



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 01:44 PM UTC

PDB ID : 8VTW / pdb\_00008vtw  
Title : Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with macrolone MCX-128 and protein Y at 2.35Å resolution  
Authors : Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.  
Deposited on : 2024-01-27  
Resolution : 2.35 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                     | : | <b>FAILED</b>                                                    |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

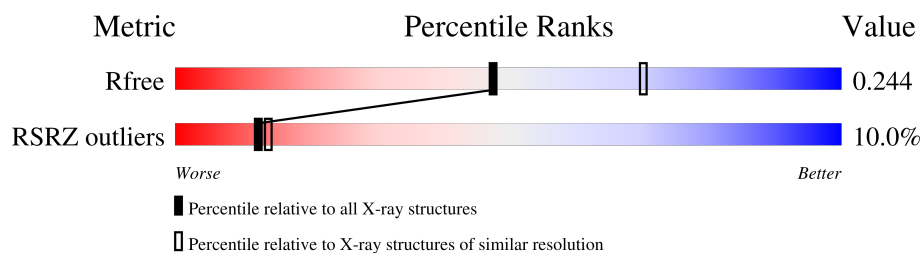
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



| Metric        | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 180053                      | 1596 (2.36-2.36)                                      |
| RSRZ outliers | 180081                      | 1598 (2.36-2.36)                                      |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | 1a    | 1675 | -         | -        | -       | X                |
| 54  | MG   | 2A    | 3245 | -         | -        | -       | X                |
| 54  | MG   | 2a    | 3047 | -         | -        | -       | X                |
| 54  | MG   | 2a    | 3058 | -         | -        | -       | X                |
| 54  | MG   | 2a    | 3080 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 296775 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    | 2872     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61869 | 27540 | 11574 | 19884 | 2871 |         |         |       |
| 1   | 2A    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61758 | 27491 | 11552 | 19850 | 2865 |         |         |       |

- 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     |
|     |       |          | 2572  | 1145 | 476 | 832 | 119 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- 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     |
|     |       |          | 2131  | 1346 | 422 | 360 | 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     |
|     |       |          | 1426  | 916 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 912 | 259 | 249 | 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    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 842 | 247 | 234 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 699 | 191 | 203 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 687 | 186 | 202 | 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     |
|     |       |          | 1121  | 722 | 208 | 187 | 4 |         |         |       |
| 9   | 2N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | 1V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 498 | 141 | 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     |
|     |       |          | 810   | 520 | 153 | 131 | 6 |         |         |       |
| 20  | 2Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1587  | 1011 | 282 | 292 | 2 |         |         |       |
| 21  | 2Z    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1557  | 995  | 274 | 286 | 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     |
|     |       |          | 650   | 401 | 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     |
|     |       |          | 754   | 475 | 148 | 130 | 1 |         |         |       |
| 23  | 21    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 149 | 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     |
|     |       |          | 592   | 368 | 119 | 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     |
|     |       |          | 546   | 346 | 96 | 99 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 536   | 342 | 98 | 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     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 27  | 25    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 32  | 1a    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14358 | 5975 | 10413 | 1500 |         |         |       |
| 32  | 2a    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32331 | 14396 | 5990 | 10441 | 1504 |         |         |       |

- 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     |
|     |       |          | 1842  | 1175 | 330 | 332 | 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     |
|     |       |          | 1558  | 979 | 305 | 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     |
|     |       |          | 1665  | 1043 | 329 | 286 | 7 |         |         |       |
| 35  | 2d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1047 | 330 | 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     |
|     |       |          | 1133  | 716 | 214 | 199 | 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     |
|     |       |          | 814   | 516 | 144 | 151 | 3 |         |         |       |
| 37  | 2f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | 1g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |
| 38  | 2g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1229  | 766 | 241 | 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     |
|     |       |          | 1098  | 694 | 210 | 192 | 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     |
|     |       |          | 986   | 625 | 193 | 168 |         |         |       |
| 40  | 2i    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 966   | 613 | 186 | 167 |         |         |       |

- 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     |
|     |       |          | 719   | 446 | 142 | 131 |         |         |       |
| 41  | 2j    | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 710   | 442 | 137 | 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     |
|     |       |          | 834   | 520 | 156 | 155 | 3 |         |         |       |

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | 1m    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 914   | 564 | 189 | 159 | 2 |         |         |       |
| 44  | 2m    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 895   | 550 | 186 | 157 | 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     |
|     |       |          | 648   | 415 | 120 | 111 | 2 |         |         |       |
| 50  | 2s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 410 | 118 | 115 | 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     |
|     |       |          | 732   | 449 | 157 | 124 | 2 |         |         |       |
| 51  | 2t    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 451 | 154 | 126 | 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 protein called Ribosome-associated inhibitor A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | 1y    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 764   | 478 | 144 | 139 | 3 |         |         |       |
| 53  | 2y    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 749   | 468 | 141 | 137 | 3 |         |         |       |

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54  | 1A    | 996      | Total | Mg  | 0       | 0       |
|     |       |          | 996   | 996 |         |         |
| 54  | 1B    | 31       | Total | Mg  | 0       | 0       |
|     |       |          | 31    | 31  |         |         |
| 54  | 1D    | 16       | Total | Mg  | 0       | 0       |
|     |       |          | 16    | 16  |         |         |
| 54  | 1E    | 11       | Total | Mg  | 0       | 0       |
|     |       |          | 11    | 11  |         |         |
| 54  | 1F    | 17       | Total | Mg  | 0       | 0       |
|     |       |          | 17    | 17  |         |         |
| 54  | 1G    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | 1H    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 54  | 1N    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | 1O    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | 1P    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | 1Q    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | 1R    | 5        | Total | Mg  | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 54  | 1T    | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 54  | 1U    | 5        | Total | Mg  | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 54  | 1V    | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 54  | 1W    | 5        | Total | Mg  | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 54  | 1X    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | 1Y    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | 1Z    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 10    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 54  | 11    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 12    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 13    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 15    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 54  | 17    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 18    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 19    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1a    | 267      | Total<br>267 | Mg<br>267 | 0       | 0       |
| 54  | 1b    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1d    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | 1e    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1f    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1g    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1h    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1i    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1l    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1m    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1n    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 1o    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |

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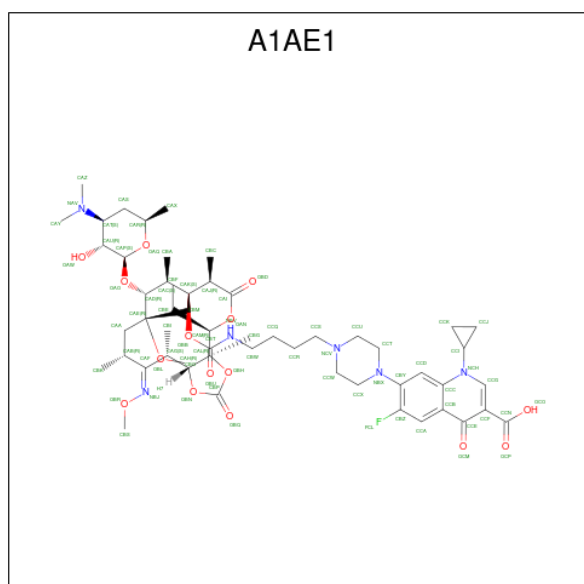
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | 1r    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 1t    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 1y    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2A    | 726      | Total<br>726 | Mg<br>726 | 0       | 0       |
| 54  | 2B    | 18       | Total<br>18  | Mg<br>18  | 0       | 0       |
| 54  | 2D    | 12       | Total<br>12  | Mg<br>12  | 0       | 0       |
| 54  | 2E    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 54  | 2F    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | 2G    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2I    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2N    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2O    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2P    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2Q    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2R    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2T    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | 2V    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 2W    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 20    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 23    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 25    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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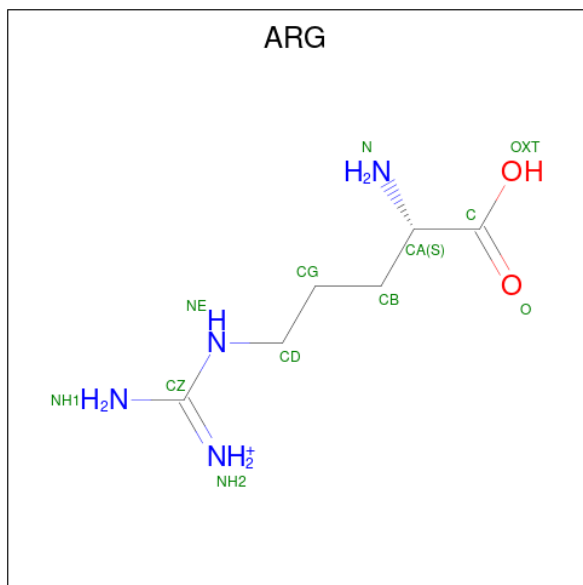
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | 27    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | 28    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2a    | 181      | Total<br>181 | Mg<br>181 | 0       | 0       |
| 54  | 2e    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2f    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | 2h    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2j    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2p    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2r    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | 2t    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 55 is 1-cyclopropyl-7-(4-{4-[(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-[[[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy]-4-ethyl-11-methoxy-14-(methoxyimino)-3a,7,9,11,13,15-hexamethyl-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl]oxy}carbonyl)amino]butyl}piperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AE1) (formula: C<sub>54</sub>H<sub>81</sub>FN<sub>6</sub>O<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



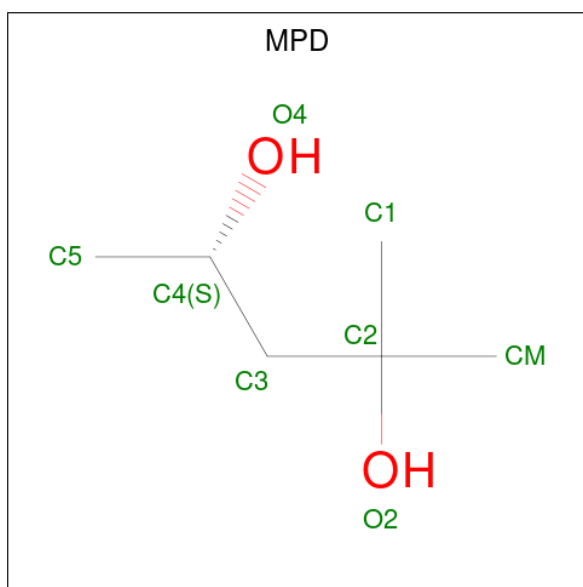
| Mol | Chain | Residues | Atoms |    |   |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|----|---------|---------|
| 55  | 1A    | 1        | Total | C  | F | N | O  | 0       | 0       |
|     |       |          | 76    | 54 | 1 | 6 | 15 |         |         |
| 55  | 2A    | 1        | Total | C  | F | N | O  | 0       | 0       |
|     |       |          | 76    | 54 | 1 | 6 | 15 |         |         |

- Molecule 56 is ARGinine (CCD ID: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 56  | 1A    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |
| 56  | 1B    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula:  $C_6H_{14}O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 57  | 1A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 1T    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 18    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 1a    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 2A    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 57  | 2B    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

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

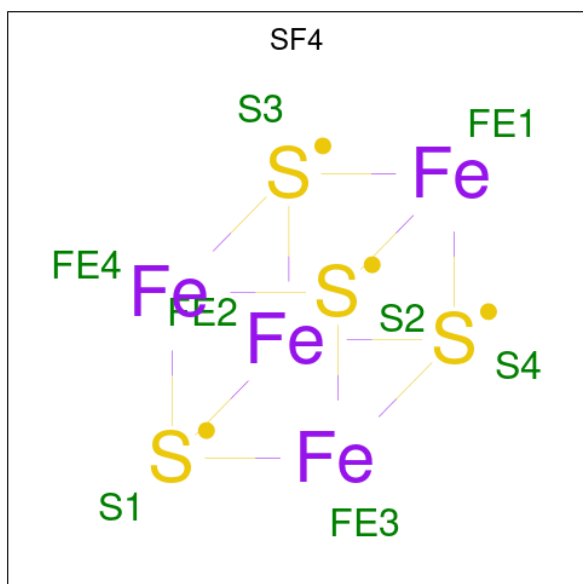
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 60 is water.

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 60  | 1A    | 3773     | Total | O    | 0       | 0       |
|     |       |          | 3773  | 3773 |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 1B    | 85       | Total<br>85  | O<br>85  | 0       | 0       |
| 60  | 1D    | 105      | Total<br>105 | O<br>105 | 0       | 0       |
| 60  | 1E    | 67       | Total<br>67  | O<br>67  | 0       | 0       |
| 60  | 1F    | 60       | Total<br>60  | O<br>60  | 0       | 0       |
| 60  | 1G    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 60  | 1H    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 60  | 1I    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 1N    | 46       | Total<br>46  | O<br>46  | 0       | 0       |
| 60  | 1O    | 26       | Total<br>26  | O<br>26  | 0       | 0       |
| 60  | 1P    | 61       | Total<br>61  | O<br>61  | 0       | 0       |
| 60  | 1Q    | 38       | Total<br>38  | O<br>38  | 0       | 0       |
| 60  | 1R    | 33       | Total<br>33  | O<br>33  | 0       | 0       |
| 60  | 1S    | 11       | Total<br>11  | O<br>11  | 0       | 0       |
| 60  | 1T    | 29       | Total<br>29  | O<br>29  | 0       | 0       |
| 60  | 1U    | 45       | Total<br>45  | O<br>45  | 0       | 0       |
| 60  | 1V    | 30       | Total<br>30  | O<br>30  | 0       | 0       |
| 60  | 1W    | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 60  | 1X    | 23       | Total<br>23  | O<br>23  | 0       | 0       |
| 60  | 1Y    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 60  | 1Z    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 60  | 10    | 22       | Total<br>22  | O<br>22  | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | 11    | 26       | Total<br>26  | O<br>26  | 0       | 0       |
| 60  | 12    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 60  | 13    | 22       | Total<br>22  | O<br>22  | 0       | 0       |
| 60  | 14    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 15    | 25       | Total<br>25  | O<br>25  | 0       | 0       |
| 60  | 16    | 16       | Total<br>16  | O<br>16  | 0       | 0       |
| 60  | 17    | 19       | Total<br>19  | O<br>19  | 0       | 0       |
| 60  | 18    | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 60  | 19    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 1a    | 446      | Total<br>446 | O<br>446 | 0       | 0       |
| 60  | 1b    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1c    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1d    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 60  | 1e    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | 1f    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1g    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 60  | 1h    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | 1j    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1l    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | 1n    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | 1o    | 4        | Total<br>4   | O<br>4   | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 60  | 1p    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 1y    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 2A    | 1939     | Total<br>1939 | O<br>1939 | 0       | 0       |
| 60  | 2B    | 31       | Total<br>31   | O<br>31   | 0       | 0       |
| 60  | 2D    | 45       | Total<br>45   | O<br>45   | 0       | 0       |
| 60  | 2E    | 23       | Total<br>23   | O<br>23   | 0       | 0       |
| 60  | 2F    | 16       | Total<br>16   | O<br>16   | 0       | 0       |
| 60  | 2G    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 60  | 2I    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 2N    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 60  | 2O    | 14       | Total<br>14   | O<br>14   | 0       | 0       |
| 60  | 2P    | 24       | Total<br>24   | O<br>24   | 0       | 0       |
| 60  | 2Q    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 60  | 2R    | 14       | Total<br>14   | O<br>14   | 0       | 0       |
| 60  | 2S    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 60  | 2T    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 60  | 2U    | 12       | Total<br>12   | O<br>12   | 0       | 0       |
| 60  | 2V    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 60  | 2W    | 15       | Total<br>15   | O<br>15   | 0       | 0       |
| 60  | 2X    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 60  | 2Z    | 3        | Total<br>3    | O<br>3    | 0       | 0       |

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| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 60  | 20    | 7        | Total | O   | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 60  | 21    | 9        | Total | O   | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 60  | 23    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | 25    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 60  | 26    | 5        | Total | O   | 0       | 0       |
|     |       |          | 5     | 5   |         |         |
| 60  | 27    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 60  | 28    | 9        | Total | O   | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 60  | 2a    | 259      | Total | O   | 0       | 0       |
|     |       |          | 259   | 259 |         |         |
| 60  | 2e    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | 2l    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 60  | 2n    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | 2o    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 60  | 2p    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 60  | 2r    | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 60  | 2t    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |

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### 3 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.60Å 449.32Å 619.65Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 124.58 – 2.35<br>124.58 – 2.35                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (124.58-2.35)<br>100.0 (124.58-2.35)                  | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.19                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.19 (at 2.34Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.2                                                | Depositor        |
| R, $R_{free}$                                                           | 0.207 , 0.243<br>0.208 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 119915 reflections (5.02%)                                  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.134                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 47.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 296775                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

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#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

48 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  | 4OC  | 2a    | 1402 | 32   | 20,23,24     | 0.76 | 0           | 25,32,35    | 0.94 | 1 (4%)      |
| 1   | PSU  | 1A    | 2605 | 1    | 18,21,22     | 1.36 | 2 (11%)     | 21,30,33    | 1.95 | 4 (19%)     |
| 32  | 2MG  | 1a    | 1207 | 32   | 23,26,27     | 1.23 | 2 (8%)      | 33,38,41    | 2.36 | 10 (30%)    |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 4OC  | 1a    | 1402 | 32    | 20,23,24     | 0.74 | 0        | 25,32,35    | 1.01 | 1 (4%)   |
| 1   | PSU  | 2A    | 2605 | 1     | 18,21,22     | 1.32 | 3 (16%)  | 21,30,33    | 1.92 | 5 (23%)  |
| 1   | PSU  | 1A    | 1911 | 1     | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1400 | 32    | 19,22,23     | 1.68 | 3 (15%)  | 26,32,35    | 1.19 | 2 (7%)   |
| 32  | 5MC  | 2a    | 1407 | 32    | 19,22,23     | 1.60 | 3 (15%)  | 26,32,35    | 1.15 | 3 (11%)  |
| 1   | PSU  | 2A    | 1911 | 1     | 18,21,22     | 1.42 | 3 (16%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 32  | UR3  | 2a    | 1498 | 32    | 19,22,23     | 1.00 | 1 (5%)   | 26,32,35    | 1.71 | 2 (7%)   |
| 32  | PSU  | 2a    | 516  | 54,32 | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 2.07 | 5 (23%)  |
| 1   | OMC  | 2A    | 1920 | 1     | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.91 | 1 (4%)   |
| 32  | MA6  | 2a    | 1518 | 32    | 23,26,27     | 0.40 | 0        | 33,38,41    | 2.01 | 9 (27%)  |
| 1   | OMC  | 1A    | 1920 | 1     | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.99 | 1 (4%)   |
| 32  | 5MC  | 1a    | 1400 | 32    | 19,22,23     | 1.81 | 3 (15%)  | 26,32,35    | 1.19 | 2 (7%)   |
| 1   | 5MU  | 2A    | 1939 | 1,54  | 19,22,23     | 1.39 | 6 (31%)  | 27,32,35    | 2.23 | 6 (22%)  |
| 1   | 5MC  | 2A    | 1962 | 1,54  | 19,22,23     | 1.61 | 3 (15%)  | 26,32,35    | 1.13 | 2 (7%)   |
| 32  | 5MC  | 1a    | 1407 | 32    | 19,22,23     | 1.80 | 3 (15%)  | 26,32,35    | 1.15 | 3 (11%)  |
| 32  | G7M  | 2a    | 527  | 32    | 23,26,27     | 1.51 | 3 (13%)  | 34,39,42    | 1.66 | 5 (14%)  |
| 32  | UR3  | 1a    | 1498 | 32    | 19,22,23     | 1.02 | 1 (5%)   | 26,32,35    | 1.84 | 4 (15%)  |
| 1   | 2MA  | 1A    | 2503 | 1,54  | 22,25,26     | 1.45 | 6 (27%)  | 32,37,40    | 2.36 | 9 (28%)  |
| 1   | OMU  | 1A    | 2552 | 1,54  | 19,22,23     | 1.21 | 3 (15%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 32  | PSU  | 1a    | 516  | 54,32 | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.87 | 4 (19%)  |
| 32  | 5MC  | 2a    | 1404 | 32    | 19,22,23     | 1.75 | 3 (15%)  | 26,32,35    | 1.17 | 3 (11%)  |
| 1   | 2MA  | 2A    | 2503 | 1,54  | 22,25,26     | 1.41 | 4 (18%)  | 32,37,40    | 2.46 | 9 (28%)  |
| 1   | OMU  | 2A    | 2552 | 1,54  | 19,22,23     | 1.15 | 2 (10%)  | 25,31,34    | 1.89 | 6 (24%)  |
| 32  | G7M  | 1a    | 527  | 54,32 | 23,26,27     | 1.51 | 4 (17%)  | 34,39,42    | 1.69 | 5 (14%)  |
| 32  | MA6  | 1a    | 1518 | 32    | 23,26,27     | 0.39 | 0        | 33,38,41    | 1.98 | 9 (27%)  |
| 1   | 5MU  | 1A    | 1915 | 1     | 19,22,23     | 1.44 | 5 (26%)  | 27,32,35    | 2.37 | 9 (33%)  |
| 32  | MA6  | 1a    | 1519 | 32    | 23,26,27     | 0.41 | 0        | 33,38,41    | 2.00 | 9 (27%)  |
| 1   | 5MU  | 2A    | 1915 | 1     | 19,22,23     | 1.45 | 4 (21%)  | 27,32,35    | 2.21 | 9 (33%)  |
| 32  | M2G  | 1a    | 966  | 32    | 24,27,28     | 1.29 | 3 (12%)  | 33,40,43    | 1.78 | 5 (15%)  |
| 32  | 5MC  | 1a    | 1404 | 32    | 19,22,23     | 1.64 | 3 (15%)  | 26,32,35    | 1.08 | 3 (11%)  |
| 43  | 0TD  | 2l    | 92   | 43    | 8,9,10       | 4.43 | 2 (25%)  | 6,11,13     | 3.95 | 2 (33%)  |
| 1   | 5MC  | 1A    | 1962 | 1     | 19,22,23     | 1.58 | 3 (15%)  | 26,32,35    | 1.15 | 4 (15%)  |
| 1   | PSU  | 1A    | 1917 | 1     | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 1.89 | 4 (19%)  |
| 1   | 5MU  | 1A    | 1939 | 1,54  | 19,22,23     | 1.46 | 5 (26%)  | 27,32,35    | 2.14 | 6 (22%)  |
| 43  | 0TD  | 1l    | 92   | 43    | 8,9,10       | 4.60 | 2 (25%)  | 6,11,13     | 4.25 | 2 (33%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | 1A    | 2251 | 1,54 | 23,26,27     | 1.30 | 3 (13%)  | 32,38,41    | 2.03 | 6 (18%)  |
| 32  | 5MC  | 1a    | 967  | 32   | 19,22,23     | 1.63 | 3 (15%)  | 26,32,35    | 1.09 | 2 (7%)   |
| 32  | 5MC  | 2a    | 967  | 32   | 19,22,23     | 1.83 | 3 (15%)  | 26,32,35    | 1.10 | 2 (7%)   |
| 1   | 5MC  | 1A    | 1942 | 1,54 | 19,22,23     | 1.57 | 3 (15%)  | 26,32,35    | 1.10 | 3 (11%)  |
| 1   | PSU  | 2A    | 1917 | 1    | 18,21,22     | 1.31 | 2 (11%)  | 21,30,33    | 2.02 | 3 (14%)  |
| 1   | 5MC  | 2A    | 1942 | 1,54 | 19,22,23     | 1.66 | 3 (15%)  | 26,32,35    | 1.24 | 2 (7%)   |
| 32  | 2MG  | 2a    | 1207 | 32   | 23,26,27     | 1.22 | 2 (8%)   | 33,38,41    | 2.19 | 7 (21%)  |
| 32  | MA6  | 2a    | 1519 | 32   | 23,26,27     | 0.40 | 0        | 33,38,41    | 2.11 | 9 (27%)  |
| 32  | M2G  | 2a    | 966  | 32   | 24,27,28     | 1.28 | 3 (12%)  | 33,40,43    | 1.81 | 5 (15%)  |
| 1   | OMG  | 2A    | 2251 | 1,54 | 23,26,27     | 1.18 | 3 (13%)  | 32,38,41    | 2.06 | 7 (21%)  |

