



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:26 PM UTC

PDB ID : 4V6G / pdb\_00004v6g  
Title : Initiation complex of 70S ribosome with two tRNAs and mRNA.  
Authors : Jenner, L.B.; Yusupova, G.; Yusupov, M.  
Deposited on : 2009-07-10  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

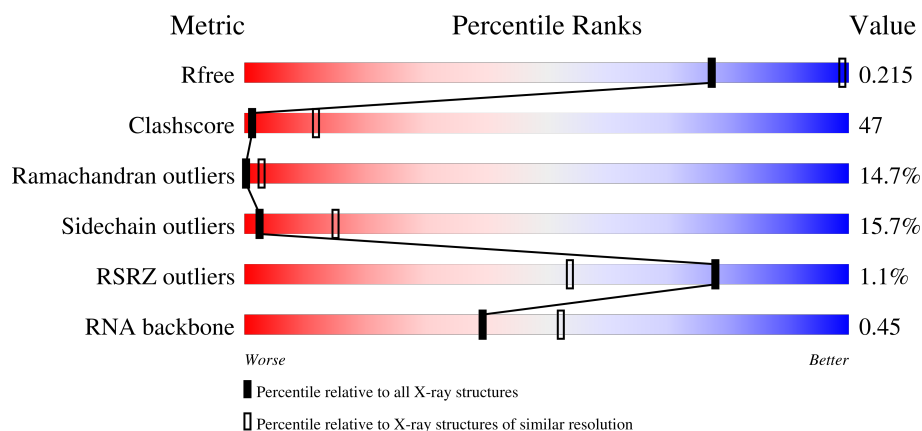
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |
| RNA backbone          | 3983                        | 1010 (3.98-3.02)                                      |

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   | AA    | 1661 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1840 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1909 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1911 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3091 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3269 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3326 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3441 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3512 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3573 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3668 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | DA    | 3682 | -         | -        | -       | X                |

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 298428 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 16S RRNA (E.COLI NUMBERING).

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1517     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32600 | 14510 | 6032 | 10541 | 1517 |         |         |       |
| 1   | CA    | 1515     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32554 | 14491 | 6025 | 10524 | 1514 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| AA    | 1542    | G        | U      | conflict | GB M26923.1 |
| CA    | 1542    | G        | U      | conflict | GB M26923.1 |

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AE    | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1223 | 343 | 344 | 5 |         |         |       |
| 2   | CE    | 237      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1924  | 1228 | 344 | 347 | 5 |         |         |       |

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AF    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |
| 3   | CF    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1011 | 313 | 280 | 1 |         |         |       |

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AG    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | CG    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AH    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1178  | 743 | 221 | 210 | 4 |         |         |       |
| 5   | CH    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AI    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | CI    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AJ    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | CJ    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AK    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | CK    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AL    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1018  | 644 | 198 | 175 | 1 |         |         |       |
| 9   | CL    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |   |         |         |       |

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AM    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |
| 10  | CM    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AN    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 560 | 171 | 167 | 3 |         |         |       |
| 11  | CN    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AO    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |
| 12  | CO    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AP    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 937   | 579 | 193 | 163 | 2 |         |         |       |
| 13  | CP    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 597 | 199 | 166 | 2 |         |         |       |

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AQ    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | CQ    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AR    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | CR    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |
| 16  | CS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AT    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 17  | CT    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AU    | 71       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 585   | 373 | 116 | 96 |         |         |       |
| 18  | CU    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AV    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 656   | 419 | 121 | 114 | 2 |         |         |       |
| 19  | CV    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 674   | 430 | 126 | 116 | 2 |         |         |       |

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AW    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | CW    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | AX    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |
| 21  | CX    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 22 is a RNA chain called TRNA FMET (UNMODIFIED BASES).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | AD    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | CC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | CD    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1640  | 732 | 298 | 534 | 76 |         |         |       |
| 22  | CB    | 65       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1385  | 618 | 250 | 453 | 64 |         |         |       |

- Molecule 23 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23  | A1    | 23       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 502   | 227 | 107 | 146 | 22 |         |         |       |
| 23  | C1    | 23       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 502   | 227 | 107 | 146 | 22 |         |         |       |

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 24  | BA    | 2885     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62134 | 27656 | 11622 | 19972 | 2884 |         |         |       |
| 24  | DA    | 2886     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62151 | 27664 | 11620 | 19982 | 2885 |         |         |       |

There are 29 discrepancies between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| BA    | ?       | -        | U      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | U      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| BA    | 654T    | A        | C      | conflict  | GB AP008226.1 |
| BA    | 1058    | U        | G      | conflict  | GB AP008226.1 |
| BA    | 1080    | A        | C      | conflict  | GB AP008226.1 |
| DA    | 161     | U        | -      | insertion | GB AP008226.1 |
| DA    | 654A    | A        | G      | conflict  | GB AP008226.1 |
| DA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| DA    | ?       | -        | G      | deletion  | GB AP008226.1 |
| DA    | ?       | -        | C      | deletion  | GB AP008226.1 |
| DA    | ?       | -        | A      | deletion  | GB AP008226.1 |
| DA    | 654L    | G        | C      | conflict  | GB AP008226.1 |
| DA    | 654T    | A        | C      | conflict  | GB AP008226.1 |
| DA    | 1058    | U        | G      | conflict  | GB AP008226.1 |
| DA    | 1080    | A        | C      | conflict  | GB AP008226.1 |

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 25  | BB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2572  | 1146 | 476 | 831 | 119 |         |         |       |
| 25  | DB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| BB    | 1M      | A        | -      | insertion | GB X01554.1 |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | BD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 26  | DD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 27  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28  | BF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |
| 28  | DF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 29  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |
| 30  | DH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 31  | DK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 32  | DM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 33  | DN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 34  | DO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 35  | DP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 36  | B0    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | D0    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 37  | BQ    | 111      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |  |         |         |       |
| 37  | DQ    | 111      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |  |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BR    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 38  | DR    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | B1    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 39  | D1    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | B2    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 40  | D2    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |
| 41  | DS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | BT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |
| 42  | DT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |
| 43  | DU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BV    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1404  | 897 | 252 | 252 | 3 |         |         |       |
| 44  | DV    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1378  | 879 | 248 | 248 | 3 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | B3    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 629   | 389 | 132 | 107 | 1 |         |         |       |
| 45  | D3    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 611   | 378 | 129 | 103 | 1 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 46  | DZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BW    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |
| 47  | DW    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | BX    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |   |         |         |       |
| 48  | DX    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |   |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | B4    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |
| 49  | D4    | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 50  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | B6    | 48       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 68 | 4 |         |         |       |
| 51  | D6    | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 424   | 264 | 87 | 69 | 4 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52  | B7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52  | D7    | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 53  | D8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54  | AA    | 440      | Total | Mg  | 0       | 0       |
|     |       |          | 440   | 440 |         |         |
| 54  | AH    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 54  | AI    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AJ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AK    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AL    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 54  | AO    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AP    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AS    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 54  | AT    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 54  | AW    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | AX    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AC    | 8        | Total | Mg  | 0       | 0       |
|     |       |          | 8     | 8   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | AD    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | A1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BA    | 683      | Total<br>683 | Mg<br>683 | 0       | 0       |
| 54  | BB    | 26       | Total<br>26  | Mg<br>26  | 0       | 0       |
| 54  | BD    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | BE    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 54  | BF    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | BG    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BH    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BK    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B0    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | BQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BR    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | B1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BT    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | BU    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | B3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | BZ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | BW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 54  | B5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | B8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CA    | 384      | Total<br>384 | Mg<br>384 | 0       | 0       |
| 54  | CG    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CH    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | CK    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | CL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CM    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CP    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 54  | CQ    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 54  | CR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CS    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | CT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | CW    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 54  | CX    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 54  | CC    | 13       | Total<br>13  | Mg<br>13  | 0       | 0       |
| 54  | CD    | 26       | Total<br>26  | Mg<br>26  | 0       | 0       |
| 54  | C1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 54  | DA    | 905      | Total<br>905 | Mg<br>905 | 0       | 0       |
| 54  | DB    | 29       | Total<br>29  | Mg<br>29  | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 54  | DD    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 54  | DE    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 54  | DF    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 54  | DG    | 3        | Total<br>3 | Mg<br>3 | 0       | 0       |
| 54  | DH    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 54  | DO    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 54  | D0    | 5        | Total<br>5 | Mg<br>5 | 0       | 0       |
| 54  | DR    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 54  | D1    | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |
| 54  | D2    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 54  | DS    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 54  | DT    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 54  | DU    | 6        | Total<br>6 | Mg<br>6 | 0       | 0       |
| 54  | D3    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 54  | DZ    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 54  | DW    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 54  | D5    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 54  | D6    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 54  | D7    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 55  | AA    | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 55  | AG    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 55  | AQ    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 55  | CG    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 55  | CQ    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.46Å 452.18Å 626.12Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 300.00 – 3.50<br>300.00 – 3.50                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.7 (300.00-3.50)<br>100.0 (300.00-3.50)                   | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.28                                                        | Depositor        |
| $R_{sym}$                                                               | 0.18                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.34 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.252<br>0.212 , 0.215                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 22133 reflections (1.88%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 71.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.113                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 61.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 298428                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 106.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.33% 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 ⓘ

### 4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | AA    | 0.38         | 0/36490        | 0.80        | 103/56951 (0.2%) |
| 1   | CA    | 0.39         | 1/36439 (0.0%) | 0.81        | 106/56872 (0.2%) |
| 2   | AE    | 0.41         | 0/1950         | 1.03        | 10/2630 (0.4%)   |
| 2   | CE    | 0.41         | 0/1959         | 1.04        | 10/2642 (0.4%)   |
| 3   | AF    | 0.45         | 0/1636         | 0.97        | 8/2205 (0.4%)    |
| 3   | CF    | 0.43         | 0/1629         | 0.92        | 1/2195 (0.0%)    |
| 4   | AG    | 0.52         | 0/1733         | 1.16        | 13/2318 (0.6%)   |
| 4   | CG    | 0.50         | 0/1733         | 1.08        | 15/2318 (0.6%)   |
| 5   | AH    | 0.47         | 0/1195         | 1.04        | 10/1609 (0.6%)   |
| 5   | CH    | 0.45         | 0/1171         | 1.01        | 9/1576 (0.6%)    |
| 6   | AI    | 0.48         | 0/856          | 0.99        | 2/1154 (0.2%)    |
| 6   | CI    | 0.49         | 0/856          | 0.97        | 3/1154 (0.3%)    |
| 7   | AJ    | 0.43         | 0/1276         | 1.06        | 10/1709 (0.6%)   |
| 7   | CJ    | 0.42         | 0/1276         | 0.90        | 1/1709 (0.1%)    |
| 8   | AK    | 0.43         | 0/1136         | 0.99        | 3/1527 (0.2%)    |
| 8   | CK    | 0.49         | 0/1136         | 1.05        | 5/1527 (0.3%)    |
| 9   | AL    | 0.41         | 0/1037         | 1.15        | 13/1389 (0.9%)   |
| 9   | CL    | 0.39         | 0/1029         | 1.03        | 9/1379 (0.7%)    |
| 10  | AM    | 0.43         | 0/814          | 1.04        | 6/1095 (0.5%)    |
| 10  | CM    | 0.46         | 0/814          | 0.91        | 1/1095 (0.1%)    |
| 11  | AN    | 0.47         | 0/916          | 1.12        | 6/1234 (0.5%)    |
| 11  | CN    | 0.46         | 0/900          | 1.05        | 6/1213 (0.5%)    |
| 12  | AO    | 0.50         | 0/991          | 1.05        | 5/1327 (0.4%)    |
| 12  | CO    | 0.55         | 0/991          | 1.74        | 11/1327 (0.8%)   |
| 13  | AP    | 0.64         | 2/947 (0.2%)   | 1.09        | 6/1270 (0.5%)    |
| 13  | CP    | 0.42         | 0/974          | 1.04        | 9/1303 (0.7%)    |
| 14  | AQ    | 0.43         | 0/501          | 1.04        | 4/664 (0.6%)     |
| 14  | CQ    | 0.50         | 0/501          | 1.10        | 5/664 (0.8%)     |
| 15  | AR    | 0.48         | 0/745          | 0.91        | 2/992 (0.2%)     |
| 15  | CR    | 0.47         | 0/745          | 1.00        | 3/992 (0.3%)     |
| 16  | AS    | 0.46         | 0/721          | 1.01        | 5/970 (0.5%)     |
| 16  | CS    | 0.45         | 0/721          | 1.03        | 4/970 (0.4%)     |

| Mol | Chain | Bond lengths |                | Bond angles |                   |
|-----|-------|--------------|----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5           |
| 17  | AT    | 0.44         | 0/847          | 1.03        | 1/1131 (0.1%)     |
| 17  | CT    | 0.42         | 0/847          | 1.06        | 6/1131 (0.5%)     |
| 18  | AU    | 0.50         | 0/590          | 1.05        | 3/782 (0.4%)      |
| 18  | CU    | 0.46         | 0/579          | 1.04        | 3/768 (0.4%)      |
| 19  | AV    | 0.47         | 0/670          | 1.04        | 6/901 (0.7%)      |
| 19  | CV    | 0.45         | 0/689          | 1.21        | 7/926 (0.8%)      |
| 20  | AW    | 0.46         | 0/765          | 1.09        | 6/1007 (0.6%)     |
| 20  | CW    | 0.41         | 0/765          | 1.09        | 5/1007 (0.5%)     |
| 21  | AX    | 0.44         | 0/221          | 0.91        | 1/288 (0.3%)      |
| 21  | CX    | 0.41         | 0/221          | 1.01        | 1/288 (0.3%)      |
| 22  | AC    | 0.38         | 1/1832 (0.1%)  | 0.79        | 6/2855 (0.2%)     |
| 22  | AD    | 0.36         | 1/1832 (0.1%)  | 0.72        | 3/2855 (0.1%)     |
| 22  | CB    | 0.37         | 1/1547 (0.1%)  | 0.74        | 2/2411 (0.1%)     |
| 22  | CC    | 0.41         | 1/1832 (0.1%)  | 0.80        | 2/2855 (0.1%)     |
| 22  | CD    | 0.35         | 1/1832 (0.1%)  | 0.66        | 1/2855 (0.0%)     |
| 23  | A1    | 0.40         | 0/567          | 0.89        | 1/884 (0.1%)      |
| 23  | C1    | 0.36         | 0/567          | 0.85        | 2/884 (0.2%)      |
| 24  | BA    | 0.45         | 8/69594 (0.0%) | 0.89        | 251/108647 (0.2%) |
| 24  | DA    | 0.47         | 0/69611        | 0.93        | 293/108670 (0.3%) |
| 25  | BB    | 0.36         | 0/2877         | 0.74        | 4/4488 (0.1%)     |
| 25  | DB    | 0.40         | 0/2878         | 0.82        | 6/4490 (0.1%)     |
| 26  | BD    | 0.60         | 0/2165         | 1.17        | 21/2919 (0.7%)    |
| 26  | DD    | 0.84         | 3/2165 (0.1%)  | 1.30        | 32/2919 (1.1%)    |
| 27  | BE    | 0.54         | 0/1601         | 1.25        | 22/2160 (1.0%)    |
| 27  | DE    | 0.62         | 0/1601         | 1.35        | 29/2160 (1.3%)    |
| 28  | BF    | 0.53         | 0/1662         | 1.13        | 13/2249 (0.6%)    |
| 28  | DF    | 0.62         | 0/1620         | 1.19        | 18/2194 (0.8%)    |
| 29  | BG    | 0.42         | 0/1499         | 1.03        | 13/2016 (0.6%)    |
| 29  | DG    | 0.47         | 0/1499         | 0.99        | 9/2016 (0.4%)     |
| 30  | BH    | 0.48         | 0/1332         | 1.14        | 13/1802 (0.7%)    |
| 30  | DH    | 0.57         | 0/1332         | 1.22        | 15/1802 (0.8%)    |
| 31  | BK    | 0.47         | 0/1151         | 1.09        | 8/1558 (0.5%)     |
| 31  | DK    | 0.54         | 0/1151         | 1.19        | 11/1558 (0.7%)    |
| 32  | BM    | 0.48         | 0/1131         | 1.05        | 3/1525 (0.2%)     |
| 32  | DM    | 0.54         | 0/1131         | 1.18        | 10/1525 (0.7%)    |
| 33  | BN    | 0.59         | 0/943          | 1.07        | 3/1269 (0.2%)     |
| 33  | DN    | 0.64         | 0/943          | 1.04        | 5/1269 (0.4%)     |
| 34  | BO    | 0.54         | 0/1162         | 1.26        | 13/1544 (0.8%)    |
| 34  | DO    | 0.63         | 1/1162 (0.1%)  | 1.37        | 17/1544 (1.1%)    |
| 35  | BP    | 0.50         | 0/1143         | 1.11        | 12/1527 (0.8%)    |
| 35  | DP    | 0.69         | 0/1143         | 1.34        | 19/1527 (1.2%)    |
| 36  | B0    | 0.57         | 0/974          | 1.05        | 3/1302 (0.2%)     |
| 36  | D0    | 0.55         | 0/982          | 1.17        | 10/1312 (0.8%)    |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 37  | BQ    | 0.42         | 0/892            | 0.99        | 4/1187 (0.3%)      |
| 37  | DQ    | 0.51         | 0/892            | 1.18        | 8/1187 (0.7%)      |
| 38  | BR    | 0.51         | 0/1155           | 1.08        | 7/1542 (0.5%)      |
| 38  | DR    | 0.56         | 0/1155           | 1.18        | 17/1542 (1.1%)     |
| 39  | B1    | 0.48         | 0/982            | 1.11        | 8/1306 (0.6%)      |
| 39  | D1    | 0.59         | 0/982            | 1.21        | 10/1306 (0.8%)     |
| 40  | B2    | 0.56         | 0/790            | 1.21        | 7/1057 (0.7%)      |
| 40  | D2    | 0.55         | 0/790            | 1.10        | 6/1057 (0.6%)      |
| 41  | BS    | 0.58         | 0/911            | 1.07        | 3/1220 (0.2%)      |
| 41  | DS    | 0.57         | 0/911            | 1.18        | 13/1220 (1.1%)     |
| 42  | BT    | 0.53         | 0/739            | 1.09        | 4/993 (0.4%)       |
| 42  | DT    | 0.62         | 0/739            | 1.14        | 5/993 (0.5%)       |
| 43  | BU    | 0.65         | 0/798            | 1.28        | 11/1064 (1.0%)     |
| 43  | DU    | 0.64         | 0/798            | 1.16        | 3/1064 (0.3%)      |
| 44  | BV    | 0.49         | 0/1435           | 1.09        | 12/1947 (0.6%)     |
| 44  | DV    | 0.60         | 1/1408 (0.1%)    | 1.07        | 10/1908 (0.5%)     |
| 45  | B3    | 0.51         | 0/637            | 1.09        | 4/848 (0.5%)       |
| 45  | D3    | 0.51         | 0/619            | 1.14        | 5/825 (0.6%)       |
| 46  | BZ    | 0.53         | 0/770            | 1.13        | 6/1022 (0.6%)      |
| 46  | DZ    | 0.58         | 0/770            | 1.20        | 9/1022 (0.9%)      |
| 47  | BW    | 0.46         | 0/583            | 1.14        | 9/771 (1.2%)       |
| 47  | DW    | 0.60         | 0/583            | 1.32        | 9/771 (1.2%)       |
| 48  | BX    | 0.45         | 0/474            | 1.17        | 6/635 (0.9%)       |
| 48  | DX    | 0.53         | 0/474            | 1.04        | 0/635              |
| 49  | B4    | 0.57         | 0/594            | 1.23        | 12/795 (1.5%)      |
| 49  | D4    | 0.46         | 0/594            | 1.24        | 10/795 (1.3%)      |
| 50  | B5    | 0.52         | 0/473            | 1.13        | 5/639 (0.8%)       |
| 50  | D5    | 0.64         | 0/473            | 1.22        | 6/639 (0.9%)       |
| 51  | B6    | 0.49         | 0/424            | 1.07        | 3/565 (0.5%)       |
| 51  | D6    | 0.53         | 0/431            | 1.06        | 3/575 (0.5%)       |
| 52  | B7    | 0.61         | 0/438            | 1.05        | 0/575              |
| 52  | D7    | 0.73         | 0/438            | 1.19        | 2/575 (0.3%)       |
| 53  | B8    | 0.61         | 0/525            | 1.36        | 10/691 (1.4%)      |
| 53  | D8    | 0.79         | 0/525            | 1.40        | 9/691 (1.3%)       |
| All | All   | 0.46         | 21/321675 (0.0%) | 0.94        | 1549/481462 (0.3%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 54                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | CA    | 0                   | 53                  |
| 22  | AC    | 0                   | 2                   |
| 22  | AD    | 0                   | 2                   |
| 22  | CD    | 0                   | 1                   |
| 23  | A1    | 0                   | 3                   |
| 23  | C1    | 0                   | 3                   |
| 24  | BA    | 0                   | 136                 |
| 24  | DA    | 0                   | 153                 |
| 25  | BB    | 0                   | 4                   |
| 25  | DB    | 0                   | 5                   |
| All | All   | 0                   | 416                 |

The worst 5 of 21 bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|--------|-------------|----------|
| 24  | BA    | 654(R) | C    | O5'-C5' | 24.60  | 1.79        | 1.42     |
| 26  | DD    | 236    | GLY  | C-N     | 14.32  | 1.53        | 1.33     |
| 24  | BA    | 654(R) | C    | N1-C2   | 14.23  | 1.68        | 1.40     |
| 26  | DD    | 239    | ARG  | CA-C    | -12.97 | 1.35        | 1.52     |
| 13  | AP    | 117    | VAL  | CA-CB   | 11.38  | 1.70        | 1.54     |

The worst 5 of 1549 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 12  | CO    | 47   | LYS  | CA-C-N      | 31.27  | 158.93      | 119.84   |
| 12  | CO    | 47   | LYS  | C-N-CA      | 31.27  | 158.93      | 119.84   |
| 24  | BA    | 945  | A    | C1'-O4'-C4' | -19.36 | 90.34       | 109.70   |
| 24  | DA    | 1379 | A    | C1'-O4'-C4' | -19.32 | 90.58       | 109.90   |
| 24  | DA    | 945  | A    | C1'-O4'-C4' | -18.84 | 91.06       | 109.90   |

There are no chirality outliers.

