | 1/1   | 0.99 | 0.04 | 16,16,16,16                 | 0     |
| 59  | MG   | 1A    | 4157 | 1/1   | 0.99 | 0.04 | 24,24,24,24                 | 0     |
| 60  | ZN   | 1Y    | 501  | 1/1   | 0.99 | 0.02 | 58,58,58,58                 | 0     |
| 59  | MG   | 1A    | 4158 | 1/1   | 0.99 | 0.07 | 20,20,20,20                 | 0     |
| 60  | ZN   | 15    | 101  | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |
| 60  | ZN   | 16    | 102  | 1/1   | 0.99 | 0.05 | 36,36,36,36                 | 0     |
| 59  | MG   | 1A    | 3662 | 1/1   | 0.99 | 0.05 | 15,15,15,15                 | 0     |
| 59  | MG   | 2A    | 3701 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 60  | ZN   | 25    | 101  | 1/1   | 0.99 | 0.03 | 49,49,49,49                 | 0     |
| 60  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.03 | 57,57,57,57                 | 0     |
| 59  | MG   | 2A    | 3644 | 1/1   | 0.99 | 0.04 | 69,69,69,69                 | 0     |
| 59  | MG   | 2A    | 3703 | 1/1   | 0.99 | 0.04 | 30,30,30,30                 | 0     |
| 61  | SF4  | 1d    | 501  | 8/8   | 0.99 | 0.06 | 52,55,64,66                 | 0     |
| 59  | MG   | 1A    | 3663 | 1/1   | 0.99 | 0.05 | 14,14,14,14                 | 0     |
| 59  | MG   | 2A    | 3646 | 1/1   | 0.99 | 0.04 | 53,53,53,53                 | 0     |
| 60  | ZN   | 1n    | 501  | 1/1   | 1.00 | 0.02 | 54,54,54,54                 | 0     |
| 59  | MG   | 1A    | 3737 | 1/1   | 1.00 | 0.03 | 34,34,34,34                 | 0     |
| 59  | MG   | 2A    | 3460 | 1/1   | 1.00 | 0.04 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3928 | 1/1   | 1.00 | 0.02 | 16,16,16,16                 | 0     |
| 59  | MG   | 2a    | 3145 | 1/1   | 1.00 | 0.04 | 45,45,45,45                 | 0     |
| 59  | MG   | 1A    | 3653 | 1/1   | 1.00 | 0.03 | 12,12,12,12                 | 0     |
| 59  | MG   | 1A    | 3010 | 1/1   | 1.00 | 0.04 | 16,16,16,16                 | 0     |
| 59  | MG   | 2A    | 3578 | 1/1   | 1.00 | 0.04 | 25,25,25,25                 | 0     |
| 59  | MG   | 1A    | 3866 | 1/1   | 1.00 | 0.05 | 15,15,15,15                 | 0     |
| 60  | ZN   | 19    | 102  | 1/1   | 1.00 | 0.07 | 40,40,40,40                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.