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  | 4OC  | 2a    | 1402 | 32    | -       | 3/9/29/30  | 0/2/2/2 |
| 1   | PSU  | 1A    | 2605 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32    | -       | 2/9/27/28  | 0/3/3/3 |
| 32  | 4OC  | 1a    | 1402 | 32    | -       | 0/9/29/30  | 0/2/2/2 |
| 1   | PSU  | 2A    | 2605 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1400 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1911 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | UR3  | 2a    | 1498 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 54,32 | -       | 2/7/25/26  | 0/2/2/2 |
| 1   | OMC  | 2A    | 1920 | 1     | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | MA6  | 2a    | 1518 | 32    | -       | 1/11/29/30 | 0/3/3/3 |
| 1   | OMC  | 1A    | 1920 | 1     | -       | 1/9/27/28  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1400 | 32    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | G7M  | 2a    | 527  | 32    | -       | 0/7/25/26  | 0/3/3/3 |
| 32  | UR3  | 1a    | 1498 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2503 | 1,54  | -       | 1/7/25/26  | 0/3/3/3 |
| 1   | OMU  | 1A    | 2552 | 1,54  | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | PSU  | 1a    | 516  | 54,32 | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 32  | 5MC  | 2a    | 1404 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 2MA  | 2A    | 2503 | 1,54  | -       | 0/7/25/26  | 0/3/3/3 |
| 1   | OMU  | 2A    | 2552 | 1,54  | -       | 0/9/27/28  | 0/2/2/2 |
| 32  | G7M  | 1a    | 527  | 54,32 | -       | 3/7/25/26  | 0/3/3/3 |
| 32  | MA6  | 1a    | 1518 | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | 5MU  | 1A    | 1915 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 32  | MA6  | 1a    | 1519 | 32    | -       | 2/11/29/30 | 0/3/3/3 |
| 1   | 5MU  | 2A    | 1915 | 1     | -       | 2/7/25/26  | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 32  | 5MC  | 1a    | 1404 | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43    | -       | 3/7/12/14  | -       |
| 1   | 5MC  | 1A    | 1962 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 43  | 0TD  | 1l    | 92   | 43    | -       | 3/7/12/14  | -       |
| 1   | OMG  | 1A    | 2251 | 1,54  | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | 5MC  | 1a    | 967  | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 5MC  | 2a    | 967  | 32    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1942 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | PSU  | 2A    | 1917 | 1     | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1942 | 1,54  | -       | 0/7/25/26  | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32    | -       | 0/9/27/28  | 0/3/3/3 |
| 32  | MA6  | 2a    | 1519 | 32    | -       | 3/11/29/30 | 0/3/3/3 |
| 32  | M2G  | 2a    | 966  | 32    | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | OMG  | 2A    | 2251 | 1,54  | -       | 0/9/27/28  | 0/3/3/3 |

The worst 5 of 118 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CB-SB | -12.44 | 1.69        | 1.82     |
| 43  | 2l    | 92   | 0TD  | CB-SB | -11.89 | 1.70        | 1.82     |
| 32  | 2a    | 967  | 5MC  | C5-C4 | 6.76   | 1.49        | 1.44     |
| 32  | 1a    | 1407 | 5MC  | C5-C4 | 6.70   | 1.49        | 1.44     |
| 32  | 1a    | 1400 | 5MC  | C5-C4 | 6.69   | 1.49        | 1.44     |

The worst 5 of 223 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 43  | 1l    | 92  | 0TD  | CSB-SB-CB | -9.98 | 84.43       | 102.36   |
| 43  | 2l    | 92  | 0TD  | CSB-SB-CB | -9.27 | 85.69       | 102.36   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 2A    | 2503 | 2MA  | C5-C4-N3 | -7.91 | 118.85      | 127.18   |
| 1   | 1A    | 2503 | 2MA  | C5-C4-N3 | -7.74 | 119.03      | 127.18   |
| 32  | 1a    | 1498 | UR3  | C4-N3-C2 | -7.32 | 118.69      | 124.58   |

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 1   | 1A    | 1915 | 5MU  | O4'-C1'-N1-C2 |
| 1   | 1A    | 1915 | 5MU  | O4'-C1'-N1-C6 |
| 32  | 1a    | 1207 | 2MG  | N1-C2-N2-CM2  |
| 32  | 1a    | 1207 | 2MG  | N3-C2-N2-CM2  |
| 43  | 1l    | 92   | 0TD  | CA-CB-SB-CSB  |

There are no ring outliers.

No monomer is involved in short contacts.

## 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 4.6 Ligand geometry [i](#)

Of 2458 ligands modelled in this entry, 2446 are monoatomic - leaving 12 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 | $\# Z  > 2$ |
| 56  | ARG   | 1B    | 232  | -    | 10,11,11     | 0.72 | 0           | 9,13,13     | 1.04 | 1 (11%)     |
| 57  | MPD   | 1T    | 207  | -    | 7,7,7        | 0.38 | 0           | 9,10,10     | 0.41 | 0           |
| 59  | SF4   | 1d    | 306  | 35   | 0,12,12      | -    | -           | -           |      |             |
| 59  | SF4   | 2d    | 501  | 35   | 0,12,12      | -    | -           | -           |      |             |
| 55  | A1AE1 | 1A    | 3996 | 54   | 82,82,82     | 2.31 | 18 (21%)    | 116,122,122 | 2.56 | 34 (29%)    |

| Mol | Type  | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|-------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |       |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | A1AE1 | 2A    | 3726 | 54   | 82,82,82     | 2.28 | 13 (15%) | 116,122,122 | 2.42 | 31 (26%) |
| 56  | ARG   | 1A    | 3998 | -    | 10,11,11     | 0.76 | 1 (10%)  | 9,13,13     | 1.12 | 1 (11%)  |
| 57  | MPD   | 18    | 103  | -    | 7,7,7        | 0.29 | 0        | 9,10,10     | 0.26 | 0        |
| 57  | MPD   | 2A    | 3728 | -    | 7,7,7        | 0.33 | 0        | 9,10,10     | 0.27 | 0        |
| 57  | MPD   | 1a    | 1868 | 32   | 7,7,7        | 0.41 | 0        | 9,10,10     | 0.61 | 0        |
| 57  | MPD   | 1A    | 3999 | -    | 7,7,7        | 0.44 | 0        | 9,10,10     | 0.32 | 0        |
| 57  | MPD   | 2B    | 219  | -    | 7,7,7        | 0.34 | 0        | 9,10,10     | 0.33 | 0        |

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   |
|-----|-------|-------|------|------|---------|---------------|---------|
| 56  | ARG   | 1B    | 232  | -    | -       | 4/11/11/11    | -       |
| 57  | MPD   | 1T    | 207  | -    | -       | 3/5/5/5       | -       |
| 59  | SF4   | 1d    | 306  | 35   | -       | -             | 0/6/5/5 |
| 59  | SF4   | 2d    | 501  | 35   | -       | -             | 0/6/5/5 |
| 55  | A1AE1 | 1A    | 3996 | 54   | -       | 16/89/132/132 | 0/7/7/7 |
| 55  | A1AE1 | 2A    | 3726 | 54   | -       | 12/89/132/132 | 0/7/7/7 |
| 56  | ARG   | 1A    | 3998 | -    | -       | 4/11/11/11    | -       |
| 57  | MPD   | 18    | 103  | -    | -       | 2/5/5/5       | -       |
| 57  | MPD   | 2A    | 3728 | -    | -       | 3/5/5/5       | -       |
| 57  | MPD   | 1a    | 1868 | 32   | -       | 4/5/5/5       | -       |
| 57  | MPD   | 1A    | 3999 | -    | -       | 2/5/5/5       | -       |
| 57  | MPD   | 2B    | 219  | -    | -       | 4/5/5/5       | -       |

The worst 5 of 32 bond length outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|-------|---------|--------|-------------|----------|
| 55  | 2A    | 3726 | A1AE1 | CAG-CAF | -12.58 | 1.41        | 1.53     |
| 55  | 1A    | 3996 | A1AE1 | CAG-CAF | -12.26 | 1.41        | 1.53     |
| 55  | 2A    | 3726 | A1AE1 | CAB-CAF | -6.47  | 1.41        | 1.52     |
| 55  | 1A    | 3996 | A1AE1 | CAB-CAF | -6.32  | 1.41        | 1.52     |
| 55  | 1A    | 3996 | A1AE1 | OBR-NBJ | 5.98   | 1.54        | 1.40     |

The worst 5 of 67 bond angle outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|-------|-------------|--------|-------------|----------|
| 55  | 2A    | 3726 | A1AE1 | CAB-CAF-NBJ | -13.01 | 116.62      | 126.21   |
| 55  | 1A    | 3996 | A1AE1 | CAB-CAF-NBJ | -11.24 | 117.93      | 126.21   |
| 55  | 1A    | 3996 | A1AE1 | CCC-NCH-CCI | 9.94   | 130.24      | 119.88   |
| 55  | 1A    | 3996 | A1AE1 | OBB-CBT-NBV | 7.72   | 123.59      | 111.01   |
| 55  | 2A    | 3726 | A1AE1 | OBB-CBT-NBV | 7.05   | 122.49      | 111.01   |

There are no chirality outliers.

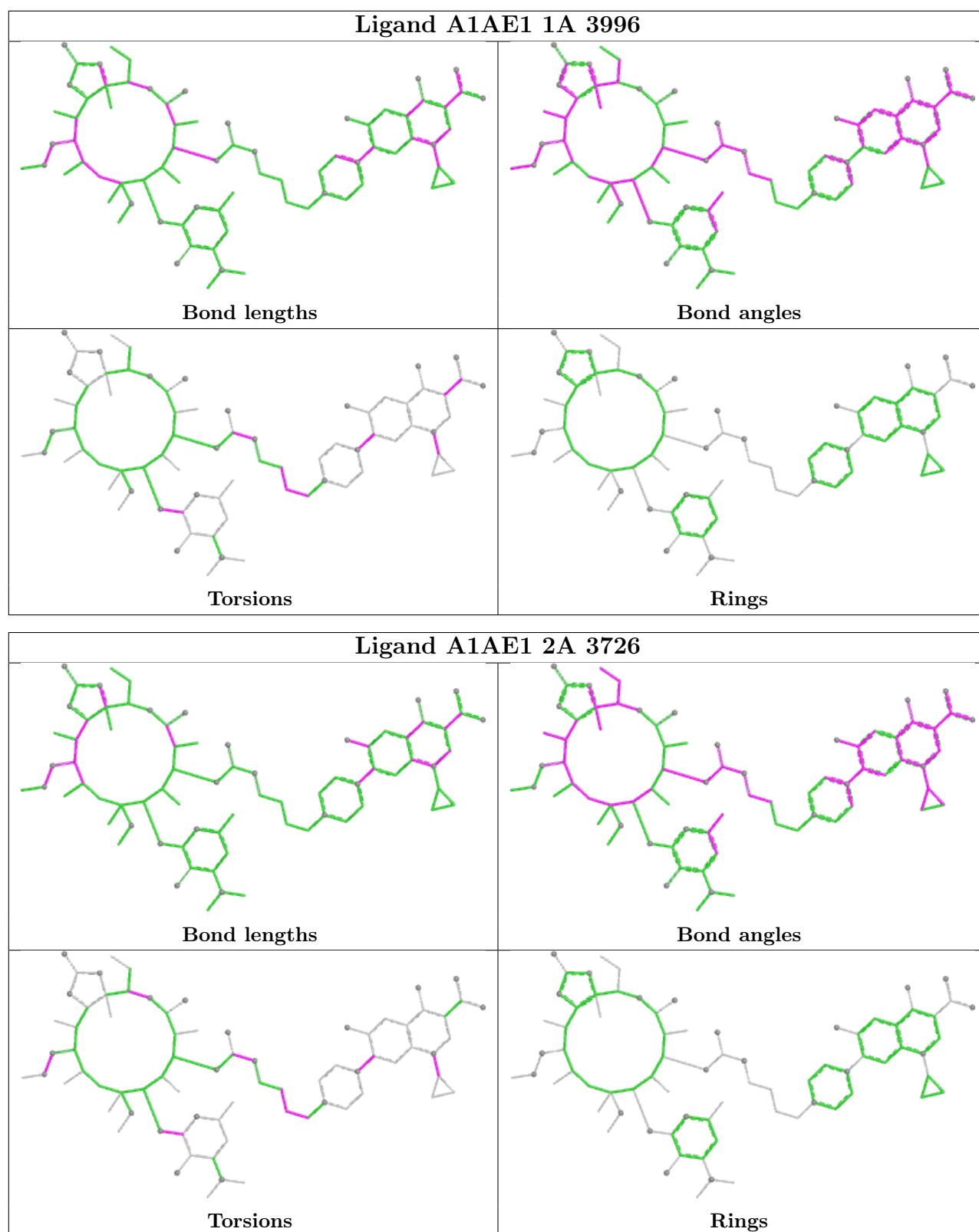
5 of 54 torsion outliers are listed below:

| Mol | Chain | Res  | Type  | Atoms           |
|-----|-------|------|-------|-----------------|
| 55  | 1A    | 3996 | A1AE1 | CCE-CCF-CCN-OCO |
| 55  | 1A    | 3996 | A1AE1 | CCE-CCF-CCN-OCF |
| 55  | 1A    | 3996 | A1AE1 | CCJ-CCI-NCH-CCG |
| 55  | 1A    | 3996 | A1AE1 | CCK-CCI-NCH-CCC |
| 55  | 1A    | 3996 | A1AE1 | CCK-CCI-NCH-CCG |

There are no ring outliers.

No monomer is involved in short contacts.

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



#### 4.7 Other polymers ⓘ

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 5 Fit of model and data ⓘ

### 5.1 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    | 2861/2915 (98%) | -0.49  | 142 (4%) 34 40 | 24, 41, 91, 102       | 0     |
| 1   | 2A    | 2856/2915 (97%) | -0.06  | 155 (5%) 31 37 | 35, 56, 93, 102       | 0     |
| 2   | 1B    | 120/121 (99%)   | -0.26  | 3 (2%) 58 64   | 35, 54, 68, 83        | 0     |
| 2   | 2B    | 120/121 (99%)   | 0.50   | 1 (0%) 82 86   | 59, 75, 82, 87        | 0     |
| 3   | 1D    | 275/276 (99%)   | -0.02  | 4 (1%) 72 77   | 25, 40, 54, 78        | 0     |
| 3   | 2D    | 275/276 (99%)   | 0.29   | 7 (2%) 58 64   | 35, 50, 61, 77        | 0     |
| 4   | 1E    | 204/206 (99%)   | 0.13   | 4 (1%) 65 70   | 24, 44, 64, 76        | 0     |
| 4   | 2E    | 204/206 (99%)   | 0.53   | 8 (3%) 43 49   | 36, 58, 72, 82        | 0     |
| 5   | 1F    | 203/210 (96%)   | 0.19   | 4 (1%) 65 70   | 24, 46, 71, 82        | 0     |
| 5   | 2F    | 203/210 (96%)   | 0.69   | 5 (2%) 58 64   | 35, 65, 78, 84        | 0     |
| 6   | 1G    | 181/182 (99%)   | 0.94   | 18 (9%) 13 14  | 52, 66, 79, 87        | 0     |
| 6   | 2G    | 181/182 (99%)   | 1.94   | 79 (43%) 0 0   | 70, 80, 86, 91        | 0     |
| 7   | 1H    | 174/180 (96%)   | 0.53   | 5 (2%) 53 60   | 44, 57, 69, 76        | 0     |
| 7   | 2H    | 173/180 (96%)   | 1.78   | 59 (34%) 1 0   | 67, 78, 85, 86        | 0     |
| 8   | 1I    | 147/148 (99%)   | 1.17   | 14 (9%) 14 16  | 44, 71, 80, 82        | 0     |
| 8   | 2I    | 146/148 (98%)   | 1.42   | 30 (20%) 2 2   | 57, 74, 82, 84        | 0     |
| 9   | 1N    | 140/140 (100%)  | 0.20   | 2 (1%) 73 78   | 31, 44, 64, 77        | 0     |
| 9   | 2N    | 140/140 (100%)  | 0.69   | 5 (3%) 46 52   | 49, 63, 75, 81        | 0     |
| 10  | 1O    | 122/122 (100%)  | 0.10   | 2 (1%) 70 76   | 32, 43, 61, 67        | 0     |
| 10  | 2O    | 122/122 (100%)  | 0.53   | 2 (1%) 70 76   | 46, 56, 68, 74        | 0     |
| 11  | 1P    | 149/150 (99%)   | 0.25   | 1 (0%) 84 87   | 24, 49, 68, 79        | 0     |
| 11  | 2P    | 149/150 (99%)   | 0.65   | 7 (4%) 36 42   | 37, 66, 79, 85        | 0     |
| 12  | 1Q    | 141/141 (100%)  | 0.21   | 0 100 100      | 33, 44, 57, 67        | 0     |
| 12  | 2Q    | 141/141 (100%)  | 0.93   | 9 (6%) 25 28   | 45, 63, 71, 79        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | 0.03   | 0 100 100      | 29, 40, 55, 63        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.46   | 1 (0%) 82 86   | 42, 53, 62, 71        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.62   | 5 (4%) 38 44   | 42, 54, 66, 73        | 0     |
| 14  | 2S    | 110/112 (98%)  | 1.47   | 24 (21%) 2 2   | 62, 71, 77, 79        | 0     |
| 15  | 1T    | 131/146 (89%)  | 0.39   | 6 (4%) 37 43   | 37, 48, 69, 85        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.72   | 6 (4%) 37 43   | 50, 60, 76, 82        | 0     |
| 16  | 1U    | 116/118 (98%)  | -0.05  | 1 (0%) 81 84   | 28, 37, 53, 69        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.72   | 3 (2%) 57 63   | 41, 58, 71, 75        | 0     |
| 17  | 1V    | 101/101 (100%) | 0.16   | 2 (1%) 65 70   | 28, 49, 64, 73        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.92   | 6 (5%) 28 32   | 42, 68, 75, 78        | 0     |
| 18  | 1W    | 112/113 (99%)  | -0.02  | 2 (1%) 67 72   | 31, 38, 57, 84        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.44   | 3 (2%) 56 63   | 39, 51, 67, 87        | 0     |
| 19  | 1X    | 95/96 (98%)    | 0.28   | 3 (3%) 50 57   | 31, 41, 65, 73        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.92   | 10 (10%) 11 13 | 47, 59, 75, 82        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.59   | 3 (2%) 55 61   | 41, 53, 69, 77        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 1.43   | 21 (19%) 3 3   | 60, 70, 77, 85        | 0     |
| 21  | 1Z    | 203/206 (98%)  | 0.83   | 13 (6%) 25 28  | 46, 61, 76, 84        | 0     |
| 21  | 2Z    | 201/206 (97%)  | 1.51   | 47 (23%) 2 1   | 64, 75, 82, 86        | 0     |
| 22  | 10    | 83/85 (97%)    | 0.61   | 8 (9%) 13 16   | 34, 42, 76, 84        | 0     |
| 22  | 20    | 83/85 (97%)    | 1.26   | 11 (13%) 7 8   | 50, 62, 76, 88        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.29   | 2 (2%) 63 68   | 31, 46, 67, 74        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.66   | 3 (3%) 51 58   | 41, 57, 74, 79        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.50   | 2 (2%) 53 60   | 38, 51, 63, 82        | 0     |
| 24  | 22    | 70/72 (97%)    | 1.02   | 4 (5%) 29 34   | 59, 69, 75, 79        | 0     |
| 25  | 13    | 59/60 (98%)    | 0.14   | 1 (1%) 69 74   | 31, 43, 67, 75        | 0     |
| 25  | 23    | 59/60 (98%)    | 0.85   | 4 (6%) 23 26   | 49, 60, 75, 79        | 0     |
| 26  | 14    | 69/71 (97%)    | 1.60   | 18 (26%) 1 1   | 63, 79, 88, 90        | 0     |
| 26  | 24    | 69/71 (97%)    | 2.40   | 47 (68%) 0 0   | 78, 85, 91, 92        | 0     |
| 27  | 15    | 59/60 (98%)    | 0.02   | 1 (1%) 69 74   | 26, 40, 61, 71        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.32   | 0 100 100      | 37, 52, 68, 77        | 0     |
| 28  | 16    | 53/54 (98%)    | 0.16   | 0 100 100      | 37, 46, 60, 66        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.71   | 2 (3%) 44 50   | 52, 61, 68, 73        | 0     |
| 29  | 17    | 48/49 (97%)     | 0.01   | 5 (10%) 11 13  | 24, 31, 54, 65        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.39   | 6 (12%) 8 9    | 36, 42, 68, 72        | 0     |
| 30  | 18    | 64/65 (98%)     | -0.17  | 0 100 100      | 31, 38, 44, 57        | 0     |
| 30  | 28    | 64/65 (98%)     | 0.57   | 2 (3%) 51 58   | 46, 54, 62, 67        | 0     |
| 31  | 19    | 37/37 (100%)    | 0.20   | 0 100 100      | 38, 46, 58, 60        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.30   | 8 (21%) 2 2    | 56, 65, 72, 75        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.29   | 58 (3%) 43 49  | 40, 68, 90, 102       | 0     |
| 32  | 2a    | 1492/1521 (98%) | 0.47   | 66 (4%) 39 45  | 47, 74, 91, 101       | 0     |
| 33  | 1b    | 231/256 (90%)   | 1.68   | 64 (27%) 1 1   | 65, 77, 84, 89        | 0     |
| 33  | 2b    | 231/256 (90%)   | 2.02   | 106 (45%) 0 0  | 71, 81, 86, 91        | 0     |
| 34  | 1c    | 206/239 (86%)   | 1.15   | 27 (13%) 7 8   | 60, 72, 82, 88        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.83   | 79 (38%) 1 0   | 71, 81, 86, 89        | 0     |
| 35  | 1d    | 208/209 (99%)   | 1.27   | 35 (16%) 4 4   | 58, 71, 78, 85        | 0     |
| 35  | 2d    | 208/209 (99%)   | 1.41   | 38 (18%) 3 3   | 62, 71, 78, 82        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.95   | 8 (5%) 31 37   | 53, 65, 74, 84        | 0     |
| 36  | 2e    | 148/162 (91%)   | 1.14   | 17 (11%) 9 11  | 55, 70, 78, 87        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.92   | 3 (3%) 52 59   | 57, 67, 74, 79        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.96   | 5 (5%) 34 40   | 58, 67, 76, 79        | 0     |
| 38  | 1g    | 155/156 (99%)   | 1.01   | 12 (7%) 19 22  | 63, 71, 79, 84        | 0     |
| 38  | 2g    | 155/156 (99%)   | 1.56   | 39 (25%) 1 1   | 70, 78, 83, 85        | 0     |
| 39  | 1h    | 137/138 (99%)   | 1.11   | 10 (7%) 21 24  | 55, 68, 74, 80        | 0     |
| 39  | 2h    | 137/138 (99%)   | 1.13   | 12 (8%) 15 18  | 60, 70, 77, 80        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.86   | 49 (38%) 1 0   | 61, 77, 83, 85        | 0     |
| 40  | 2i    | 126/128 (98%)   | 2.46   | 77 (61%) 0 0   | 71, 82, 86, 89        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.69   | 32 (32%) 1 0   | 60, 77, 84, 87        | 0     |
| 41  | 2j    | 96/105 (91%)    | 2.56   | 65 (67%) 0 0   | 73, 82, 87, 91        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.93   | 8 (7%) 22 25   | 46, 65, 75, 80        | 0     |
| 42  | 2k    | 114/129 (88%)   | 1.14   | 14 (12%) 8 10  | 57, 70, 79, 82        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.88   | 13 (10%) 11 13 | 49, 60, 70, 74        | 0     |
| 43  | 2l    | 121/132 (91%)   | 1.05   | 13 (10%) 11 13 | 56, 66, 73, 77        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 116/126 (92%)     | 1.31   | 16 (13%) 6 7    | 62, 75, 80, 84        | 0     |
| 44  | 2m    | 114/126 (90%)     | 1.78   | 34 (29%) 1 1    | 73, 81, 85, 88        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.20   | 8 (13%) 7 8     | 63, 70, 78, 81        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.51   | 37 (61%) 0 0    | 72, 79, 84, 90        | 0     |
| 46  | 1o    | 88/89 (98%)       | 1.10   | 7 (7%) 18 21    | 49, 67, 76, 79        | 0     |
| 46  | 2o    | 88/89 (98%)       | 1.16   | 9 (10%) 12 13   | 58, 70, 78, 82        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.96   | 40 (48%) 0 0    | 60, 71, 80, 84        | 0     |
| 47  | 2p    | 82/88 (93%)       | 1.46   | 17 (20%) 2 2    | 63, 69, 78, 85        | 0     |
| 48  | 1q    | 99/105 (94%)      | 1.32   | 14 (14%) 6 7    | 56, 69, 77, 79        | 0     |
| 48  | 2q    | 99/105 (94%)      | 1.10   | 8 (8%) 18 20    | 57, 68, 76, 79        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.97   | 6 (8%) 15 18    | 58, 65, 77, 83        | 0     |
| 49  | 2r    | 68/88 (77%)       | 1.00   | 4 (5%) 28 32    | 63, 70, 79, 83        | 0     |
| 50  | 1s    | 83/93 (89%)       | 1.59   | 22 (26%) 1 1    | 65, 76, 81, 85        | 0     |
| 50  | 2s    | 83/93 (89%)       | 2.21   | 48 (57%) 0 0    | 77, 84, 88, 91        | 0     |
| 51  | 1t    | 96/106 (90%)      | 1.57   | 23 (23%) 2 1    | 61, 71, 80, 82        | 0     |
| 51  | 2t    | 98/106 (92%)      | 1.22   | 14 (14%) 6 7    | 60, 69, 80, 82        | 0     |
| 52  | 1u    | 23/27 (85%)       | 1.58   | 8 (34%) 1 0     | 66, 71, 75, 77        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.82   | 17 (73%) 0 0    | 76, 78, 82, 82        | 0     |
| 53  | 1y    | 97/113 (85%)      | 1.12   | 12 (12%) 8 9    | 54, 64, 74, 81        | 0     |
| 53  | 2y    | 96/113 (84%)      | 1.88   | 34 (35%) 1 0    | 67, 76, 83, 84        | 0     |
| All | All   | 20778/21468 (96%) | 0.54   | 2074 (9%) 12 14 | 24, 63, 85, 102       | 0     |