5 of 416 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 30  | U    | Sidechain |
| 1   | AA    | 47  | C    | Sidechain |
| 1   | AA    | 49  | U    | Sidechain |
| 1   | AA    | 51  | A    | Sidechain |
| 1   | AA    | 82  | U    | Sidechain |



## 4.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32600 | 0        | 16446    | 1810    | 2            |
| 1   | CA    | 32554 | 0        | 16428    | 1782    | 16           |
| 2   | AE    | 1915  | 0        | 1969     | 392     | 0            |
| 2   | CE    | 1924  | 0        | 1975     | 312     | 0            |
| 3   | AF    | 1612  | 0        | 1677     | 318     | 0            |
| 3   | CF    | 1605  | 0        | 1668     | 221     | 0            |
| 4   | AG    | 1703  | 0        | 1764     | 272     | 0            |
| 4   | CG    | 1703  | 0        | 1763     | 260     | 0            |
| 5   | AH    | 1178  | 0        | 1233     | 157     | 0            |
| 5   | CH    | 1155  | 0        | 1213     | 148     | 0            |
| 6   | AI    | 843   | 0        | 857      | 112     | 0            |
| 6   | CI    | 843   | 0        | 857      | 108     | 0            |
| 7   | AJ    | 1257  | 0        | 1296     | 187     | 0            |
| 7   | CJ    | 1257  | 0        | 1296     | 166     | 0            |
| 8   | AK    | 1116  | 0        | 1177     | 157     | 0            |
| 8   | CK    | 1116  | 0        | 1177     | 160     | 0            |
| 9   | AL    | 1018  | 0        | 1049     | 223     | 0            |
| 9   | CL    | 1010  | 0        | 1037     | 166     | 0            |
| 10  | AM    | 801   | 0        | 849      | 158     | 0            |
| 10  | CM    | 801   | 0        | 849      | 151     | 0            |
| 11  | AN    | 901   | 0        | 926      | 126     | 0            |
| 11  | CN    | 885   | 0        | 904      | 112     | 0            |
| 12  | AO    | 975   | 0        | 1062     | 141     | 0            |
| 12  | CO    | 975   | 0        | 1062     | 116     | 0            |
| 13  | AP    | 937   | 0        | 995      | 211     | 0            |
| 13  | CP    | 964   | 0        | 1034     | 164     | 0            |
| 14  | AQ    | 492   | 0        | 529      | 71      | 0            |
| 14  | CQ    | 492   | 0        | 529      | 100     | 0            |
| 15  | AR    | 734   | 0        | 771      | 104     | 0            |
| 15  | CR    | 734   | 0        | 771      | 88      | 0            |
| 16  | AS    | 705   | 0        | 725      | 78      | 0            |
| 16  | CS    | 705   | 0        | 725      | 134     | 0            |
| 17  | AT    | 834   | 0        | 904      | 65      | 0            |
| 17  | CT    | 834   | 0        | 904      | 87      | 0            |
| 18  | AU    | 585   | 0        | 657      | 106     | 0            |
| 18  | CU    | 574   | 0        | 644      | 82      | 0            |
| 19  | AV    | 656   | 0        | 678      | 176     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | CV    | 674   | 0        | 699      | 143     | 0            |
| 20  | AW    | 763   | 0        | 861      | 92      | 0            |
| 20  | CW    | 763   | 0        | 861      | 128     | 0            |
| 21  | AX    | 217   | 0        | 234      | 35      | 0            |
| 21  | CX    | 217   | 0        | 234      | 34      | 0            |
| 22  | AC    | 1640  | 0        | 836      | 71      | 0            |
| 22  | AD    | 1640  | 0        | 836      | 119     | 0            |
| 22  | CB    | 1385  | 0        | 704      | 65      | 0            |
| 22  | CC    | 1640  | 0        | 836      | 41      | 0            |
| 22  | CD    | 1640  | 0        | 834      | 97      | 0            |
| 23  | A1    | 502   | 0        | 253      | 40      | 0            |
| 23  | C1    | 502   | 0        | 253      | 38      | 0            |
| 24  | BA    | 62134 | 0        | 31302    | 3013    | 2            |
| 24  | DA    | 62151 | 0        | 31309    | 2783    | 0            |
| 25  | BB    | 2572  | 0        | 1305     | 184     | 0            |
| 25  | DB    | 2573  | 0        | 1305     | 139     | 0            |
| 26  | BD    | 2115  | 0        | 2195     | 321     | 0            |
| 26  | DD    | 2115  | 0        | 2195     | 351     | 0            |
| 27  | BE    | 1568  | 0        | 1634     | 294     | 0            |
| 27  | DE    | 1568  | 0        | 1634     | 301     | 0            |
| 28  | BF    | 1627  | 0        | 1680     | 277     | 0            |
| 28  | DF    | 1585  | 0        | 1632     | 204     | 0            |
| 29  | BG    | 1474  | 0        | 1535     | 277     | 0            |
| 29  | DG    | 1474  | 0        | 1535     | 222     | 0            |
| 30  | BH    | 1307  | 0        | 1382     | 335     | 16           |
| 30  | DH    | 1307  | 0        | 1382     | 239     | 0            |
| 31  | BK    | 1136  | 0        | 1223     | 216     | 0            |
| 31  | DK    | 1136  | 0        | 1223     | 218     | 0            |
| 32  | BM    | 1104  | 0        | 1180     | 144     | 0            |
| 32  | DM    | 1104  | 0        | 1180     | 208     | 0            |
| 33  | BN    | 933   | 0        | 996      | 120     | 0            |
| 33  | DN    | 933   | 0        | 996      | 133     | 0            |
| 34  | BO    | 1145  | 0        | 1228     | 271     | 0            |
| 34  | DO    | 1145  | 0        | 1228     | 272     | 0            |
| 35  | BP    | 1122  | 0        | 1179     | 251     | 0            |
| 35  | DP    | 1122  | 0        | 1179     | 163     | 0            |
| 36  | B0    | 960   | 0        | 1021     | 129     | 0            |
| 36  | D0    | 968   | 0        | 1033     | 120     | 0            |
| 37  | BQ    | 882   | 0        | 943      | 172     | 0            |
| 37  | DQ    | 882   | 0        | 943      | 172     | 0            |
| 38  | BR    | 1141  | 0        | 1202     | 165     | 0            |
| 38  | DR    | 1141  | 0        | 1202     | 165     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 39  | B1    | 964   | 0        | 1022     | 167     | 0            |
| 39  | D1    | 964   | 0        | 1022     | 141     | 0            |
| 40  | B2    | 779   | 0        | 852      | 196     | 0            |
| 40  | D2    | 779   | 0        | 851      | 140     | 0            |
| 41  | BS    | 900   | 0        | 964      | 115     | 0            |
| 41  | DS    | 900   | 0        | 964      | 109     | 0            |
| 42  | BT    | 725   | 0        | 778      | 92      | 0            |
| 42  | DT    | 725   | 0        | 778      | 76      | 0            |
| 43  | BU    | 785   | 0        | 878      | 216     | 0            |
| 43  | DU    | 785   | 0        | 878      | 170     | 0            |
| 44  | BV    | 1404  | 0        | 1437     | 327     | 0            |
| 44  | DV    | 1378  | 0        | 1407     | 245     | 0            |
| 45  | B3    | 629   | 0        | 650      | 78      | 0            |
| 45  | D3    | 611   | 0        | 631      | 63      | 0            |
| 46  | BZ    | 763   | 0        | 848      | 111     | 0            |
| 46  | DZ    | 763   | 0        | 848      | 147     | 0            |
| 47  | BW    | 581   | 0        | 629      | 114     | 0            |
| 47  | DW    | 581   | 0        | 629      | 89      | 0            |
| 48  | BX    | 469   | 0        | 518      | 41      | 0            |
| 48  | DX    | 469   | 0        | 518      | 45      | 0            |
| 49  | B4    | 581   | 0        | 573      | 171     | 0            |
| 49  | D4    | 581   | 0        | 574      | 168     | 0            |
| 50  | B5    | 459   | 0        | 480      | 53      | 0            |
| 50  | D5    | 459   | 0        | 480      | 80      | 0            |
| 51  | B6    | 417   | 0        | 441      | 96      | 0            |
| 51  | D6    | 424   | 0        | 450      | 100     | 0            |
| 52  | B7    | 430   | 0        | 480      | 57      | 0            |
| 52  | D7    | 430   | 0        | 480      | 50      | 0            |
| 53  | B8    | 517   | 0        | 582      | 143     | 0            |
| 53  | D8    | 517   | 0        | 582      | 115     | 0            |
| 54  | A1    | 1     | 0        | 0        | 0       | 0            |
| 54  | AA    | 440   | 0        | 0        | 0       | 0            |
| 54  | AC    | 8     | 0        | 0        | 0       | 0            |
| 54  | AD    | 3     | 0        | 0        | 0       | 0            |
| 54  | AH    | 2     | 0        | 0        | 0       | 0            |
| 54  | AI    | 1     | 0        | 0        | 0       | 0            |
| 54  | AJ    | 1     | 0        | 0        | 0       | 0            |
| 54  | AK    | 1     | 0        | 0        | 0       | 0            |
| 54  | AL    | 2     | 0        | 0        | 0       | 0            |
| 54  | AO    | 1     | 0        | 0        | 0       | 0            |
| 54  | AP    | 1     | 0        | 0        | 0       | 0            |
| 54  | AQ    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54  | AS    | 2     | 0        | 0        | 0       | 0            |
| 54  | AT    | 2     | 0        | 0        | 0       | 0            |
| 54  | AW    | 4     | 0        | 0        | 0       | 0            |
| 54  | AX    | 1     | 0        | 0        | 0       | 0            |
| 54  | B0    | 2     | 0        | 0        | 0       | 0            |
| 54  | B1    | 1     | 0        | 0        | 0       | 0            |
| 54  | B3    | 2     | 0        | 0        | 0       | 0            |
| 54  | B4    | 1     | 0        | 0        | 0       | 0            |
| 54  | B5    | 1     | 0        | 0        | 0       | 0            |
| 54  | B6    | 1     | 0        | 0        | 0       | 0            |
| 54  | B8    | 1     | 0        | 0        | 0       | 0            |
| 54  | BA    | 683   | 0        | 0        | 0       | 0            |
| 54  | BB    | 26    | 0        | 0        | 0       | 0            |
| 54  | BD    | 2     | 0        | 0        | 0       | 0            |
| 54  | BE    | 7     | 0        | 0        | 0       | 0            |
| 54  | BF    | 2     | 0        | 0        | 0       | 0            |
| 54  | BG    | 1     | 0        | 0        | 0       | 0            |
| 54  | BH    | 1     | 0        | 0        | 0       | 0            |
| 54  | BK    | 1     | 0        | 0        | 0       | 0            |
| 54  | BO    | 1     | 0        | 0        | 0       | 0            |
| 54  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 54  | BR    | 2     | 0        | 0        | 0       | 0            |
| 54  | BT    | 2     | 0        | 0        | 0       | 0            |
| 54  | BU    | 5     | 0        | 0        | 0       | 0            |
| 54  | BW    | 1     | 0        | 0        | 0       | 0            |
| 54  | BZ    | 1     | 0        | 0        | 0       | 0            |
| 54  | C1    | 1     | 0        | 0        | 0       | 0            |
| 54  | CA    | 384   | 0        | 0        | 0       | 0            |
| 54  | CC    | 13    | 0        | 0        | 0       | 0            |
| 54  | CD    | 26    | 0        | 0        | 0       | 0            |
| 54  | CG    | 1     | 0        | 0        | 0       | 0            |
| 54  | CH    | 2     | 0        | 0        | 0       | 0            |
| 54  | CK    | 2     | 0        | 0        | 0       | 0            |
| 54  | CL    | 1     | 0        | 0        | 0       | 0            |
| 54  | CM    | 1     | 0        | 0        | 0       | 0            |
| 54  | CP    | 4     | 0        | 0        | 0       | 0            |
| 54  | CQ    | 3     | 0        | 0        | 0       | 0            |
| 54  | CR    | 1     | 0        | 0        | 0       | 0            |
| 54  | CS    | 2     | 0        | 0        | 0       | 0            |
| 54  | CT    | 1     | 0        | 0        | 0       | 0            |
| 54  | CW    | 5     | 0        | 0        | 0       | 0            |
| 54  | CX    | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 54  | D0    | 5      | 0        | 0        | 0       | 0            |
| 54  | D1    | 6      | 0        | 0        | 0       | 0            |
| 54  | D2    | 1      | 0        | 0        | 0       | 0            |
| 54  | D3    | 4      | 0        | 0        | 0       | 0            |
| 54  | D5    | 1      | 0        | 0        | 0       | 0            |
| 54  | D6    | 2      | 0        | 0        | 0       | 0            |
| 54  | D7    | 1      | 0        | 0        | 0       | 0            |
| 54  | DA    | 905    | 0        | 0        | 0       | 0            |
| 54  | DB    | 29     | 0        | 0        | 0       | 0            |
| 54  | DD    | 3      | 0        | 0        | 0       | 0            |
| 54  | DE    | 3      | 0        | 0        | 0       | 0            |
| 54  | DF    | 1      | 0        | 0        | 0       | 0            |
| 54  | DG    | 3      | 0        | 0        | 0       | 0            |
| 54  | DH    | 4      | 0        | 0        | 0       | 0            |
| 54  | DO    | 5      | 0        | 0        | 0       | 0            |
| 54  | DR    | 2      | 0        | 0        | 0       | 0            |
| 54  | DS    | 1      | 0        | 0        | 0       | 0            |
| 54  | DT    | 2      | 0        | 0        | 0       | 0            |
| 54  | DU    | 6      | 0        | 0        | 0       | 0            |
| 54  | DW    | 2      | 0        | 0        | 0       | 0            |
| 54  | DZ    | 2      | 0        | 0        | 0       | 0            |
| 55  | AA    | 2      | 0        | 0        | 0       | 0            |
| 55  | AG    | 1      | 0        | 0        | 0       | 0            |
| 55  | AQ    | 1      | 0        | 0        | 0       | 0            |
| 55  | CG    | 1      | 0        | 0        | 0       | 0            |
| 55  | CQ    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 298428 | 0        | 200046   | 23495   | 18           |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

The worst 5 of 23495 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DH:127:GLU:CG   | 30:DH:128:PRO:HD3  | 1.36                     | 1.52              |
| 24:BA:654(R):C:C2  | 24:BA:654(R):C:C5' | 1.96                     | 1.45              |
| 24:DA:1378:A:O2'   | 24:DA:1379:A:C5'   | 1.64                     | 1.44              |
| 49:B4:12:ALA:CB    | 49:B4:23:GLU:O     | 1.68                     | 1.41              |
| 24:BA:654(R):C:C5' | 24:BA:654(R):C:C4  | 2.07                     | 1.38              |

The worst 5 of 18 symmetry-related close contacts are listed below. The label for Atom-2 includes

the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1            | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 30:BH:125:VAL:CG2 | 1:CA:84:U:N1[3_545]  | 1.00                     | 1.20              |
| 30:BH:125:VAL:CG2 | 1:CA:84:U:C6[3_545]  | 1.17                     | 1.03              |
| 30:BH:126:PRO:CD  | 1:CA:82:U:O3'[3_545] | 1.41                     | 0.79              |
| 30:BH:126:PRO:CG  | 1:CA:84:U:O5'[3_545] | 1.57                     | 0.63              |
| 30:BH:126:PRO:CG  | 1:CA:84:U:P[3_545]   | 1.60                     | 0.60              |

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

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AE    | 234/256 (91%) | 128 (55%) | 55 (24%) | 51 (22%) | 0           | 1  |
| 2   | CE    | 235/256 (92%) | 153 (65%) | 52 (22%) | 30 (13%) | 0           | 3  |
| 3   | AF    | 204/239 (85%) | 119 (58%) | 49 (24%) | 36 (18%) | 0           | 1  |
| 3   | CF    | 203/239 (85%) | 128 (63%) | 56 (28%) | 19 (9%)  | 0           | 6  |
| 4   | AG    | 206/209 (99%) | 117 (57%) | 56 (27%) | 33 (16%) | 0           | 2  |
| 4   | CG    | 206/209 (99%) | 133 (65%) | 51 (25%) | 22 (11%) | 0           | 5  |
| 5   | AH    | 152/162 (94%) | 103 (68%) | 34 (22%) | 15 (10%) | 0           | 6  |
| 5   | CH    | 149/162 (92%) | 103 (69%) | 31 (21%) | 15 (10%) | 0           | 6  |
| 6   | AI    | 99/101 (98%)  | 71 (72%)  | 21 (21%) | 7 (7%)   | 1           | 10 |
| 6   | CI    | 99/101 (98%)  | 66 (67%)  | 24 (24%) | 9 (9%)   | 0           | 7  |
| 7   | AJ    | 153/156 (98%) | 95 (62%)  | 42 (28%) | 16 (10%) | 0           | 5  |
| 7   | CJ    | 153/156 (98%) | 102 (67%) | 36 (24%) | 15 (10%) | 0           | 6  |
| 8   | AK    | 136/138 (99%) | 98 (72%)  | 29 (21%) | 9 (7%)   | 1           | 11 |
| 8   | CK    | 136/138 (99%) | 92 (68%)  | 29 (21%) | 15 (11%) | 0           | 5  |
| 9   | AL    | 126/128 (98%) | 71 (56%)  | 36 (29%) | 19 (15%) | 0           | 2  |
| 9   | CL    | 125/128 (98%) | 77 (62%)  | 32 (26%) | 16 (13%) | 0           | 3  |
| 10  | AM    | 97/105 (92%)  | 67 (69%)  | 20 (21%) | 10 (10%) | 0           | 5  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 10  | CM    | 97/105 (92%)  | 68 (70%)  | 19 (20%) | 10 (10%) | 0           | 5  |
| 11  | AN    | 119/129 (92%) | 76 (64%)  | 29 (24%) | 14 (12%) | 0           | 4  |
| 11  | CN    | 117/129 (91%) | 87 (74%)  | 21 (18%) | 9 (8%)   | 1           | 8  |
| 12  | AO    | 123/132 (93%) | 80 (65%)  | 22 (18%) | 21 (17%) | 0           | 2  |
| 12  | CO    | 123/132 (93%) | 85 (69%)  | 24 (20%) | 14 (11%) | 0           | 5  |
| 13  | AP    | 116/126 (92%) | 62 (53%)  | 23 (20%) | 31 (27%) | 0           | 0  |
| 13  | CP    | 119/126 (94%) | 71 (60%)  | 27 (23%) | 21 (18%) | 0           | 1  |
| 14  | AQ    | 58/61 (95%)   | 37 (64%)  | 15 (26%) | 6 (10%)  | 0           | 5  |
| 14  | CQ    | 58/61 (95%)   | 33 (57%)  | 15 (26%) | 10 (17%) | 0           | 2  |
| 15  | AR    | 86/89 (97%)   | 55 (64%)  | 27 (31%) | 4 (5%)   | 2           | 17 |
| 15  | CR    | 86/89 (97%)   | 61 (71%)  | 19 (22%) | 6 (7%)   | 1           | 10 |
| 16  | AS    | 82/88 (93%)   | 57 (70%)  | 16 (20%) | 9 (11%)  | 0           | 5  |
| 16  | CS    | 82/88 (93%)   | 48 (58%)  | 23 (28%) | 11 (13%) | 0           | 3  |
| 17  | AT    | 98/105 (93%)  | 75 (76%)  | 17 (17%) | 6 (6%)   | 1           | 12 |
| 17  | CT    | 98/105 (93%)  | 75 (76%)  | 15 (15%) | 8 (8%)   | 0           | 8  |
| 18  | AU    | 69/88 (78%)   | 42 (61%)  | 21 (30%) | 6 (9%)   | 0           | 7  |
| 18  | CU    | 68/88 (77%)   | 46 (68%)  | 14 (21%) | 8 (12%)  | 0           | 4  |
| 19  | AV    | 80/93 (86%)   | 43 (54%)  | 20 (25%) | 17 (21%) | 0           | 1  |
| 19  | CV    | 82/93 (88%)   | 46 (56%)  | 18 (22%) | 18 (22%) | 0           | 1  |
| 20  | AW    | 97/106 (92%)  | 54 (56%)  | 26 (27%) | 17 (18%) | 0           | 2  |
| 20  | CW    | 97/106 (92%)  | 63 (65%)  | 16 (16%) | 18 (19%) | 0           | 1  |
| 21  | AX    | 23/27 (85%)   | 15 (65%)  | 7 (30%)  | 1 (4%)   | 2           | 18 |
| 21  | CX    | 23/27 (85%)   | 15 (65%)  | 4 (17%)  | 4 (17%)  | 0           | 2  |
| 26  | BD    | 270/276 (98%) | 193 (72%) | 46 (17%) | 31 (12%) | 0           | 5  |
| 26  | DD    | 270/276 (98%) | 204 (76%) | 46 (17%) | 20 (7%)  | 1           | 9  |
| 27  | BE    | 203/206 (98%) | 114 (56%) | 46 (23%) | 43 (21%) | 0           | 1  |
| 27  | DE    | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0           | 1  |
| 28  | BF    | 206/210 (98%) | 137 (66%) | 45 (22%) | 24 (12%) | 0           | 4  |
| 28  | DF    | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 0           | 6  |
| 29  | BG    | 179/182 (98%) | 114 (64%) | 39 (22%) | 26 (14%) | 0           | 3  |
| 29  | DG    | 179/182 (98%) | 120 (67%) | 38 (21%) | 21 (12%) | 0           | 4  |

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| Mol | Chain | Analysed      | Favoured | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 30  | BH    | 168/180 (93%) | 60 (36%) | 54 (32%) | 54 (32%) | 0           | 0  |
| 30  | DH    | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0           | 1  |
| 31  | BK    | 144/148 (97%) | 77 (54%) | 45 (31%) | 22 (15%) | 0           | 2  |
| 31  | DK    | 144/148 (97%) | 80 (56%) | 36 (25%) | 28 (19%) | 0           | 1  |
| 32  | BM    | 136/140 (97%) | 88 (65%) | 29 (21%) | 19 (14%) | 0           | 3  |
| 32  | DM    | 136/140 (97%) | 84 (62%) | 30 (22%) | 22 (16%) | 0           | 2  |
| 33  | BN    | 120/122 (98%) | 96 (80%) | 17 (14%) | 7 (6%)   | 1           | 13 |
| 33  | DN    | 120/122 (98%) | 90 (75%) | 21 (18%) | 9 (8%)   | 1           | 9  |
| 34  | BO    | 148/150 (99%) | 80 (54%) | 32 (22%) | 36 (24%) | 0           | 0  |
| 34  | DO    | 148/150 (99%) | 97 (66%) | 19 (13%) | 32 (22%) | 0           | 1  |
| 35  | BP    | 139/141 (99%) | 96 (69%) | 24 (17%) | 19 (14%) | 0           | 3  |
| 35  | DP    | 139/141 (99%) | 94 (68%) | 30 (22%) | 15 (11%) | 0           | 5  |
| 36  | B0    | 115/118 (98%) | 73 (64%) | 31 (27%) | 11 (10%) | 0           | 6  |
| 36  | D0    | 116/118 (98%) | 82 (71%) | 20 (17%) | 14 (12%) | 0           | 4  |
| 37  | BQ    | 109/112 (97%) | 58 (53%) | 32 (29%) | 19 (17%) | 0           | 2  |
| 37  | DQ    | 109/112 (97%) | 62 (57%) | 28 (26%) | 19 (17%) | 0           | 2  |
| 38  | BR    | 135/146 (92%) | 94 (70%) | 31 (23%) | 10 (7%)  | 1           | 9  |
| 38  | DR    | 135/146 (92%) | 83 (62%) | 32 (24%) | 20 (15%) | 0           | 2  |
| 39  | B1    | 115/118 (98%) | 81 (70%) | 22 (19%) | 12 (10%) | 0           | 5  |
| 39  | D1    | 115/118 (98%) | 87 (76%) | 19 (16%) | 9 (8%)   | 1           | 8  |
| 40  | B2    | 99/101 (98%)  | 67 (68%) | 12 (12%) | 20 (20%) | 0           | 1  |
| 40  | D2    | 99/101 (98%)  | 73 (74%) | 16 (16%) | 10 (10%) | 0           | 6  |
| 41  | BS    | 111/113 (98%) | 79 (71%) | 20 (18%) | 12 (11%) | 0           | 5  |
| 41  | DS    | 111/113 (98%) | 75 (68%) | 22 (20%) | 14 (13%) | 0           | 4  |
| 42  | BT    | 90/96 (94%)   | 63 (70%) | 18 (20%) | 9 (10%)  | 0           | 6  |
| 42  | DT    | 90/96 (94%)   | 77 (86%) | 8 (9%)   | 5 (6%)   | 1           | 13 |
| 43  | BU    | 100/110 (91%) | 37 (37%) | 29 (29%) | 34 (34%) | 0           | 0  |
| 43  | DU    | 100/110 (91%) | 57 (57%) | 17 (17%) | 26 (26%) | 0           | 0  |
| 44  | BV    | 174/206 (84%) | 85 (49%) | 43 (25%) | 46 (26%) | 0           | 0  |
| 44  | DV    | 170/206 (82%) | 91 (54%) | 40 (24%) | 39 (23%) | 0           | 1  |
| 45  | B3    | 78/85 (92%)   | 54 (69%) | 13 (17%) | 11 (14%) | 0           | 3  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 45  | D3    | 75/85 (88%)       | 56 (75%)   | 13 (17%)   | 6 (8%)     | 1           | 8  |
| 46  | BZ    | 95/98 (97%)       | 66 (70%)   | 17 (18%)   | 12 (13%)   | 0           | 4  |
| 46  | DZ    | 95/98 (97%)       | 64 (67%)   | 20 (21%)   | 11 (12%)   | 0           | 4  |
| 47  | BW    | 67/72 (93%)       | 43 (64%)   | 12 (18%)   | 12 (18%)   | 0           | 1  |
| 47  | DW    | 67/72 (93%)       | 46 (69%)   | 12 (18%)   | 9 (13%)    | 0           | 3  |
| 48  | BX    | 57/60 (95%)       | 51 (90%)   | 4 (7%)     | 2 (4%)     | 3           | 23 |
| 48  | DX    | 57/60 (95%)       | 45 (79%)   | 9 (16%)    | 3 (5%)     | 1           | 14 |
| 49  | B4    | 69/71 (97%)       | 33 (48%)   | 10 (14%)   | 26 (38%)   | 0           | 0  |
| 49  | D4    | 69/71 (97%)       | 23 (33%)   | 20 (29%)   | 26 (38%)   | 0           | 0  |
| 50  | B5    | 57/60 (95%)       | 37 (65%)   | 14 (25%)   | 6 (10%)    | 0           | 5  |
| 50  | D5    | 57/60 (95%)       | 33 (58%)   | 9 (16%)    | 15 (26%)   | 0           | 0  |
| 51  | B6    | 46/54 (85%)       | 9 (20%)    | 11 (24%)   | 26 (56%)   | 0           | 0  |
| 51  | D6    | 47/54 (87%)       | 15 (32%)   | 18 (38%)   | 14 (30%)   | 0           | 0  |
| 52  | B7    | 47/49 (96%)       | 36 (77%)   | 9 (19%)    | 2 (4%)     | 2           | 18 |
| 52  | D7    | 47/49 (96%)       | 37 (79%)   | 7 (15%)    | 3 (6%)     | 1           | 11 |
| 53  | B8    | 62/65 (95%)       | 37 (60%)   | 14 (23%)   | 11 (18%)   | 0           | 1  |
| 53  | D8    | 62/65 (95%)       | 36 (58%)   | 15 (24%)   | 11 (18%)   | 0           | 1  |
| All | All   | 11381/12054 (94%) | 7244 (64%) | 2468 (22%) | 1669 (15%) | 0           | 3  |

5 of 1669 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AE    | 8   | LYS  |
| 2   | AE    | 17  | PHE  |
| 2   | AE    | 20  | GLU  |
| 2   | AE    | 23  | ARG  |
| 2   | AE    | 29  | ALA  |

#### 4.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | AE    | 204/220 (93%)  | 169 (83%) | 35 (17%) | 2           | 12 |
| 2   | CE    | 205/220 (93%)  | 181 (88%) | 24 (12%) | 5           | 24 |
| 3   | AF    | 160/188 (85%)  | 139 (87%) | 21 (13%) | 4           | 20 |
| 3   | CF    | 159/188 (85%)  | 144 (91%) | 15 (9%)  | 8           | 31 |
| 4   | AG    | 180/181 (99%)  | 153 (85%) | 27 (15%) | 3           | 17 |
| 4   | CG    | 180/181 (99%)  | 161 (89%) | 19 (11%) | 6           | 27 |
| 5   | AH    | 119/123 (97%)  | 99 (83%)  | 20 (17%) | 2           | 13 |
| 5   | CH    | 116/123 (94%)  | 104 (90%) | 12 (10%) | 7           | 28 |
| 6   | AI    | 90/90 (100%)   | 79 (88%)  | 11 (12%) | 5           | 22 |
| 6   | CI    | 90/90 (100%)   | 76 (84%)  | 14 (16%) | 2           | 15 |
| 7   | AJ    | 126/127 (99%)  | 114 (90%) | 12 (10%) | 8           | 31 |
| 7   | CJ    | 126/127 (99%)  | 113 (90%) | 13 (10%) | 7           | 28 |
| 8   | AK    | 119/119 (100%) | 108 (91%) | 11 (9%)  | 8           | 32 |
| 8   | CK    | 119/119 (100%) | 106 (89%) | 13 (11%) | 6           | 26 |
| 9   | AL    | 99/99 (100%)   | 80 (81%)  | 19 (19%) | 1           | 8  |
| 9   | CL    | 98/99 (99%)    | 84 (86%)  | 14 (14%) | 3           | 18 |
| 10  | AM    | 89/92 (97%)    | 80 (90%)  | 9 (10%)  | 7           | 28 |
| 10  | CM    | 89/92 (97%)    | 81 (91%)  | 8 (9%)   | 9           | 32 |
| 11  | AN    | 92/99 (93%)    | 80 (87%)  | 12 (13%) | 4           | 21 |
| 11  | CN    | 90/99 (91%)    | 82 (91%)  | 8 (9%)   | 9           | 32 |
| 12  | AO    | 104/109 (95%)  | 91 (88%)  | 13 (12%) | 4           | 22 |
| 12  | CO    | 104/109 (95%)  | 86 (83%)  | 18 (17%) | 2           | 11 |
| 13  | AP    | 94/101 (93%)   | 77 (82%)  | 17 (18%) | 2           | 10 |
| 13  | CP    | 97/101 (96%)   | 83 (86%)  | 14 (14%) | 3           | 18 |
| 14  | AQ    | 49/50 (98%)    | 44 (90%)  | 5 (10%)  | 7           | 28 |
| 14  | CQ    | 49/50 (98%)    | 42 (86%)  | 7 (14%)  | 3           | 18 |
| 15  | AR    | 79/80 (99%)    | 74 (94%)  | 5 (6%)   | 16          | 42 |
| 15  | CR    | 79/80 (99%)    | 71 (90%)  | 8 (10%)  | 7           | 28 |
| 16  | AS    | 72/74 (97%)    | 61 (85%)  | 11 (15%) | 3           | 16 |
| 16  | CS    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 6           | 25 |
| 17  | AT    | 95/97 (98%)    | 86 (90%)  | 9 (10%)  | 8           | 31 |
| 17  | CT    | 95/97 (98%)    | 86 (90%)  | 9 (10%)  | 8           | 31 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 18  | AU    | 62/77 (80%)    | 55 (89%)  | 7 (11%)  | 5           | 25  |
| 18  | CU    | 61/77 (79%)    | 52 (85%)  | 9 (15%)  | 3           | 17  |
| 19  | AV    | 71/80 (89%)    | 61 (86%)  | 10 (14%) | 3           | 18  |
| 19  | CV    | 73/80 (91%)    | 62 (85%)  | 11 (15%) | 3           | 16  |
| 20  | AW    | 76/82 (93%)    | 64 (84%)  | 12 (16%) | 2           | 15  |
| 20  | CW    | 76/82 (93%)    | 68 (90%)  | 8 (10%)  | 6           | 27  |
| 21  | AX    | 20/22 (91%)    | 18 (90%)  | 2 (10%)  | 7           | 28  |
| 21  | CX    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 26  | BD    | 214/218 (98%)  | 181 (85%) | 33 (15%) | 2           | 16  |
| 26  | DD    | 214/218 (98%)  | 174 (81%) | 40 (19%) | 1           | 9   |
| 27  | BE    | 165/166 (99%)  | 135 (82%) | 30 (18%) | 2           | 10  |
| 27  | DE    | 165/166 (99%)  | 125 (76%) | 40 (24%) | 1           | 4   |
| 28  | BF    | 165/166 (99%)  | 144 (87%) | 21 (13%) | 4           | 21  |
| 28  | DF    | 161/166 (97%)  | 137 (85%) | 24 (15%) | 3           | 17  |
| 29  | BG    | 155/156 (99%)  | 138 (89%) | 17 (11%) | 6           | 26  |
| 29  | DG    | 155/156 (99%)  | 135 (87%) | 20 (13%) | 4           | 21  |
| 30  | BH    | 142/148 (96%)  | 111 (78%) | 31 (22%) | 1           | 6   |
| 30  | DH    | 142/148 (96%)  | 112 (79%) | 30 (21%) | 1           | 6   |
| 31  | BK    | 122/124 (98%)  | 105 (86%) | 17 (14%) | 3           | 19  |
| 31  | DK    | 122/124 (98%)  | 93 (76%)  | 29 (24%) | 1           | 4   |
| 32  | BM    | 117/119 (98%)  | 100 (86%) | 17 (14%) | 3           | 17  |
| 32  | DM    | 117/119 (98%)  | 96 (82%)  | 21 (18%) | 2           | 10  |
| 33  | BN    | 100/100 (100%) | 86 (86%)  | 14 (14%) | 3           | 19  |
| 33  | DN    | 100/100 (100%) | 89 (89%)  | 11 (11%) | 6           | 26  |
| 34  | BO    | 116/116 (100%) | 83 (72%)  | 33 (28%) | 0           | 2   |
| 34  | DO    | 116/116 (100%) | 88 (76%)  | 28 (24%) | 1           | 4   |
| 35  | BP    | 111/111 (100%) | 91 (82%)  | 20 (18%) | 2           | 10  |
| 35  | DP    | 111/111 (100%) | 93 (84%)  | 18 (16%) | 2           | 14  |
| 36  | B0    | 100/101 (99%)  | 86 (86%)  | 14 (14%) | 3           | 19  |
| 36  | D0    | 101/101 (100%) | 84 (83%)  | 17 (17%) | 2           | 13  |
| 37  | BQ    | 87/88 (99%)    | 75 (86%)  | 12 (14%) | 3           | 19  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 37  | DQ    | 87/88 (99%)   | 73 (84%)  | 14 (16%) | 2           | 14 |
| 38  | BR    | 120/127 (94%) | 98 (82%)  | 22 (18%) | 2           | 10 |
| 38  | DR    | 120/127 (94%) | 98 (82%)  | 22 (18%) | 2           | 10 |
| 39  | B1    | 93/94 (99%)   | 81 (87%)  | 12 (13%) | 4           | 21 |
| 39  | D1    | 93/94 (99%)   | 81 (87%)  | 12 (13%) | 4           | 21 |
| 40  | B2    | 82/82 (100%)  | 67 (82%)  | 15 (18%) | 2           | 10 |
| 40  | D2    | 82/82 (100%)  | 65 (79%)  | 17 (21%) | 1           | 6  |
| 41  | BS    | 92/92 (100%)  | 77 (84%)  | 15 (16%) | 2           | 14 |
| 41  | DS    | 92/92 (100%)  | 76 (83%)  | 16 (17%) | 2           | 11 |
| 42  | BT    | 74/78 (95%)   | 62 (84%)  | 12 (16%) | 2           | 14 |
| 42  | DT    | 74/78 (95%)   | 60 (81%)  | 14 (19%) | 1           | 9  |
| 43  | BU    | 85/91 (93%)   | 65 (76%)  | 20 (24%) | 1           | 4  |
| 43  | DU    | 85/91 (93%)   | 66 (78%)  | 19 (22%) | 1           | 5  |
| 44  | BV    | 155/179 (87%) | 121 (78%) | 34 (22%) | 1           | 5  |
| 44  | DV    | 152/179 (85%) | 121 (80%) | 31 (20%) | 1           | 7  |
| 45  | B3    | 63/67 (94%)   | 54 (86%)  | 9 (14%)  | 3           | 18 |
| 45  | D3    | 62/67 (92%)   | 55 (89%)  | 7 (11%)  | 5           | 25 |
| 46  | BZ    | 82/83 (99%)   | 66 (80%)  | 16 (20%) | 1           | 8  |
| 46  | DZ    | 82/83 (99%)   | 70 (85%)  | 12 (15%) | 3           | 17 |
| 47  | BW    | 64/67 (96%)   | 55 (86%)  | 9 (14%)  | 3           | 18 |
| 47  | DW    | 64/67 (96%)   | 56 (88%)  | 8 (12%)  | 4           | 22 |
| 48  | BX    | 51/52 (98%)   | 41 (80%)  | 10 (20%) | 1           | 8  |
| 48  | DX    | 51/52 (98%)   | 41 (80%)  | 10 (20%) | 1           | 8  |
| 49  | B4    | 63/63 (100%)  | 46 (73%)  | 17 (27%) | 0           | 3  |
| 49  | D4    | 63/63 (100%)  | 46 (73%)  | 17 (27%) | 0           | 3  |
| 50  | B5    | 51/52 (98%)   | 45 (88%)  | 6 (12%)  | 5           | 23 |
| 50  | D5    | 51/52 (98%)   | 39 (76%)  | 12 (24%) | 1           | 4  |
| 51  | B6    | 47/52 (90%)   | 31 (66%)  | 16 (34%) | 0           | 2  |
| 51  | D6    | 48/52 (92%)   | 36 (75%)  | 12 (25%) | 0           | 4  |
| 52  | B7    | 42/42 (100%)  | 33 (79%)  | 9 (21%)  | 1           | 6  |
| 52  | D7    | 42/42 (100%)  | 37 (88%)  | 5 (12%)  | 5           | 23 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 53  | B8    | 54/55 (98%)     | 43 (80%)   | 11 (20%)   | 1           | 7  |
| 53  | D8    | 54/55 (98%)     | 40 (74%)   | 14 (26%)   | 0           | 3  |
| All | All   | 9616/9998 (96%) | 8104 (84%) | 1512 (16%) | 2           | 15 |

5 of 1512 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CP    | 70  | LEU  |
| 31  | DK    | 1   | MET  |
| 16  | CS    | 71  | ARG  |
| 13  | CP    | 66  | LEU  |
| 27  | DE    | 26  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 320 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DF    | 69  | HIS  |
| 40  | D2    | 89  | GLN  |
| 29  | DG    | 121 | ASN  |
| 34  | DO    | 9   | ASN  |
| 44  | DV    | 151 | HIS  |

#### 4.3.3 RNA ⓘ

| Mol | Chain | Analysed         | Backbone Outliers | Pucker Outliers |
|-----|-------|------------------|-------------------|-----------------|
| 1   | AA    | 1516/1244 (121%) | 342 (22%)         | 139 (9%)        |
| 1   | CA    | 1514/1244 (121%) | 320 (21%)         | 133 (8%)        |
| 22  | AC    | 77/77 (100%)     | 15 (19%)          | 5 (6%)          |
| 22  | AD    | 76/77 (98%)      | 28 (36%)          | 6 (7%)          |
| 22  | CB    | 64/77 (83%)      | 15 (23%)          | 3 (4%)          |
| 22  | CC    | 76/77 (98%)      | 15 (19%)          | 8 (10%)         |
| 22  | CD    | 76/77 (98%)      | 11 (14%)          | 1 (1%)          |
| 23  | A1    | 22/25 (88%)      | 10 (45%)          | 3 (13%)         |
| 23  | C1    | 22/25 (88%)      | 9 (40%)           | 5 (22%)         |
| 24  | BA    | 2884/2898 (99%)  | 770 (26%)         | 325 (11%)       |
| 24  | DA    | 2884/2898 (99%)  | 790 (27%)         | 354 (12%)       |
| 25  | BB    | 119/122 (97%)    | 25 (21%)          | 3 (2%)          |
| 25  | DB    | 119/122 (97%)    | 22 (18%)          | 6 (5%)          |
| All | All   | 9449/8963 (105%) | 2372 (25%)        | 991 (10%)       |

5 of 2372 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 4   | U    |
| 1   | AA    | 5   | U    |
| 1   | AA    | 6   | G    |
| 1   | AA    | 8   | A    |
| 1   | AA    | 9   | G    |

5 of 991 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | BA    | 2713 | A    |
| 24  | DA    | 1962 | C    |
| 1   | CA    | 975  | A    |
| 24  | DA    | 1936 | A    |
| 24  | DA    | 2497 | A    |

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

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 4.6 Ligand geometry [i](#)

Of 2659 ligands modelled in this entry, 2659 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