The worst 5 of 2074 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | 2n    | 2    | ALA  | 10.5 |
| 22  | 10    | 7    | LEU  | 8.6  |
| 1   | 1A    | 1087 | G    | 8.4  |
| 22  | 20    | 7    | LEU  | 7.6  |
| 45  | 1n    | 2    | ALA  | 7.5  |

## 5.2 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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.84 | 0.12 | 75,83,86,99                | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.85 | 0.12 | 79,85,90,93                | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.86 | 0.13 | 72,80,85,91                | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.88 | 0.15 | 60,72,82,86                | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.89 | 0.13 | 62,69,72,79                | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.90 | 0.10 | 72,76,89,91                | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.90 | 0.10 | 68,73,78,83                | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.91 | 0.14 | 66,72,81,88                | 0     |
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.92 | 0.10 | 66,72,79,82                | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.92 | 0.10 | 71,75,79,82                | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.93 | 0.09 | 62,67,74,76                | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.94 | 0.12 | 53,61,68,72                | 0     |
| 32  | G7M  | 2a    | 527  | 24/25 | 0.94 | 0.10 | 62,68,73,75                | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.94 | 0.09 | 57,67,70,71                | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.94 | 0.12 | 60,67,74,78                | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.94 | 0.09 | 65,72,75,76                | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.94 | 0.10 | 62,68,73,74                | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.95 | 0.13 | 63,69,72,75                | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.95 | 0.09 | 55,60,65,67                | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.95 | 0.10 | 55,63,68,70                | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.95 | 0.10 | 58,63,66,68                | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.95 | 0.10 | 55,63,69,74                | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.96 | 0.10 | 46,57,62,64                | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.96 | 0.10 | 52,57,62,63                | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.96 | 0.10 | 50,55,57,68                | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.96 | 0.10 | 43,49,53,55                | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.96 | 0.09 | 59,65,71,75                | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.96 | 0.10 | 47,56,59,64                | 0     |
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.96 | 0.08 | 47,53,57,59                | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.96 | 0.10 | 48,53,56,59                | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.96 | 0.11 | 54,62,67,70                | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.96 | 0.10 | 43,51,56,57                | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.97 | 0.09 | 42,48,54,64                | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.97 | 0.10 | 40,44,47,49                | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.08 | 33,39,43,47                | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.97 | 0.07 | 36,39,46,48                | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.07 | 36,42,44,50                | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.97 | 0.10 | 43,51,54,58                | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.07 | 34,39,42,47                | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.97 | 0.10 | 55,61,65,66                | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.97 | 0.09 | 52,60,63,64                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.98 | 0.07 | 29,34,37,39                 | 0     |
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.98 | 0.07 | 26,31,34,42                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.07 | 26,33,35,36                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.98 | 0.07 | 33,40,44,47                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.07 | 25,32,39,40                 | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.06 | 22,28,29,32                 | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.98 | 0.07 | 37,43,46,47                 | 0     |