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   | AA    | 1244/1244 (100%) | -0.33  | 10 (0%) 82 60 | 66, 115, 203, 251     | 0     |
| 1   | CA    | 1242/1244 (99%)  | -0.28  | 17 (1%) 73 48 | 47, 111, 202, 247     | 0     |
| 2   | AE    | 236/256 (92%)    | -0.11  | 3 (1%) 75 50  | 111, 152, 183, 188    | 0     |
| 2   | CE    | 237/256 (92%)    | -0.10  | 0 100 100     | 108, 138, 175, 185    | 0     |
| 3   | AF    | 206/239 (86%)    | 0.23   | 2 (0%) 79 56  | 116, 134, 171, 178    | 0     |
| 3   | CF    | 205/239 (85%)    | -0.19  | 1 (0%) 87 68  | 98, 128, 150, 160     | 0     |
| 4   | AG    | 208/209 (99%)    | 0.34   | 8 (3%) 44 24  | 72, 106, 128, 137     | 0     |
| 4   | CG    | 208/209 (99%)    | 0.15   | 3 (1%) 73 48  | 95, 116, 136, 143     | 0     |
| 5   | AH    | 154/162 (95%)    | 0.02   | 0 100 100     | 89, 109, 139, 163     | 0     |
| 5   | CH    | 151/162 (93%)    | -0.08  | 0 100 100     | 84, 105, 132, 157     | 0     |
| 6   | AI    | 101/101 (100%)   | -0.15  | 0 100 100     | 85, 106, 121, 138     | 0     |
| 6   | CI    | 101/101 (100%)   | 0.32   | 3 (2%) 52 30  | 80, 109, 119, 139     | 0     |
| 7   | AJ    | 155/156 (99%)    | -0.18  | 1 (0%) 85 65  | 105, 129, 150, 160    | 0     |
| 7   | CJ    | 155/156 (99%)    | -0.05  | 0 100 100     | 98, 121, 141, 157     | 0     |
| 8   | AK    | 138/138 (100%)   | -0.24  | 0 100 100     | 91, 114, 126, 131     | 0     |
| 8   | CK    | 138/138 (100%)   | -0.21  | 0 100 100     | 83, 109, 121, 123     | 0     |
| 9   | AL    | 128/128 (100%)   | -0.22  | 0 100 100     | 109, 150, 168, 173    | 0     |
| 9   | CL    | 127/128 (99%)    | -0.17  | 0 100 100     | 98, 138, 160, 169     | 0     |
| 10  | AM    | 99/105 (94%)     | -0.08  | 0 100 100     | 118, 152, 168, 172    | 0     |
| 10  | CM    | 99/105 (94%)     | -0.21  | 0 100 100     | 111, 147, 168, 175    | 0     |
| 11  | AN    | 121/129 (93%)    | -0.10  | 0 100 100     | 88, 110, 140, 155     | 0     |
| 11  | CN    | 119/129 (92%)    | 0.04   | 2 (1%) 69 43  | 79, 102, 128, 146     | 0     |
| 12  | AO    | 125/132 (94%)    | 0.06   | 0 100 100     | 77, 96, 115, 148      | 0     |
| 12  | CO    | 125/132 (94%)    | -0.05  | 1 (0%) 82 60  | 72, 90, 115, 150      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | AP    | 118/126 (93%)   | 0.15   | 1 (0%) 82 60  | 114, 146, 169, 172    | 0     |
| 13  | CP    | 121/126 (96%)   | 0.32   | 7 (5%) 29 17  | 95, 132, 150, 153     | 0     |
| 14  | AQ    | 60/61 (98%)     | -0.04  | 0 100 100     | 119, 134, 148, 152    | 0     |
| 14  | CQ    | 60/61 (98%)     | -0.26  | 0 100 100     | 97, 116, 127, 129     | 0     |
| 15  | AR    | 88/89 (98%)     | -0.20  | 1 (1%) 78 54  | 80, 102, 125, 136     | 0     |
| 15  | CR    | 88/89 (98%)     | -0.04  | 1 (1%) 78 54  | 77, 103, 122, 127     | 0     |
| 16  | AS    | 84/88 (95%)     | -0.12  | 0 100 100     | 86, 97, 118, 150      | 0     |
| 16  | CS    | 84/88 (95%)     | -0.15  | 1 (1%) 76 52  | 95, 112, 140, 156     | 0     |
| 17  | AT    | 100/105 (95%)   | 0.06   | 1 (1%) 79 56  | 81, 104, 130, 155     | 0     |
| 17  | CT    | 100/105 (95%)   | 0.35   | 3 (3%) 52 30  | 82, 109, 125, 144     | 0     |
| 18  | AU    | 71/88 (80%)     | -0.33  | 0 100 100     | 87, 107, 135, 141     | 0     |
| 18  | CU    | 70/88 (79%)     | 0.10   | 0 100 100     | 84, 107, 125, 125     | 0     |
| 19  | AV    | 82/93 (88%)     | 0.30   | 3 (3%) 45 25  | 130, 159, 169, 170    | 0     |
| 19  | CV    | 84/93 (90%)     | 0.23   | 0 100 100     | 118, 134, 149, 152    | 0     |
| 20  | AW    | 99/106 (93%)    | -0.05  | 0 100 100     | 88, 106, 149, 157     | 0     |
| 20  | CW    | 99/106 (93%)    | -0.11  | 0 100 100     | 96, 119, 148, 155     | 0     |
| 21  | AX    | 25/27 (92%)     | -0.07  | 0 100 100     | 143, 151, 161, 165    | 0     |
| 21  | CX    | 25/27 (92%)     | -0.32  | 0 100 100     | 101, 131, 147, 158    | 0     |
| 22  | AC    | 77/77 (100%)    | -0.43  | 0 100 100     | 76, 119, 153, 162     | 0     |
| 22  | AD    | 77/77 (100%)    | -0.21  | 0 100 100     | 111, 217, 236, 246    | 0     |
| 22  | CB    | 65/77 (84%)     | 0.24   | 1 (1%) 72 47  | 133, 199, 226, 234    | 0     |
| 22  | CC    | 77/77 (100%)    | -0.34  | 1 (1%) 75 50  | 68, 99, 133, 139      | 0     |
| 22  | CD    | 77/77 (100%)    | 0.11   | 1 (1%) 75 50  | 105, 210, 222, 228    | 0     |
| 23  | A1    | 23/25 (92%)     | 0.36   | 1 (4%) 40 21  | 101, 193, 235, 240    | 0     |
| 23  | C1    | 23/25 (92%)     | 0.11   | 0 100 100     | 87, 180, 239, 241     | 0     |
| 24  | BA    | 2885/2898 (99%) | -0.38  | 9 (0%) 90 76  | 53, 90, 211, 243      | 0     |
| 24  | DA    | 2886/2898 (99%) | -0.44  | 24 (0%) 82 60 | 35, 74, 192, 231      | 0     |
| 25  | BB    | 120/122 (98%)   | -0.43  | 0 100 100     | 103, 144, 169, 214    | 0     |
| 25  | DB    | 120/122 (98%)   | -0.43  | 1 (0%) 82 60  | 77, 106, 126, 157     | 0     |
| 26  | BD    | 272/276 (98%)   | 0.16   | 2 (0%) 84 63  | 50, 78, 97, 112       | 0     |
| 26  | DD    | 272/276 (98%)   | 0.16   | 5 (1%) 67 42  | 44, 63, 84, 100       | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 27  | BE    | 205/206 (99%)  | 0.20   | 8 (3%) 43 23 | 60, 93, 138, 151      | 0     |
| 27  | DE    | 205/206 (99%)  | -0.06  | 0 100 100    | 48, 84, 123, 139      | 0     |
| 28  | BF    | 208/210 (99%)  | 0.08   | 2 (0%) 79 56 | 62, 98, 158, 176      | 0     |
| 28  | DF    | 202/210 (96%)  | -0.28  | 3 (1%) 72 47 | 40, 74, 112, 125      | 0     |
| 29  | BG    | 181/182 (99%)  | 0.10   | 1 (0%) 85 65 | 120, 144, 163, 175    | 0     |
| 29  | DG    | 181/182 (99%)  | 0.35   | 8 (4%) 39 21 | 86, 109, 136, 146     | 0     |
| 30  | BH    | 170/180 (94%)  | 0.26   | 3 (1%) 67 42 | 121, 169, 203, 209    | 0     |
| 30  | DH    | 170/180 (94%)  | 0.05   | 2 (1%) 76 52 | 75, 101, 123, 131     | 0     |
| 31  | BK    | 146/148 (98%)  | 0.08   | 0 100 100    | 82, 122, 143, 151     | 0     |
| 31  | DK    | 146/148 (98%)  | 0.12   | 3 (2%) 63 38 | 68, 112, 127, 142     | 0     |
| 32  | BM    | 138/140 (98%)  | -0.02  | 0 100 100    | 80, 105, 124, 129     | 0     |
| 32  | DM    | 138/140 (98%)  | -0.14  | 3 (2%) 62 37 | 66, 84, 116, 123      | 0     |
| 33  | BN    | 122/122 (100%) | 0.10   | 0 100 100    | 69, 86, 99, 105       | 0     |
| 33  | DN    | 122/122 (100%) | -0.19  | 0 100 100    | 50, 77, 90, 95        | 0     |
| 34  | BO    | 150/150 (100%) | -0.29  | 1 (0%) 84 63 | 67, 106, 135, 158     | 0     |
| 34  | DO    | 150/150 (100%) | -0.13  | 0 100 100    | 45, 88, 114, 138      | 0     |
| 35  | BP    | 141/141 (100%) | 0.05   | 3 (2%) 63 38 | 82, 105, 134, 178     | 0     |
| 35  | DP    | 141/141 (100%) | 0.08   | 3 (2%) 63 38 | 62, 86, 107, 131      | 0     |
| 36  | B0    | 117/118 (99%)  | -0.08  | 3 (2%) 57 33 | 54, 80, 102, 119      | 0     |
| 36  | D0    | 118/118 (100%) | -0.08  | 0 100 100    | 54, 80, 98, 107       | 0     |
| 37  | BQ    | 111/112 (99%)  | -0.44  | 0 100 100    | 113, 132, 155, 167    | 0     |
| 37  | DQ    | 111/112 (99%)  | -0.09  | 1 (0%) 81 58 | 82, 97, 130, 139      | 0     |
| 38  | BR    | 137/146 (93%)  | 0.19   | 5 (3%) 46 25 | 77, 93, 148, 177      | 0     |
| 38  | DR    | 137/146 (93%)  | 0.03   | 3 (2%) 62 37 | 71, 89, 136, 157      | 0     |
| 39  | B1    | 117/118 (99%)  | -0.20  | 2 (1%) 69 43 | 68, 94, 135, 155      | 0     |
| 39  | D1    | 117/118 (99%)  | -0.30  | 0 100 100    | 53, 69, 104, 130      | 0     |
| 40  | B2    | 101/101 (100%) | 0.12   | 0 100 100    | 64, 118, 132, 136     | 0     |
| 40  | D2    | 101/101 (100%) | 0.12   | 3 (2%) 52 30 | 52, 97, 117, 126      | 0     |
| 41  | BS    | 113/113 (100%) | -0.06  | 0 100 100    | 67, 80, 101, 141      | 0     |
| 41  | DS    | 113/113 (100%) | -0.21  | 3 (2%) 56 33 | 53, 70, 100, 142      | 0     |
| 42  | BT    | 92/96 (95%)    | 0.10   | 2 (2%) 62 37 | 73, 89, 111, 121      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------|-----|-----|-----------------------|-------|
| 42  | DT    | 92/96 (95%)       | -0.07  | 3 (3%)   | 49  | 28  | 54, 70, 91, 103       | 0     |
| 43  | BU    | 102/110 (92%)     | 0.56   | 7 (6%)   | 23  | 14  | 79, 106, 161, 172     | 0     |
| 43  | DU    | 102/110 (92%)     | 0.07   | 4 (3%)   | 43  | 23  | 67, 93, 134, 144      | 0     |
| 44  | BV    | 176/206 (85%)     | -0.01  | 0        | 100 | 100 | 113, 142, 185, 190    | 0     |
| 44  | DV    | 172/206 (83%)     | 0.44   | 8 (4%)   | 36  | 20  | 90, 126, 184, 190     | 0     |
| 45  | B3    | 80/85 (94%)       | -0.57  | 0        | 100 | 100 | 84, 99, 113, 119      | 0     |
| 45  | D3    | 77/85 (90%)       | -0.32  | 1 (1%)   | 75  | 50  | 67, 81, 100, 115      | 0     |
| 46  | BZ    | 97/98 (98%)       | 0.29   | 6 (6%)   | 26  | 16  | 67, 91, 149, 174      | 0     |
| 46  | DZ    | 97/98 (98%)       | 0.08   | 4 (4%)   | 41  | 22  | 48, 78, 141, 158      | 0     |
| 47  | BW    | 69/72 (95%)       | 0.05   | 1 (1%)   | 73  | 48  | 80, 105, 125, 140     | 0     |
| 47  | DW    | 69/72 (95%)       | -0.06  | 0        | 100 | 100 | 60, 83, 105, 122      | 0     |
| 48  | BX    | 59/60 (98%)       | -0.31  | 0        | 100 | 100 | 83, 107, 129, 134     | 0     |
| 48  | DX    | 59/60 (98%)       | -0.06  | 0        | 100 | 100 | 64, 84, 110, 124      | 0     |
| 49  | B4    | 71/71 (100%)      | 0.61   | 6 (8%)   | 16  | 11  | 164, 193, 208, 211    | 0     |
| 49  | D4    | 71/71 (100%)      | 0.70   | 2 (2%)   | 55  | 32  | 128, 160, 185, 188    | 0     |
| 50  | B5    | 59/60 (98%)       | 0.40   | 5 (8%)   | 16  | 11  | 56, 91, 168, 177      | 0     |
| 50  | D5    | 59/60 (98%)       | 0.00   | 2 (3%)   | 48  | 27  | 46, 86, 186, 190      | 0     |
| 51  | B6    | 48/54 (88%)       | -0.23  | 0        | 100 | 100 | 138, 153, 169, 175    | 0     |
| 51  | D6    | 49/54 (90%)       | 0.48   | 1 (2%)   | 65  | 39  | 132, 146, 156, 162    | 0     |
| 52  | B7    | 49/49 (100%)      | -0.18  | 1 (2%)   | 65  | 39  | 51, 68, 116, 148      | 0     |
| 52  | D7    | 49/49 (100%)      | -0.24  | 1 (2%)   | 65  | 39  | 40, 49, 109, 135      | 0     |
| 53  | B8    | 64/65 (98%)       | -0.25  | 0        | 100 | 100 | 77, 93, 114, 152      | 0     |
| 53  | D8    | 64/65 (98%)       | -0.11  | 0        | 100 | 100 | 53, 72, 100, 127      | 0     |
| All | All   | 20489/21017 (97%) | -0.15  | 228 (1%) | 78  | 54  | 35, 102, 179, 251     | 0     |

The worst 5 of 228 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 50  | B5    | 2    | ALA  | 6.7  |
| 40  | D2    | 36   | PRO  | 5.7  |
| 13  | CP    | 119  | GLY  | 5.5  |
| 1   | CA    | 345  | C    | 5.0  |
| 24  | BA    | 2798 | C    | 4.7  |