### 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3670 | 1/1   | 0.45 | 0.25 | 84,84,84,84                 | 0     |
| 54  | MG   | 2a    | 3119 | 1/1   | 0.47 | 0.23 | 93,93,93,93                 | 0     |
| 54  | MG   | 1A    | 3625 | 1/1   | 0.48 | 0.26 | 84,84,84,84                 | 0     |
| 54  | MG   | 2a    | 3155 | 1/1   | 0.58 | 0.28 | 95,95,95,95                 | 0     |
| 54  | MG   | 1a    | 1675 | 1/1   | 0.59 | 0.40 | 84,84,84,84                 | 0     |
| 54  | MG   | 1A    | 3946 | 1/1   | 0.59 | 0.21 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3464 | 1/1   | 0.60 | 0.30 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3658 | 1/1   | 0.62 | 0.28 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3452 | 1/1   | 0.62 | 0.19 | 82,82,82,82                 | 0     |
| 54  | MG   | 1A    | 3411 | 1/1   | 0.63 | 0.17 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3577 | 1/1   | 0.63 | 0.15 | 79,79,79,79                 | 0     |
| 54  | MG   | 2A    | 3454 | 1/1   | 0.64 | 0.24 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3763 | 1/1   | 0.65 | 0.36 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3717 | 1/1   | 0.65 | 0.15 | 88,88,88,88                 | 0     |
| 54  | MG   | 1A    | 3680 | 1/1   | 0.66 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3854 | 1/1   | 0.66 | 0.27 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1830 | 1/1   | 0.66 | 0.36 | 85,85,85,85                 | 0     |
| 54  | MG   | 2A    | 3656 | 1/1   | 0.67 | 0.29 | 83,83,83,83                 | 0     |
| 54  | MG   | 1A    | 3925 | 1/1   | 0.67 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1740 | 1/1   | 0.68 | 0.19 | 93,93,93,93                 | 0     |
| 54  | MG   | 2A    | 3421 | 1/1   | 0.68 | 0.23 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1774 | 1/1   | 0.68 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | 2A    | 3704 | 1/1   | 0.69 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3508 | 1/1   | 0.69 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 2B    | 215  | 1/1   | 0.69 | 0.20 | 84,84,84,84                 | 0     |
| 54  | MG   | 1A    | 3491 | 1/1   | 0.69 | 0.22 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3581 | 1/1   | 0.69 | 0.21 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3675 | 1/1   | 0.70 | 0.18 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3566 | 1/1   | 0.70 | 0.28 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3986 | 1/1   | 0.70 | 0.28 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3628 | 1/1   | 0.70 | 0.22 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3008 | 1/1   | 0.70 | 0.33 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3624 | 1/1   | 0.70 | 0.17 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3403 | 1/1   | 0.70 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3964 | 1/1   | 0.71 | 0.28 | 78,78,78,78                 | 0     |
| 54  | MG   | 1a    | 1825 | 1/1   | 0.71 | 0.23 | 69,69,69,69                 | 0     |
| 54  | MG   | 1B    | 207  | 1/1   | 0.71 | 0.30 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3295 | 1/1   | 0.71 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3518 | 1/1   | 0.72 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1781 | 1/1   | 0.72 | 0.31 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3775 | 1/1   | 0.72 | 0.21 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1751 | 1/1   | 0.72 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | 2A    | 3458 | 1/1   | 0.72 | 0.30 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3256 | 1/1   | 0.72 | 0.32 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3146 | 1/1   | 0.73 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3855 | 1/1   | 0.73 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | 1b    | 301  | 1/1   | 0.73 | 0.23 | 83,83,83,83                 | 0     |
| 54  | MG   | 2A    | 3681 | 1/1   | 0.73 | 0.33 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3416 | 1/1   | 0.73 | 0.37 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1676 | 1/1   | 0.74 | 0.16 | 83,83,83,83                 | 0     |
| 54  | MG   | 1a    | 1788 | 1/1   | 0.74 | 0.19 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3707 | 1/1   | 0.74 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1812 | 1/1   | 0.74 | 0.23 | 82,82,82,82                 | 0     |
| 54  | MG   | 2A    | 3497 | 1/1   | 0.74 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | 2I    | 201  | 1/1   | 0.74 | 0.22 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3659 | 1/1   | 0.74 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3666 | 1/1   | 0.74 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | 1B    | 228  | 1/1   | 0.74 | 0.24 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3348 | 1/1   | 0.75 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3380 | 1/1   | 0.75 | 0.26 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3661 | 1/1   | 0.75 | 0.20 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1623 | 1/1   | 0.75 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3958 | 1/1   | 0.75 | 0.23 | 85,85,85,85                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3607 | 1/1   | 0.75 | 0.20 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3306 | 1/1   | 0.75 | 0.40 | 81,81,81,81                 | 0     |
| 54  | MG   | 1a    | 1854 | 1/1   | 0.75 | 0.19 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3370 | 1/1   | 0.75 | 0.22 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3024 | 1/1   | 0.75 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3076 | 1/1   | 0.75 | 0.32 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3660 | 1/1   | 0.75 | 0.24 | 73,73,73,73                 | 0     |
| 54  | MG   | 2a    | 3022 | 1/1   | 0.75 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | 1T    | 202  | 1/1   | 0.75 | 0.28 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1785 | 1/1   | 0.75 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | 2h    | 201  | 1/1   | 0.75 | 0.27 | 84,84,84,84                 | 0     |
| 54  | MG   | 1a    | 1708 | 1/1   | 0.76 | 0.28 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1842 | 1/1   | 0.76 | 0.30 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3421 | 1/1   | 0.76 | 0.18 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3754 | 1/1   | 0.76 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | 1h    | 201  | 1/1   | 0.76 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3283 | 1/1   | 0.76 | 0.24 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3937 | 1/1   | 0.76 | 0.33 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3079 | 1/1   | 0.76 | 0.30 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3499 | 1/1   | 0.76 | 0.24 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3533 | 1/1   | 0.76 | 0.26 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1640 | 1/1   | 0.76 | 0.22 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3279 | 1/1   | 0.76 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3080 | 1/1   | 0.76 | 0.53 | 85,85,85,85                 | 0     |
| 54  | MG   | 1A    | 3815 | 1/1   | 0.76 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3657 | 1/1   | 0.76 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3169 | 1/1   | 0.76 | 0.35 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3833 | 1/1   | 0.76 | 0.14 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3152 | 1/1   | 0.77 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3297 | 1/1   | 0.77 | 0.39 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3047 | 1/1   | 0.77 | 0.46 | 76,76,76,76                 | 0     |
| 54  | MG   | 2a    | 3069 | 1/1   | 0.77 | 0.21 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3696 | 1/1   | 0.77 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3269 | 1/1   | 0.77 | 0.26 | 78,78,78,78                 | 0     |
| 54  | MG   | 1a    | 1759 | 1/1   | 0.77 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | 1A    | 3602 | 1/1   | 0.77 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3903 | 1/1   | 0.77 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1811 | 1/1   | 0.78 | 0.19 | 79,79,79,79                 | 0     |
| 54  | MG   | 2A    | 3702 | 1/1   | 0.78 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3668 | 1/1   | 0.78 | 0.26 | 79,79,79,79                 | 0     |
| 54  | MG   | 1a    | 1821 | 1/1   | 0.78 | 0.19 | 79,79,79,79                 | 0     |
| 54  | MG   | 2A    | 3235 | 1/1   | 0.78 | 0.33 | 77,77,77,77                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3245 | 1/1   | 0.78 | 0.41 | 73,73,73,73                 | 0     |
| 54  | MG   | 1B    | 231  | 1/1   | 0.78 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3293 | 1/1   | 0.78 | 0.39 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3016 | 1/1   | 0.78 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1834 | 1/1   | 0.78 | 0.21 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3305 | 1/1   | 0.78 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3965 | 1/1   | 0.78 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1636 | 1/1   | 0.78 | 0.30 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3980 | 1/1   | 0.78 | 0.24 | 80,80,80,80                 | 0     |
| 54  | MG   | 2a    | 3145 | 1/1   | 0.78 | 0.33 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3744 | 1/1   | 0.78 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3805 | 1/1   | 0.78 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3453 | 1/1   | 0.78 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 1B    | 225  | 1/1   | 0.79 | 0.15 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1798 | 1/1   | 0.79 | 0.21 | 81,81,81,81                 | 0     |
| 54  | MG   | 2B    | 207  | 1/1   | 0.79 | 0.29 | 79,79,79,79                 | 0     |
| 54  | MG   | 2B    | 211  | 1/1   | 0.79 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 1B    | 227  | 1/1   | 0.79 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3349 | 1/1   | 0.79 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3366 | 1/1   | 0.79 | 0.34 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3311 | 1/1   | 0.79 | 0.31 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3826 | 1/1   | 0.79 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3034 | 1/1   | 0.79 | 0.14 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3584 | 1/1   | 0.79 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3981 | 1/1   | 0.79 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3450 | 1/1   | 0.79 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3090 | 1/1   | 0.79 | 0.31 | 75,75,75,75                 | 0     |
| 54  | MG   | 2a    | 3098 | 1/1   | 0.79 | 0.31 | 82,82,82,82                 | 0     |
| 54  | MG   | 1A    | 3185 | 1/1   | 0.79 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3266 | 1/1   | 0.79 | 0.32 | 77,77,77,77                 | 0     |
| 54  | MG   | 1a    | 1663 | 1/1   | 0.79 | 0.29 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3470 | 1/1   | 0.79 | 0.24 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3475 | 1/1   | 0.79 | 0.21 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3509 | 1/1   | 0.80 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3526 | 1/1   | 0.80 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3530 | 1/1   | 0.80 | 0.16 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3569 | 1/1   | 0.80 | 0.21 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3052 | 1/1   | 0.80 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | 2a    | 3058 | 1/1   | 0.80 | 0.43 | 83,83,83,83                 | 0     |
| 54  | MG   | 2A    | 3703 | 1/1   | 0.80 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1782 | 1/1   | 0.80 | 0.20 | 86,86,86,86                 | 0     |
| 54  | MG   | 1d    | 305  | 1/1   | 0.80 | 0.11 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3536 | 1/1   | 0.80 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3412 | 1/1   | 0.80 | 0.23 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3302 | 1/1   | 0.80 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3320 | 1/1   | 0.80 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3431 | 1/1   | 0.80 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3176 | 1/1   | 0.80 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3757 | 1/1   | 0.80 | 0.21 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3123 | 1/1   | 0.81 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | 2B    | 217  | 1/1   | 0.81 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | 1A    | 3027 | 1/1   | 0.81 | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1817 | 1/1   | 0.81 | 0.19 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3632 | 1/1   | 0.81 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3018 | 1/1   | 0.81 | 0.38 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3616 | 1/1   | 0.81 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3251 | 1/1   | 0.81 | 0.41 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3562 | 1/1   | 0.81 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3886 | 1/1   | 0.81 | 0.12 | 31,31,31,31                 | 0     |
| 54  | MG   | 2a    | 3053 | 1/1   | 0.81 | 0.26 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3116 | 1/1   | 0.81 | 0.30 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3758 | 1/1   | 0.81 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 1B    | 230  | 1/1   | 0.81 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3480 | 1/1   | 0.81 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3486 | 1/1   | 0.81 | 0.20 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3631 | 1/1   | 0.81 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3579 | 1/1   | 0.81 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3790 | 1/1   | 0.81 | 0.24 | 83,83,83,83                 | 0     |
| 54  | MG   | 1A    | 3426 | 1/1   | 0.81 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3586 | 1/1   | 0.81 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3267 | 1/1   | 0.81 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | 2A    | 3145 | 1/1   | 0.82 | 0.37 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3302 | 1/1   | 0.82 | 0.29 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3201 | 1/1   | 0.82 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3713 | 1/1   | 0.82 | 0.19 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1650 | 1/1   | 0.82 | 0.35 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3477 | 1/1   | 0.82 | 0.12 | 81,81,81,81                 | 0     |
| 54  | MG   | 1a    | 1801 | 1/1   | 0.82 | 0.28 | 71,71,71,71                 | 0     |
| 54  | MG   | 2B    | 213  | 1/1   | 0.82 | 0.25 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3676 | 1/1   | 0.82 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3445 | 1/1   | 0.82 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3498 | 1/1   | 0.82 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3250 | 1/1   | 0.82 | 0.44 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1687 | 1/1   | 0.82 | 0.23 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1692 | 1/1   | 0.82 | 0.42 | 75,75,75,75                 | 0     |
| 54  | MG   | 2a    | 3021 | 1/1   | 0.82 | 0.33 | 79,79,79,79                 | 0     |
| 54  | MG   | 1a    | 1698 | 1/1   | 0.82 | 0.37 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3557 | 1/1   | 0.82 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3802 | 1/1   | 0.82 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3346 | 1/1   | 0.82 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3743 | 1/1   | 0.82 | 0.13 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 3056 | 1/1   | 0.82 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1853 | 1/1   | 0.82 | 0.24 | 77,77,77,77                 | 0     |
| 54  | MG   | 1a    | 1745 | 1/1   | 0.82 | 0.44 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3600 | 1/1   | 0.82 | 0.25 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3082 | 1/1   | 0.82 | 0.32 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3084 | 1/1   | 0.82 | 0.30 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3822 | 1/1   | 0.82 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | 1E    | 305  | 1/1   | 0.82 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | 2a    | 3100 | 1/1   | 0.82 | 0.25 | 87,87,87,87                 | 0     |
| 54  | MG   | 2A    | 3417 | 1/1   | 0.82 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1780 | 1/1   | 0.82 | 0.24 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3046 | 1/1   | 0.82 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3166 | 1/1   | 0.82 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3198 | 1/1   | 0.82 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3201 | 1/1   | 0.82 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3850 | 1/1   | 0.82 | 0.11 | 33,33,33,33                 | 0     |
| 56  | ARG  | 1A    | 3998 | 12/12 | 0.82 | 0.20 | 56,69,76,77                 | 0     |
| 57  | MPD  | 1T    | 207  | 8/8   | 0.82 | 0.25 | 67,74,79,79                 | 0     |
| 57  | MPD  | 2B    | 219  | 8/8   | 0.82 | 0.29 | 59,68,74,77                 | 0     |
| 54  | MG   | 1a    | 1662 | 1/1   | 0.83 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3503 | 1/1   | 0.83 | 0.24 | 76,76,76,76                 | 0     |
| 54  | MG   | 1g    | 202  | 1/1   | 0.83 | 0.27 | 80,80,80,80                 | 0     |
| 54  | MG   | 2D    | 308  | 1/1   | 0.83 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3569 | 1/1   | 0.83 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3608 | 1/1   | 0.83 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3955 | 1/1   | 0.83 | 0.38 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3381 | 1/1   | 0.83 | 0.13 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3407 | 1/1   | 0.83 | 0.30 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1790 | 1/1   | 0.83 | 0.13 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3029 | 1/1   | 0.83 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3616 | 1/1   | 0.83 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3191 | 1/1   | 0.83 | 0.27 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3088 | 1/1   | 0.83 | 0.25 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3639 | 1/1   | 0.83 | 0.19 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3285 | 1/1   | 0.83 | 0.23 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3683 | 1/1   | 0.83 | 0.27 | 42,42,42,42                 | 0     |
| 54  | MG   | 2a    | 3062 | 1/1   | 0.83 | 0.34 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1702 | 1/1   | 0.83 | 0.45 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3184 | 1/1   | 0.83 | 0.40 | 81,81,81,81                 | 0     |
| 54  | MG   | 1a    | 1707 | 1/1   | 0.83 | 0.23 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3662 | 1/1   | 0.83 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3455 | 1/1   | 0.83 | 0.16 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3457 | 1/1   | 0.83 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3462 | 1/1   | 0.83 | 0.16 | 73,73,73,73                 | 0     |
| 54  | MG   | 2a    | 3108 | 1/1   | 0.83 | 0.19 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3683 | 1/1   | 0.83 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 2a    | 3138 | 1/1   | 0.83 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3696 | 1/1   | 0.83 | 0.09 | 84,84,84,84                 | 0     |
| 54  | MG   | 1a    | 1728 | 1/1   | 0.83 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3160 | 1/1   | 0.83 | 0.27 | 82,82,82,82                 | 0     |
| 54  | MG   | 1T    | 205  | 1/1   | 0.83 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | 1Z    | 301  | 1/1   | 0.83 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3721 | 1/1   | 0.83 | 0.26 | 57,57,57,57                 | 0     |
| 54  | MG   | 2f    | 202  | 1/1   | 0.83 | 0.20 | 81,81,81,81                 | 0     |
| 54  | MG   | 1a    | 1846 | 1/1   | 0.83 | 0.30 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3409 | 1/1   | 0.83 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | 1B    | 203  | 1/1   | 0.83 | 0.28 | 72,72,72,72                 | 0     |
| 57  | MPD  | 1a    | 1868 | 8/8   | 0.83 | 0.18 | 53,67,74,76                 | 0     |
| 54  | MG   | 1A    | 3437 | 1/1   | 0.83 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | 1r    | 101  | 1/1   | 0.84 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3475 | 1/1   | 0.84 | 0.10 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3437 | 1/1   | 0.84 | 0.24 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3438 | 1/1   | 0.84 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3446 | 1/1   | 0.84 | 0.17 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3361 | 1/1   | 0.84 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3632 | 1/1   | 0.84 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3651 | 1/1   | 0.84 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3770 | 1/1   | 0.84 | 0.18 | 70,70,70,70                 | 0     |
| 54  | MG   | 2B    | 209  | 1/1   | 0.84 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3109 | 1/1   | 0.84 | 0.26 | 67,67,67,67                 | 0     |
| 54  | MG   | 2B    | 212  | 1/1   | 0.84 | 0.30 | 79,79,79,79                 | 0     |
| 54  | MG   | 2A    | 3115 | 1/1   | 0.84 | 0.30 | 71,71,71,71                 | 0     |
| 54  | MG   | 2B    | 214  | 1/1   | 0.84 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1653 | 1/1   | 0.84 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3498 | 1/1   | 0.84 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3663 | 1/1   | 0.84 | 0.10 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3166 | 1/1   | 0.84 | 0.28 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1807 | 1/1   | 0.84 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | 2A    | 3483 | 1/1   | 0.84 | 0.21 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1808 | 1/1   | 0.84 | 0.20 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1809 | 1/1   | 0.84 | 0.25 | 82,82,82,82                 | 0     |
| 54  | MG   | 1A    | 3436 | 1/1   | 0.84 | 0.13 | 81,81,81,81                 | 0     |
| 54  | MG   | 1A    | 3515 | 1/1   | 0.84 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3305 | 1/1   | 0.84 | 0.30 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3046 | 1/1   | 0.84 | 0.23 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3504 | 1/1   | 0.84 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3050 | 1/1   | 0.84 | 0.37 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3508 | 1/1   | 0.84 | 0.23 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3817 | 1/1   | 0.84 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1824 | 1/1   | 0.84 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3280 | 1/1   | 0.84 | 0.25 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3552 | 1/1   | 0.84 | 0.23 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3281 | 1/1   | 0.84 | 0.15 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3414 | 1/1   | 0.84 | 0.15 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3102 | 1/1   | 0.84 | 0.16 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3692 | 1/1   | 0.84 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3088 | 1/1   | 0.84 | 0.40 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3586 | 1/1   | 0.84 | 0.17 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1841 | 1/1   | 0.84 | 0.15 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3558 | 1/1   | 0.84 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 1B    | 229  | 1/1   | 0.84 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3636 | 1/1   | 0.84 | 0.20 | 84,84,84,84                 | 0     |
| 54  | MG   | 2A    | 3353 | 1/1   | 0.84 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3641 | 1/1   | 0.84 | 0.27 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3652 | 1/1   | 0.84 | 0.46 | 83,83,83,83                 | 0     |
| 54  | MG   | 2a    | 3157 | 1/1   | 0.84 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | 2a    | 3158 | 1/1   | 0.84 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1850 | 1/1   | 0.84 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3374 | 1/1   | 0.84 | 0.21 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3379 | 1/1   | 0.84 | 0.17 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1730 | 1/1   | 0.84 | 0.19 | 82,82,82,82                 | 0     |
| 54  | MG   | 1A    | 3612 | 1/1   | 0.84 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3728 | 1/1   | 0.84 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3663 | 1/1   | 0.84 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3870 | 1/1   | 0.84 | 0.29 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3560 | 1/1   | 0.84 | 0.19 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3423 | 1/1   | 0.84 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3148 | 1/1   | 0.85 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | 1V    | 203  | 1/1   | 0.85 | 0.22 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2B    | 205  | 1/1   | 0.85 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1W    | 204  | 1/1   | 0.85 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3185 | 1/1   | 0.85 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3451 | 1/1   | 0.85 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3217 | 1/1   | 0.85 | 0.31 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3224 | 1/1   | 0.85 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3232 | 1/1   | 0.85 | 0.48 | 75,75,75,75                 | 0     |
| 54  | MG   | 10    | 107  | 1/1   | 0.85 | 0.19 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1749 | 1/1   | 0.85 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3665 | 1/1   | 0.85 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 2G    | 201  | 1/1   | 0.85 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3572 | 1/1   | 0.85 | 0.15 | 38,38,38,38                 | 0     |
| 54  | MG   | 1B    | 220  | 1/1   | 0.85 | 0.18 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3274 | 1/1   | 0.85 | 0.48 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1775 | 1/1   | 0.85 | 0.19 | 80,80,80,80                 | 0     |
| 54  | MG   | 2a    | 3020 | 1/1   | 0.85 | 0.28 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1776 | 1/1   | 0.85 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3541 | 1/1   | 0.85 | 0.20 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3582 | 1/1   | 0.85 | 0.13 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3033 | 1/1   | 0.85 | 0.23 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3952 | 1/1   | 0.85 | 0.19 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 3036 | 1/1   | 0.85 | 0.24 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3557 | 1/1   | 0.85 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1671 | 1/1   | 0.85 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3061 | 1/1   | 0.85 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3032 | 1/1   | 0.85 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3466 | 1/1   | 0.85 | 0.10 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3354 | 1/1   | 0.85 | 0.11 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3047 | 1/1   | 0.85 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3063 | 1/1   | 0.85 | 0.29 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3627 | 1/1   | 0.85 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3079 | 1/1   | 0.85 | 0.40 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3375 | 1/1   | 0.85 | 0.12 | 65,65,65,65                 | 0     |
| 54  | MG   | 1D    | 314  | 1/1   | 0.85 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3634 | 1/1   | 0.85 | 0.33 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1691 | 1/1   | 0.85 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3186 | 1/1   | 0.85 | 0.33 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3384 | 1/1   | 0.85 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3386 | 1/1   | 0.85 | 0.21 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3394 | 1/1   | 0.85 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 3111 | 1/1   | 0.85 | 0.22 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3118 | 1/1   | 0.85 | 0.22 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3404 | 1/1   | 0.85 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3122 | 1/1   | 0.85 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3095 | 1/1   | 0.85 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3102 | 1/1   | 0.85 | 0.32 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 3152 | 1/1   | 0.85 | 0.31 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3414 | 1/1   | 0.85 | 0.14 | 86,86,86,86                 | 0     |
| 54  | MG   | 1F    | 313  | 1/1   | 0.85 | 0.36 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3113 | 1/1   | 0.85 | 0.20 | 83,83,83,83                 | 0     |
| 54  | MG   | 1a    | 1699 | 1/1   | 0.85 | 0.40 | 75,75,75,75                 | 0     |
| 54  | MG   | 2a    | 3162 | 1/1   | 0.85 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3118 | 1/1   | 0.85 | 0.18 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3167 | 1/1   | 0.85 | 0.30 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3120 | 1/1   | 0.85 | 0.23 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3682 | 1/1   | 0.85 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 1P    | 202  | 1/1   | 0.85 | 0.27 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3368 | 1/1   | 0.85 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3450 | 1/1   | 0.85 | 0.20 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3451 | 1/1   | 0.85 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3792 | 1/1   | 0.85 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MPD  | 2A    | 3728 | 8/8   | 0.85 | 0.22 | 51,65,69,71                 | 0     |
| 54  | MG   | 2A    | 3147 | 1/1   | 0.85 | 0.31 | 84,84,84,84                 | 0     |
| 54  | MG   | 2A    | 3276 | 1/1   | 0.86 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3501 | 1/1   | 0.86 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3936 | 1/1   | 0.86 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3489 | 1/1   | 0.86 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3493 | 1/1   | 0.86 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 1T    | 204  | 1/1   | 0.86 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3506 | 1/1   | 0.86 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 2V    | 203  | 1/1   | 0.86 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | 20    | 102  | 1/1   | 0.86 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3943 | 1/1   | 0.86 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3501 | 1/1   | 0.86 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3303 | 1/1   | 0.86 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3574 | 1/1   | 0.86 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3331 | 1/1   | 0.86 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3041 | 1/1   | 0.86 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3023 | 1/1   | 0.86 | 0.37 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3043 | 1/1   | 0.86 | 0.35 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3442 | 1/1   | 0.86 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3539 | 1/1   | 0.86 | 0.21 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3035 | 1/1   | 0.86 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3444 | 1/1   | 0.86 | 0.15 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3037 | 1/1   | 0.86 | 0.29 | 80,80,80,80                 | 0     |
| 54  | MG   | 2a    | 3043 | 1/1   | 0.86 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | 15    | 108  | 1/1   | 0.86 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3362 | 1/1   | 0.86 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1611 | 1/1   | 0.86 | 0.30 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3373 | 1/1   | 0.86 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3670 | 1/1   | 0.86 | 0.17 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3083 | 1/1   | 0.86 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3084 | 1/1   | 0.86 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3043 | 1/1   | 0.86 | 0.24 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3525 | 1/1   | 0.86 | 0.24 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3363 | 1/1   | 0.86 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3238 | 1/1   | 0.86 | 0.12 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3637 | 1/1   | 0.86 | 0.13 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3391 | 1/1   | 0.86 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1656 | 1/1   | 0.86 | 0.13 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3982 | 1/1   | 0.86 | 0.23 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3249 | 1/1   | 0.86 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3544 | 1/1   | 0.86 | 0.16 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3545 | 1/1   | 0.86 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 1B    | 213  | 1/1   | 0.86 | 0.24 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1677 | 1/1   | 0.86 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3837 | 1/1   | 0.86 | 0.21 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3464 | 1/1   | 0.86 | 0.10 | 28,28,28,28                 | 0     |
| 54  | MG   | 2a    | 3135 | 1/1   | 0.86 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3435 | 1/1   | 0.86 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3738 | 1/1   | 0.86 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1697 | 1/1   | 0.86 | 0.29 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3445 | 1/1   | 0.86 | 0.27 | 76,76,76,76                 | 0     |
| 54  | MG   | 1a    | 1832 | 1/1   | 0.86 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3189 | 1/1   | 0.86 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3192 | 1/1   | 0.86 | 0.32 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3398 | 1/1   | 0.86 | 0.28 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3867 | 1/1   | 0.86 | 0.11 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3427 | 1/1   | 0.86 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3184 | 1/1   | 0.86 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3014 | 1/1   | 0.86 | 0.28 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3721 | 1/1   | 0.86 | 0.15 | 81,81,81,81                 | 0     |
| 54  | MG   | 2B    | 204  | 1/1   | 0.86 | 0.16 | 80,80,80,80                 | 0     |
| 54  | MG   | 2r    | 101  | 1/1   | 0.86 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1719 | 1/1   | 0.86 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3912 | 1/1   | 0.86 | 0.17 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1855 | 1/1   | 0.86 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1860 | 1/1   | 0.86 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3923 | 1/1   | 0.86 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3521 | 1/1   | 0.87 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3371 | 1/1   | 0.87 | 0.26 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3926 | 1/1   | 0.87 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3712 | 1/1   | 0.87 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3618 | 1/1   | 0.87 | 0.23 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3477 | 1/1   | 0.87 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 1a    | 1814 | 1/1   | 0.87 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3232 | 1/1   | 0.87 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | 1a    | 1683 | 1/1   | 0.87 | 0.32 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1684 | 1/1   | 0.87 | 0.37 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3456 | 1/1   | 0.87 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3497 | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3318 | 1/1   | 0.87 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1F    | 311  | 1/1   | 0.87 | 0.26 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3466 | 1/1   | 0.87 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1694 | 1/1   | 0.87 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1840 | 1/1   | 0.87 | 0.23 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3476 | 1/1   | 0.87 | 0.18 | 59,59,59,59                 | 0     |
| 54  | MG   | 2E    | 306  | 1/1   | 0.87 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3246 | 1/1   | 0.87 | 0.28 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3739 | 1/1   | 0.87 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3252 | 1/1   | 0.87 | 0.27 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3366 | 1/1   | 0.87 | 0.13 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3003 | 1/1   | 0.87 | 0.32 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3550 | 1/1   | 0.87 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1848 | 1/1   | 0.87 | 0.17 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1700 | 1/1   | 0.87 | 0.30 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3589 | 1/1   | 0.87 | 0.17 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1704 | 1/1   | 0.87 | 0.12 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3598 | 1/1   | 0.87 | 0.22 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3502 | 1/1   | 0.87 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3233 | 1/1   | 0.87 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1865 | 1/1   | 0.87 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1717 | 1/1   | 0.87 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1d    | 302  | 1/1   | 0.87 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3522 | 1/1   | 0.87 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3308 | 1/1   | 0.87 | 0.20 | 81,81,81,81                 | 0     |
| 54  | MG   | 2A    | 3314 | 1/1   | 0.87 | 0.20 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3535 | 1/1   | 0.87 | 0.23 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1V    | 204  | 1/1   | 0.87 | 0.29 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1723 | 1/1   | 0.87 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG   | 1a    | 1726 | 1/1   | 0.87 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3565 | 1/1   | 0.87 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3333 | 1/1   | 0.87 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3571 | 1/1   | 0.87 | 0.15 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3575 | 1/1   | 0.87 | 0.16 | 38,38,38,38                 | 0     |
| 54  | MG   | 2a    | 3066 | 1/1   | 0.87 | 0.35 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3576 | 1/1   | 0.87 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | 1t    | 201  | 1/1   | 0.87 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3984 | 1/1   | 0.87 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3869 | 1/1   | 0.87 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 1l    | 104  | 1/1   | 0.87 | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3626 | 1/1   | 0.87 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3997 | 1/1   | 0.87 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 2a    | 3092 | 1/1   | 0.87 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3096 | 1/1   | 0.87 | 0.26 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1603 | 1/1   | 0.87 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | 1a    | 1752 | 1/1   | 0.87 | 0.11 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3102 | 1/1   | 0.87 | 0.22 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3633 | 1/1   | 0.87 | 0.22 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1605 | 1/1   | 0.87 | 0.26 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1763 | 1/1   | 0.87 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1773 | 1/1   | 0.87 | 0.13 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3120 | 1/1   | 0.87 | 0.22 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3080 | 1/1   | 0.87 | 0.27 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 3127 | 1/1   | 0.87 | 0.18 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3385 | 1/1   | 0.87 | 0.16 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3081 | 1/1   | 0.87 | 0.34 | 66,66,66,66                 | 0     |
| 54  | MG   | 1B    | 202  | 1/1   | 0.87 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1617 | 1/1   | 0.87 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3396 | 1/1   | 0.87 | 0.15 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3768 | 1/1   | 0.87 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3406 | 1/1   | 0.87 | 0.19 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1779 | 1/1   | 0.87 | 0.21 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1627 | 1/1   | 0.87 | 0.42 | 71,71,71,71                 | 0     |
| 54  | MG   | 1B    | 206  | 1/1   | 0.87 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3669 | 1/1   | 0.87 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1637 | 1/1   | 0.87 | 0.49 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3671 | 1/1   | 0.87 | 0.30 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3420 | 1/1   | 0.87 | 0.16 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3469 | 1/1   | 0.87 | 0.12 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1B    | 218  | 1/1   | 0.87 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3692 | 1/1   | 0.87 | 0.25 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3781 | 1/1   | 0.87 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3697 | 1/1   | 0.87 | 0.13 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3701 | 1/1   | 0.87 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1659 | 1/1   | 0.87 | 0.22 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3795 | 1/1   | 0.88 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3424 | 1/1   | 0.88 | 0.16 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1862 | 1/1   | 0.88 | 0.11 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1645 | 1/1   | 0.88 | 0.31 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1762 | 1/1   | 0.88 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3621 | 1/1   | 0.88 | 0.23 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1766 | 1/1   | 0.88 | 0.29 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1768 | 1/1   | 0.88 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3812 | 1/1   | 0.88 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 1l    | 202  | 1/1   | 0.88 | 0.25 | 78,78,78,78                 | 0     |
| 54  | MG   | 1n    | 101  | 1/1   | 0.88 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3701 | 1/1   | 0.88 | 0.09 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3947 | 1/1   | 0.88 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 1y    | 201  | 1/1   | 0.88 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3001 | 1/1   | 0.88 | 0.15 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3317 | 1/1   | 0.88 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3520 | 1/1   | 0.88 | 0.24 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3483 | 1/1   | 0.88 | 0.13 | 37,37,37,37                 | 0     |
| 54  | MG   | 1E    | 309  | 1/1   | 0.88 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3033 | 1/1   | 0.88 | 0.37 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1668 | 1/1   | 0.88 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3489 | 1/1   | 0.88 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3446 | 1/1   | 0.88 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 1F    | 314  | 1/1   | 0.88 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3560 | 1/1   | 0.88 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3364 | 1/1   | 0.88 | 0.28 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3049 | 1/1   | 0.88 | 0.34 | 76,76,76,76                 | 0     |