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 54  | MG   | CA    | 1847 | 1/1   | -0.36 | 0.30 | 133,133,133,133            | 0     |
| 54  | MG   | DA    | 3794 | 1/1   | -0.22 | 0.27 | 142,142,142,142            | 0     |
| 54  | MG   | AA    | 1909 | 1/1   | -0.20 | 0.43 | 128,128,128,128            | 0     |
| 54  | MG   | DA    | 3791 | 1/1   | -0.07 | 0.30 | 114,114,114,114            | 0     |
| 54  | MG   | DA    | 3802 | 1/1   | -0.03 | 0.26 | 138,138,138,138            | 0     |
| 54  | MG   | AA    | 2004 | 1/1   | 0.07  | 0.25 | 124,124,124,124            | 0     |
| 54  | MG   | AA    | 1834 | 1/1   | 0.08  | 0.27 | 183,183,183,183            | 0     |
| 54  | MG   | DA    | 3792 | 1/1   | 0.08  | 0.21 | 157,157,157,157            | 0     |
| 54  | MG   | CA    | 1848 | 1/1   | 0.09  | 0.20 | 130,130,130,130            | 0     |
| 54  | MG   | CA    | 1947 | 1/1   | 0.10  | 0.33 | 205,205,205,205            | 0     |
| 54  | MG   | DA    | 3463 | 1/1   | 0.11  | 0.34 | 155,155,155,155            | 0     |
| 54  | MG   | AA    | 1911 | 1/1   | 0.14  | 0.40 | 104,104,104,104            | 0     |
| 54  | MG   | BA    | 3283 | 1/1   | 0.15  | 0.24 | 126,126,126,126            | 0     |
| 54  | MG   | AA    | 1882 | 1/1   | 0.16  | 0.20 | 134,134,134,134            | 0     |
| 54  | MG   | AA    | 1915 | 1/1   | 0.16  | 0.18 | 172,172,172,172            | 0     |
| 54  | MG   | BA    | 3468 | 1/1   | 0.16  | 0.20 | 110,110,110,110            | 0     |
| 54  | MG   | BB    | 226  | 1/1   | 0.16  | 0.21 | 146,146,146,146            | 0     |
| 54  | MG   | BA    | 3297 | 1/1   | 0.18  | 0.17 | 131,131,131,131            | 0     |
| 54  | MG   | AA    | 1949 | 1/1   | 0.19  | 0.22 | 122,122,122,122            | 0     |
| 54  | MG   | DA    | 3049 | 1/1   | 0.20  | 0.38 | 114,114,114,114            | 0     |
| 54  | MG   | DA    | 3570 | 1/1   | 0.20  | 0.36 | 152,152,152,152            | 0     |
| 54  | MG   | BA    | 3471 | 1/1   | 0.21  | 0.23 | 156,156,156,156            | 0     |
| 54  | MG   | AA    | 2014 | 1/1   | 0.21  | 0.20 | 175,175,175,175            | 0     |
| 54  | MG   | BA    | 3554 | 1/1   | 0.22  | 0.15 | 122,122,122,122            | 0     |
| 54  | MG   | AA    | 1932 | 1/1   | 0.23  | 0.29 | 122,122,122,122            | 0     |
| 54  | MG   | AA    | 1622 | 1/1   | 0.23  | 0.21 | 78,78,78,78                | 0     |
| 54  | MG   | AA    | 1887 | 1/1   | 0.24  | 0.18 | 161,161,161,161            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1956 | 1/1   | 0.24 | 0.11 | 217,217,217,217             | 0     |
| 54  | MG   | AA    | 1805 | 1/1   | 0.24 | 0.32 | 109,109,109,109             | 0     |
| 54  | MG   | DU    | 202  | 1/1   | 0.24 | 0.24 | 139,139,139,139             | 0     |
| 54  | MG   | AD    | 102  | 1/1   | 0.25 | 0.08 | 120,120,120,120             | 0     |
| 54  | MG   | AA    | 2030 | 1/1   | 0.26 | 0.36 | 188,188,188,188             | 0     |
| 54  | MG   | AA    | 1789 | 1/1   | 0.26 | 0.29 | 128,128,128,128             | 0     |
| 54  | MG   | CA    | 1824 | 1/1   | 0.27 | 0.18 | 156,156,156,156             | 0     |
| 54  | MG   | AA    | 1865 | 1/1   | 0.27 | 0.30 | 140,140,140,140             | 0     |
| 54  | MG   | DA    | 3790 | 1/1   | 0.27 | 0.25 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1800 | 1/1   | 0.27 | 0.36 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3512 | 1/1   | 0.28 | 0.41 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1709 | 1/1   | 0.30 | 0.19 | 130,130,130,130             | 0     |
| 54  | MG   | BA    | 3571 | 1/1   | 0.30 | 0.17 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3417 | 1/1   | 0.30 | 0.14 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1835 | 1/1   | 0.32 | 0.33 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1861 | 1/1   | 0.32 | 0.16 | 120,120,120,120             | 0     |
| 54  | MG   | CA    | 1741 | 1/1   | 0.32 | 0.29 | 123,123,123,123             | 0     |
| 54  | MG   | CA    | 1878 | 1/1   | 0.32 | 0.17 | 133,133,133,133             | 0     |
| 54  | MG   | AA    | 1761 | 1/1   | 0.34 | 0.23 | 136,136,136,136             | 0     |
| 54  | MG   | DA    | 3491 | 1/1   | 0.34 | 0.35 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3232 | 1/1   | 0.35 | 0.14 | 99,99,99,99                 | 0     |
| 54  | MG   | BH    | 201  | 1/1   | 0.35 | 0.28 | 193,193,193,193             | 0     |
| 54  | MG   | AA    | 1910 | 1/1   | 0.35 | 0.29 | 103,103,103,103             | 0     |
| 54  | MG   | AA    | 1840 | 1/1   | 0.35 | 0.46 | 132,132,132,132             | 0     |
| 54  | MG   | AA    | 1706 | 1/1   | 0.35 | 0.32 | 143,143,143,143             | 0     |
| 54  | MG   | DB    | 227  | 1/1   | 0.36 | 0.28 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1806 | 1/1   | 0.36 | 0.21 | 118,118,118,118             | 0     |
| 54  | MG   | DA    | 3597 | 1/1   | 0.37 | 0.32 | 168,168,168,168             | 0     |
| 54  | MG   | AA    | 2038 | 1/1   | 0.37 | 0.24 | 116,116,116,116             | 0     |
| 54  | MG   | DA    | 3188 | 1/1   | 0.37 | 0.37 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1808 | 1/1   | 0.37 | 0.25 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3440 | 1/1   | 0.38 | 0.40 | 118,118,118,118             | 0     |
| 54  | MG   | BA    | 2912 | 1/1   | 0.38 | 0.12 | 138,138,138,138             | 0     |
| 54  | MG   | DA    | 3520 | 1/1   | 0.38 | 0.22 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3694 | 1/1   | 0.39 | 0.30 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3631 | 1/1   | 0.39 | 0.22 | 118,118,118,118             | 0     |
| 54  | MG   | DA    | 3675 | 1/1   | 0.40 | 0.28 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1860 | 1/1   | 0.40 | 0.31 | 127,127,127,127             | 0     |
| 54  | MG   | CA    | 1963 | 1/1   | 0.40 | 0.19 | 145,145,145,145             | 0     |
| 54  | MG   | DA    | 3303 | 1/1   | 0.41 | 0.33 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1878 | 1/1   | 0.41 | 0.19 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3499 | 1/1   | 0.41 | 0.19 | 114,114,114,114             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3181 | 1/1   | 0.42 | 0.38 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1903 | 1/1   | 0.42 | 0.33 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3464 | 1/1   | 0.43 | 0.23 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3293 | 1/1   | 0.43 | 0.28 | 134,134,134,134             | 0     |
| 54  | MG   | BA    | 3414 | 1/1   | 0.43 | 0.28 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 2007 | 1/1   | 0.43 | 0.21 | 119,119,119,119             | 0     |
| 54  | MG   | CA    | 1912 | 1/1   | 0.43 | 0.23 | 127,127,127,127             | 0     |
| 54  | MG   | AA    | 1816 | 1/1   | 0.44 | 0.30 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1719 | 1/1   | 0.44 | 0.35 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1782 | 1/1   | 0.44 | 0.21 | 123,123,123,123             | 0     |
| 54  | MG   | BA    | 3376 | 1/1   | 0.44 | 0.24 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3656 | 1/1   | 0.44 | 0.29 | 136,136,136,136             | 0     |
| 54  | MG   | AA    | 1958 | 1/1   | 0.44 | 0.19 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3246 | 1/1   | 0.44 | 0.29 | 101,101,101,101             | 0     |
| 54  | MG   | CA    | 1846 | 1/1   | 0.45 | 0.25 | 129,129,129,129             | 0     |
| 54  | MG   | BA    | 3555 | 1/1   | 0.45 | 0.16 | 119,119,119,119             | 0     |
| 54  | MG   | CA    | 1813 | 1/1   | 0.45 | 0.16 | 127,127,127,127             | 0     |
| 54  | MG   | BA    | 3320 | 1/1   | 0.45 | 0.31 | 101,101,101,101             | 0     |
| 54  | MG   | CC    | 110  | 1/1   | 0.46 | 0.10 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3671 | 1/1   | 0.46 | 0.23 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1680 | 1/1   | 0.46 | 0.19 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3688 | 1/1   | 0.46 | 0.24 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3561 | 1/1   | 0.46 | 0.34 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3743 | 1/1   | 0.46 | 0.29 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3136 | 1/1   | 0.46 | 0.28 | 111,111,111,111             | 0     |
| 54  | MG   | AA    | 1913 | 1/1   | 0.46 | 0.23 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 2913 | 1/1   | 0.46 | 0.12 | 115,115,115,115             | 0     |
| 54  | MG   | DA    | 3573 | 1/1   | 0.46 | 0.43 | 124,124,124,124             | 0     |
| 54  | MG   | DA    | 3587 | 1/1   | 0.46 | 0.31 | 134,134,134,134             | 0     |
| 54  | MG   | DB    | 221  | 1/1   | 0.46 | 0.14 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3368 | 1/1   | 0.46 | 0.27 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3430 | 1/1   | 0.46 | 0.33 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3465 | 1/1   | 0.47 | 0.32 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1840 | 1/1   | 0.47 | 0.23 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3712 | 1/1   | 0.47 | 0.26 | 138,138,138,138             | 0     |
| 54  | MG   | AA    | 1666 | 1/1   | 0.47 | 0.26 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1653 | 1/1   | 0.48 | 0.16 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1775 | 1/1   | 0.48 | 0.35 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3575 | 1/1   | 0.48 | 0.20 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3018 | 1/1   | 0.48 | 0.34 | 109,109,109,109             | 0     |
| 54  | MG   | CA    | 1975 | 1/1   | 0.48 | 0.17 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3569 | 1/1   | 0.48 | 0.15 | 137,137,137,137             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1812 | 1/1   | 0.48 | 0.22 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3788 | 1/1   | 0.49 | 0.20 | 111,111,111,111             | 0     |
| 54  | MG   | AA    | 1780 | 1/1   | 0.49 | 0.28 | 95,95,95,95                 | 0     |
| 54  | MG   | CA    | 1818 | 1/1   | 0.49 | 0.17 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1655 | 1/1   | 0.49 | 0.21 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3422 | 1/1   | 0.49 | 0.31 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1735 | 1/1   | 0.49 | 0.22 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3245 | 1/1   | 0.49 | 0.12 | 128,128,128,128             | 0     |
| 54  | MG   | BF    | 302  | 1/1   | 0.49 | 0.28 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3265 | 1/1   | 0.49 | 0.23 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3266 | 1/1   | 0.50 | 0.29 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3433 | 1/1   | 0.50 | 0.24 | 109,109,109,109             | 0     |
| 54  | MG   | CS    | 102  | 1/1   | 0.50 | 0.23 | 119,119,119,119             | 0     |
| 54  | MG   | CA    | 1866 | 1/1   | 0.50 | 0.28 | 118,118,118,118             | 0     |
| 54  | MG   | AT    | 201  | 1/1   | 0.50 | 0.26 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3378 | 1/1   | 0.50 | 0.11 | 129,129,129,129             | 0     |
| 54  | MG   | DA    | 3704 | 1/1   | 0.50 | 0.20 | 134,134,134,134             | 0     |
| 54  | MG   | BA    | 3400 | 1/1   | 0.50 | 0.20 | 117,117,117,117             | 0     |
| 54  | MG   | BA    | 3080 | 1/1   | 0.50 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3267 | 1/1   | 0.51 | 0.39 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3479 | 1/1   | 0.51 | 0.22 | 119,119,119,119             | 0     |
| 54  | MG   | DA    | 3091 | 1/1   | 0.51 | 0.40 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3528 | 1/1   | 0.51 | 0.24 | 80,80,80,80                 | 0     |
| 54  | MG   | AJ    | 201  | 1/1   | 0.51 | 0.13 | 116,116,116,116             | 0     |
| 54  | MG   | AA    | 2003 | 1/1   | 0.51 | 0.17 | 128,128,128,128             | 0     |
| 54  | MG   | DB    | 208  | 1/1   | 0.51 | 0.13 | 135,135,135,135             | 0     |
| 54  | MG   | AA    | 1954 | 1/1   | 0.51 | 0.28 | 108,108,108,108             | 0     |
| 54  | MG   | CA    | 1888 | 1/1   | 0.51 | 0.14 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3470 | 1/1   | 0.51 | 0.30 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3336 | 1/1   | 0.52 | 0.35 | 127,127,127,127             | 0     |
| 54  | MG   | DA    | 3134 | 1/1   | 0.52 | 0.34 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3422 | 1/1   | 0.52 | 0.27 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3517 | 1/1   | 0.53 | 0.25 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3432 | 1/1   | 0.53 | 0.17 | 115,115,115,115             | 0     |
| 54  | MG   | CA    | 1707 | 1/1   | 0.53 | 0.14 | 106,106,106,106             | 0     |
| 54  | MG   | CA    | 1727 | 1/1   | 0.53 | 0.12 | 131,131,131,131             | 0     |
| 54  | MG   | AA    | 1993 | 1/1   | 0.53 | 0.19 | 134,134,134,134             | 0     |
| 54  | MG   | BA    | 3572 | 1/1   | 0.53 | 0.27 | 106,106,106,106             | 0     |
| 54  | MG   | CA    | 1788 | 1/1   | 0.53 | 0.28 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3441 | 1/1   | 0.53 | 0.42 | 116,116,116,116             | 0     |
| 54  | MG   | DA    | 3618 | 1/1   | 0.53 | 0.33 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1956 | 1/1   | 0.53 | 0.22 | 118,118,118,118             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AL    | 202  | 1/1   | 0.53 | 0.09 | 129,129,129,129             | 0     |
| 54  | MG   | AA    | 1696 | 1/1   | 0.53 | 0.23 | 134,134,134,134             | 0     |
| 54  | MG   | BQ    | 201  | 1/1   | 0.53 | 0.10 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1830 | 1/1   | 0.53 | 0.18 | 135,135,135,135             | 0     |
| 54  | MG   | CW    | 205  | 1/1   | 0.54 | 0.20 | 143,143,143,143             | 0     |
| 54  | MG   | DA    | 3611 | 1/1   | 0.54 | 0.31 | 112,112,112,112             | 0     |
| 54  | MG   | AA    | 1937 | 1/1   | 0.54 | 0.30 | 95,95,95,95                 | 0     |
| 54  | MG   | CA    | 1910 | 1/1   | 0.54 | 0.14 | 130,130,130,130             | 0     |
| 54  | MG   | DA    | 3738 | 1/1   | 0.54 | 0.15 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1964 | 1/1   | 0.54 | 0.30 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1858 | 1/1   | 0.54 | 0.27 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3311 | 1/1   | 0.54 | 0.22 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1747 | 1/1   | 0.55 | 0.27 | 89,89,89,89                 | 0     |
| 54  | MG   | DB    | 213  | 1/1   | 0.55 | 0.25 | 133,133,133,133             | 0     |
| 54  | MG   | CA    | 1759 | 1/1   | 0.55 | 0.24 | 113,113,113,113             | 0     |
| 54  | MG   | DB    | 222  | 1/1   | 0.55 | 0.19 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1815 | 1/1   | 0.55 | 0.34 | 105,105,105,105             | 0     |
| 54  | MG   | DG    | 203  | 1/1   | 0.55 | 0.30 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3472 | 1/1   | 0.55 | 0.30 | 111,111,111,111             | 0     |
| 54  | MG   | CA    | 1722 | 1/1   | 0.56 | 0.22 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3746 | 1/1   | 0.56 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3594 | 1/1   | 0.56 | 0.17 | 123,123,123,123             | 0     |
| 54  | MG   | CA    | 1942 | 1/1   | 0.56 | 0.14 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 2911 | 1/1   | 0.56 | 0.08 | 120,120,120,120             | 0     |
| 54  | MG   | AA    | 2024 | 1/1   | 0.56 | 0.27 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1971 | 1/1   | 0.56 | 0.13 | 123,123,123,123             | 0     |
| 54  | MG   | AA    | 1872 | 1/1   | 0.56 | 0.13 | 108,108,108,108             | 0     |
| 54  | MG   | AA    | 1826 | 1/1   | 0.56 | 0.34 | 108,108,108,108             | 0     |
| 54  | MG   | AA    | 1919 | 1/1   | 0.56 | 0.35 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3527 | 1/1   | 0.56 | 0.30 | 127,127,127,127             | 0     |
| 54  | MG   | AA    | 1727 | 1/1   | 0.56 | 0.22 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3205 | 1/1   | 0.56 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | AW    | 203  | 1/1   | 0.56 | 0.27 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1687 | 1/1   | 0.56 | 0.27 | 138,138,138,138             | 0     |
| 54  | MG   | DA    | 3238 | 1/1   | 0.57 | 0.33 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3375 | 1/1   | 0.57 | 0.12 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3515 | 1/1   | 0.57 | 0.19 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1966 | 1/1   | 0.57 | 0.18 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1794 | 1/1   | 0.57 | 0.18 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1862 | 1/1   | 0.57 | 0.12 | 112,112,112,112             | 0     |
| 54  | MG   | AT    | 202  | 1/1   | 0.57 | 0.19 | 111,111,111,111             | 0     |
| 54  | MG   | DA    | 3532 | 1/1   | 0.57 | 0.18 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3278 | 1/1   | 0.57 | 0.23 | 119,119,119,119             | 0     |
| 54  | MG   | BB    | 225  | 1/1   | 0.57 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3281 | 1/1   | 0.58 | 0.18 | 123,123,123,123             | 0     |
| 54  | MG   | DB    | 201  | 1/1   | 0.58 | 0.26 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3076 | 1/1   | 0.58 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3450 | 1/1   | 0.58 | 0.20 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 2023 | 1/1   | 0.58 | 0.10 | 112,112,112,112             | 0     |
| 54  | MG   | CA    | 1704 | 1/1   | 0.58 | 0.18 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 2029 | 1/1   | 0.58 | 0.36 | 127,127,127,127             | 0     |
| 54  | MG   | DA    | 3269 | 1/1   | 0.58 | 0.44 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3477 | 1/1   | 0.58 | 0.14 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3644 | 1/1   | 0.59 | 0.35 | 106,106,106,106             | 0     |
| 54  | MG   | CR    | 101  | 1/1   | 0.59 | 0.26 | 117,117,117,117             | 0     |
| 54  | MG   | BA    | 3335 | 1/1   | 0.59 | 0.36 | 86,86,86,86                 | 0     |
| 54  | MG   | DB    | 229  | 1/1   | 0.59 | 0.24 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1689 | 1/1   | 0.59 | 0.22 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3328 | 1/1   | 0.59 | 0.23 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1904 | 1/1   | 0.60 | 0.20 | 121,121,121,121             | 0     |
| 54  | MG   | CA    | 1897 | 1/1   | 0.60 | 0.16 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1939 | 1/1   | 0.60 | 0.20 | 118,118,118,118             | 0     |
| 54  | MG   | DA    | 3451 | 1/1   | 0.60 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3301 | 1/1   | 0.60 | 0.25 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1742 | 1/1   | 0.60 | 0.14 | 124,124,124,124             | 0     |
| 54  | MG   | CA    | 1841 | 1/1   | 0.60 | 0.18 | 119,119,119,119             | 0     |
| 54  | MG   | CA    | 1748 | 1/1   | 0.60 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1868 | 1/1   | 0.60 | 0.13 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3321 | 1/1   | 0.60 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3299 | 1/1   | 0.60 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1664 | 1/1   | 0.60 | 0.20 | 69,69,69,69                 | 0     |
| 54  | MG   | AA    | 2017 | 1/1   | 0.60 | 0.14 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3368 | 1/1   | 0.60 | 0.25 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1720 | 1/1   | 0.60 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3410 | 1/1   | 0.60 | 0.28 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3570 | 1/1   | 0.60 | 0.20 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3725 | 1/1   | 0.60 | 0.28 | 132,132,132,132             | 0     |
| 54  | MG   | BA    | 3520 | 1/1   | 0.61 | 0.19 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1733 | 1/1   | 0.61 | 0.27 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3682 | 1/1   | 0.61 | 0.49 | 141,141,141,141             | 0     |
| 54  | MG   | AA    | 1899 | 1/1   | 0.61 | 0.15 | 112,112,112,112             | 0     |
| 54  | MG   | AA    | 1762 | 1/1   | 0.61 | 0.27 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1657 | 1/1   | 0.61 | 0.23 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3226 | 1/1   | 0.61 | 0.24 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3235 | 1/1   | 0.61 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1886 | 1/1   | 0.61 | 0.22 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1957 | 1/1   | 0.61 | 0.15 | 82,82,82,82                 | 0     |
| 54  | MG   | AH    | 201  | 1/1   | 0.61 | 0.20 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3574 | 1/1   | 0.61 | 0.12 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3105 | 1/1   | 0.61 | 0.18 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1928 | 1/1   | 0.62 | 0.23 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3716 | 1/1   | 0.62 | 0.21 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3503 | 1/1   | 0.62 | 0.16 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1944 | 1/1   | 0.62 | 0.15 | 99,99,99,99                 | 0     |
| 54  | MG   | AA    | 1799 | 1/1   | 0.62 | 0.13 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1750 | 1/1   | 0.62 | 0.20 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1629 | 1/1   | 0.62 | 0.25 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3789 | 1/1   | 0.62 | 0.23 | 118,118,118,118             | 0     |
| 54  | MG   | DB    | 228  | 1/1   | 0.62 | 0.32 | 116,116,116,116             | 0     |
| 54  | MG   | CA    | 1810 | 1/1   | 0.62 | 0.17 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1662 | 1/1   | 0.62 | 0.19 | 100,100,100,100             | 0     |
| 54  | MG   | AW    | 201  | 1/1   | 0.62 | 0.25 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3424 | 1/1   | 0.63 | 0.30 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3719 | 1/1   | 0.63 | 0.20 | 116,116,116,116             | 0     |
| 54  | MG   | DA    | 3668 | 1/1   | 0.63 | 0.46 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3196 | 1/1   | 0.63 | 0.25 | 106,106,106,106             | 0     |
| 54  | MG   | CC    | 102  | 1/1   | 0.63 | 0.09 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1881 | 1/1   | 0.63 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3785 | 1/1   | 0.63 | 0.27 | 117,117,117,117             | 0     |
| 54  | MG   | CP    | 204  | 1/1   | 0.63 | 0.19 | 137,137,137,137             | 0     |
| 54  | MG   | DA    | 3569 | 1/1   | 0.63 | 0.25 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3699 | 1/1   | 0.63 | 0.29 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1852 | 1/1   | 0.63 | 0.28 | 111,111,111,111             | 0     |
| 54  | MG   | BA    | 3394 | 1/1   | 0.63 | 0.19 | 121,121,121,121             | 0     |
| 54  | MG   | BA    | 3358 | 1/1   | 0.64 | 0.21 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3771 | 1/1   | 0.64 | 0.24 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1876 | 1/1   | 0.64 | 0.12 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1641 | 1/1   | 0.64 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3285 | 1/1   | 0.64 | 0.07 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3293 | 1/1   | 0.64 | 0.13 | 111,111,111,111             | 0     |
| 54  | MG   | AA    | 1926 | 1/1   | 0.64 | 0.17 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3326 | 1/1   | 0.64 | 0.41 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3518 | 1/1   | 0.64 | 0.13 | 78,78,78,78                 | 0     |
| 54  | MG   | CD    | 108  | 1/1   | 0.64 | 0.10 | 174,174,174,174             | 0     |
| 54  | MG   | DA    | 3357 | 1/1   | 0.64 | 0.19 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3242 | 1/1   | 0.64 | 0.18 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1829 | 1/1   | 0.64 | 0.14 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3573 | 1/1   | 0.64 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1724 | 1/1   | 0.64 | 0.35 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3490 | 1/1   | 0.64 | 0.21 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 2034 | 1/1   | 0.64 | 0.23 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1893 | 1/1   | 0.64 | 0.26 | 95,95,95,95                 | 0     |
| 54  | MG   | DF    | 301  | 1/1   | 0.64 | 0.20 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3423 | 1/1   | 0.64 | 0.19 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1787 | 1/1   | 0.64 | 0.21 | 147,147,147,147             | 0     |
| 54  | MG   | BA    | 3201 | 1/1   | 0.65 | 0.17 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1653 | 1/1   | 0.65 | 0.32 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1986 | 1/1   | 0.65 | 0.11 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3360 | 1/1   | 0.65 | 0.23 | 117,117,117,117             | 0     |
| 54  | MG   | BA    | 3223 | 1/1   | 0.65 | 0.24 | 88,88,88,88                 | 0     |
| 54  | MG   | BB    | 208  | 1/1   | 0.65 | 0.11 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1866 | 1/1   | 0.65 | 0.23 | 117,117,117,117             | 0     |
| 54  | MG   | AA    | 1857 | 1/1   | 0.65 | 0.29 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3799 | 1/1   | 0.65 | 0.10 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1739 | 1/1   | 0.65 | 0.12 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3129 | 1/1   | 0.65 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1617 | 1/1   | 0.65 | 0.26 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1904 | 1/1   | 0.65 | 0.33 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3713 | 1/1   | 0.65 | 0.25 | 144,144,144,144             | 0     |
| 54  | MG   | DA    | 3592 | 1/1   | 0.65 | 0.24 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3177 | 1/1   | 0.65 | 0.23 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3034 | 1/1   | 0.65 | 0.26 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3318 | 1/1   | 0.65 | 0.26 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1704 | 1/1   | 0.65 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3628 | 1/1   | 0.65 | 0.21 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3751 | 1/1   | 0.65 | 0.21 | 101,101,101,101             | 0     |
| 55  | ZN   | AA    | 2041 | 1/1   | 0.65 | 0.12 | 262,262,262,262             | 0     |
| 54  | MG   | AA    | 1850 | 1/1   | 0.66 | 0.31 | 112,112,112,112             | 0     |
| 54  | MG   | AA    | 1992 | 1/1   | 0.66 | 0.12 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1945 | 1/1   | 0.66 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1931 | 1/1   | 0.66 | 0.23 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 2907 | 1/1   | 0.66 | 0.15 | 106,106,106,106             | 0     |
| 54  | MG   | CA    | 1922 | 1/1   | 0.66 | 0.28 | 116,116,116,116             | 0     |
| 54  | MG   | DA    | 3018 | 1/1   | 0.66 | 0.32 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1928 | 1/1   | 0.66 | 0.09 | 122,122,122,122             | 0     |
| 54  | MG   | AA    | 1737 | 1/1   | 0.66 | 0.14 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3537 | 1/1   | 0.66 | 0.31 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3142 | 1/1   | 0.66 | 0.22 | 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   | BA    | 3382 | 1/1   | 0.66 | 0.21 | 123,123,123,123             | 0     |
| 54  | MG   | DA    | 3363 | 1/1   | 0.66 | 0.27 | 113,113,113,113             | 0     |
| 54  | MG   | AO    | 201  | 1/1   | 0.66 | 0.20 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3652 | 1/1   | 0.66 | 0.21 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3770 | 1/1   | 0.66 | 0.25 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3379 | 1/1   | 0.66 | 0.28 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1768 | 1/1   | 0.66 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | BR    | 201  | 1/1   | 0.66 | 0.23 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3049 | 1/1   | 0.67 | 0.32 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1971 | 1/1   | 0.67 | 0.20 | 116,116,116,116             | 0     |
| 54  | MG   | BA    | 3071 | 1/1   | 0.67 | 0.17 | 74,74,74,74                 | 0     |
| 54  | MG   | AI    | 201  | 1/1   | 0.67 | 0.24 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1870 | 1/1   | 0.67 | 0.12 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1985 | 1/1   | 0.67 | 0.08 | 131,131,131,131             | 0     |
| 54  | MG   | AA    | 1853 | 1/1   | 0.67 | 0.14 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1906 | 1/1   | 0.67 | 0.21 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1867 | 1/1   | 0.67 | 0.28 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1821 | 1/1   | 0.67 | 0.13 | 141,141,141,141             | 0     |
| 54  | MG   | CA    | 1762 | 1/1   | 0.67 | 0.19 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3008 | 1/1   | 0.67 | 0.19 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3724 | 1/1   | 0.67 | 0.20 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1999 | 1/1   | 0.67 | 0.20 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1661 | 1/1   | 0.67 | 0.19 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3107 | 1/1   | 0.67 | 0.27 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3186 | 1/1   | 0.67 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | BB    | 213  | 1/1   | 0.67 | 0.10 | 122,122,122,122             | 0     |