| 54  | MG   | 1O    | 201  | 1/1   | 0.88 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3146 | 1/1   | 0.88 | 0.35 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3649 | 1/1   | 0.88 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3377 | 1/1   | 0.88 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 2a    | 3048 | 1/1   | 0.88 | 0.27 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3378 | 1/1   | 0.88 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3051 | 1/1   | 0.88 | 0.28 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3585 | 1/1   | 0.88 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3608 | 1/1   | 0.88 | 0.13 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1803 | 1/1   | 0.88 | 0.22 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3136 | 1/1   | 0.88 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3059 | 1/1   | 0.88 | 0.40 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3662 | 1/1   | 0.88 | 0.11 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3063 | 1/1   | 0.88 | 0.12 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3454 | 1/1   | 0.88 | 0.16 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3553 | 1/1   | 0.88 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3072 | 1/1   | 0.88 | 0.39 | 70,70,70,70                 | 0     |
| 54  | MG   | 2a    | 3077 | 1/1   | 0.88 | 0.26 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3099 | 1/1   | 0.88 | 0.42 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3393 | 1/1   | 0.88 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3994 | 1/1   | 0.88 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3432 | 1/1   | 0.88 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3086 | 1/1   | 0.88 | 0.41 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3398 | 1/1   | 0.88 | 0.26 | 63,63,63,63                 | 0     |
| 54  | MG   | 10    | 108  | 1/1   | 0.88 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1819 | 1/1   | 0.88 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1820 | 1/1   | 0.88 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3395 | 1/1   | 0.88 | 0.20 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3897 | 1/1   | 0.88 | 0.14 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 3101 | 1/1   | 0.88 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3141 | 1/1   | 0.88 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 17    | 105  | 1/1   | 0.88 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 1B    | 204  | 1/1   | 0.88 | 0.25 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3426 | 1/1   | 0.88 | 0.13 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3430 | 1/1   | 0.88 | 0.23 | 79,79,79,79                 | 0     |
| 54  | MG   | 1A    | 3255 | 1/1   | 0.88 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3121 | 1/1   | 0.88 | 0.32 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3911 | 1/1   | 0.88 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3159 | 1/1   | 0.88 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | 1a    | 1836 | 1/1   | 0.88 | 0.18 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 3136 | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3444 | 1/1   | 0.88 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3401 | 1/1   | 0.88 | 0.27 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3684 | 1/1   | 0.88 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3686 | 1/1   | 0.88 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3688 | 1/1   | 0.88 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3922 | 1/1   | 0.88 | 0.13 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3175 | 1/1   | 0.88 | 0.37 | 75,75,75,75                 | 0     |
| 54  | MG   | 2a    | 3161 | 1/1   | 0.88 | 0.29 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1845 | 1/1   | 0.88 | 0.31 | 76,76,76,76                 | 0     |
| 54  | MG   | 2a    | 3163 | 1/1   | 0.88 | 0.23 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1629 | 1/1   | 0.88 | 0.28 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3209 | 1/1   | 0.88 | 0.28 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1847 | 1/1   | 0.88 | 0.24 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3218 | 1/1   | 0.88 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3178 | 1/1   | 0.88 | 0.15 | 77,77,77,77                 | 0     |
| 54  | MG   | 1a    | 1735 | 1/1   | 0.88 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | 1a    | 1849 | 1/1   | 0.88 | 0.28 | 78,78,78,78                 | 0     |
| 54  | MG   | 2j    | 201  | 1/1   | 0.88 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1631 | 1/1   | 0.88 | 0.33 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3242 | 1/1   | 0.88 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3718 | 1/1   | 0.88 | 0.22 | 76,76,76,76                 | 0     |
| 54  | MG   | 1a    | 1634 | 1/1   | 0.88 | 0.25 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3522 | 1/1   | 0.88 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3250 | 1/1   | 0.88 | 0.43 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3031 | 1/1   | 0.89 | 0.28 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3797 | 1/1   | 0.89 | 0.21 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3476 | 1/1   | 0.89 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3685 | 1/1   | 0.89 | 0.23 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1757 | 1/1   | 0.89 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3202 | 1/1   | 0.89 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 15    | 103  | 1/1   | 0.89 | 0.25 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3387 | 1/1   | 0.89 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3807 | 1/1   | 0.89 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3376 | 1/1   | 0.89 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 1a    | 1602 | 1/1   | 0.89 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3070 | 1/1   | 0.89 | 0.26 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3075 | 1/1   | 0.89 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3688 | 1/1   | 0.89 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3301 | 1/1   | 0.89 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3966 | 1/1   | 0.89 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3714 | 1/1   | 0.89 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3411 | 1/1   | 0.89 | 0.33 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3974 | 1/1   | 0.89 | 0.31 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1777 | 1/1   | 0.89 | 0.25 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3415 | 1/1   | 0.89 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3979 | 1/1   | 0.89 | 0.19 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3821 | 1/1   | 0.89 | 0.23 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3622 | 1/1   | 0.89 | 0.20 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3011 | 1/1   | 0.89 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3581 | 1/1   | 0.89 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1787 | 1/1   | 0.89 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3985 | 1/1   | 0.89 | 0.23 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3835 | 1/1   | 0.89 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1791 | 1/1   | 0.89 | 0.21 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3442 | 1/1   | 0.89 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | 2D    | 309  | 1/1   | 0.89 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | 1a    | 1792 | 1/1   | 0.89 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3121 | 1/1   | 0.89 | 0.22 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1638 | 1/1   | 0.89 | 0.24 | 78,78,78,78                 | 0     |
| 54  | MG   | 2T    | 203  | 1/1   | 0.89 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3126 | 1/1   | 0.89 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3132 | 1/1   | 0.89 | 0.29 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3140 | 1/1   | 0.89 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3626 | 1/1   | 0.89 | 0.16 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 3014 | 1/1   | 0.89 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1644 | 1/1   | 0.89 | 0.29 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1805 | 1/1   | 0.89 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3845 | 1/1   | 0.89 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3848 | 1/1   | 0.89 | 0.13 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3158 | 1/1   | 0.89 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3463 | 1/1   | 0.89 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3148 | 1/1   | 0.89 | 0.21 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 3031 | 1/1   | 0.89 | 0.34 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3160 | 1/1   | 0.89 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3163 | 1/1   | 0.89 | 0.21 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1654 | 1/1   | 0.89 | 0.28 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3168 | 1/1   | 0.89 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3175 | 1/1   | 0.89 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3040 | 1/1   | 0.89 | 0.35 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3177 | 1/1   | 0.89 | 0.25 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3045 | 1/1   | 0.89 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3851 | 1/1   | 0.89 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3039 | 1/1   | 0.89 | 0.13 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3188 | 1/1   | 0.89 | 0.41 | 76,76,76,76                 | 0     |
| 54  | MG   | 1a    | 1815 | 1/1   | 0.89 | 0.11 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3494 | 1/1   | 0.89 | 0.12 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3496 | 1/1   | 0.89 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3741 | 1/1   | 0.89 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3866 | 1/1   | 0.89 | 0.11 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3205 | 1/1   | 0.89 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | 1B    | 215  | 1/1   | 0.89 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3742 | 1/1   | 0.89 | 0.15 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1823 | 1/1   | 0.89 | 0.09 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3633 | 1/1   | 0.89 | 0.13 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3228 | 1/1   | 0.89 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3230 | 1/1   | 0.89 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1B    | 221  | 1/1   | 0.89 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1826 | 1/1   | 0.89 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3241 | 1/1   | 0.89 | 0.29 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3640 | 1/1   | 0.89 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3531 | 1/1   | 0.89 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3872 | 1/1   | 0.89 | 0.12 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3878 | 1/1   | 0.89 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3089 | 1/1   | 0.89 | 0.17 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3249 | 1/1   | 0.89 | 0.31 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3555 | 1/1   | 0.89 | 0.15 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3880 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3645 | 1/1   | 0.89 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3887 | 1/1   | 0.89 | 0.20 | 52,52,52,52                 | 0     |
| 54  | MG   | 1D    | 301  | 1/1   | 0.89 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | 1D    | 309  | 1/1   | 0.89 | 0.28 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3890 | 1/1   | 0.89 | 0.20 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3546 | 1/1   | 0.89 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 2a    | 3113 | 1/1   | 0.89 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3548 | 1/1   | 0.89 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3580 | 1/1   | 0.89 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3760 | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1703 | 1/1   | 0.89 | 0.33 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3658 | 1/1   | 0.89 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3125 | 1/1   | 0.89 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3625 | 1/1   | 0.89 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | 1F    | 316  | 1/1   | 0.89 | 0.24 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3304 | 1/1   | 0.89 | 0.16 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1709 | 1/1   | 0.89 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1714 | 1/1   | 0.89 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3311 | 1/1   | 0.89 | 0.19 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3461 | 1/1   | 0.89 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3369 | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3322 | 1/1   | 0.89 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1T    | 201  | 1/1   | 0.89 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3342 | 1/1   | 0.89 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3650 | 1/1   | 0.89 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | 1d    | 303  | 1/1   | 0.89 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3413 | 1/1   | 0.89 | 0.15 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3927 | 1/1   | 0.89 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3173 | 1/1   | 0.89 | 0.21 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3175 | 1/1   | 0.89 | 0.27 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3603 | 1/1   | 0.89 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1731 | 1/1   | 0.89 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3438 | 1/1   | 0.89 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1738 | 1/1   | 0.89 | 0.26 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3940 | 1/1   | 0.89 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 2p    | 101  | 1/1   | 0.89 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | 1t    | 202  | 1/1   | 0.89 | 0.15 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3091 | 1/1   | 0.89 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1746 | 1/1   | 0.89 | 0.11 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3017 | 1/1   | 0.89 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3674 | 1/1   | 0.89 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3945 | 1/1   | 0.89 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3962 | 1/1   | 0.90 | 0.23 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3016 | 1/1   | 0.90 | 0.22 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3243 | 1/1   | 0.90 | 0.29 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3244 | 1/1   | 0.90 | 0.33 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1679 | 1/1   | 0.90 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1682 | 1/1   | 0.90 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3429 | 1/1   | 0.90 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | 1R    | 205  | 1/1   | 0.90 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1795 | 1/1   | 0.90 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3722 | 1/1   | 0.90 | 0.18 | 70,70,70,70                 | 0     |
| 54  | MG   | 2B    | 201  | 1/1   | 0.90 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1796 | 1/1   | 0.90 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3253 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3467 | 1/1   | 0.90 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3469 | 1/1   | 0.90 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3853 | 1/1   | 0.90 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3473 | 1/1   | 0.90 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3258 | 1/1   | 0.90 | 0.43 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1689 | 1/1   | 0.90 | 0.33 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3270 | 1/1   | 0.90 | 0.41 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3599 | 1/1   | 0.90 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3552 | 1/1   | 0.90 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3485 | 1/1   | 0.90 | 0.15 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3050 | 1/1   | 0.90 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | 2E    | 307  | 1/1   | 0.90 | 0.09 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3058 | 1/1   | 0.90 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3490 | 1/1   | 0.90 | 0.28 | 70,70,70,70                 | 0     |
| 54  | MG   | 2N    | 201  | 1/1   | 0.90 | 0.13 | 77,77,77,77                 | 0     |
| 54  | MG   | 2Q    | 202  | 1/1   | 0.90 | 0.16 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3492 | 1/1   | 0.90 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3976 | 1/1   | 0.90 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3978 | 1/1   | 0.90 | 0.13 | 81,81,81,81                 | 0     |
| 54  | MG   | 25    | 101  | 1/1   | 0.90 | 0.18 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3298 | 1/1   | 0.90 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3004 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3856 | 1/1   | 0.90 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3011 | 1/1   | 0.90 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3761 | 1/1   | 0.90 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3036 | 1/1   | 0.90 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3500 | 1/1   | 0.90 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3270 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3276 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3771 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 13    | 102  | 1/1   | 0.90 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3315 | 1/1   | 0.90 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3773 | 1/1   | 0.90 | 0.27 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3517 | 1/1   | 0.90 | 0.27 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3519 | 1/1   | 0.90 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3321 | 1/1   | 0.90 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3521 | 1/1   | 0.90 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3989 | 1/1   | 0.90 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3039 | 1/1   | 0.90 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3325 | 1/1   | 0.90 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3527 | 1/1   | 0.90 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3096 | 1/1   | 0.90 | 0.22 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3097 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3345 | 1/1   | 0.90 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3879 | 1/1   | 0.90 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3545 | 1/1   | 0.90 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3100 | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3351 | 1/1   | 0.90 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3350 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3055 | 1/1   | 0.90 | 0.11 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3439 | 1/1   | 0.90 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3057 | 1/1   | 0.90 | 0.20 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3563 | 1/1   | 0.90 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 1a    | 1604 | 1/1   | 0.90 | 0.25 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1829 | 1/1   | 0.90 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3783 | 1/1   | 0.90 | 0.13 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3574 | 1/1   | 0.90 | 0.10 | 82,82,82,82                 | 0     |
| 54  | MG   | 2a    | 3067 | 1/1   | 0.90 | 0.45 | 78,78,78,78                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3615 | 1/1   | 0.90 | 0.09 | 25,25,25,25                 | 0     |
| 54  | MG   | 2A    | 3372 | 1/1   | 0.90 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1833 | 1/1   | 0.90 | 0.19 | 77,77,77,77                 | 0     |
| 54  | MG   | 2a    | 3078 | 1/1   | 0.90 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3565 | 1/1   | 0.90 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3470 | 1/1   | 0.90 | 0.13 | 39,39,39,39                 | 0     |
| 54  | MG   | 1a    | 1837 | 1/1   | 0.90 | 0.22 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3595 | 1/1   | 0.90 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3604 | 1/1   | 0.90 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3905 | 1/1   | 0.90 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3609 | 1/1   | 0.90 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3909 | 1/1   | 0.90 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3619 | 1/1   | 0.90 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3093 | 1/1   | 0.90 | 0.28 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3472 | 1/1   | 0.90 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 1B    | 219  | 1/1   | 0.90 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3382 | 1/1   | 0.90 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3356 | 1/1   | 0.90 | 0.22 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1747 | 1/1   | 0.90 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 3106 | 1/1   | 0.90 | 0.21 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3804 | 1/1   | 0.90 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3109 | 1/1   | 0.90 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3387 | 1/1   | 0.90 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3112 | 1/1   | 0.90 | 0.15 | 83,83,83,83                 | 0     |
| 54  | MG   | 2A    | 3635 | 1/1   | 0.90 | 0.08 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3155 | 1/1   | 0.90 | 0.27 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3162 | 1/1   | 0.90 | 0.35 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3638 | 1/1   | 0.90 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1643 | 1/1   | 0.90 | 0.25 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1758 | 1/1   | 0.90 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3125 | 1/1   | 0.90 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3539 | 1/1   | 0.90 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3169 | 1/1   | 0.90 | 0.31 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3654 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3627 | 1/1   | 0.90 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3628 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3409 | 1/1   | 0.90 | 0.28 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3729 | 1/1   | 0.90 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3156 | 1/1   | 0.90 | 0.26 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1867 | 1/1   | 0.90 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3733 | 1/1   | 0.90 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3159 | 1/1   | 0.90 | 0.26 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3629 | 1/1   | 0.90 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1658 | 1/1   | 0.90 | 0.22 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3668 | 1/1   | 0.90 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3256 | 1/1   | 0.90 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3420 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3204 | 1/1   | 0.90 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3673 | 1/1   | 0.90 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3170 | 1/1   | 0.90 | 0.30 | 77,77,77,77                 | 0     |
| 54  | MG   | 2a    | 3172 | 1/1   | 0.90 | 0.23 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3423 | 1/1   | 0.90 | 0.25 | 72,72,72,72                 | 0     |
| 54  | MG   | 2a    | 3174 | 1/1   | 0.90 | 0.26 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3675 | 1/1   | 0.90 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1660 | 1/1   | 0.90 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3449 | 1/1   | 0.90 | 0.08 | 31,31,31,31                 | 0     |
| 54  | MG   | 1i    | 201  | 1/1   | 0.90 | 0.23 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3163 | 1/1   | 0.90 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3220 | 1/1   | 0.90 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3492 | 1/1   | 0.90 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3953 | 1/1   | 0.90 | 0.25 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3367 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1783 | 1/1   | 0.90 | 0.14 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3234 | 1/1   | 0.90 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3448 | 1/1   | 0.90 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3592 | 1/1   | 0.90 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1727 | 1/1   | 0.91 | 0.12 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3580 | 1/1   | 0.91 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3350 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 12    | 101  | 1/1   | 0.91 | 0.13 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3971 | 1/1   | 0.91 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3113 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3077 | 1/1   | 0.91 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3238 | 1/1   | 0.91 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 2B    | 202  | 1/1   | 0.91 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | 1a    | 1743 | 1/1   | 0.91 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3296 | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3472 | 1/1   | 0.91 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 2B    | 208  | 1/1   | 0.91 | 0.31 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1601 | 1/1   | 0.91 | 0.11 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3852 | 1/1   | 0.91 | 0.18 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3543 | 1/1   | 0.91 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3634 | 1/1   | 0.91 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3587 | 1/1   | 0.91 | 0.10 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3482 | 1/1   | 0.91 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1753 | 1/1   | 0.91 | 0.24 | 70,70,70,70                 | 0     |
| 54  | MG   | 2D    | 303  | 1/1   | 0.91 | 0.35 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3484 | 1/1   | 0.91 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1607 | 1/1   | 0.91 | 0.09 | 71,71,71,71                 | 0     |
| 54  | MG   | 2D    | 312  | 1/1   | 0.91 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1608 | 1/1   | 0.91 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3746 | 1/1   | 0.91 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 1a    | 1760 | 1/1   | 0.91 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3003 | 1/1   | 0.91 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3749 | 1/1   | 0.91 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3643 | 1/1   | 0.91 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | 1a    | 1764 | 1/1   | 0.91 | 0.14 | 75,75,75,75                 | 0     |
| 54  | MG   | 2V    | 201  | 1/1   | 0.91 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3025 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1765 | 1/1   | 0.91 | 0.19 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3755 | 1/1   | 0.91 | 0.19 | 47,47,47,47                 | 0     |
| 54  | MG   | 28    | 101  | 1/1   | 0.91 | 0.20 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3991 | 1/1   | 0.91 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3282 | 1/1   | 0.91 | 0.30 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3005 | 1/1   | 0.91 | 0.26 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3007 | 1/1   | 0.91 | 0.52 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3034 | 1/1   | 0.91 | 0.30 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3756 | 1/1   | 0.91 | 0.13 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3117 | 1/1   | 0.91 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3505 | 1/1   | 0.91 | 0.25 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3507 | 1/1   | 0.91 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3019 | 1/1   | 0.91 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3875 | 1/1   | 0.91 | 0.12 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3876 | 1/1   | 0.91 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3511 | 1/1   | 0.91 | 0.09 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3365 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 2a    | 3024 | 1/1   | 0.91 | 0.15 | 73,73,73,73                 | 0     |
| 54  | MG   | 2a    | 3028 | 1/1   | 0.91 | 0.24 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3597 | 1/1   | 0.91 | 0.13 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3052 | 1/1   | 0.91 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3312 | 1/1   | 0.91 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3656 | 1/1   | 0.91 | 0.25 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3033 | 1/1   | 0.91 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 1B    | 214  | 1/1   | 0.91 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3529 | 1/1   | 0.91 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3767 | 1/1   | 0.91 | 0.10 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3266 | 1/1   | 0.91 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | 2a    | 3041 | 1/1   | 0.91 | 0.29 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3077 | 1/1   | 0.91 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1786 | 1/1   | 0.91 | 0.08 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3340 | 1/1   | 0.91 | 0.27 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3547 | 1/1   | 0.91 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3550 | 1/1   | 0.91 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3494 | 1/1   | 0.91 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3902 | 1/1   | 0.91 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3082 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3304 | 1/1   | 0.91 | 0.27 | 65,65,65,65                 | 0     |
| 54  | MG   | 1B    | 224  | 1/1   | 0.91 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3904 | 1/1   | 0.91 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3089 | 1/1   | 0.91 | 0.34 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3570 | 1/1   | 0.91 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3096 | 1/1   | 0.91 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3355 | 1/1   | 0.91 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3358 | 1/1   | 0.91 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | 2a    | 3064 | 1/1   | 0.91 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3212 | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3778 | 1/1   | 0.91 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3098 | 1/1   | 0.91 | 0.20 | 69,69,69,69                 | 0     |
| 54  | MG   | 1a    | 1670 | 1/1   | 0.91 | 0.40 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3074 | 1/1   | 0.91 | 0.25 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3502 | 1/1   | 0.91 | 0.08 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1672 | 1/1   | 0.91 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3597 | 1/1   | 0.91 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1806 | 1/1   | 0.91 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3607 | 1/1   | 0.91 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1673 | 1/1   | 0.91 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3085 | 1/1   | 0.91 | 0.27 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3919 | 1/1   | 0.91 | 0.18 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3612 | 1/1   | 0.91 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3116 | 1/1   | 0.91 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3425 | 1/1   | 0.91 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 1D    | 303  | 1/1   | 0.91 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1678 | 1/1   | 0.91 | 0.32 | 74,74,74,74                 | 0     |
| 54  | MG   | 1A    | 3179 | 1/1   | 0.91 | 0.24 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3678 | 1/1   | 0.91 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | 2a    | 3099 | 1/1   | 0.91 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1816 | 1/1   | 0.91 | 0.12 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3139 | 1/1   | 0.91 | 0.22 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3512 | 1/1   | 0.91 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3796 | 1/1   | 0.91 | 0.09 | 17,17,17,17                 | 0     |
| 54  | MG   | 1A    | 3934 | 1/1   | 0.91 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3137 | 1/1   | 0.91 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3567 | 1/1   | 0.91 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3062 | 1/1   | 0.91 | 0.24 | 54,54,54,54                 | 0     |
| 54  | MG   | 1N    | 203  | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3646 | 1/1   | 0.91 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3648 | 1/1   | 0.91 | 0.22 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1696 | 1/1   | 0.91 | 0.26 | 82,82,82,82                 | 0     |
| 54  | MG   | 1a    | 1827 | 1/1   | 0.91 | 0.26 | 81,81,81,81                 | 0     |
| 54  | MG   | 2A    | 3410 | 1/1   | 0.91 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3941 | 1/1   | 0.91 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3942 | 1/1   | 0.91 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | 1P    | 204  | 1/1   | 0.91 | 0.14 | 80,80,80,80                 | 0     |
| 54  | MG   | 2A    | 3167 | 1/1   | 0.91 | 0.28 | 66,66,66,66                 | 0     |
| 54  | MG   | 1Q    | 202  | 1/1   | 0.91 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3142 | 1/1   | 0.91 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3693 | 1/1   | 0.91 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3146 | 1/1   | 0.91 | 0.18 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3173 | 1/1   | 0.91 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 3153 | 1/1   | 0.91 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | 2a    | 3154 | 1/1   | 0.91 | 0.12 | 85,85,85,85                 | 0     |
| 54  | MG   | 2A    | 3664 | 1/1   | 0.91 | 0.21 | 76,76,76,76                 | 0     |
| 54  | MG   | 1A    | 3623 | 1/1   | 0.91 | 0.31 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3422 | 1/1   | 0.91 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3698 | 1/1   | 0.91 | 0.17 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3183 | 1/1   | 0.91 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3468 | 1/1   | 0.91 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3705 | 1/1   | 0.91 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3432 | 1/1   | 0.91 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3433 | 1/1   | 0.91 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 2a    | 3165 | 1/1   | 0.91 | 0.27 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3677 | 1/1   | 0.91 | 0.27 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3679 | 1/1   | 0.91 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | 2a    | 3168 | 1/1   | 0.91 | 0.29 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3680 | 1/1   | 0.91 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3391 | 1/1   | 0.91 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 1a    | 1712 | 1/1   | 0.91 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3722 | 1/1   | 0.91 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3439 | 1/1   | 0.91 | 0.32 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3441 | 1/1   | 0.91 | 0.14 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3200 | 1/1   | 0.91 | 0.34 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3723 | 1/1   | 0.91 | 0.27 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3203 | 1/1   | 0.91 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | 1Y    | 201  | 1/1   | 0.91 | 0.09 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1722 | 1/1   | 0.91 | 0.13 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3724 | 1/1   | 0.91 | 0.17 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3212 | 1/1   | 0.91 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3213 | 1/1   | 0.91 | 0.27 | 64,64,64,64                 | 0     |
| 56  | ARG  | 1B    | 232  | 12/12 | 0.91 | 0.12 | 37,47,60,63                 | 0     |
| 54  | MG   | 1a    | 1725 | 1/1   | 0.91 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3706 | 1/1   | 0.91 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3284 | 1/1   | 0.91 | 0.18 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3709 | 1/1   | 0.91 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1646 | 1/1   | 0.92 | 0.31 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3048 | 1/1   | 0.92 | 0.28 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3377 | 1/1   | 0.92 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3900 | 1/1   | 0.92 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3381 | 1/1   | 0.92 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3053 | 1/1   | 0.92 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1655 | 1/1   | 0.92 | 0.15 | 75,75,75,75                 | 0     |
| 54  | MG   | 2D    | 310  | 1/1   | 0.92 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | 2D    | 311  | 1/1   | 0.92 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3062 | 1/1   | 0.92 | 0.23 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1784 | 1/1   | 0.92 | 0.11 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3671 | 1/1   | 0.92 | 0.13 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3073 | 1/1   | 0.92 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3672 | 1/1   | 0.92 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3776 | 1/1   | 0.92 | 0.19 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3605 | 1/1   | 0.92 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2R    | 202  | 1/1   | 0.92 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | 2T    | 202  | 1/1   | 0.92 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3910 | 1/1   | 0.92 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG   | 2T    | 204  | 1/1   | 0.92 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3510 | 1/1   | 0.92 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3321 | 1/1   | 0.92 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | 20    | 101  | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3514 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 1a    | 1665 | 1/1   | 0.92 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1666 | 1/1   | 0.92 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3002 | 1/1   | 0.92 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | 1a    | 1667 | 1/1   | 0.92 | 0.41 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3323 | 1/1   | 0.92 | 0.09 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3324 | 1/1   | 0.92 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3322 | 1/1   | 0.92 | 0.11 | 28,28,28,28                 | 0     |
| 54  | MG   | 1a    | 1799 | 1/1   | 0.92 | 0.15 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3336 | 1/1   | 0.92 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3012 | 1/1   | 0.92 | 0.30 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3610 | 1/1   | 0.92 | 0.09 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3094 | 1/1   | 0.92 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3921 | 1/1   | 0.92 | 0.08 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3611 | 1/1   | 0.92 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3347 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3685 | 1/1   | 0.92 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 1D    | 312  | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3287 | 1/1   | 0.92 | 0.17 | 41,41,41,41                 | 0     |
| 54  | MG   | 1E    | 301  | 1/1   | 0.92 | 0.27 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3496 | 1/1   | 0.92 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3343 | 1/1   | 0.92 | 0.11 | 69,69,69,69                 | 0     |
| 54  | MG   | 1E    | 310  | 1/1   | 0.92 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 1F    | 309  | 1/1   | 0.92 | 0.33 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3929 | 1/1   | 0.92 | 0.12 | 85,85,85,85                 | 0     |
| 54  | MG   | 2A    | 3117 | 1/1   | 0.92 | 0.22 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3368 | 1/1   | 0.92 | 0.08 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3369 | 1/1   | 0.92 | 0.11 | 72,72,72,72                 | 0     |
| 54  | MG   | 1F    | 312  | 1/1   | 0.92 | 0.13 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3031 | 1/1   | 0.92 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3620 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3806 | 1/1   | 0.92 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3124 | 1/1   | 0.92 | 0.21 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3583 | 1/1   | 0.92 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3041 | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3588 | 1/1   | 0.92 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1695 | 1/1   | 0.92 | 0.27 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3811 | 1/1   | 0.92 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3405 | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3814 | 1/1   | 0.92 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3716 | 1/1   | 0.92 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3503 | 1/1   | 0.92 | 0.06 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3407 | 1/1   | 0.92 | 0.12 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3613 | 1/1   | 0.92 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3353 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3061 | 1/1   | 0.92 | 0.14 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3388 | 1/1   | 0.92 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3155 | 1/1   | 0.92 | 0.11 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3156 | 1/1   | 0.92 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3121 | 1/1   | 0.92 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3829 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3068 | 1/1   | 0.92 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3630 | 1/1   | 0.92 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3070 | 1/1   | 0.92 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3300 | 1/1   | 0.92 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3401 | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3578 | 1/1   | 0.92 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1V    | 206  | 1/1   | 0.92 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3164 | 1/1   | 0.92 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3408 | 1/1   | 0.92 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3081 | 1/1   | 0.92 | 0.43 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3165 | 1/1   | 0.92 | 0.27 | 74,74,74,74                 | 0     |
| 54  | MG   | 2a    | 3083 | 1/1   | 0.92 | 0.20 | 57,57,57,57                 | 0     |
| 54  | MG   | 1W    | 201  | 1/1   | 0.92 | 0.27 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3836 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3643 | 1/1   | 0.92 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3644 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3730 | 1/1   | 0.92 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3732 | 1/1   | 0.92 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 10    | 102  | 1/1   | 0.92 | 0.18 | 53,53,53,53                 | 0     |