| 54  | MG   | DA    | 3376 | 1/1   | 0.67 | 0.20 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3660 | 1/1   | 0.67 | 0.29 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3781 | 1/1   | 0.67 | 0.24 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1716 | 1/1   | 0.68 | 0.10 | 110,110,110,110             | 0     |
| 54  | MG   | AA    | 1742 | 1/1   | 0.68 | 0.19 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3509 | 1/1   | 0.68 | 0.11 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1821 | 1/1   | 0.68 | 0.17 | 104,104,104,104             | 0     |
| 54  | MG   | CD    | 107  | 1/1   | 0.68 | 0.18 | 122,122,122,122             | 0     |
| 54  | MG   | CA    | 1908 | 1/1   | 0.68 | 0.23 | 128,128,128,128             | 0     |
| 54  | MG   | AA    | 1997 | 1/1   | 0.68 | 0.18 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3351 | 1/1   | 0.68 | 0.07 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 2036 | 1/1   | 0.68 | 0.14 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1894 | 1/1   | 0.68 | 0.25 | 103,103,103,103             | 0     |
| 54  | MG   | AA    | 1959 | 1/1   | 0.68 | 0.20 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3281 | 1/1   | 0.68 | 0.23 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1849 | 1/1   | 0.68 | 0.24 | 92,92,92,92                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1965 | 1/1   | 0.68 | 0.20 | 117,117,117,117             | 0     |
| 54  | MG   | DB    | 220  | 1/1   | 0.68 | 0.13 | 122,122,122,122             | 0     |
| 54  | MG   | AA    | 1633 | 1/1   | 0.68 | 0.22 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3219 | 1/1   | 0.68 | 0.26 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1644 | 1/1   | 0.68 | 0.27 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1602 | 1/1   | 0.68 | 0.28 | 53,53,53,53                 | 0     |
| 54  | MG   | BB    | 204  | 1/1   | 0.68 | 0.17 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1698 | 1/1   | 0.68 | 0.19 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1955 | 1/1   | 0.68 | 0.25 | 103,103,103,103             | 0     |
| 54  | MG   | AA    | 1632 | 1/1   | 0.68 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | CW    | 202  | 1/1   | 0.68 | 0.23 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3374 | 1/1   | 0.69 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1775 | 1/1   | 0.69 | 0.17 | 99,99,99,99                 | 0     |
| 54  | MG   | CA    | 1664 | 1/1   | 0.69 | 0.16 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3401 | 1/1   | 0.69 | 0.13 | 182,182,182,182             | 0     |
| 54  | MG   | DA    | 3588 | 1/1   | 0.69 | 0.15 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1786 | 1/1   | 0.69 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3419 | 1/1   | 0.69 | 0.30 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3159 | 1/1   | 0.69 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1950 | 1/1   | 0.69 | 0.20 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3612 | 1/1   | 0.69 | 0.14 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3437 | 1/1   | 0.69 | 0.15 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1957 | 1/1   | 0.69 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1917 | 1/1   | 0.69 | 0.36 | 132,132,132,132             | 0     |
| 54  | MG   | AD    | 101  | 1/1   | 0.69 | 0.12 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1804 | 1/1   | 0.69 | 0.13 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3270 | 1/1   | 0.69 | 0.34 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1682 | 1/1   | 0.69 | 0.31 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1811 | 1/1   | 0.69 | 0.21 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3487 | 1/1   | 0.69 | 0.24 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1924 | 1/1   | 0.69 | 0.17 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1728 | 1/1   | 0.69 | 0.21 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1606 | 1/1   | 0.69 | 0.19 | 70,70,70,70                 | 0     |
| 54  | MG   | CC    | 103  | 1/1   | 0.69 | 0.10 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1863 | 1/1   | 0.69 | 0.36 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1929 | 1/1   | 0.69 | 0.18 | 124,124,124,124             | 0     |
| 54  | MG   | BA    | 3582 | 1/1   | 0.69 | 0.10 | 133,133,133,133             | 0     |
| 54  | MG   | DA    | 3010 | 1/1   | 0.69 | 0.26 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1851 | 1/1   | 0.69 | 0.20 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1924 | 1/1   | 0.69 | 0.09 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1843 | 1/1   | 0.69 | 0.32 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1934 | 1/1   | 0.70 | 0.14 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3085 | 1/1   | 0.70 | 0.29 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3749 | 1/1   | 0.70 | 0.12 | 102,102,102,102             | 0     |
| 54  | MG   | CK    | 202  | 1/1   | 0.70 | 0.19 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3546 | 1/1   | 0.70 | 0.25 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3327 | 1/1   | 0.70 | 0.28 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3390 | 1/1   | 0.70 | 0.21 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3474 | 1/1   | 0.70 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3495 | 1/1   | 0.70 | 0.26 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3501 | 1/1   | 0.70 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1935 | 1/1   | 0.70 | 0.18 | 94,94,94,94                 | 0     |
| 54  | MG   | CW    | 203  | 1/1   | 0.70 | 0.10 | 111,111,111,111             | 0     |
| 54  | MG   | DA    | 3205 | 1/1   | 0.70 | 0.26 | 115,115,115,115             | 0     |
| 54  | MG   | DA    | 3369 | 1/1   | 0.70 | 0.27 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3217 | 1/1   | 0.70 | 0.27 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1747 | 1/1   | 0.70 | 0.23 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3805 | 1/1   | 0.70 | 0.22 | 90,90,90,90                 | 0     |
| 54  | MG   | BB    | 216  | 1/1   | 0.70 | 0.11 | 83,83,83,83                 | 0     |
| 54  | MG   | DB    | 204  | 1/1   | 0.70 | 0.14 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3691 | 1/1   | 0.70 | 0.20 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3562 | 1/1   | 0.70 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | DB    | 218  | 1/1   | 0.70 | 0.17 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3243 | 1/1   | 0.70 | 0.23 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3563 | 1/1   | 0.70 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1685 | 1/1   | 0.70 | 0.21 | 96,96,96,96                 | 0     |
| 54  | MG   | AC    | 101  | 1/1   | 0.70 | 0.08 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1819 | 1/1   | 0.70 | 0.11 | 98,98,98,98                 | 0     |
| 54  | MG   | CA    | 1828 | 1/1   | 0.70 | 0.18 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3517 | 1/1   | 0.70 | 0.16 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3444 | 1/1   | 0.70 | 0.25 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3728 | 1/1   | 0.70 | 0.15 | 123,123,123,123             | 0     |
| 54  | MG   | BA    | 3161 | 1/1   | 0.70 | 0.25 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3765 | 1/1   | 0.71 | 0.19 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3223 | 1/1   | 0.71 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3498 | 1/1   | 0.71 | 0.19 | 107,107,107,107             | 0     |
| 54  | MG   | BA    | 3154 | 1/1   | 0.71 | 0.25 | 117,117,117,117             | 0     |
| 54  | MG   | AA    | 1802 | 1/1   | 0.71 | 0.17 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3377 | 1/1   | 0.71 | 0.17 | 111,111,111,111             | 0     |
| 54  | MG   | CD    | 110  | 1/1   | 0.71 | 0.13 | 102,102,102,102             | 0     |
| 54  | MG   | CD    | 124  | 1/1   | 0.71 | 0.14 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3669 | 1/1   | 0.71 | 0.13 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1960 | 1/1   | 0.71 | 0.21 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3413 | 1/1   | 0.71 | 0.32 | 99,99,99,99                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1832 | 1/1   | 0.71 | 0.23 | 91,91,91,91                 | 0     |
| 54  | MG   | BU    | 204  | 1/1   | 0.71 | 0.20 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1850 | 1/1   | 0.71 | 0.11 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3535 | 1/1   | 0.71 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3433 | 1/1   | 0.71 | 0.24 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3437 | 1/1   | 0.71 | 0.29 | 107,107,107,107             | 0     |
| 54  | MG   | DB    | 209  | 1/1   | 0.71 | 0.34 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1938 | 1/1   | 0.71 | 0.34 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3117 | 1/1   | 0.71 | 0.16 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3454 | 1/1   | 0.71 | 0.13 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3580 | 1/1   | 0.71 | 0.19 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1925 | 1/1   | 0.71 | 0.19 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1651 | 1/1   | 0.71 | 0.26 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1930 | 1/1   | 0.71 | 0.15 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3193 | 1/1   | 0.71 | 0.31 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1725 | 1/1   | 0.71 | 0.29 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1933 | 1/1   | 0.71 | 0.22 | 98,98,98,98                 | 0     |
| 54  | MG   | D1    | 201  | 1/1   | 0.71 | 0.28 | 83,83,83,83                 | 0     |
| 54  | MG   | D2    | 201  | 1/1   | 0.71 | 0.12 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1886 | 1/1   | 0.71 | 0.12 | 120,120,120,120             | 0     |
| 54  | MG   | AA    | 1918 | 1/1   | 0.71 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3784 | 1/1   | 0.72 | 0.29 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1674 | 1/1   | 0.72 | 0.19 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3478 | 1/1   | 0.72 | 0.27 | 127,127,127,127             | 0     |
| 54  | MG   | DA    | 3670 | 1/1   | 0.72 | 0.21 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1982 | 1/1   | 0.72 | 0.05 | 126,126,126,126             | 0     |
| 54  | MG   | DA    | 3088 | 1/1   | 0.72 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1735 | 1/1   | 0.72 | 0.24 | 108,108,108,108             | 0     |
| 54  | MG   | AA    | 1947 | 1/1   | 0.72 | 0.26 | 119,119,119,119             | 0     |
| 54  | MG   | DA    | 3797 | 1/1   | 0.72 | 0.29 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3127 | 1/1   | 0.72 | 0.29 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3800 | 1/1   | 0.72 | 0.11 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1629 | 1/1   | 0.72 | 0.26 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1634 | 1/1   | 0.72 | 0.33 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3512 | 1/1   | 0.72 | 0.24 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3710 | 1/1   | 0.72 | 0.11 | 106,106,106,106             | 0     |
| 54  | MG   | DB    | 205  | 1/1   | 0.72 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3132 | 1/1   | 0.72 | 0.28 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1656 | 1/1   | 0.72 | 0.17 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3365 | 1/1   | 0.72 | 0.14 | 107,107,107,107             | 0     |
| 54  | MG   | CA    | 1761 | 1/1   | 0.72 | 0.13 | 129,129,129,129             | 0     |
| 54  | MG   | AA    | 1730 | 1/1   | 0.72 | 0.26 | 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   | BA    | 3441 | 1/1   | 0.72 | 0.11 | 144,144,144,144             | 0     |
| 54  | MG   | AX    | 101  | 1/1   | 0.72 | 0.14 | 107,107,107,107             | 0     |
| 54  | MG   | BA    | 3240 | 1/1   | 0.72 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3625 | 1/1   | 0.72 | 0.19 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3626 | 1/1   | 0.72 | 0.29 | 109,109,109,109             | 0     |
| 54  | MG   | CA    | 1697 | 1/1   | 0.72 | 0.33 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3385 | 1/1   | 0.72 | 0.30 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3151 | 1/1   | 0.72 | 0.30 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1995 | 1/1   | 0.72 | 0.15 | 142,142,142,142             | 0     |
| 54  | MG   | CA    | 1705 | 1/1   | 0.72 | 0.14 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1940 | 1/1   | 0.72 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3393 | 1/1   | 0.73 | 0.11 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1828 | 1/1   | 0.73 | 0.07 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3442 | 1/1   | 0.73 | 0.16 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3793 | 1/1   | 0.73 | 0.14 | 108,108,108,108             | 0     |
| 54  | MG   | CA    | 1903 | 1/1   | 0.73 | 0.19 | 134,134,134,134             | 0     |
| 54  | MG   | BA    | 3264 | 1/1   | 0.73 | 0.18 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1643 | 1/1   | 0.73 | 0.12 | 124,124,124,124             | 0     |
| 54  | MG   | BA    | 3473 | 1/1   | 0.73 | 0.17 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3168 | 1/1   | 0.73 | 0.32 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1668 | 1/1   | 0.73 | 0.38 | 107,107,107,107             | 0     |
| 54  | MG   | CA    | 1771 | 1/1   | 0.73 | 0.21 | 101,101,101,101             | 0     |
| 54  | MG   | CA    | 1918 | 1/1   | 0.73 | 0.10 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1699 | 1/1   | 0.73 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1923 | 1/1   | 0.73 | 0.16 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3613 | 1/1   | 0.73 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3496 | 1/1   | 0.73 | 0.22 | 69,69,69,69                 | 0     |
| 54  | MG   | DB    | 217  | 1/1   | 0.73 | 0.12 | 122,122,122,122             | 0     |
| 54  | MG   | CA    | 1776 | 1/1   | 0.73 | 0.12 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1611 | 1/1   | 0.73 | 0.26 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1754 | 1/1   | 0.73 | 0.21 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1804 | 1/1   | 0.73 | 0.27 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1712 | 1/1   | 0.73 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | CD    | 112  | 1/1   | 0.73 | 0.07 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1842 | 1/1   | 0.73 | 0.17 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1927 | 1/1   | 0.73 | 0.27 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1760 | 1/1   | 0.73 | 0.21 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 2033 | 1/1   | 0.73 | 0.22 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1844 | 1/1   | 0.73 | 0.13 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3525 | 1/1   | 0.73 | 0.09 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3673 | 1/1   | 0.73 | 0.09 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3233 | 1/1   | 0.74 | 0.12 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1640 | 1/1   | 0.74 | 0.19 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3773 | 1/1   | 0.74 | 0.18 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3146 | 1/1   | 0.74 | 0.08 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3415 | 1/1   | 0.74 | 0.37 | 89,89,89,89                 | 0     |
| 54  | MG   | AC    | 102  | 1/1   | 0.74 | 0.24 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1649 | 1/1   | 0.74 | 0.29 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1746 | 1/1   | 0.74 | 0.29 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 2015 | 1/1   | 0.74 | 0.18 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1914 | 1/1   | 0.74 | 0.16 | 109,109,109,109             | 0     |
| 54  | MG   | CA    | 1753 | 1/1   | 0.74 | 0.14 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 2905 | 1/1   | 0.74 | 0.09 | 136,136,136,136             | 0     |
| 54  | MG   | BA    | 3500 | 1/1   | 0.74 | 0.17 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3084 | 1/1   | 0.74 | 0.33 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3116 | 1/1   | 0.74 | 0.34 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3505 | 1/1   | 0.74 | 0.35 | 114,114,114,114             | 0     |
| 54  | MG   | CA    | 1667 | 1/1   | 0.74 | 0.08 | 93,93,93,93                 | 0     |
| 54  | MG   | BB    | 207  | 1/1   | 0.74 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1968 | 1/1   | 0.74 | 0.12 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3169 | 1/1   | 0.74 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3185 | 1/1   | 0.74 | 0.29 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 2018 | 1/1   | 0.74 | 0.14 | 117,117,117,117             | 0     |
| 54  | MG   | CA    | 1875 | 1/1   | 0.74 | 0.15 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3515 | 1/1   | 0.74 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3434 | 1/1   | 0.74 | 0.17 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3212 | 1/1   | 0.74 | 0.22 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 2020 | 1/1   | 0.74 | 0.15 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3720 | 1/1   | 0.74 | 0.30 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 2021 | 1/1   | 0.74 | 0.11 | 108,108,108,108             | 0     |
| 54  | MG   | CA    | 1898 | 1/1   | 0.74 | 0.18 | 122,122,122,122             | 0     |
| 54  | MG   | DA    | 3228 | 1/1   | 0.74 | 0.24 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1706 | 1/1   | 0.74 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3130 | 1/1   | 0.74 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1953 | 1/1   | 0.74 | 0.14 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1888 | 1/1   | 0.74 | 0.15 | 114,114,114,114             | 0     |
| 54  | MG   | DA    | 3449 | 1/1   | 0.74 | 0.15 | 95,95,95,95                 | 0     |
| 54  | MG   | DU    | 201  | 1/1   | 0.74 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3764 | 1/1   | 0.74 | 0.10 | 108,108,108,108             | 0     |
| 54  | MG   | DU    | 205  | 1/1   | 0.74 | 0.09 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1718 | 1/1   | 0.74 | 0.22 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3624 | 1/1   | 0.75 | 0.16 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1715 | 1/1   | 0.75 | 0.25 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3493 | 1/1   | 0.75 | 0.26 | 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   | BA    | 3118 | 1/1   | 0.75 | 0.17 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1797 | 1/1   | 0.75 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1699 | 1/1   | 0.75 | 0.17 | 95,95,95,95                 | 0     |
| 54  | MG   | CA    | 1964 | 1/1   | 0.75 | 0.07 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3195 | 1/1   | 0.75 | 0.11 | 124,124,124,124             | 0     |
| 54  | MG   | AK    | 201  | 1/1   | 0.75 | 0.27 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3133 | 1/1   | 0.75 | 0.22 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1801 | 1/1   | 0.75 | 0.28 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1654 | 1/1   | 0.75 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | CP    | 201  | 1/1   | 0.75 | 0.32 | 118,118,118,118             | 0     |
| 54  | MG   | CA    | 1660 | 1/1   | 0.75 | 0.14 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3388 | 1/1   | 0.75 | 0.18 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3137 | 1/1   | 0.75 | 0.36 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3456 | 1/1   | 0.75 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3195 | 1/1   | 0.75 | 0.28 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1740 | 1/1   | 0.75 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1915 | 1/1   | 0.75 | 0.18 | 133,133,133,133             | 0     |
| 54  | MG   | CA    | 1754 | 1/1   | 0.75 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3542 | 1/1   | 0.75 | 0.19 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1979 | 1/1   | 0.75 | 0.15 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3237 | 1/1   | 0.75 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3715 | 1/1   | 0.75 | 0.17 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3081 | 1/1   | 0.75 | 0.28 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3227 | 1/1   | 0.75 | 0.26 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1765 | 1/1   | 0.75 | 0.23 | 118,118,118,118             | 0     |
| 54  | MG   | DB    | 224  | 1/1   | 0.75 | 0.12 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1612 | 1/1   | 0.75 | 0.27 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3581 | 1/1   | 0.75 | 0.14 | 139,139,139,139             | 0     |
| 54  | MG   | AA    | 1734 | 1/1   | 0.75 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | CD    | 121  | 1/1   | 0.75 | 0.13 | 112,112,112,112             | 0     |
| 54  | MG   | CD    | 122  | 1/1   | 0.75 | 0.07 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3254 | 1/1   | 0.75 | 0.28 | 101,101,101,101             | 0     |
| 54  | MG   | D1    | 205  | 1/1   | 0.75 | 0.15 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1604 | 1/1   | 0.75 | 0.26 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1960 | 1/1   | 0.75 | 0.19 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3283 | 1/1   | 0.75 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3284 | 1/1   | 0.75 | 0.22 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3464 | 1/1   | 0.75 | 0.28 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3617 | 1/1   | 0.76 | 0.26 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3467 | 1/1   | 0.76 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1763 | 1/1   | 0.76 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1621 | 1/1   | 0.76 | 0.19 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1917 | 1/1   | 0.76 | 0.12 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 2910 | 1/1   | 0.76 | 0.05 | 149,149,149,149             | 0     |
| 54  | MG   | DA    | 3630 | 1/1   | 0.76 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 2027 | 1/1   | 0.76 | 0.25 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3355 | 1/1   | 0.76 | 0.11 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 1902 | 1/1   | 0.76 | 0.11 | 107,107,107,107             | 0     |
| 54  | MG   | BA    | 3138 | 1/1   | 0.76 | 0.22 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3499 | 1/1   | 0.76 | 0.19 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1637 | 1/1   | 0.76 | 0.19 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3580 | 1/1   | 0.76 | 0.13 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3348 | 1/1   | 0.76 | 0.21 | 99,99,99,99                 | 0     |
| 54  | MG   | BB    | 201  | 1/1   | 0.76 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3465 | 1/1   | 0.76 | 0.08 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3803 | 1/1   | 0.76 | 0.08 | 99,99,99,99                 | 0     |
| 54  | MG   | AC    | 106  | 1/1   | 0.76 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | CD    | 120  | 1/1   | 0.76 | 0.11 | 110,110,110,110             | 0     |
| 54  | MG   | AA    | 1841 | 1/1   | 0.76 | 0.16 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3690 | 1/1   | 0.76 | 0.21 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3400 | 1/1   | 0.76 | 0.20 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1880 | 1/1   | 0.76 | 0.15 | 130,130,130,130             | 0     |
| 54  | MG   | DA    | 3534 | 1/1   | 0.76 | 0.24 | 86,86,86,86                 | 0     |
| 54  | MG   | BB    | 212  | 1/1   | 0.76 | 0.15 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3115 | 1/1   | 0.76 | 0.15 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1758 | 1/1   | 0.76 | 0.15 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3036 | 1/1   | 0.76 | 0.21 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 3167 | 1/1   | 0.76 | 0.35 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3072 | 1/1   | 0.76 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | BE    | 307  | 1/1   | 0.76 | 0.35 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3579 | 1/1   | 0.76 | 0.24 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3275 | 1/1   | 0.76 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3380 | 1/1   | 0.76 | 0.28 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1976 | 1/1   | 0.76 | 0.10 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1983 | 1/1   | 0.76 | 0.09 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3491 | 1/1   | 0.76 | 0.22 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3126 | 1/1   | 0.76 | 0.25 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3301 | 1/1   | 0.76 | 0.17 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 2016 | 1/1   | 0.76 | 0.29 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3130 | 1/1   | 0.76 | 0.36 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3466 | 1/1   | 0.76 | 0.15 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1882 | 1/1   | 0.77 | 0.16 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1671 | 1/1   | 0.77 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1814 | 1/1   | 0.77 | 0.30 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3024 | 1/1   | 0.77 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3037 | 1/1   | 0.77 | 0.19 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3430 | 1/1   | 0.77 | 0.15 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3261 | 1/1   | 0.77 | 0.26 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1974 | 1/1   | 0.77 | 0.12 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3078 | 1/1   | 0.77 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1820 | 1/1   | 0.77 | 0.19 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1622 | 1/1   | 0.77 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3568 | 1/1   | 0.77 | 0.14 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3535 | 1/1   | 0.77 | 0.08 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1984 | 1/1   | 0.77 | 0.19 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1741 | 1/1   | 0.77 | 0.18 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1610 | 1/1   | 0.77 | 0.26 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1895 | 1/1   | 0.77 | 0.12 | 133,133,133,133             | 0     |
| 54  | MG   | CA    | 1772 | 1/1   | 0.77 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3457 | 1/1   | 0.77 | 0.11 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1896 | 1/1   | 0.77 | 0.18 | 93,93,93,93                 | 0     |
| 54  | MG   | DB    | 215  | 1/1   | 0.77 | 0.22 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3718 | 1/1   | 0.77 | 0.26 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1765 | 1/1   | 0.77 | 0.22 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1655 | 1/1   | 0.77 | 0.17 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1849 | 1/1   | 0.77 | 0.18 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3082 | 1/1   | 0.77 | 0.18 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1885 | 1/1   | 0.77 | 0.08 | 113,113,113,113             | 0     |
| 54  | MG   | CC    | 105  | 1/1   | 0.77 | 0.23 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3356 | 1/1   | 0.77 | 0.24 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1744 | 1/1   | 0.77 | 0.19 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3015 | 1/1   | 0.77 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3493 | 1/1   | 0.77 | 0.18 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3511 | 1/1   | 0.77 | 0.08 | 140,140,140,140             | 0     |
| 54  | MG   | BA    | 3373 | 1/1   | 0.77 | 0.30 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1676 | 1/1   | 0.77 | 0.24 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3370 | 1/1   | 0.77 | 0.20 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1876 | 1/1   | 0.77 | 0.12 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1839 | 1/1   | 0.77 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1689 | 1/1   | 0.77 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | AA    | 1607 | 1/1   | 0.78 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1694 | 1/1   | 0.78 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | CS    | 101  | 1/1   | 0.78 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | BE    | 306  | 1/1   | 0.78 | 0.12 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3462 | 1/1   | 0.78 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1695 | 1/1   | 0.78 | 0.16 | 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   | DA    | 3727 | 1/1   | 0.78 | 0.33 | 106,106,106,106             | 0     |
| 54  | MG   | CA    | 1916 | 1/1   | 0.78 | 0.13 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 3315 | 1/1   | 0.78 | 0.19 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3202 | 1/1   | 0.78 | 0.30 | 49,49,49,49                 | 0     |
| 54  | MG   | CA    | 1845 | 1/1   | 0.78 | 0.21 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3404 | 1/1   | 0.78 | 0.26 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1864 | 1/1   | 0.78 | 0.23 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3412 | 1/1   | 0.78 | 0.20 | 105,105,105,105             | 0     |
| 54  | MG   | CC    | 107  | 1/1   | 0.78 | 0.14 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3766 | 1/1   | 0.78 | 0.15 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1809 | 1/1   | 0.78 | 0.17 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3402 | 1/1   | 0.78 | 0.21 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3591 | 1/1   | 0.78 | 0.11 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3403 | 1/1   | 0.78 | 0.25 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1661 | 1/1   | 0.78 | 0.45 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1929 | 1/1   | 0.78 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3609 | 1/1   | 0.78 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3610 | 1/1   | 0.78 | 0.20 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3439 | 1/1   | 0.78 | 0.32 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1781 | 1/1   | 0.78 | 0.29 | 118,118,118,118             | 0     |
| 54  | MG   | CA    | 1938 | 1/1   | 0.78 | 0.22 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1855 | 1/1   | 0.78 | 0.12 | 99,99,99,99                 | 0     |
| 54  | MG   | AA    | 2022 | 1/1   | 0.78 | 0.10 | 117,117,117,117             | 0     |
| 54  | MG   | AA    | 1746 | 1/1   | 0.78 | 0.18 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3352 | 1/1   | 0.78 | 0.11 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3271 | 1/1   | 0.78 | 0.39 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1713 | 1/1   | 0.78 | 0.23 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3629 | 1/1   | 0.78 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1874 | 1/1   | 0.78 | 0.08 | 144,144,144,144             | 0     |
| 54  | MG   | BA    | 3106 | 1/1   | 0.78 | 0.33 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3059 | 1/1   | 0.78 | 0.32 | 58,58,58,58                 | 0     |
| 54  | MG   | AA    | 1676 | 1/1   | 0.78 | 0.16 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 2967 | 1/1   | 0.78 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 2005 | 1/1   | 0.78 | 0.10 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3661 | 1/1   | 0.78 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3666 | 1/1   | 0.78 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1980 | 1/1   | 0.78 | 0.08 | 136,136,136,136             | 0     |
| 54  | MG   | DA    | 3480 | 1/1   | 0.78 | 0.12 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3310 | 1/1   | 0.78 | 0.28 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 2011 | 1/1   | 0.78 | 0.23 | 120,120,120,120             | 0     |
| 54  | MG   | DA    | 3317 | 1/1   | 0.78 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3094 | 1/1   | 0.78 | 0.16 | 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   | DA    | 3323 | 1/1   | 0.78 | 0.17 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3683 | 1/1   | 0.78 | 0.16 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1925 | 1/1   | 0.78 | 0.11 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3109 | 1/1   | 0.78 | 0.35 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1889 | 1/1   | 0.78 | 0.13 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3349 | 1/1   | 0.78 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1978 | 1/1   | 0.78 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3446 | 1/1   | 0.78 | 0.14 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3448 | 1/1   | 0.78 | 0.07 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1729 | 1/1   | 0.78 | 0.14 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1749 | 1/1   | 0.78 | 0.18 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3156 | 1/1   | 0.78 | 0.32 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3536 | 1/1   | 0.79 | 0.16 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3538 | 1/1   | 0.79 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3445 | 1/1   | 0.79 | 0.25 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3386 | 1/1   | 0.79 | 0.15 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1831 | 1/1   | 0.79 | 0.17 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3255 | 1/1   | 0.79 | 0.14 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3387 | 1/1   | 0.79 | 0.26 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3087 | 1/1   | 0.79 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3740 | 1/1   | 0.79 | 0.19 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1972 | 1/1   | 0.79 | 0.17 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3217 | 1/1   | 0.79 | 0.24 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3747 | 1/1   | 0.79 | 0.17 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3459 | 1/1   | 0.79 | 0.14 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3342 | 1/1   | 0.79 | 0.32 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3761 | 1/1   | 0.79 | 0.10 | 112,112,112,112             | 0     |
| 54  | MG   | CD    | 106  | 1/1   | 0.79 | 0.10 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3226 | 1/1   | 0.79 | 0.16 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3343 | 1/1   | 0.79 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1907 | 1/1   | 0.79 | 0.12 | 106,106,106,106             | 0     |
| 54  | MG   | BA    | 3409 | 1/1   | 0.79 | 0.14 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3435 | 1/1   | 0.79 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1932 | 1/1   | 0.79 | 0.12 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1937 | 1/1   | 0.79 | 0.17 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3273 | 1/1   | 0.79 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG   | BZ    | 101  | 1/1   | 0.79 | 0.12 | 92,92,92,92                 | 0     |
| 54  | MG   | AC    | 103  | 1/1   | 0.79 | 0.09 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 2981 | 1/1   | 0.79 | 0.26 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3447 | 1/1   | 0.79 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 2991 | 1/1   | 0.79 | 0.31 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3450 | 1/1   | 0.79 | 0.19 | 98,98,98,98                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3051 | 1/1   | 0.79 | 0.26 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1616 | 1/1   | 0.79 | 0.14 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1952 | 1/1   | 0.79 | 0.18 | 134,134,134,134             | 0     |
| 54  | MG   | BA    | 3367 | 1/1   | 0.79 | 0.27 | 111,111,111,111             | 0     |
| 54  | MG   | AA    | 1759 | 1/1   | 0.79 | 0.24 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3295 | 1/1   | 0.79 | 0.22 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3645 | 1/1   | 0.79 | 0.35 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3647 | 1/1   | 0.79 | 0.18 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3483 | 1/1   | 0.79 | 0.13 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1800 | 1/1   | 0.79 | 0.14 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3488 | 1/1   | 0.79 | 0.15 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1965 | 1/1   | 0.79 | 0.19 | 92,92,92,92                 | 0     |
| 54  | MG   | CA    | 1730 | 1/1   | 0.79 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3089 | 1/1   | 0.79 | 0.29 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1969 | 1/1   | 0.79 | 0.12 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1733 | 1/1   | 0.79 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3370 | 1/1   | 0.79 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1736 | 1/1   | 0.79 | 0.17 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3328 | 1/1   | 0.79 | 0.18 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1892 | 1/1   | 0.79 | 0.08 | 99,99,99,99                 | 0     |
| 54  | MG   | DB    | 225  | 1/1   | 0.79 | 0.17 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3343 | 1/1   | 0.79 | 0.18 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3284 | 1/1   | 0.79 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 2028 | 1/1   | 0.79 | 0.18 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1817 | 1/1   | 0.79 | 0.26 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3132 | 1/1   | 0.79 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | DH    | 201  | 1/1   | 0.79 | 0.21 | 77,77,77,77                 | 0     |
| 54  | MG   | D0    | 204  | 1/1   | 0.79 | 0.08 | 95,95,95,95                 | 0     |
| 54  | MG   | CG    | 301  | 1/1   | 0.79 | 0.39 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 2987 | 1/1   | 0.79 | 0.27 | 57,57,57,57                 | 0     |
| 54  | MG   | CM    | 201  | 1/1   | 0.79 | 0.09 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1855 | 1/1   | 0.79 | 0.18 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1748 | 1/1   | 0.79 | 0.10 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1771 | 1/1   | 0.79 | 0.22 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1911 | 1/1   | 0.79 | 0.08 | 123,123,123,123             | 0     |
| 54  | MG   | AA    | 1680 | 1/1   | 0.80 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1899 | 1/1   | 0.80 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3741 | 1/1   | 0.80 | 0.17 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1977 | 1/1   | 0.80 | 0.10 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1659 | 1/1   | 0.80 | 0.15 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1845 | 1/1   | 0.80 | 0.13 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3294 | 1/1   | 0.80 | 0.19 | 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   | BB    | 215  | 1/1   | 0.80 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3104 | 1/1   | 0.80 | 0.25 | 79,79,79,79                 | 0     |
| 54  | MG   | AS    | 101  | 1/1   | 0.80 | 0.34 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1751 | 1/1   | 0.80 | 0.12 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1826 | 1/1   | 0.80 | 0.20 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3124 | 1/1   | 0.80 | 0.16 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1752 | 1/1   | 0.80 | 0.15 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3279 | 1/1   | 0.80 | 0.21 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1930 | 1/1   | 0.80 | 0.23 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3627 | 1/1   | 0.80 | 0.08 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1757 | 1/1   | 0.80 | 0.07 | 79,79,79,79                 | 0     |
| 54  | MG   | BD    | 302  | 1/1   | 0.80 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3365 | 1/1   | 0.80 | 0.15 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3335 | 1/1   | 0.80 | 0.33 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3142 | 1/1   | 0.80 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1990 | 1/1   | 0.80 | 0.12 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 2031 | 1/1   | 0.80 | 0.23 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3350 | 1/1   | 0.80 | 0.18 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 2943 | 1/1   | 0.80 | 0.23 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3559 | 1/1   | 0.80 | 0.20 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3286 | 1/1   | 0.80 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1963 | 1/1   | 0.80 | 0.25 | 103,103,103,103             | 0     |
| 54  | MG   | CA    | 1854 | 1/1   | 0.80 | 0.27 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3364 | 1/1   | 0.80 | 0.28 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1831 | 1/1   | 0.80 | 0.12 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1883 | 1/1   | 0.80 | 0.11 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3198 | 1/1   | 0.80 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3302 | 1/1   | 0.80 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1920 | 1/1   | 0.80 | 0.12 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 3495 | 1/1   | 0.80 | 0.48 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1645 | 1/1   | 0.80 | 0.22 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3256 | 1/1   | 0.80 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3502 | 1/1   | 0.80 | 0.12 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1728 | 1/1   | 0.80 | 0.28 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3396 | 1/1   | 0.80 | 0.11 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1648 | 1/1   | 0.80 | 0.28 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3705 | 1/1   | 0.80 | 0.18 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3706 | 1/1   | 0.80 | 0.11 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3708 | 1/1   | 0.80 | 0.19 | 152,152,152,152             | 0     |
| 54  | MG   | CA    | 1805 | 1/1   | 0.80 | 0.12 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3559 | 1/1   | 0.80 | 0.22 | 103,103,103,103             | 0     |
| 54  | MG   | DD    | 301  | 1/1   | 0.80 | 0.31 | 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   | AA    | 1898 | 1/1   | 0.80 | 0.07 | 102,102,102,102             | 0     |
| 54  | MG   | DG    | 201  | 1/1   | 0.80 | 0.25 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3014 | 1/1   | 0.80 | 0.40 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3334 | 1/1   | 0.80 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1642 | 1/1   | 0.80 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3415 | 1/1   | 0.80 | 0.26 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1695 | 1/1   | 0.80 | 0.25 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3722 | 1/1   | 0.80 | 0.14 | 166,166,166,166             | 0     |
| 54  | MG   | CA    | 1895 | 1/1   | 0.80 | 0.11 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3268 | 1/1   | 0.80 | 0.37 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1973 | 1/1   | 0.80 | 0.11 | 116,116,116,116             | 0     |
| 54  | MG   | BB    | 209  | 1/1   | 0.80 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 2991 | 1/1   | 0.81 | 0.19 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 2992 | 1/1   | 0.81 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 2996 | 1/1   | 0.81 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3345 | 1/1   | 0.81 | 0.10 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1732 | 1/1   | 0.81 | 0.15 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3732 | 1/1   | 0.81 | 0.27 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1970 | 1/1   | 0.81 | 0.19 | 98,98,98,98                 | 0     |
| 54  | MG   | CC    | 112  | 1/1   | 0.81 | 0.11 | 88,88,88,88                 | 0     |
| 54  | MG   | AW    | 204  | 1/1   | 0.81 | 0.17 | 105,105,105,105             | 0     |
| 54  | MG   | AA    | 1798 | 1/1   | 0.81 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1919 | 1/1   | 0.81 | 0.13 | 112,112,112,112             | 0     |
| 54  | MG   | AA    | 1838 | 1/1   | 0.81 | 0.33 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1978 | 1/1   | 0.81 | 0.07 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3152 | 1/1   | 0.81 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | BG    | 201  | 1/1   | 0.81 | 0.10 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3762 | 1/1   | 0.81 | 0.12 | 119,119,119,119             | 0     |
| 54  | MG   | AA    | 2012 | 1/1   | 0.81 | 0.11 | 117,117,117,117             | 0     |
| 54  | MG   | B0    | 201  | 1/1   | 0.81 | 0.21 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 2965 | 1/1   | 0.81 | 0.28 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3447 | 1/1   | 0.81 | 0.10 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3526 | 1/1   | 0.81 | 0.08 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3534 | 1/1   | 0.81 | 0.15 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1603 | 1/1   | 0.81 | 0.31 | 54,54,54,54                 | 0     |
| 54  | MG   | AA    | 2037 | 1/1   | 0.81 | 0.15 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3541 | 1/1   | 0.81 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1609 | 1/1   | 0.81 | 0.28 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3456 | 1/1   | 0.81 | 0.39 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3544 | 1/1   | 0.81 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3545 | 1/1   | 0.81 | 0.13 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1808 | 1/1   | 0.81 | 0.10 | 92,92,92,92                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3073 | 1/1   | 0.81 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3641 | 1/1   | 0.81 | 0.19 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1633 | 1/1   | 0.81 | 0.25 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1750 | 1/1   | 0.81 | 0.10 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1634 | 1/1   | 0.81 | 0.19 | 54,54,54,54                 | 0     |
| 54  | MG   | AA    | 1637 | 1/1   | 0.81 | 0.33 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1638 | 1/1   | 0.81 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1967 | 1/1   | 0.81 | 0.08 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1830 | 1/1   | 0.81 | 0.19 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3665 | 1/1   | 0.81 | 0.27 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1631 | 1/1   | 0.81 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 1901 | 1/1   | 0.81 | 0.15 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1781 | 1/1   | 0.81 | 0.25 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3298 | 1/1   | 0.81 | 0.14 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1833 | 1/1   | 0.81 | 0.19 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3109 | 1/1   | 0.81 | 0.19 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3398 | 1/1   | 0.81 | 0.10 | 131,131,131,131             | 0     |
| 54  | MG   | DA    | 3506 | 1/1   | 0.81 | 0.26 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3476 | 1/1   | 0.81 | 0.15 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3686 | 1/1   | 0.81 | 0.15 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1883 | 1/1   | 0.81 | 0.07 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1923 | 1/1   | 0.81 | 0.19 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3516 | 1/1   | 0.81 | 0.14 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3141 | 1/1   | 0.81 | 0.12 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3319 | 1/1   | 0.81 | 0.29 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3581 | 1/1   | 0.81 | 0.23 | 125,125,125,125             | 0     |
| 54  | MG   | BA    | 3116 | 1/1   | 0.81 | 0.31 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1674 | 1/1   | 0.81 | 0.15 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1847 | 1/1   | 0.81 | 0.18 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1906 | 1/1   | 0.81 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | DO    | 203  | 1/1   | 0.81 | 0.23 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3711 | 1/1   | 0.81 | 0.12 | 102,102,102,102             | 0     |
| 54  | MG   | DA    | 3371 | 1/1   | 0.81 | 0.20 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3187 | 1/1   | 0.81 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3125 | 1/1   | 0.81 | 0.11 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1694 | 1/1   | 0.81 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3557 | 1/1   | 0.81 | 0.19 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1798 | 1/1   | 0.81 | 0.14 | 112,112,112,112             | 0     |
| 54  | MG   | D3    | 104  | 1/1   | 0.81 | 0.08 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3492 | 1/1   | 0.81 | 0.08 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1701 | 1/1   | 0.82 | 0.26 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1644 | 1/1   | 0.82 | 0.19 | 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   | AA    | 1663 | 1/1   | 0.82 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3445 | 1/1   | 0.82 | 0.20 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3745 | 1/1   | 0.82 | 0.18 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3357 | 1/1   | 0.82 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1852 | 1/1   | 0.82 | 0.23 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3313 | 1/1   | 0.82 | 0.09 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3314 | 1/1   | 0.82 | 0.12 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3754 | 1/1   | 0.82 | 0.24 | 99,99,99,99                 | 0     |
| 54  | MG   | AA    | 1998 | 1/1   | 0.82 | 0.17 | 98,98,98,98                 | 0     |
| 54  | MG   | CX    | 101  | 1/1   | 0.82 | 0.13 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1814 | 1/1   | 0.82 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1614 | 1/1   | 0.82 | 0.26 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3089 | 1/1   | 0.82 | 0.32 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1658 | 1/1   | 0.82 | 0.24 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1941 | 1/1   | 0.82 | 0.10 | 93,93,93,93                 | 0     |
| 54  | MG   | AA    | 1708 | 1/1   | 0.82 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3179 | 1/1   | 0.82 | 0.19 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3473 | 1/1   | 0.82 | 0.19 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3474 | 1/1   | 0.82 | 0.33 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3642 | 1/1   | 0.82 | 0.18 | 81,81,81,81                 | 0     |
| 54  | MG   | BB    | 217  | 1/1   | 0.82 | 0.22 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3199 | 1/1   | 0.82 | 0.30 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1679 | 1/1   | 0.82 | 0.13 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3490 | 1/1   | 0.82 | 0.23 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3655 | 1/1   | 0.82 | 0.17 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3377 | 1/1   | 0.82 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | BE    | 301  | 1/1   | 0.82 | 0.13 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3290 | 1/1   | 0.82 | 0.05 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3359 | 1/1   | 0.82 | 0.18 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3361 | 1/1   | 0.82 | 0.26 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1824 | 1/1   | 0.82 | 0.22 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1864 | 1/1   | 0.82 | 0.23 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3206 | 1/1   | 0.82 | 0.19 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 2995 | 1/1   | 0.82 | 0.23 | 52,52,52,52                 | 0     |
| 54  | MG   | AA    | 1710 | 1/1   | 0.82 | 0.12 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1711 | 1/1   | 0.82 | 0.36 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3681 | 1/1   | 0.82 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | DB    | 212  | 1/1   | 0.82 | 0.22 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1890 | 1/1   | 0.82 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1648 | 1/1   | 0.82 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | BT    | 102  | 1/1   | 0.82 | 0.14 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3472 | 1/1   | 0.82 | 0.09 | 125,125,125,125             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3232 | 1/1   | 0.82 | 0.18 | 67,67,67,67                 | 0     |
| 54  | MG   | AC    | 107  | 1/1   | 0.82 | 0.14 | 114,114,114,114             | 0     |
| 54  | MG   | CA    | 1711 | 1/1   | 0.82 | 0.34 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1650 | 1/1   | 0.82 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3397 | 1/1   | 0.82 | 0.23 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3324 | 1/1   | 0.82 | 0.26 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3247 | 1/1   | 0.82 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3135 | 1/1   | 0.82 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3405 | 1/1   | 0.82 | 0.16 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3407 | 1/1   | 0.82 | 0.24 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3411 | 1/1   | 0.82 | 0.21 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3567 | 1/1   | 0.82 | 0.22 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1779 | 1/1   | 0.82 | 0.06 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 2904 | 1/1   | 0.82 | 0.07 | 101,101,101,101             | 0     |
| 54  | MG   | CA    | 1631 | 1/1   | 0.82 | 0.25 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3064 | 1/1   | 0.82 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3278 | 1/1   | 0.82 | 0.17 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3069 | 1/1   | 0.82 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1635 | 1/1   | 0.82 | 0.32 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3106 | 1/1   | 0.82 | 0.20 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3421 | 1/1   | 0.82 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1638 | 1/1   | 0.82 | 0.23 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1740 | 1/1   | 0.82 | 0.08 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3086 | 1/1   | 0.83 | 0.15 | 50,50,50,50                 | 0     |
| 54  | MG   | CA    | 1662 | 1/1   | 0.83 | 0.15 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1981 | 1/1   | 0.83 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | CA    | 1663 | 1/1   | 0.83 | 0.25 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3583 | 1/1   | 0.83 | 0.24 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3438 | 1/1   | 0.83 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3438 | 1/1   | 0.83 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | B0    | 202  | 1/1   | 0.83 | 0.28 | 111,111,111,111             | 0     |
| 54  | MG   | CA    | 1913 | 1/1   | 0.83 | 0.10 | 101,101,101,101             | 0     |
| 54  | MG   | AD    | 103  | 1/1   | 0.83 | 0.11 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 2981 | 1/1   | 0.83 | 0.20 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3598 | 1/1   | 0.83 | 0.07 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3336 | 1/1   | 0.83 | 0.13 | 88,88,88,88                 | 0     |
| 54  | MG   | CQ    | 102  | 1/1   | 0.83 | 0.16 | 111,111,111,111             | 0     |
| 54  | MG   | DA    | 3306 | 1/1   | 0.83 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3448 | 1/1   | 0.83 | 0.21 | 103,103,103,103             | 0     |
| 54  | MG   | CQ    | 103  | 1/1   | 0.83 | 0.12 | 122,122,122,122             | 0     |
| 54  | MG   | BA    | 3221 | 1/1   | 0.83 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3094 | 1/1   | 0.83 | 0.14 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3622 | 1/1   | 0.83 | 0.28 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3145 | 1/1   | 0.83 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3315 | 1/1   | 0.83 | 0.25 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3780 | 1/1   | 0.83 | 0.11 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1875 | 1/1   | 0.83 | 0.10 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3783 | 1/1   | 0.83 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3575 | 1/1   | 0.83 | 0.11 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1612 | 1/1   | 0.83 | 0.11 | 37,37,37,37                 | 0     |
| 54  | MG   | DA    | 3136 | 1/1   | 0.83 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3455 | 1/1   | 0.83 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3509 | 1/1   | 0.83 | 0.15 | 107,107,107,107             | 0     |
| 54  | MG   | BA    | 3056 | 1/1   | 0.83 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3057 | 1/1   | 0.83 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3063 | 1/1   | 0.83 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | CC    | 109  | 1/1   | 0.83 | 0.20 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3478 | 1/1   | 0.83 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1678 | 1/1   | 0.83 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3481 | 1/1   | 0.83 | 0.23 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3362 | 1/1   | 0.83 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | AS    | 102  | 1/1   | 0.83 | 0.22 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1946 | 1/1   | 0.83 | 0.09 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1790 | 1/1   | 0.83 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3469 | 1/1   | 0.83 | 0.18 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1720 | 1/1   | 0.83 | 0.10 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1608 | 1/1   | 0.83 | 0.29 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1922 | 1/1   | 0.83 | 0.35 | 94,94,94,94                 | 0     |