| 54  | MG   | 10    | 106  | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | 2a    | 3095 | 1/1   | 0.92 | 0.37 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3653 | 1/1   | 0.92 | 0.20 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3970 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3419 | 1/1   | 0.92 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3179 | 1/1   | 0.92 | 0.35 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3181 | 1/1   | 0.92 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3166 | 1/1   | 0.92 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 10    | 109  | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3107 | 1/1   | 0.92 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3735 | 1/1   | 0.92 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3520 | 1/1   | 0.92 | 0.16 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3463 | 1/1   | 0.92 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3190 | 1/1   | 0.92 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1864 | 1/1   | 0.92 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | 2a    | 3114 | 1/1   | 0.92 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3115 | 1/1   | 0.92 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3195 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3436 | 1/1   | 0.92 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1736 | 1/1   | 0.92 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3672 | 1/1   | 0.92 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | 1a    | 1866 | 1/1   | 0.92 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 2a    | 3124 | 1/1   | 0.92 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3202 | 1/1   | 0.92 | 0.34 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3210 | 1/1   | 0.92 | 0.19 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3583 | 1/1   | 0.92 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3638 | 1/1   | 0.92 | 0.25 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3207 | 1/1   | 0.92 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | 19    | 101  | 1/1   | 0.92 | 0.16 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3524 | 1/1   | 0.92 | 0.26 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3010 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1748 | 1/1   | 0.92 | 0.36 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3644 | 1/1   | 0.92 | 0.18 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3054 | 1/1   | 0.92 | 0.25 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3988 | 1/1   | 0.92 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 1n    | 102  | 1/1   | 0.92 | 0.21 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3695 | 1/1   | 0.92 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 1o    | 101  | 1/1   | 0.92 | 0.25 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3060 | 1/1   | 0.92 | 0.08 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3699 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3459 | 1/1   | 0.92 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3871 | 1/1   | 0.92 | 0.09 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3992 | 1/1   | 0.92 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3237 | 1/1   | 0.92 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3705 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3873 | 1/1   | 0.92 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 1B    | 201  | 1/1   | 0.92 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3012 | 1/1   | 0.92 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3655 | 1/1   | 0.92 | 0.15 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3317 | 1/1   | 0.92 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3022 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3716 | 1/1   | 0.92 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3596 | 1/1   | 0.92 | 0.25 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3542 | 1/1   | 0.92 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3002 | 1/1   | 0.92 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 2e    | 201  | 1/1   | 0.92 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | 2f    | 201  | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1772 | 1/1   | 0.92 | 0.08 | 64,64,64,64                 | 0     |
| 54  | MG   | 1B    | 208  | 1/1   | 0.92 | 0.34 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3255 | 1/1   | 0.92 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | 2B    | 203  | 1/1   | 0.92 | 0.31 | 68,68,68,68                 | 0     |
| 54  | MG   | 1B    | 210  | 1/1   | 0.92 | 0.10 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3040 | 1/1   | 0.92 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3264 | 1/1   | 0.92 | 0.42 | 72,72,72,72                 | 0     |
| 57  | MPD  | 1A    | 3999 | 8/8   | 0.92 | 0.20 | 50,53,61,63                 | 0     |
| 54  | MG   | 1A    | 3765 | 1/1   | 0.92 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3373 | 1/1   | 0.92 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3491 | 1/1   | 0.92 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3115 | 1/1   | 0.92 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3718 | 1/1   | 0.93 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 2F    | 302  | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1620 | 1/1   | 0.93 | 0.22 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1733 | 1/1   | 0.93 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3220 | 1/1   | 0.93 | 0.18 | 65,65,65,65                 | 0     |
| 54  | MG   | 2P    | 201  | 1/1   | 0.93 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | 2P    | 202  | 1/1   | 0.93 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 2Q    | 201  | 1/1   | 0.93 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3138 | 1/1   | 0.93 | 0.42 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1625 | 1/1   | 0.93 | 0.11 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3231 | 1/1   | 0.93 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3575 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3532 | 1/1   | 0.93 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1851 | 1/1   | 0.93 | 0.25 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1852 | 1/1   | 0.93 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 2W    | 202  | 1/1   | 0.93 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3544 | 1/1   | 0.93 | 0.08 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3363 | 1/1   | 0.93 | 0.19 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1742 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1630 | 1/1   | 0.93 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3152 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3090 | 1/1   | 0.93 | 0.21 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3371 | 1/1   | 0.93 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3559 | 1/1   | 0.93 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1856 | 1/1   | 0.93 | 0.18 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3157 | 1/1   | 0.93 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3009 | 1/1   | 0.93 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1858 | 1/1   | 0.93 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3567 | 1/1   | 0.93 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3013 | 1/1   | 0.93 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3931 | 1/1   | 0.93 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3396 | 1/1   | 0.93 | 0.16 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1863 | 1/1   | 0.93 | 0.09 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3448 | 1/1   | 0.93 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3056 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3635 | 1/1   | 0.93 | 0.20 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1641 | 1/1   | 0.93 | 0.31 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3579 | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3057 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1755 | 1/1   | 0.93 | 0.08 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3830 | 1/1   | 0.93 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3030 | 1/1   | 0.93 | 0.30 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3172 | 1/1   | 0.93 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3118 | 1/1   | 0.93 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3390 | 1/1   | 0.93 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3596 | 1/1   | 0.93 | 0.15 | 40,40,40,40                 | 0     |
| 54  | MG   | 1f    | 201  | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 1D    | 313  | 1/1   | 0.93 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3038 | 1/1   | 0.93 | 0.17 | 74,74,74,74                 | 0     |
| 54  | MG   | 1a    | 1649 | 1/1   | 0.93 | 0.37 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3180 | 1/1   | 0.93 | 0.30 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3944 | 1/1   | 0.93 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3611 | 1/1   | 0.93 | 0.13 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3400 | 1/1   | 0.93 | 0.22 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3737 | 1/1   | 0.93 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3402 | 1/1   | 0.93 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3403 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3620 | 1/1   | 0.93 | 0.20 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3622 | 1/1   | 0.93 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3624 | 1/1   | 0.93 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3642 | 1/1   | 0.93 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 3054 | 1/1   | 0.93 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3405 | 1/1   | 0.93 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3519 | 1/1   | 0.93 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3186 | 1/1   | 0.93 | 0.26 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3069 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1o    | 102  | 1/1   | 0.93 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3846 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3191 | 1/1   | 0.93 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3188 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3413 | 1/1   | 0.93 | 0.30 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3065 | 1/1   | 0.93 | 0.28 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3194 | 1/1   | 0.93 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3647 | 1/1   | 0.93 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3960 | 1/1   | 0.93 | 0.13 | 65,65,65,65                 | 0     |
| 54  | MG   | 1y    | 202  | 1/1   | 0.93 | 0.17 | 80,80,80,80                 | 0     |
| 54  | MG   | 1A    | 3460 | 1/1   | 0.93 | 0.06 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3002 | 1/1   | 0.93 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3073 | 1/1   | 0.93 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3359 | 1/1   | 0.93 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3647 | 1/1   | 0.93 | 0.16 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3010 | 1/1   | 0.93 | 0.13 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3748 | 1/1   | 0.93 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3651 | 1/1   | 0.93 | 0.08 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1778 | 1/1   | 0.93 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3211 | 1/1   | 0.93 | 0.26 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3299 | 1/1   | 0.93 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3655 | 1/1   | 0.93 | 0.12 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3967 | 1/1   | 0.93 | 0.15 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3968 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3595 | 1/1   | 0.93 | 0.26 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3219 | 1/1   | 0.93 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | 1Q    | 204  | 1/1   | 0.93 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 1R    | 204  | 1/1   | 0.93 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3412 | 1/1   | 0.93 | 0.14 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3972 | 1/1   | 0.93 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3665 | 1/1   | 0.93 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3253 | 1/1   | 0.93 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3254 | 1/1   | 0.93 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3042 | 1/1   | 0.93 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3154 | 1/1   | 0.93 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3044 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 3105 | 1/1   | 0.93 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3449 | 1/1   | 0.93 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1680 | 1/1   | 0.93 | 0.19 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3303 | 1/1   | 0.93 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1794 | 1/1   | 0.93 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3110 | 1/1   | 0.93 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3122 | 1/1   | 0.93 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 1V    | 205  | 1/1   | 0.93 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3247 | 1/1   | 0.93 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1686 | 1/1   | 0.93 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3473 | 1/1   | 0.93 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3054 | 1/1   | 0.93 | 0.25 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3460 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3055 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3056 | 1/1   | 0.93 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3687 | 1/1   | 0.93 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3262 | 1/1   | 0.93 | 0.28 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1690 | 1/1   | 0.93 | 0.20 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3053 | 1/1   | 0.93 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 2a    | 3133 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1X    | 101  | 1/1   | 0.93 | 0.09 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3130 | 1/1   | 0.93 | 0.22 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3769 | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3139 | 1/1   | 0.93 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | 2a    | 3141 | 1/1   | 0.93 | 0.21 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3316 | 1/1   | 0.93 | 0.11 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1810 | 1/1   | 0.93 | 0.08 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3551 | 1/1   | 0.93 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3148 | 1/1   | 0.93 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3151 | 1/1   | 0.93 | 0.07 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3485 | 1/1   | 0.93 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3478 | 1/1   | 0.93 | 0.08 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3774 | 1/1   | 0.93 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3993 | 1/1   | 0.93 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3289 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3710 | 1/1   | 0.93 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3290 | 1/1   | 0.93 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3291 | 1/1   | 0.93 | 0.13 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3294 | 1/1   | 0.93 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1701 | 1/1   | 0.93 | 0.43 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3487 | 1/1   | 0.93 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3892 | 1/1   | 0.93 | 0.22 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3164 | 1/1   | 0.93 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3169 | 1/1   | 0.93 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3093 | 1/1   | 0.93 | 0.17 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3725 | 1/1   | 0.93 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3727 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1705 | 1/1   | 0.93 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1822 | 1/1   | 0.93 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3310 | 1/1   | 0.93 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3172 | 1/1   | 0.93 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3689 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3434 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3561 | 1/1   | 0.93 | 0.12 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3493 | 1/1   | 0.93 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1715 | 1/1   | 0.93 | 0.26 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3379 | 1/1   | 0.93 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3112 | 1/1   | 0.93 | 0.44 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3273 | 1/1   | 0.93 | 0.25 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3702 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3704 | 1/1   | 0.93 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3385 | 1/1   | 0.93 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3337 | 1/1   | 0.93 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3513 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3715 | 1/1   | 0.93 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3515 | 1/1   | 0.93 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1610 | 1/1   | 0.93 | 0.25 | 59,59,59,59                 | 0     |
| 54  | MG   | 2E    | 304  | 1/1   | 0.93 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3386 | 1/1   | 0.93 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3254 | 1/1   | 0.94 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3221 | 1/1   | 0.94 | 0.28 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3487 | 1/1   | 0.94 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3358 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3479 | 1/1   | 0.94 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1606 | 1/1   | 0.94 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3416 | 1/1   | 0.94 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3734 | 1/1   | 0.94 | 0.13 | 65,65,65,65                 | 0     |
| 54  | MG   | 2D    | 305  | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2D    | 307  | 1/1   | 0.94 | 0.21 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3272 | 1/1   | 0.94 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3495 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 1a    | 1609 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3226 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3277 | 1/1   | 0.94 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 2E    | 303  | 1/1   | 0.94 | 0.44 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1769 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | 1a    | 1770 | 1/1   | 0.94 | 0.28 | 65,65,65,65                 | 0     |
| 54  | MG   | 1a    | 1771 | 1/1   | 0.94 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3289 | 1/1   | 0.94 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3283 | 1/1   | 0.94 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3287 | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1616 | 1/1   | 0.94 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3362 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3490 | 1/1   | 0.94 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3293 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3173 | 1/1   | 0.94 | 0.21 | 42,42,42,42                 | 0     |
| 54  | MG   | 2R    | 201  | 1/1   | 0.94 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3858 | 1/1   | 0.94 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3512 | 1/1   | 0.94 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3862 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3066 | 1/1   | 0.94 | 0.08 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3641 | 1/1   | 0.94 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3364 | 1/1   | 0.94 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3518 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3868 | 1/1   | 0.94 | 0.07 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3294 | 1/1   | 0.94 | 0.18 | 38,38,38,38                 | 0     |
| 54  | MG   | 20    | 103  | 1/1   | 0.94 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3745 | 1/1   | 0.94 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3139 | 1/1   | 0.94 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3176 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | 1a    | 1639 | 1/1   | 0.94 | 0.12 | 73,73,73,73                 | 0     |
| 54  | MG   | 1A    | 3431 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3751 | 1/1   | 0.94 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3006 | 1/1   | 0.94 | 0.13 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3320 | 1/1   | 0.94 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | 1B    | 212  | 1/1   | 0.94 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3534 | 1/1   | 0.94 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3648 | 1/1   | 0.94 | 0.42 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3234 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3090 | 1/1   | 0.94 | 0.17 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3178 | 1/1   | 0.94 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3327 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3330 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3551 | 1/1   | 0.94 | 0.08 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3143 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3553 | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3332 | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3556 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3180 | 1/1   | 0.94 | 0.19 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3027 | 1/1   | 0.94 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1797 | 1/1   | 0.94 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | 1a    | 1651 | 1/1   | 0.94 | 0.33 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3372 | 1/1   | 0.94 | 0.20 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1800 | 1/1   | 0.94 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3888 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3101 | 1/1   | 0.94 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3659 | 1/1   | 0.94 | 0.34 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3106 | 1/1   | 0.94 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3008 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3896 | 1/1   | 0.94 | 0.06 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3509 | 1/1   | 0.94 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3898 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3578 | 1/1   | 0.94 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2a    | 3042 | 1/1   | 0.94 | 0.13 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1661 | 1/1   | 0.94 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3092 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3443 | 1/1   | 0.94 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | 1a    | 1664 | 1/1   | 0.94 | 0.29 | 75,75,75,75                 | 0     |
| 54  | MG   | 2A    | 3365 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3591 | 1/1   | 0.94 | 0.11 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3591 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3592 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3669 | 1/1   | 0.94 | 0.14 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3516 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3370 | 1/1   | 0.94 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3601 | 1/1   | 0.94 | 0.11 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3906 | 1/1   | 0.94 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3772 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3134 | 1/1   | 0.94 | 0.14 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3012 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | 1D    | 316  | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3100 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1674 | 1/1   | 0.94 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3001 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3617 | 1/1   | 0.94 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | 1E    | 308  | 1/1   | 0.94 | 0.14 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3261 | 1/1   | 0.94 | 0.14 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3621 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3777 | 1/1   | 0.94 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3623 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3149 | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3150 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3151 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1F    | 305  | 1/1   | 0.94 | 0.21 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3153 | 1/1   | 0.94 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3193 | 1/1   | 0.94 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3779 | 1/1   | 0.94 | 0.13 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3523 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3682 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3395 | 1/1   | 0.94 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1685 | 1/1   | 0.94 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3265 | 1/1   | 0.94 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | 2a    | 3087 | 1/1   | 0.94 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3399 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3791 | 1/1   | 0.94 | 0.13 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1F    | 317  | 1/1   | 0.94 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3091 | 1/1   | 0.94 | 0.34 | 62,62,62,62                 | 0     |
| 54  | MG   | 1H    | 201  | 1/1   | 0.94 | 0.11 | 70,70,70,70                 | 0     |
| 54  | MG   | 1N    | 202  | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3645 | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3390 | 1/1   | 0.94 | 0.05 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3793 | 1/1   | 0.94 | 0.18 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3686 | 1/1   | 0.94 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3527 | 1/1   | 0.94 | 0.11 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3161 | 1/1   | 0.94 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3801 | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3174 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 1R    | 202  | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3691 | 1/1   | 0.94 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3128 | 1/1   | 0.94 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3035 | 1/1   | 0.94 | 0.11 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3540 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1T    | 203  | 1/1   | 0.94 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1859 | 1/1   | 0.94 | 0.07 | 70,70,70,70                 | 0     |
| 54  | MG   | 2A    | 3418 | 1/1   | 0.94 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3397 | 1/1   | 0.94 | 0.10 | 29,29,29,29                 | 0     |
| 54  | MG   | 1a    | 1706 | 1/1   | 0.94 | 0.25 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3323 | 1/1   | 0.94 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | 1T    | 206  | 1/1   | 0.94 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3667 | 1/1   | 0.94 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 1U    | 201  | 1/1   | 0.94 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3948 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 3123 | 1/1   | 0.94 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 1a    | 1713 | 1/1   | 0.94 | 0.23 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3193 | 1/1   | 0.94 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3949 | 1/1   | 0.94 | 0.06 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3326 | 1/1   | 0.94 | 0.05 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3434 | 1/1   | 0.94 | 0.07 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3197 | 1/1   | 0.94 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3205 | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | 1d    | 304  | 1/1   | 0.94 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3619 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 1e    | 201  | 1/1   | 0.94 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3440 | 1/1   | 0.94 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3708 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1g    | 201  | 1/1   | 0.94 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | 1W    | 205  | 1/1   | 0.94 | 0.20 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3959 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3210 | 1/1   | 0.94 | 0.23 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3818 | 1/1   | 0.94 | 0.11 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3689 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3961 | 1/1   | 0.94 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3694 | 1/1   | 0.94 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 10    | 101  | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1729 | 1/1   | 0.94 | 0.08 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3820 | 1/1   | 0.94 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 10    | 103  | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 10    | 104  | 1/1   | 0.94 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3712 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3085 | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3825 | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3231 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3346 | 1/1   | 0.94 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3461 | 1/1   | 0.94 | 0.08 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3233 | 1/1   | 0.94 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3408 | 1/1   | 0.94 | 0.12 | 29,29,29,29                 | 0     |
| 54  | MG   | 2a    | 3171 | 1/1   | 0.94 | 0.27 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3549 | 1/1   | 0.94 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3237 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1744 | 1/1   | 0.94 | 0.16 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3468 | 1/1   | 0.94 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | 2A    | 3008 | 1/1   | 0.94 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 2a    | 3177 | 1/1   | 0.94 | 0.14 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3832 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3471 | 1/1   | 0.94 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | 15    | 106  | 1/1   | 0.94 | 0.30 | 74,74,74,74                 | 0     |
| 54  | MG   | 2A    | 3723 | 1/1   | 0.94 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3724 | 1/1   | 0.94 | 0.32 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3474 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3211 | 1/1   | 0.94 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG   | 15    | 109  | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 17    | 104  | 1/1   | 0.94 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3975 | 1/1   | 0.94 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG   | 18    | 102  | 1/1   | 0.94 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3171 | 1/1   | 0.94 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | 2B    | 206  | 1/1   | 0.94 | 0.14 | 84,84,84,84                 | 0     |
| 54  | MG   | 1A    | 3050 | 1/1   | 0.94 | 0.23 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3843 | 1/1   | 0.94 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3467 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3063 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3347 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3333 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3335 | 1/1   | 0.95 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | 2F    | 301  | 1/1   | 0.95 | 0.27 | 46,46,46,46                 | 0     |
| 54  | MG   | 1U    | 205  | 1/1   | 0.95 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | 2F    | 303  | 1/1   | 0.95 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3037 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3236 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3410 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3542 | 1/1   | 0.95 | 0.13 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3343 | 1/1   | 0.95 | 0.16 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3344 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3125 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3141 | 1/1   | 0.95 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3129 | 1/1   | 0.95 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1831 | 1/1   | 0.95 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3727 | 1/1   | 0.95 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3135 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3351 | 1/1   | 0.95 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3137 | 1/1   | 0.95 | 0.16 | 59,59,59,59                 | 0     |
| 54  | MG   | 2W    | 201  | 1/1   | 0.95 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | 1W    | 202  | 1/1   | 0.95 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3354 | 1/1   | 0.95 | 0.14 | 28,28,28,28                 | 0     |
| 54  | MG   | 2A    | 3561 | 1/1   | 0.95 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3168 | 1/1   | 0.95 | 0.22 | 42,42,42,42                 | 0     |
| 54  | MG   | 23    | 101  | 1/1   | 0.95 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3357 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 27    | 102  | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3143 | 1/1   | 0.95 | 0.27 | 52,52,52,52                 | 0     |
| 54  | MG   | 2a    | 3001 | 1/1   | 0.95 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3478 | 1/1   | 0.95 | 0.06 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3840 | 1/1   | 0.95 | 0.08 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3415 | 1/1   | 0.95 | 0.05 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3573 | 1/1   | 0.95 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | 2A    | 3367 | 1/1   | 0.95 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3556 | 1/1   | 0.95 | 0.20 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3480 | 1/1   | 0.95 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3295 | 1/1   | 0.95 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 10    | 105  | 1/1   | 0.95 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3417 | 1/1   | 0.95 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3244 | 1/1   | 0.95 | 0.10 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3154 | 1/1   | 0.95 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 1a    | 1711 | 1/1   | 0.95 | 0.21 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3376 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3740 | 1/1   | 0.95 | 0.06 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3360 | 1/1   | 0.95 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 11    | 101  | 1/1   | 0.95 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3594 | 1/1   | 0.95 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 11    | 102  | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | 1a    | 1716 | 1/1   | 0.95 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3161 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3598 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3383 | 1/1   | 0.95 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3603 | 1/1   | 0.95 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 11    | 103  | 1/1   | 0.95 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3605 | 1/1   | 0.95 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | 1a    | 1718 | 1/1   | 0.95 | 0.13 | 78,78,78,78                 | 0     |
| 54  | MG   | 1A    | 3108 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1721 | 1/1   | 0.95 | 0.15 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3197 | 1/1   | 0.95 | 0.34 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3170 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | 13    | 103  | 1/1   | 0.95 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3614 | 1/1   | 0.95 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3568 | 1/1   | 0.95 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3123 | 1/1   | 0.95 | 0.25 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3052 | 1/1   | 0.95 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1d    | 301  | 1/1   | 0.95 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3573 | 1/1   | 0.95 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 17    | 102  | 1/1   | 0.95 | 0.17 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3650 | 1/1   | 0.95 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3049 | 1/1   | 0.95 | 0.29 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3752 | 1/1   | 0.95 | 0.08 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3753 | 1/1   | 0.95 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3182 | 1/1   | 0.95 | 0.35 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3495 | 1/1   | 0.95 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 19    | 102  | 1/1   | 0.95 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3150 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3576 | 1/1   | 0.95 | 0.22 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3187 | 1/1   | 0.95 | 0.11 | 50,50,50,50                 | 0     |
| 54  | MG   | 1h    | 202  | 1/1   | 0.95 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3151 | 1/1   | 0.95 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 1B    | 205  | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 1m    | 201  | 1/1   | 0.95 | 0.07 | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3093 | 1/1   | 0.95 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3264 | 1/1   | 0.95 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | 1n    | 103  | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3642 | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3435 | 1/1   | 0.95 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3177 | 1/1   | 0.95 | 0.22 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3883 | 1/1   | 0.95 | 0.19 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3504 | 1/1   | 0.95 | 0.09 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3312 | 1/1   | 0.95 | 0.30 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3313 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3649 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 3075 | 1/1   | 0.95 | 0.43 | 68,68,68,68                 | 0     |
| 54  | MG   | 1a    | 1754 | 1/1   | 0.95 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3315 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 1a    | 1756 | 1/1   | 0.95 | 0.11 | 71,71,71,71                 | 0     |
| 54  | MG   | 1A    | 3511 | 1/1   | 0.95 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | 1a    | 1622 | 1/1   | 0.95 | 0.18 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3894 | 1/1   | 0.95 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3213 | 1/1   | 0.95 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3014 | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3214 | 1/1   | 0.95 | 0.21 | 53,53,53,53                 | 0     |
| 54  | MG   | 1a    | 1761 | 1/1   | 0.95 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1B    | 222  | 1/1   | 0.95 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | 1a    | 1628 | 1/1   | 0.95 | 0.21 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3023 | 1/1   | 0.95 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3673 | 1/1   | 0.95 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3225 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3226 | 1/1   | 0.95 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3513 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 2a    | 3094 | 1/1   | 0.95 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3030 | 1/1   | 0.95 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3094 | 1/1   | 0.95 | 0.21 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1767 | 1/1   | 0.95 | 0.13 | 71,71,71,71                 | 0     |
| 54  | MG   | 1a    | 1632 | 1/1   | 0.95 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3593 | 1/1   | 0.95 | 0.18 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3036 | 1/1   | 0.95 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3038 | 1/1   | 0.95 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | 2a    | 3103 | 1/1   | 0.95 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3104 | 1/1   | 0.95 | 0.07 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3039 | 1/1   | 0.95 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3240 | 1/1   | 0.95 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3678 | 1/1   | 0.95 | 0.10 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1635 | 1/1   | 0.95 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3378 | 1/1   | 0.95 | 0.05 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3047 | 1/1   | 0.95 | 0.32 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3224 | 1/1   | 0.95 | 0.22 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3157 | 1/1   | 0.95 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3780 | 1/1   | 0.95 | 0.26 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3228 | 1/1   | 0.95 | 0.24 | 52,52,52,52                 | 0     |
| 54  | MG   | 1D    | 311  | 1/1   | 0.95 | 0.21 | 45,45,45,45                 | 0     |
| 54  | MG   | 2a    | 3116 | 1/1   | 0.95 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3687 | 1/1   | 0.95 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3784 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3051 | 1/1   | 0.95 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | 2A    | 3690 | 1/1   | 0.95 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3918 | 1/1   | 0.95 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3693 | 1/1   | 0.95 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3785 | 1/1   | 0.95 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3920 | 1/1   | 0.95 | 0.09 | 68,68,68,68                 | 0     |
| 54  | MG   | 1A    | 3788 | 1/1   | 0.95 | 0.11 | 58,58,58,58                 | 0     |
| 54  | MG   | 2a    | 3128 | 1/1   | 0.95 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG   | 2a    | 3130 | 1/1   | 0.95 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3278 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3698 | 1/1   | 0.95 | 0.08 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3259 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3260 | 1/1   | 0.95 | 0.33 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3261 | 1/1   | 0.95 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3282 | 1/1   | 0.95 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3329 | 1/1   | 0.95 | 0.11 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3331 | 1/1   | 0.95 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1657 | 1/1   | 0.95 | 0.24 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3273 | 1/1   | 0.95 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3150 | 1/1   | 0.95 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | 2A    | 3708 | 1/1   | 0.95 | 0.07 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3067 | 1/1   | 0.95 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3275 | 1/1   | 0.95 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | 2A    | 3711 | 1/1   | 0.95 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3068 | 1/1   | 0.95 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3182 | 1/1   | 0.95 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3694 | 1/1   | 0.95 | 0.20 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3715 | 1/1   | 0.95 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3695 | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3800 | 1/1   | 0.95 | 0.08 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3529 | 1/1   | 0.95 | 0.06 | 40,40,40,40                 | 0     |

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| Mol | Type  | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|-------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG    | 2A    | 3719 | 1/1   | 0.95 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG    | 1F    | 315  | 1/1   | 0.95 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG    | 1A    | 3335 | 1/1   | 0.95 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG    | 2A    | 3288 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG    | 1A    | 3938 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG    | 1G    | 202  | 1/1   | 0.95 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG    | 1A    | 3699 | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG    | 1A    | 3535 | 1/1   | 0.95 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG    | 1a    | 1802 | 1/1   | 0.95 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG    | 1a    | 1669 | 1/1   | 0.95 | 0.16 | 69,69,69,69                 | 0     |
| 54  | MG    | 1A    | 3336 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG    | 1A    | 3537 | 1/1   | 0.95 | 0.27 | 61,61,61,61                 | 0     |
| 54  | MG    | 1A    | 3809 | 1/1   | 0.95 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG    | 1A    | 3810 | 1/1   | 0.95 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG    | 1Q    | 201  | 1/1   | 0.95 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG    | 1A    | 3538 | 1/1   | 0.95 | 0.21 | 36,36,36,36                 | 0     |
| 54  | MG    | 2B    | 210  | 1/1   | 0.95 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG    | 2a    | 3180 | 1/1   | 0.95 | 0.18 | 65,65,65,65                 | 0     |
| 54  | MG    | 1Q    | 203  | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG    | 1A    | 3706 | 1/1   | 0.95 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG    | 1A    | 3707 | 1/1   | 0.95 | 0.08 | 57,57,57,57                 | 0     |
| 54  | MG    | 1A    | 3342 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG    | 1A    | 3950 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG    | 1A    | 3951 | 1/1   | 0.95 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG    | 2B    | 218  | 1/1   | 0.95 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG    | 2t    | 201  | 1/1   | 0.95 | 0.12 | 49,49,49,49                 | 0     |
| 55  | A1AE1 | 2A    | 3726 | 76/76 | 0.95 | 0.11 | 38,48,54,60                 | 0     |
| 54  | MG    | 2A    | 3107 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG    | 2A    | 3108 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG    | 1a    | 1818 | 1/1   | 0.95 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG    | 1A    | 3710 | 1/1   | 0.95 | 0.07 | 58,58,58,58                 | 0     |
| 57  | MPD   | 18    | 103  | 8/8   | 0.95 | 0.12 | 36,45,46,51                 | 0     |
| 54  | MG    | 1A    | 3158 | 1/1   | 0.95 | 0.31 | 57,57,57,57                 | 0     |
| 54  | MG    | 2A    | 3114 | 1/1   | 0.95 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG    | 1A    | 3819 | 1/1   | 0.95 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG    | 2V    | 202  | 1/1   | 0.96 | 0.29 | 49,49,49,49                 | 0     |
| 54  | MG    | 1A    | 3045 | 1/1   | 0.96 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG    | 1A    | 3190 | 1/1   | 0.96 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG    | 1A    | 3954 | 1/1   | 0.96 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG    | 2A    | 3198 | 1/1   | 0.96 | 0.21 | 43,43,43,43                 | 0     |
| 54  | MG    | 2A    | 3199 | 1/1   | 0.96 | 0.23 | 48,48,48,48                 | 0     |
| 54  | MG    | 1A    | 3064 | 1/1   | 0.96 | 0.22 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1R    | 203  | 1/1   | 0.96 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3956 | 1/1   | 0.96 | 0.05 | 50,50,50,50                 | 0     |
| 54  | MG   | 27    | 101  | 1/1   | 0.96 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3570 | 1/1   | 0.96 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3392 | 1/1   | 0.96 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3593 | 1/1   | 0.96 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3068 | 1/1   | 0.96 | 0.26 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3839 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3206 | 1/1   | 0.96 | 0.16 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3194 | 1/1   | 0.96 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3397 | 1/1   | 0.96 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3841 | 1/1   | 0.96 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3963 | 1/1   | 0.96 | 0.12 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3842 | 1/1   | 0.96 | 0.06 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3307 | 1/1   | 0.96 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 2A    | 3606 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3654 | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3430 | 1/1   | 0.96 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3216 | 1/1   | 0.96 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3017 | 1/1   | 0.96 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3747 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1681 | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3308 | 1/1   | 0.96 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3657 | 1/1   | 0.96 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3577 | 1/1   | 0.96 | 0.08 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3973 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3196 | 1/1   | 0.96 | 0.31 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3059 | 1/1   | 0.96 | 0.32 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3059 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3259 | 1/1   | 0.96 | 0.08 | 67,67,67,67                 | 0     |
| 54  | MG   | 2A    | 3064 | 1/1   | 0.96 | 0.28 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3070 | 1/1   | 0.96 | 0.24 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3507 | 1/1   | 0.96 | 0.06 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3098 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1693 | 1/1   | 0.96 | 0.17 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3071 | 1/1   | 0.96 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3629 | 1/1   | 0.96 | 0.05 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3239 | 1/1   | 0.96 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3631 | 1/1   | 0.96 | 0.06 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3072 | 1/1   | 0.96 | 0.36 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3133 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3424 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3134 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3044 | 1/1   | 0.96 | 0.13 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3428 | 1/1   | 0.96 | 0.05 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3429 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3207 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3075 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3640 | 1/1   | 0.96 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3078 | 1/1   | 0.96 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3764 | 1/1   | 0.96 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3987 | 1/1   | 0.96 | 0.17 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3248 | 1/1   | 0.96 | 0.05 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3588 | 1/1   | 0.96 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3766 | 1/1   | 0.96 | 0.14 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3076 | 1/1   | 0.96 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3106 | 1/1   | 0.96 | 0.17 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3087 | 1/1   | 0.96 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3677 | 1/1   | 0.96 | 0.23 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3877 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | 2A    | 3443 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3995 | 1/1   | 0.96 | 0.08 | 57,57,57,57                 | 0     |
| 54  | MG   | 2A    | 3257 | 1/1   | 0.96 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3382 | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3679 | 1/1   | 0.96 | 0.07 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3383 | 1/1   | 0.96 | 0.08 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3174 | 1/1   | 0.96 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | 15    | 107  | 1/1   | 0.96 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3265 | 1/1   | 0.96 | 0.38 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 3071 | 1/1   | 0.96 | 0.12 | 60,60,60,60                 | 0     |
| 54  | MG   | 1a    | 1835 | 1/1   | 0.96 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3267 | 1/1   | 0.96 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3884 | 1/1   | 0.96 | 0.05 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3271 | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3457 | 1/1   | 0.96 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3327 | 1/1   | 0.96 | 0.08 | 14,14,14,14                 | 0     |
| 54  | MG   | 1a    | 1838 | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1839 | 1/1   | 0.96 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3105 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3275 | 1/1   | 0.96 | 0.35 | 43,43,43,43                 | 0     |
| 54  | MG   | 17    | 103  | 1/1   | 0.96 | 0.19 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3452 | 1/1   | 0.96 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3453 | 1/1   | 0.96 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 1B    | 209  | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1720 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3215 | 1/1   | 0.96 | 0.27 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3601 | 1/1   | 0.96 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3526 | 1/1   | 0.96 | 0.25 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3455 | 1/1   | 0.96 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3456 | 1/1   | 0.96 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3532 | 1/1   | 0.96 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3219 | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3534 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3789 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3296 | 1/1   | 0.96 | 0.06 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3393 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3299 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3301 | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3691 | 1/1   | 0.96 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | 1a    | 1732 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3107 | 1/1   | 0.96 | 0.24 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3131 | 1/1   | 0.96 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3488 | 1/1   | 0.96 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3614 | 1/1   | 0.96 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3306 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3462 | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1737 | 1/1   | 0.96 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | 1a    | 1615 | 1/1   | 0.96 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | 1A    | 3703 | 1/1   | 0.96 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3313 | 1/1   | 0.96 | 0.06 | 57,57,57,57                 | 0     |
| 54  | MG   | 1a    | 1741 | 1/1   | 0.96 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3004 | 1/1   | 0.96 | 0.08 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1618 | 1/1   | 0.96 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3319 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1a    | 1619 | 1/1   | 0.96 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3913 | 1/1   | 0.96 | 0.06 | 81,81,81,81                 | 0     |
| 54  | MG   | 1A    | 3915 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3337 | 1/1   | 0.96 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3799 | 1/1   | 0.96 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | 1e    | 202  | 1/1   | 0.96 | 0.09 | 68,68,68,68                 | 0     |
| 54  | MG   | 2A    | 3506 | 1/1   | 0.96 | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | 2a    | 3126 | 1/1   | 0.96 | 0.10 | 63,63,63,63                 | 0     |
| 54  | MG   | 2A    | 3326 | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3339 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3328 | 1/1   | 0.96 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3399 | 1/1   | 0.96 | 0.06 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3341 | 1/1   | 0.96 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3079 | 1/1   | 0.96 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3924 | 1/1   | 0.96 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3114 | 1/1   | 0.96 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG   | 1l    | 201  | 1/1   | 0.96 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3713 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 2a    | 3144 | 1/1   | 0.96 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | 2A    | 3338 | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3714 | 1/1   | 0.96 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | 1E    | 306  | 1/1   | 0.96 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3406 | 1/1   | 0.96 | 0.08 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3930 | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3523 | 1/1   | 0.96 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3344 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3932 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3528 | 1/1   | 0.96 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3286 | 1/1   | 0.96 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1642 | 1/1   | 0.96 | 0.16 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3227 | 1/1   | 0.96 | 0.13 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3080 | 1/1   | 0.96 | 0.25 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3081 | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3048 | 1/1   | 0.96 | 0.21 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3537 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | 2B    | 216  | 1/1   | 0.96 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3170 | 1/1   | 0.96 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | 2A    | 3540 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3171 | 1/1   | 0.96 | 0.14 | 56,56,56,56                 | 0     |
| 54  | MG   | 2D    | 304  | 1/1   | 0.96 | 0.22 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3543 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3356 | 1/1   | 0.96 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3183 | 1/1   | 0.96 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3359 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3548 | 1/1   | 0.96 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3355 | 1/1   | 0.96 | 0.06 | 18,18,18,18                 | 0     |
| 54  | MG   | 2A    | 3005 | 1/1   | 0.96 | 0.10 | 55,55,55,55                 | 0     |
| 54  | MG   | 2A    | 3006 | 1/1   | 0.96 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3176 | 1/1   | 0.96 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3481 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3044 | 1/1   | 0.96 | 0.04 | 33,33,33,33                 | 0     |
| 54  | MG   | 2a    | 3179 | 1/1   | 0.96 | 0.08 | 82,82,82,82                 | 0     |
| 54  | MG   | 1G    | 203  | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 2a    | 3181 | 1/1   | 0.96 | 0.14 | 57,57,57,57                 | 0     |

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| Mol | Type  | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|-------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG    | 2A    | 3013 | 1/1   | 0.96 | 0.06 | 22,22,22,22                 | 0     |
| 54  | MG    | 1A    | 3119 | 1/1   | 0.96 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG    | 1H    | 202  | 1/1   | 0.96 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG    | 2A    | 3562 | 1/1   | 0.96 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG    | 1N    | 201  | 1/1   | 0.96 | 0.14 | 43,43,43,43                 | 0     |
| 54  | MG    | 2O    | 3701 | 1/1   | 0.96 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG    | 2A    | 3018 | 1/1   | 0.96 | 0.21 | 46,46,46,46                 | 0     |
| 54  | MG    | 2A    | 3019 | 1/1   | 0.96 | 0.25 | 50,50,50,50                 | 0     |
| 55  | A1AE1 | 1A    | 3996 | 76/76 | 0.96 | 0.09 | 21,36,46,56                 | 0     |
| 54  | MG    | 1A    | 3824 | 1/1   | 0.96 | 0.16 | 38,38,38,38                 | 0     |
| 54  | MG    | 1A    | 3156 | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG    | 1A    | 3419 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 54  | MG    | 2A    | 3572 | 1/1   | 0.96 | 0.08 | 54,54,54,54                 | 0     |
| 54  | MG    | 2T    | 201  | 1/1   | 0.96 | 0.28 | 65,65,65,65                 | 0     |
| 54  | MG    | 1A    | 3187 | 1/1   | 0.96 | 0.17 | 41,41,41,41                 | 0     |
| 54  | MG    | 2A    | 3026 | 1/1   | 0.96 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG    | 1A    | 3240 | 1/1   | 0.96 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG    | 1A    | 3831 | 1/1   | 0.96 | 0.06 | 57,57,57,57                 | 0     |
| 54  | MG    | 2A    | 3178 | 1/1   | 0.97 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG    | 1A    | 3531 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG    | 1A    | 3604 | 1/1   | 0.97 | 0.08 | 23,23,23,23                 | 0     |
| 54  | MG    | 1a    | 1613 | 1/1   | 0.97 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG    | 1a    | 1614 | 1/1   | 0.97 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG    | 1A    | 3046 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 54  | MG    | 2A    | 3009 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG    | 1A    | 3022 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG    | 2A    | 3011 | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 54  | MG    | 1A    | 3229 | 1/1   | 0.97 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG    | 1A    | 3907 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG    | 1A    | 3908 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG    | 2A    | 3582 | 1/1   | 0.97 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG    | 1A    | 3609 | 1/1   | 0.97 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG    | 1A    | 3230 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG    | 1A    | 3404 | 1/1   | 0.97 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG    | 1a    | 1624 | 1/1   | 0.97 | 0.09 | 47,47,47,47                 | 0     |
| 54  | MG    | 2A    | 3021 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 54  | MG    | 2A    | 3389 | 1/1   | 0.97 | 0.12 | 43,43,43,43                 | 0     |
| 54  | MG    | 1A    | 3794 | 1/1   | 0.97 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG    | 1a    | 1626 | 1/1   | 0.97 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG    | 1A    | 3099 | 1/1   | 0.97 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG    | 1D    | 302  | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG    | 2a    | 3010 | 1/1   | 0.97 | 0.06 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3914 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG   | 1D    | 305  | 1/1   | 0.97 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1D    | 307  | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3189 | 1/1   | 0.97 | 0.20 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1633 | 1/1   | 0.97 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | 1D    | 310  | 1/1   | 0.97 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3035 | 1/1   | 0.97 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3917 | 1/1   | 0.97 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 2A    | 3208 | 1/1   | 0.97 | 0.31 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3288 | 1/1   | 0.97 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3348 | 1/1   | 0.97 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3617 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1D    | 315  | 1/1   | 0.97 | 0.07 | 60,60,60,60                 | 0     |
| 54  | MG   | 2a    | 3025 | 1/1   | 0.97 | 0.12 | 56,56,56,56                 | 0     |
| 54  | MG   | 2a    | 3026 | 1/1   | 0.97 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | 2A    | 3615 | 1/1   | 0.97 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3349 | 1/1   | 0.97 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3127 | 1/1   | 0.97 | 0.19 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3215 | 1/1   | 0.97 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | 1E    | 303  | 1/1   | 0.97 | 0.25 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3045 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3803 | 1/1   | 0.97 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3474 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3023 | 1/1   | 0.97 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3711 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1647 | 1/1   | 0.97 | 0.18 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3235 | 1/1   | 0.97 | 0.21 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3227 | 1/1   | 0.97 | 0.34 | 50,50,50,50                 | 0     |
| 54  | MG   | 1a    | 1789 | 1/1   | 0.97 | 0.07 | 73,73,73,73                 | 0     |
| 54  | MG   | 1E    | 311  | 1/1   | 0.97 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | 1F    | 302  | 1/1   | 0.97 | 0.15 | 39,39,39,39                 | 0     |
| 54  | MG   | 1a    | 1652 | 1/1   | 0.97 | 0.08 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3928 | 1/1   | 0.97 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | 1F    | 306  | 1/1   | 0.97 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3425 | 1/1   | 0.97 | 0.08 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3192 | 1/1   | 0.97 | 0.21 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3060 | 1/1   | 0.97 | 0.08 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3061 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3547 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3026 | 1/1   | 0.97 | 0.27 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3104 | 1/1   | 0.97 | 0.20 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3065 | 1/1   | 0.97 | 0.17 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3717 | 1/1   | 0.97 | 0.04 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3935 | 1/1   | 0.97 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3105 | 1/1   | 0.97 | 0.12 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3069 | 1/1   | 0.97 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3719 | 1/1   | 0.97 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | 2a    | 3060 | 1/1   | 0.97 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | 1G    | 201  | 1/1   | 0.97 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3243 | 1/1   | 0.97 | 0.11 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3016 | 1/1   | 0.97 | 0.27 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3074 | 1/1   | 0.97 | 0.04 | 40,40,40,40                 | 0     |
| 54  | MG   | 1G    | 204  | 1/1   | 0.97 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3484 | 1/1   | 0.97 | 0.05 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3555 | 1/1   | 0.97 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3726 | 1/1   | 0.97 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | 2A    | 3447 | 1/1   | 0.97 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3823 | 1/1   | 0.97 | 0.06 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3246 | 1/1   | 0.97 | 0.21 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3486 | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3082 | 1/1   | 0.97 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3827 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3828 | 1/1   | 0.97 | 0.04 | 46,46,46,46                 | 0     |
| 54  | MG   | 2a    | 3076 | 1/1   | 0.97 | 0.24 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3263 | 1/1   | 0.97 | 0.18 | 58,58,58,58                 | 0     |
| 54  | MG   | 2A    | 3085 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3636 | 1/1   | 0.97 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3731 | 1/1   | 0.97 | 0.12 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3637 | 1/1   | 0.97 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | 2A    | 3269 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3422 | 1/1   | 0.97 | 0.05 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3200 | 1/1   | 0.97 | 0.18 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3138 | 1/1   | 0.97 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3563 | 1/1   | 0.97 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | 1A    | 3957 | 1/1   | 0.97 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3030 | 1/1   | 0.97 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3676 | 1/1   | 0.97 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1828 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3838 | 1/1   | 0.97 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3278 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3112 | 1/1   | 0.97 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3206 | 1/1   | 0.97 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3142 | 1/1   | 0.97 | 0.15 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3103 | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3104 | 1/1   | 0.97 | 0.27 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3284 | 1/1   | 0.97 | 0.04 | 51,51,51,51                 | 0     |
| 54  | MG   | 2A    | 3285 | 1/1   | 0.97 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | 1A    | 3260 | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | 1U    | 202  | 1/1   | 0.97 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3208 | 1/1   | 0.97 | 0.26 | 42,42,42,42                 | 0     |
| 54  | MG   | 1V    | 201  | 1/1   | 0.97 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1V    | 202  | 1/1   | 0.97 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3110 | 1/1   | 0.97 | 0.32 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3111 | 1/1   | 0.97 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3571 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3086 | 1/1   | 0.97 | 0.21 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3847 | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3652 | 1/1   | 0.97 | 0.17 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3300 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3653 | 1/1   | 0.97 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3700 | 1/1   | 0.97 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 1a    | 1844 | 1/1   | 0.97 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3263 | 1/1   | 0.97 | 0.23 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3087 | 1/1   | 0.97 | 0.27 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3088 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3122 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3374 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3309 | 1/1   | 0.97 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3505 | 1/1   | 0.97 | 0.08 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3375 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3977 | 1/1   | 0.97 | 0.21 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3128 | 1/1   | 0.97 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3319 | 1/1   | 0.97 | 0.12 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3130 | 1/1   | 0.97 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | 2a    | 3129 | 1/1   | 0.97 | 0.09 | 76,76,76,76                 | 0     |
| 54  | MG   | 2A    | 3316 | 1/1   | 0.97 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3859 | 1/1   | 0.97 | 0.04 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3318 | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3661 | 1/1   | 0.97 | 0.06 | 64,64,64,64                 | 0     |
| 54  | MG   | 2a    | 3137 | 1/1   | 0.97 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3133 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1710 | 1/1   | 0.97 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | 2a    | 3140 | 1/1   | 0.97 | 0.06 | 72,72,72,72                 | 0     |
| 54  | MG   | 2A    | 3720 | 1/1   | 0.97 | 0.07 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3441 | 1/1   | 0.97 | 0.04 | 27,27,27,27                 | 0     |
| 54  | MG   | 2a    | 3143 | 1/1   | 0.97 | 0.07 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1857 | 1/1   | 0.97 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | 1A    | 3018 | 1/1   | 0.97 | 0.18 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3983 | 1/1   | 0.97 | 0.23 | 41,41,41,41                 | 0     |
| 54  | MG   | 2a    | 3147 | 1/1   | 0.97 | 0.08 | 77,77,77,77                 | 0     |
| 54  | MG   | 2A    | 3516 | 1/1   | 0.97 | 0.06 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3055 | 1/1   | 0.97 | 0.04 | 49,49,49,49                 | 0     |
| 54  | MG   | 1a    | 1861 | 1/1   | 0.97 | 0.07 | 78,78,78,78                 | 0     |
| 54  | MG   | 2A    | 3142 | 1/1   | 0.97 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3666 | 1/1   | 0.97 | 0.05 | 61,61,61,61                 | 0     |
| 54  | MG   | 2A    | 3144 | 1/1   | 0.97 | 0.24 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3762 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3268 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3524 | 1/1   | 0.97 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3525 | 1/1   | 0.97 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3380 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3514 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3990 | 1/1   | 0.97 | 0.08 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3218 | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3339 | 1/1   | 0.97 | 0.06 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3325 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 54  | MG   | 15    | 102  | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | 2A    | 3533 | 1/1   | 0.97 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3181 | 1/1   | 0.97 | 0.18 | 45,45,45,45                 | 0     |
| 54  | MG   | 15    | 104  | 1/1   | 0.97 | 0.27 | 39,39,39,39                 | 0     |
| 54  | MG   | 15    | 105  | 1/1   | 0.97 | 0.21 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3538 | 1/1   | 0.97 | 0.06 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3674 | 1/1   | 0.97 | 0.19 | 52,52,52,52                 | 0     |
| 54  | MG   | 2D    | 306  | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3384 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3541 | 1/1   | 0.97 | 0.05 | 59,59,59,59                 | 0     |
| 54  | MG   | 1A    | 3590 | 1/1   | 0.97 | 0.23 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3881 | 1/1   | 0.97 | 0.04 | 20,20,20,20                 | 0     |
| 54  | MG   | 1A    | 3020 | 1/1   | 0.97 | 0.27 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3153 | 1/1   | 0.97 | 0.21 | 42,42,42,42                 | 0     |
| 54  | MG   | 2E    | 301  | 1/1   | 0.97 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3352 | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3073 | 1/1   | 0.97 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3332 | 1/1   | 0.97 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 18    | 101  | 1/1   | 0.97 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3034 | 1/1   | 0.97 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | 1a    | 1739 | 1/1   | 0.97 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | 2A    | 3554 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3279 | 1/1   | 0.97 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3891 | 1/1   | 0.97 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3280 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3281 | 1/1   | 0.97 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | 1B    | 211  | 1/1   | 0.97 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3895 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3528 | 1/1   | 0.97 | 0.05 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3338 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3564 | 1/1   | 0.97 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3782 | 1/1   | 0.97 | 0.15 | 48,48,48,48                 | 0     |
| 54  | MG   | 1B    | 216  | 1/1   | 0.97 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3568 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3530 | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 58  | ZN   | 2Y    | 501  | 1/1   | 0.97 | 0.05 | 91,91,91,91                 | 0     |
| 58  | ZN   | 24    | 501  | 1/1   | 0.97 | 0.15 | 122,122,122,122             | 0     |
| 54  | MG   | 1F    | 310  | 1/1   | 0.98 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3559 | 1/1   | 0.98 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3307 | 1/1   | 0.98 | 0.04 | 30,30,30,30                 | 0     |
| 54  | MG   | 2A    | 3007 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3067 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3006 | 1/1   | 0.98 | 0.05 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3124 | 1/1   | 0.98 | 0.23 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3214 | 1/1   | 0.98 | 0.19 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3340 | 1/1   | 0.98 | 0.06 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3736 | 1/1   | 0.98 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 2a    | 3032 | 1/1   | 0.98 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3834 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3479 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3015 | 1/1   | 0.98 | 0.14 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3646 | 1/1   | 0.98 | 0.04 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3488 | 1/1   | 0.98 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | 1a    | 1648 | 1/1   | 0.98 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | 1A    | 3051 | 1/1   | 0.98 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3020 | 1/1   | 0.98 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3660 | 1/1   | 0.98 | 0.06 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3277 | 1/1   | 0.98 | 0.06 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3216 | 1/1   | 0.98 | 0.16 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3015 | 1/1   | 0.98 | 0.12 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3345 | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3095 | 1/1   | 0.98 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3129 | 1/1   | 0.98 | 0.04 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3027 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3329 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3028 | 1/1   | 0.98 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3418 | 1/1   | 0.98 | 0.04 | 17,17,17,17                 | 0     |
| 54  | MG   | 1P    | 203  | 1/1   | 0.98 | 0.03 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3071 | 1/1   | 0.98 | 0.22 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3334 | 1/1   | 0.98 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3222 | 1/1   | 0.98 | 0.25 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3499 | 1/1   | 0.98 | 0.08 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3849 | 1/1   | 0.98 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3750 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3037 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3500 | 1/1   | 0.98 | 0.05 | 28,28,28,28                 | 0     |
| 54  | MG   | 1A    | 3131 | 1/1   | 0.98 | 0.08 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3225 | 1/1   | 0.98 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3352 | 1/1   | 0.98 | 0.04 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3969 | 1/1   | 0.98 | 0.03 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3097 | 1/1   | 0.98 | 0.23 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3664 | 1/1   | 0.98 | 0.12 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3857 | 1/1   | 0.98 | 0.15 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3072 | 1/1   | 0.98 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3038 | 1/1   | 0.98 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3759 | 1/1   | 0.98 | 0.05 | 47,47,47,47                 | 0     |
| 54  | MG   | 1a    | 1804 | 1/1   | 0.98 | 0.06 | 72,72,72,72                 | 0     |
| 54  | MG   | 1A    | 3865 | 1/1   | 0.98 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | 1U    | 203  | 1/1   | 0.98 | 0.24 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3196 | 1/1   | 0.98 | 0.28 | 50,50,50,50                 | 0     |
| 54  | MG   | 1U    | 204  | 1/1   | 0.98 | 0.22 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3074 | 1/1   | 0.98 | 0.14 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3291 | 1/1   | 0.98 | 0.22 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3292 | 1/1   | 0.98 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3510 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3057 | 1/1   | 0.98 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3101 | 1/1   | 0.98 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 1a    | 1813 | 1/1   | 0.98 | 0.04 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3028 | 1/1   | 0.98 | 0.24 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3140 | 1/1   | 0.98 | 0.23 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3103 | 1/1   | 0.98 | 0.17 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3040 | 1/1   | 0.98 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | 1W    | 203  | 1/1   | 0.98 | 0.13 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3594 | 1/1   | 0.98 | 0.22 | 36,36,36,36                 | 0     |
| 54  | MG   | 1a    | 1688 | 1/1   | 0.98 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | 1A    | 3298 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 2A    | 3536 | 1/1   | 0.98 | 0.04 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3029 | 1/1   | 0.98 | 0.19 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3145 | 1/1   | 0.98 | 0.23 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3681 | 1/1   | 0.98 | 0.22 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3078 | 1/1   | 0.98 | 0.25 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3882 | 1/1   | 0.98 | 0.04 | 43,43,43,43                 | 0     |
| 54  | MG   | 2a    | 3097 | 1/1   | 0.98 | 0.05 | 67,67,67,67                 | 0     |
| 54  | MG   | 1A    | 3147 | 1/1   | 0.98 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3239 | 1/1   | 0.98 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3885 | 1/1   | 0.98 | 0.06 | 54,54,54,54                 | 0     |
| 54  | MG   | 2A    | 3221 | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3546 | 1/1   | 0.98 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3222 | 1/1   | 0.98 | 0.09 | 43,43,43,43                 | 0     |
| 54  | MG   | 2A    | 3223 | 1/1   | 0.98 | 0.11 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3021 | 1/1   | 0.98 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3242 | 1/1   | 0.98 | 0.23 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3149 | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3889 | 1/1   | 0.98 | 0.05 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3058 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3229 | 1/1   | 0.98 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3690 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3110 | 1/1   | 0.98 | 0.23 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3309 | 1/1   | 0.98 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | 11    | 105  | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3310 | 1/1   | 0.98 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3086 | 1/1   | 0.98 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3236 | 1/1   | 0.98 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | 13    | 101  | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3013 | 1/1   | 0.98 | 0.08 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3786 | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3787 | 1/1   | 0.98 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 2A    | 3091 | 1/1   | 0.98 | 0.06 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3092 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3899 | 1/1   | 0.98 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3195 | 1/1   | 0.98 | 0.16 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3901 | 1/1   | 0.98 | 0.06 | 70,70,70,70                 | 0     |
| 54  | MG   | 2D    | 301  | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 2D    | 302  | 1/1   | 0.98 | 0.11 | 55,55,55,55                 | 0     |
| 54  | MG   | 1A    | 3251 | 1/1   | 0.98 | 0.20 | 49,49,49,49                 | 0     |
| 54  | MG   | 2a    | 3131 | 1/1   | 0.98 | 0.04 | 77,77,77,77                 | 0     |
| 54  | MG   | 1A    | 3697 | 1/1   | 0.98 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3314 | 1/1   | 0.98 | 0.08 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3613 | 1/1   | 0.98 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | 17    | 101  | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3700 | 1/1   | 0.98 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3252 | 1/1   | 0.98 | 0.07 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3032 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 1B    | 223  | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1724 | 1/1   | 0.98 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3584 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | 2E    | 302  | 1/1   | 0.98 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3083 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 54  | MG   | 2A    | 3587 | 1/1   | 0.98 | 0.05 | 57,57,57,57                 | 0     |
| 54  | MG   | 1A    | 3017 | 1/1   | 0.98 | 0.30 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3798 | 1/1   | 0.98 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3024 | 1/1   | 0.98 | 0.06 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3257 | 1/1   | 0.98 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3258 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3388 | 1/1   | 0.98 | 0.08 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3916 | 1/1   | 0.98 | 0.05 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3709 | 1/1   | 0.98 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3389 | 1/1   | 0.98 | 0.09 | 27,27,27,27                 | 0     |
| 54  | MG   | 2A    | 3599 | 1/1   | 0.98 | 0.05 | 24,24,24,24                 | 0     |
| 54  | MG   | 2A    | 3600 | 1/1   | 0.98 | 0.06 | 55,55,55,55                 | 0     |
| 54  | MG   | 1D    | 304  | 1/1   | 0.98 | 0.05 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3602 | 1/1   | 0.98 | 0.04 | 44,44,44,44                 | 0     |
| 54  | MG   | 2A    | 3268 | 1/1   | 0.98 | 0.14 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3025 | 1/1   | 0.98 | 0.21 | 38,38,38,38                 | 0     |
| 54  | MG   | 1D    | 306  | 1/1   | 0.98 | 0.10 | 20,20,20,20                 | 0     |
| 54  | MG   | 2A    | 3119 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3049 | 1/1   | 0.98 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3392 | 1/1   | 0.98 | 0.08 | 27,27,27,27                 | 0     |
| 54  | MG   | 1a    | 1612 | 1/1   | 0.98 | 0.13 | 31,31,31,31                 | 0     |
| 54  | MG   | 2A    | 3610 | 1/1   | 0.98 | 0.04 | 64,64,64,64                 | 0     |
| 54  | MG   | 1A    | 3808 | 1/1   | 0.98 | 0.03 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3203 | 1/1   | 0.98 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | 1A    | 3204 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3159 | 1/1   | 0.98 | 0.16 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3127 | 1/1   | 0.98 | 0.18 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3089 | 1/1   | 0.98 | 0.04 | 19,19,19,19                 | 0     |
| 54  | MG   | 1A    | 3630 | 1/1   | 0.98 | 0.06 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3618 | 1/1   | 0.98 | 0.04 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3330 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | 1A    | 3816 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 27    | 103  | 1/1   | 0.98 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | 1a    | 1750 | 1/1   | 0.98 | 0.06 | 63,63,63,63                 | 0     |
| 54  | MG   | 1E    | 302  | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3720 | 1/1   | 0.98 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3120 | 1/1   | 0.98 | 0.03 | 38,38,38,38                 | 0     |
| 54  | MG   | 2A    | 3136 | 1/1   | 0.98 | 0.08 | 40,40,40,40                 | 0     |
| 54  | MG   | 1A    | 3400 | 1/1   | 0.98 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 1E    | 307  | 1/1   | 0.98 | 0.05 | 46,46,46,46                 | 0     |
| 54  | MG   | 2A    | 3292 | 1/1   | 0.98 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3933 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3065 | 1/1   | 0.98 | 0.28 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3209 | 1/1   | 0.98 | 0.25 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3725 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 54  | MG   | 2A    | 3297 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3334 | 1/1   | 0.98 | 0.13 | 45,45,45,45                 | 0     |
| 54  | MG   | 1F    | 303  | 1/1   | 0.98 | 0.17 | 37,37,37,37                 | 0     |
| 54  | MG   | 2a    | 3015 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | 1A    | 3167 | 1/1   | 0.98 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3482 | 1/1   | 0.98 | 0.09 | 27,27,27,27                 | 0     |
| 54  | MG   | 1F    | 307  | 1/1   | 0.98 | 0.16 | 29,29,29,29                 | 0     |
| 54  | MG   | 1A    | 3639 | 1/1   | 0.98 | 0.08 | 39,39,39,39                 | 0     |
| 58  | ZN   | 14    | 501  | 1/1   | 0.98 | 0.07 | 110,110,110,110             | 0     |
| 54  | MG   | 2A    | 3465 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3004 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 58  | ZN   | 25    | 102  | 1/1   | 0.98 | 0.03 | 69,69,69,69                 | 0     |
| 58  | ZN   | 29    | 501  | 1/1   | 0.98 | 0.04 | 71,71,71,71                 | 0     |
| 58  | ZN   | 2n    | 501  | 1/1   | 0.98 | 0.05 | 90,90,90,90                 | 0     |
| 59  | SF4  | 1d    | 306  | 8/8   | 0.98 | 0.06 | 64,69,73,76                 | 0     |
| 59  | SF4  | 2d    | 501  | 8/8   | 0.98 | 0.06 | 68,78,83,88                 | 0     |
| 54  | MG   | 1E    | 304  | 1/1   | 0.99 | 0.14 | 36,36,36,36                 | 0     |
| 54  | MG   | 1A    | 3893 | 1/1   | 0.99 | 0.05 | 58,58,58,58                 | 0     |
| 54  | MG   | 1A    | 3394 | 1/1   | 0.99 | 0.05 | 24,24,24,24                 | 0     |
| 54  | MG   | 2E    | 305  | 1/1   | 0.99 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3844 | 1/1   | 0.99 | 0.08 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3667 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3465 | 1/1   | 0.99 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | 1A    | 3135 | 1/1   | 0.99 | 0.06 | 36,36,36,36                 | 0     |
| 54  | MG   | 2a    | 3132 | 1/1   | 0.99 | 0.06 | 70,70,70,70                 | 0     |
| 54  | MG   | 1A    | 3428 | 1/1   | 0.99 | 0.05 | 15,15,15,15                 | 0     |
| 54  | MG   | 2a    | 3134 | 1/1   | 0.99 | 0.10 | 54,54,54,54                 | 0     |
| 54  | MG   | 2F    | 304  | 1/1   | 0.99 | 0.22 | 48,48,48,48                 | 0     |
| 54  | MG   | 1F    | 301  | 1/1   | 0.99 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1a    | 1621 | 1/1   | 0.99 | 0.03 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3005 | 1/1   | 0.99 | 0.08 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3066 | 1/1   | 0.99 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG   | 1F    | 304  | 1/1   | 0.99 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3042 | 1/1   | 0.99 | 0.04 | 23,23,23,23                 | 0     |
| 54  | MG   | 1A    | 3126 | 1/1   | 0.99 | 0.25 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3433 | 1/1   | 0.99 | 0.03 | 28,28,28,28                 | 0     |
| 54  | MG   | 1F    | 308  | 1/1   | 0.99 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3009 | 1/1   | 0.99 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3003 | 1/1   | 0.99 | 0.03 | 27,27,27,27                 | 0     |
| 54  | MG   | 1A    | 3402 | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3084 | 1/1   | 0.99 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | 2a    | 3149 | 1/1   | 0.99 | 0.04 | 56,56,56,56                 | 0     |
| 54  | MG   | 1A    | 3554 | 1/1   | 0.99 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | 1A    | 3109 | 1/1   | 0.99 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | 2A    | 3471 | 1/1   | 0.99 | 0.07 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3860 | 1/1   | 0.99 | 0.03 | 46,46,46,46                 | 0     |
| 54  | MG   | 1B    | 217  | 1/1   | 0.99 | 0.04 | 47,47,47,47                 | 0     |
| 54  | MG   | 1A    | 3861 | 1/1   | 0.99 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | 2A    | 3549 | 1/1   | 0.99 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3262 | 1/1   | 0.99 | 0.35 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3144 | 1/1   | 0.99 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | 1A    | 3864 | 1/1   | 0.99 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3517 | 1/1   | 0.99 | 0.03 | 25,25,25,25                 | 0     |
| 54  | MG   | 1A    | 3684 | 1/1   | 0.99 | 0.02 | 42,42,42,42                 | 0     |
| 54  | MG   | 1A    | 3440 | 1/1   | 0.99 | 0.07 | 33,33,33,33                 | 0     |
| 54  | MG   | 2A    | 3481 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3019 | 1/1   | 0.99 | 0.21 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3160 | 1/1   | 0.99 | 0.15 | 30,30,30,30                 | 0     |
| 54  | MG   | 15    | 101  | 1/1   | 0.99 | 0.14 | 32,32,32,32                 | 0     |
| 54  | MG   | 1B    | 226  | 1/1   | 0.99 | 0.04 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3132 | 1/1   | 0.99 | 0.09 | 23,23,23,23                 | 0     |
| 54  | MG   | 2A    | 3341 | 1/1   | 0.99 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | 1N    | 204  | 1/1   | 0.99 | 0.02 | 53,53,53,53                 | 0     |
| 54  | MG   | 1A    | 3162 | 1/1   | 0.99 | 0.18 | 33,33,33,33                 | 0     |
| 54  | MG   | 1P    | 201  | 1/1   | 0.99 | 0.25 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3290 | 1/1   | 0.99 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3564 | 1/1   | 0.99 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | 1A    | 3874 | 1/1   | 0.99 | 0.04 | 58,58,58,58                 | 0     |
| 54  | MG   | 1a    | 1843 | 1/1   | 0.99 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3606 | 1/1   | 0.99 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | 1A    | 3199 | 1/1   | 0.99 | 0.08 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3447 | 1/1   | 0.99 | 0.05 | 60,60,60,60                 | 0     |
| 54  | MG   | 1A    | 3111 | 1/1   | 0.99 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | 1R    | 201  | 1/1   | 0.99 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | 1A    | 3241 | 1/1   | 0.99 | 0.17 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3427 | 1/1   | 0.99 | 0.02 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3286 | 1/1   | 0.99 | 0.08 | 65,65,65,65                 | 0     |
| 54  | MG   | 1A    | 3164 | 1/1   | 0.99 | 0.09 | 32,32,32,32                 | 0     |
| 54  | MG   | 2A    | 3357 | 1/1   | 0.99 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | 1A    | 3165 | 1/1   | 0.99 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | 1D    | 308  | 1/1   | 0.99 | 0.17 | 37,37,37,37                 | 0     |
| 54  | MG   | 2A    | 3361 | 1/1   | 0.99 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | 2A    | 3585 | 1/1   | 0.99 | 0.06 | 44,44,44,44                 | 0     |
| 54  | MG   | 1A    | 3324 | 1/1   | 0.99 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3223 | 1/1   | 0.99 | 0.15 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3245 | 1/1   | 0.99 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | 2A    | 3589 | 1/1   | 0.99 | 0.05 | 48,48,48,48                 | 0     |
| 54  | MG   | 2A    | 3590 | 1/1   | 0.99 | 0.10 | 63,63,63,63                 | 0     |
| 54  | MG   | 1A    | 3007 | 1/1   | 0.99 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | 1A    | 3328 | 1/1   | 0.99 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3029 | 1/1   | 0.99 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | 1a    | 1793 | 1/1   | 0.99 | 0.04 | 77,77,77,77                 | 0     |
| 58  | ZN   | 1Y    | 202  | 1/1   | 0.99 | 0.04 | 62,62,62,62                 | 0     |
| 54  | MG   | 1A    | 3271 | 1/1   | 0.99 | 0.06 | 24,24,24,24                 | 0     |
| 58  | ZN   | 15    | 110  | 1/1   | 0.99 | 0.03 | 59,59,59,59                 | 0     |
| 58  | ZN   | 16    | 501  | 1/1   | 0.99 | 0.06 | 45,45,45,45                 | 0     |
| 58  | ZN   | 19    | 103  | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 58  | ZN   | 1n    | 104  | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 54  | MG   | 2a    | 3117 | 1/1   | 0.99 | 0.10 | 75,75,75,75                 | 0     |
| 54  | MG   | 1A    | 3459 | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |
| 54  | MG   | 1A    | 3272 | 1/1   | 0.99 | 0.10 | 19,19,19,19                 | 0     |
| 58  | ZN   | 26    | 501  | 1/1   | 0.99 | 0.03 | 61,61,61,61                 | 0     |
| 54  | MG   | 1A    | 3247 | 1/1   | 0.99 | 0.22 | 33,33,33,33                 | 0     |
| 54  | MG   | 1a    | 1734 | 1/1   | 0.99 | 0.08 | 45,45,45,45                 | 0     |
| 54  | MG   | 1A    | 3274 | 1/1   | 0.99 | 0.10 | 38,38,38,38                 | 0     |
| 54  | MG   | 1A    | 3248 | 1/1   | 0.99 | 0.20 | 31,31,31,31                 | 0     |
| 54  | MG   | 1A    | 3458 | 1/1   | 1.00 | 0.02 | 54,54,54,54                 | 0     |
| 54  | MG   | 1A    | 3813 | 1/1   | 1.00 | 0.04 | 24,24,24,24                 | 0     |
| 54  | MG   | 1A    | 3217 | 1/1   | 1.00 | 0.01 | 30,30,30,30                 | 0     |
| 54  | MG   | 1A    | 3939 | 1/1   | 1.00 | 0.06 | 36,36,36,36                 | 0     |
| 54  | MG   | 2A    | 3558 | 1/1   | 1.00 | 0.03 | 41,41,41,41                 | 0     |
| 54  | MG   | 2A    | 3566 | 1/1   | 1.00 | 0.04 | 53,53,53,53                 | 0     |
| 54  | MG   | 2A    | 3360 | 1/1   | 1.00 | 0.05 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | 1A    | 3863 | 1/1   | 1.00 | 0.06 | 54,54,54,54                 | 0     |

## 5.5 Other polymers [i](#)

There are no such residues in this entry.