| 54  | MG   | DB    | 211  | 1/1   | 0.83 | 0.18 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1958 | 1/1   | 0.83 | 0.11 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3211 | 1/1   | 0.83 | 0.07 | 71,71,71,71                 | 0     |
| 54  | MG   | DB    | 214  | 1/1   | 0.83 | 0.08 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1647 | 1/1   | 0.83 | 0.21 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3216 | 1/1   | 0.83 | 0.17 | 88,88,88,88                 | 0     |
| 54  | MG   | CA    | 1962 | 1/1   | 0.83 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3184 | 1/1   | 0.83 | 0.29 | 116,116,116,116             | 0     |
| 54  | MG   | CA    | 1806 | 1/1   | 0.83 | 0.14 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3008 | 1/1   | 0.83 | 0.15 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3539 | 1/1   | 0.83 | 0.21 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3381 | 1/1   | 0.83 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3317 | 1/1   | 0.83 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3017 | 1/1   | 0.83 | 0.19 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3543 | 1/1   | 0.83 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1976 | 1/1   | 0.83 | 0.13 | 86,86,86,86                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3398 | 1/1   | 0.83 | 0.35 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1860 | 1/1   | 0.83 | 0.12 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3038 | 1/1   | 0.83 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3548 | 1/1   | 0.83 | 0.17 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3043 | 1/1   | 0.83 | 0.16 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3048 | 1/1   | 0.83 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3262 | 1/1   | 0.83 | 0.17 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3565 | 1/1   | 0.83 | 0.14 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3263 | 1/1   | 0.83 | 0.29 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1792 | 1/1   | 0.83 | 0.28 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 2954 | 1/1   | 0.83 | 0.23 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3325 | 1/1   | 0.83 | 0.26 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3723 | 1/1   | 0.83 | 0.23 | 106,106,106,106             | 0     |
| 54  | MG   | BA    | 3558 | 1/1   | 0.83 | 0.11 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3735 | 1/1   | 0.84 | 0.07 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1959 | 1/1   | 0.84 | 0.09 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3276 | 1/1   | 0.84 | 0.09 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1803 | 1/1   | 0.84 | 0.20 | 100,100,100,100             | 0     |
| 54  | MG   | BA    | 3002 | 1/1   | 0.84 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 2956 | 1/1   | 0.84 | 0.22 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3158 | 1/1   | 0.84 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3557 | 1/1   | 0.84 | 0.22 | 131,131,131,131             | 0     |
| 54  | MG   | BA    | 3227 | 1/1   | 0.84 | 0.26 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3468 | 1/1   | 0.84 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3204 | 1/1   | 0.84 | 0.36 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3003 | 1/1   | 0.84 | 0.21 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3497 | 1/1   | 0.84 | 0.22 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 2035 | 1/1   | 0.84 | 0.22 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1756 | 1/1   | 0.84 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | BK    | 201  | 1/1   | 0.84 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3768 | 1/1   | 0.84 | 0.28 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3568 | 1/1   | 0.84 | 0.05 | 123,123,123,123             | 0     |
| 54  | MG   | BA    | 3169 | 1/1   | 0.84 | 0.28 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3032 | 1/1   | 0.84 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3774 | 1/1   | 0.84 | 0.23 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3238 | 1/1   | 0.84 | 0.24 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3016 | 1/1   | 0.84 | 0.24 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3230 | 1/1   | 0.84 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | CA    | 1666 | 1/1   | 0.84 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | CA    | 1822 | 1/1   | 0.84 | 0.12 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3237 | 1/1   | 0.84 | 0.23 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3507 | 1/1   | 0.84 | 0.11 | 80,80,80,80                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1672 | 1/1   | 0.84 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3502 | 1/1   | 0.84 | 0.19 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3504 | 1/1   | 0.84 | 0.12 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3241 | 1/1   | 0.84 | 0.23 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3068 | 1/1   | 0.84 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | CL    | 201  | 1/1   | 0.84 | 0.09 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3798 | 1/1   | 0.84 | 0.20 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3514 | 1/1   | 0.84 | 0.11 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 2988 | 1/1   | 0.84 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | BA    | 3577 | 1/1   | 0.84 | 0.09 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1690 | 1/1   | 0.84 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3804 | 1/1   | 0.84 | 0.14 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1607 | 1/1   | 0.84 | 0.21 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3402 | 1/1   | 0.84 | 0.17 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3526 | 1/1   | 0.84 | 0.18 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3677 | 1/1   | 0.84 | 0.10 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3092 | 1/1   | 0.84 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3248 | 1/1   | 0.84 | 0.07 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3409 | 1/1   | 0.84 | 0.31 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3032 | 1/1   | 0.84 | 0.33 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1905 | 1/1   | 0.84 | 0.21 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3689 | 1/1   | 0.84 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3143 | 1/1   | 0.84 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3263 | 1/1   | 0.84 | 0.17 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3539 | 1/1   | 0.84 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3533 | 1/1   | 0.84 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 2019 | 1/1   | 0.84 | 0.06 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3555 | 1/1   | 0.84 | 0.25 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3556 | 1/1   | 0.84 | 0.15 | 183,183,183,183             | 0     |
| 54  | MG   | DA    | 3125 | 1/1   | 0.84 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3709 | 1/1   | 0.84 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3429 | 1/1   | 0.84 | 0.17 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 2001 | 1/1   | 0.84 | 0.14 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3477 | 1/1   | 0.84 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1784 | 1/1   | 0.84 | 0.23 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3150 | 1/1   | 0.84 | 0.27 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1863 | 1/1   | 0.84 | 0.05 | 121,121,121,121             | 0     |
| 54  | MG   | DA    | 3717 | 1/1   | 0.84 | 0.14 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3268 | 1/1   | 0.84 | 0.25 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3050 | 1/1   | 0.84 | 0.21 | 67,67,67,67                 | 0     |
| 54  | MG   | DR    | 202  | 1/1   | 0.84 | 0.23 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1871 | 1/1   | 0.84 | 0.07 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3383 | 1/1   | 0.84 | 0.15 | 63,63,63,63                 | 0     |
| 54  | MG   | CA    | 1955 | 1/1   | 0.84 | 0.33 | 102,102,102,102             | 0     |
| 54  | MG   | BB    | 220  | 1/1   | 0.84 | 0.20 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1827 | 1/1   | 0.84 | 0.18 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3322 | 1/1   | 0.84 | 0.15 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1723 | 1/1   | 0.84 | 0.10 | 111,111,111,111             | 0     |
| 54  | MG   | CD    | 115  | 1/1   | 0.84 | 0.17 | 106,106,106,106             | 0     |
| 54  | MG   | B1    | 201  | 1/1   | 0.85 | 0.11 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3412 | 1/1   | 0.85 | 0.12 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3173 | 1/1   | 0.85 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1701 | 1/1   | 0.85 | 0.12 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3733 | 1/1   | 0.85 | 0.16 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1789 | 1/1   | 0.85 | 0.13 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1951 | 1/1   | 0.85 | 0.14 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3436 | 1/1   | 0.85 | 0.09 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1749 | 1/1   | 0.85 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1871 | 1/1   | 0.85 | 0.08 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3081 | 1/1   | 0.85 | 0.24 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3347 | 1/1   | 0.85 | 0.24 | 99,99,99,99                 | 0     |
| 54  | MG   | CA    | 1708 | 1/1   | 0.85 | 0.13 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3185 | 1/1   | 0.85 | 0.13 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3443 | 1/1   | 0.85 | 0.34 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1651 | 1/1   | 0.85 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 2961 | 1/1   | 0.85 | 0.30 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3601 | 1/1   | 0.85 | 0.19 | 95,95,95,95                 | 0     |
| 54  | MG   | CK    | 201  | 1/1   | 0.85 | 0.23 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3103 | 1/1   | 0.85 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1901 | 1/1   | 0.85 | 0.10 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3274 | 1/1   | 0.85 | 0.23 | 116,116,116,116             | 0     |
| 54  | MG   | BA    | 3121 | 1/1   | 0.85 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 2013 | 1/1   | 0.85 | 0.13 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3110 | 1/1   | 0.85 | 0.15 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3061 | 1/1   | 0.85 | 0.19 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3120 | 1/1   | 0.85 | 0.35 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1770 | 1/1   | 0.85 | 0.16 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1724 | 1/1   | 0.85 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3506 | 1/1   | 0.85 | 0.15 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3319 | 1/1   | 0.85 | 0.15 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3321 | 1/1   | 0.85 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3216 | 1/1   | 0.85 | 0.26 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1627 | 1/1   | 0.85 | 0.23 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1825 | 1/1   | 0.85 | 0.10 | 95,95,95,95                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1675 | 1/1   | 0.85 | 0.16 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3070 | 1/1   | 0.85 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1604 | 1/1   | 0.85 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | BB    | 210  | 1/1   | 0.85 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3229 | 1/1   | 0.85 | 0.15 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3488 | 1/1   | 0.85 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3379 | 1/1   | 0.85 | 0.18 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3074 | 1/1   | 0.85 | 0.16 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1832 | 1/1   | 0.85 | 0.09 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1702 | 1/1   | 0.85 | 0.22 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1649 | 1/1   | 0.85 | 0.15 | 84,84,84,84                 | 0     |
| 54  | MG   | CC    | 113  | 1/1   | 0.85 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | CD    | 104  | 1/1   | 0.85 | 0.07 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3314 | 1/1   | 0.85 | 0.15 | 76,76,76,76                 | 0     |
| 54  | MG   | BB    | 222  | 1/1   | 0.85 | 0.07 | 93,93,93,93                 | 0     |
| 54  | MG   | BB    | 224  | 1/1   | 0.85 | 0.06 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3536 | 1/1   | 0.85 | 0.23 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3508 | 1/1   | 0.85 | 0.28 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1783 | 1/1   | 0.85 | 0.35 | 90,90,90,90                 | 0     |
| 54  | MG   | A1    | 101  | 1/1   | 0.85 | 0.10 | 102,102,102,102             | 0     |
| 54  | MG   | CD    | 116  | 1/1   | 0.85 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3540 | 1/1   | 0.85 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1948 | 1/1   | 0.85 | 0.10 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1949 | 1/1   | 0.85 | 0.19 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1693 | 1/1   | 0.85 | 0.06 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1624 | 1/1   | 0.85 | 0.23 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3218 | 1/1   | 0.85 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3698 | 1/1   | 0.85 | 0.23 | 89,89,89,89                 | 0     |
| 54  | MG   | CA    | 1953 | 1/1   | 0.85 | 0.26 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3244 | 1/1   | 0.85 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3529 | 1/1   | 0.85 | 0.33 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3389 | 1/1   | 0.85 | 0.27 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1794 | 1/1   | 0.85 | 0.19 | 93,93,93,93                 | 0     |
| 54  | MG   | CA    | 1861 | 1/1   | 0.85 | 0.07 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3006 | 1/1   | 0.85 | 0.26 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3020 | 1/1   | 0.85 | 0.12 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3550 | 1/1   | 0.85 | 0.13 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3553 | 1/1   | 0.85 | 0.23 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3027 | 1/1   | 0.85 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | CA    | 1870 | 1/1   | 0.85 | 0.18 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3240 | 1/1   | 0.85 | 0.17 | 58,58,58,58                 | 0     |
| 54  | MG   | AA    | 1891 | 1/1   | 0.85 | 0.17 | 93,93,93,93                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1975 | 1/1   | 0.85 | 0.09 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3562 | 1/1   | 0.85 | 0.33 | 75,75,75,75                 | 0     |
| 54  | MG   | DU    | 203  | 1/1   | 0.85 | 0.15 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1696 | 1/1   | 0.85 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3249 | 1/1   | 0.85 | 0.26 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3256 | 1/1   | 0.85 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3302 | 1/1   | 0.86 | 0.23 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1714 | 1/1   | 0.86 | 0.12 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3305 | 1/1   | 0.86 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | B3    | 102  | 1/1   | 0.86 | 0.07 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3730 | 1/1   | 0.86 | 0.10 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3576 | 1/1   | 0.86 | 0.07 | 109,109,109,109             | 0     |
| 54  | MG   | AA    | 1897 | 1/1   | 0.86 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1652 | 1/1   | 0.86 | 0.17 | 82,82,82,82                 | 0     |
| 54  | MG   | CD    | 109  | 1/1   | 0.86 | 0.07 | 89,89,89,89                 | 0     |
| 54  | MG   | AA    | 1698 | 1/1   | 0.86 | 0.33 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3189 | 1/1   | 0.86 | 0.26 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3316 | 1/1   | 0.86 | 0.16 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 3589 | 1/1   | 0.86 | 0.30 | 136,136,136,136             | 0     |
| 54  | MG   | BA    | 3514 | 1/1   | 0.86 | 0.09 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 2032 | 1/1   | 0.86 | 0.10 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3593 | 1/1   | 0.86 | 0.12 | 97,97,97,97                 | 0     |
| 54  | MG   | AA    | 1996 | 1/1   | 0.86 | 0.15 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3752 | 1/1   | 0.86 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3455 | 1/1   | 0.86 | 0.07 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3583 | 1/1   | 0.86 | 0.05 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1792 | 1/1   | 0.86 | 0.22 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3462 | 1/1   | 0.86 | 0.15 | 80,80,80,80                 | 0     |
| 54  | MG   | CD    | 123  | 1/1   | 0.86 | 0.06 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3518 | 1/1   | 0.86 | 0.35 | 134,134,134,134             | 0     |
| 54  | MG   | DA    | 2951 | 1/1   | 0.86 | 0.22 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1795 | 1/1   | 0.86 | 0.09 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3332 | 1/1   | 0.86 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3772 | 1/1   | 0.86 | 0.19 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3200 | 1/1   | 0.86 | 0.19 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3523 | 1/1   | 0.86 | 0.11 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3471 | 1/1   | 0.86 | 0.26 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1900 | 1/1   | 0.86 | 0.07 | 102,102,102,102             | 0     |
| 54  | MG   | CA    | 1801 | 1/1   | 0.86 | 0.13 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1639 | 1/1   | 0.86 | 0.34 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3007 | 1/1   | 0.86 | 0.18 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 2921 | 1/1   | 0.86 | 0.19 | 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   | BB    | 211  | 1/1   | 0.86 | 0.11 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3207 | 1/1   | 0.86 | 0.11 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3272 | 1/1   | 0.86 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3405 | 1/1   | 0.86 | 0.17 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3489 | 1/1   | 0.86 | 0.36 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3214 | 1/1   | 0.86 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 2923 | 1/1   | 0.86 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3650 | 1/1   | 0.86 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3144 | 1/1   | 0.86 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | BB    | 221  | 1/1   | 0.86 | 0.07 | 106,106,106,106             | 0     |
| 54  | MG   | AA    | 1773 | 1/1   | 0.86 | 0.13 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1817 | 1/1   | 0.86 | 0.09 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3280 | 1/1   | 0.86 | 0.08 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3044 | 1/1   | 0.86 | 0.07 | 114,114,114,114             | 0     |
| 54  | MG   | DA    | 3063 | 1/1   | 0.86 | 0.14 | 34,34,34,34                 | 0     |
| 54  | MG   | DB    | 203  | 1/1   | 0.86 | 0.32 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3359 | 1/1   | 0.86 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3505 | 1/1   | 0.86 | 0.22 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1942 | 1/1   | 0.86 | 0.14 | 128,128,128,128             | 0     |
| 54  | MG   | BA    | 3228 | 1/1   | 0.86 | 0.05 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1636 | 1/1   | 0.86 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3386 | 1/1   | 0.86 | 0.28 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 2972 | 1/1   | 0.86 | 0.26 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3494 | 1/1   | 0.86 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3394 | 1/1   | 0.86 | 0.13 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1983 | 1/1   | 0.86 | 0.11 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1834 | 1/1   | 0.86 | 0.16 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3519 | 1/1   | 0.86 | 0.18 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3292 | 1/1   | 0.86 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | AA    | 1764 | 1/1   | 0.86 | 0.08 | 96,96,96,96                 | 0     |
| 54  | MG   | DA    | 3097 | 1/1   | 0.86 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3098 | 1/1   | 0.86 | 0.22 | 65,65,65,65                 | 0     |
| 54  | MG   | AA    | 2026 | 1/1   | 0.86 | 0.29 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3501 | 1/1   | 0.86 | 0.06 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3703 | 1/1   | 0.86 | 0.12 | 99,99,99,99                 | 0     |
| 54  | MG   | AL    | 201  | 1/1   | 0.86 | 0.13 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1683 | 1/1   | 0.86 | 0.15 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3276 | 1/1   | 0.86 | 0.20 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1684 | 1/1   | 0.86 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3279 | 1/1   | 0.86 | 0.28 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3414 | 1/1   | 0.86 | 0.19 | 70,70,70,70                 | 0     |
| 54  | MG   | D0    | 203  | 1/1   | 0.86 | 0.11 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3544 | 1/1   | 0.86 | 0.17 | 87,87,87,87                 | 0     |
| 54  | MG   | BR    | 202  | 1/1   | 0.86 | 0.12 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3417 | 1/1   | 0.86 | 0.08 | 120,120,120,120             | 0     |
| 54  | MG   | D1    | 202  | 1/1   | 0.86 | 0.19 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3114 | 1/1   | 0.86 | 0.16 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1941 | 1/1   | 0.86 | 0.07 | 88,88,88,88                 | 0     |
| 54  | MG   | DS    | 201  | 1/1   | 0.86 | 0.18 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3285 | 1/1   | 0.86 | 0.22 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1822 | 1/1   | 0.86 | 0.13 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3122 | 1/1   | 0.86 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1769 | 1/1   | 0.86 | 0.12 | 81,81,81,81                 | 0     |
| 54  | MG   | BT    | 101  | 1/1   | 0.86 | 0.16 | 65,65,65,65                 | 0     |
| 54  | MG   | DZ    | 102  | 1/1   | 0.86 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3066 | 1/1   | 0.86 | 0.29 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 2987 | 1/1   | 0.87 | 0.23 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 3739 | 1/1   | 0.87 | 0.10 | 127,127,127,127             | 0     |
| 54  | MG   | DA    | 2989 | 1/1   | 0.87 | 0.20 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3489 | 1/1   | 0.87 | 0.10 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3596 | 1/1   | 0.87 | 0.21 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3235 | 1/1   | 0.87 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1613 | 1/1   | 0.87 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | AP    | 201  | 1/1   | 0.87 | 0.15 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3603 | 1/1   | 0.87 | 0.21 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3605 | 1/1   | 0.87 | 0.15 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 2935 | 1/1   | 0.87 | 0.21 | 46,46,46,46                 | 0     |
| 54  | MG   | CA    | 1829 | 1/1   | 0.87 | 0.09 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3387 | 1/1   | 0.87 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1823 | 1/1   | 0.87 | 0.29 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3214 | 1/1   | 0.87 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1846 | 1/1   | 0.87 | 0.25 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1833 | 1/1   | 0.87 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1879 | 1/1   | 0.87 | 0.09 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1722 | 1/1   | 0.87 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3220 | 1/1   | 0.87 | 0.15 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3287 | 1/1   | 0.87 | 0.25 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3041 | 1/1   | 0.87 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | CA    | 1842 | 1/1   | 0.87 | 0.08 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3778 | 1/1   | 0.87 | 0.10 | 97,97,97,97                 | 0     |
| 54  | MG   | CA    | 1844 | 1/1   | 0.87 | 0.12 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1774 | 1/1   | 0.87 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3492 | 1/1   | 0.87 | 0.19 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3373 | 1/1   | 0.87 | 0.13 | 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   | DA    | 3056 | 1/1   | 0.87 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3057 | 1/1   | 0.87 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3451 | 1/1   | 0.87 | 0.22 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3378 | 1/1   | 0.87 | 0.08 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3453 | 1/1   | 0.87 | 0.29 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1813 | 1/1   | 0.87 | 0.24 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3654 | 1/1   | 0.87 | 0.06 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3382 | 1/1   | 0.87 | 0.22 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3795 | 1/1   | 0.87 | 0.09 | 112,112,112,112             | 0     |
| 54  | MG   | BA    | 2978 | 1/1   | 0.87 | 0.24 | 47,47,47,47                 | 0     |
| 54  | MG   | AA    | 1753 | 1/1   | 0.87 | 0.17 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 2982 | 1/1   | 0.87 | 0.28 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3123 | 1/1   | 0.87 | 0.30 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3567 | 1/1   | 0.87 | 0.08 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1934 | 1/1   | 0.87 | 0.19 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1935 | 1/1   | 0.87 | 0.06 | 136,136,136,136             | 0     |
| 54  | MG   | CA    | 1936 | 1/1   | 0.87 | 0.09 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3510 | 1/1   | 0.87 | 0.13 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3124 | 1/1   | 0.87 | 0.23 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3160 | 1/1   | 0.87 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3270 | 1/1   | 0.87 | 0.16 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3218 | 1/1   | 0.87 | 0.06 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1715 | 1/1   | 0.87 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3416 | 1/1   | 0.87 | 0.13 | 74,74,74,74                 | 0     |
| 54  | MG   | CC    | 111  | 1/1   | 0.87 | 0.08 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3127 | 1/1   | 0.87 | 0.33 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1869 | 1/1   | 0.87 | 0.06 | 98,98,98,98                 | 0     |
| 54  | MG   | CD    | 103  | 1/1   | 0.87 | 0.08 | 113,113,113,113             | 0     |
| 54  | MG   | DB    | 216  | 1/1   | 0.87 | 0.11 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3318 | 1/1   | 0.87 | 0.14 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3521 | 1/1   | 0.87 | 0.31 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3696 | 1/1   | 0.87 | 0.08 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3292 | 1/1   | 0.87 | 0.12 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3540 | 1/1   | 0.87 | 0.25 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1951 | 1/1   | 0.87 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1646 | 1/1   | 0.87 | 0.24 | 66,66,66,66                 | 0     |
| 54  | MG   | CA    | 1665 | 1/1   | 0.87 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3297 | 1/1   | 0.87 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1954 | 1/1   | 0.87 | 0.08 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3524 | 1/1   | 0.87 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | AA    | 1818 | 1/1   | 0.87 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3560 | 1/1   | 0.87 | 0.15 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1879 | 1/1   | 0.87 | 0.23 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1669 | 1/1   | 0.87 | 0.27 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1744 | 1/1   | 0.87 | 0.08 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3135 | 1/1   | 0.87 | 0.23 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3176 | 1/1   | 0.87 | 0.18 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3137 | 1/1   | 0.87 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3428 | 1/1   | 0.87 | 0.06 | 93,93,93,93                 | 0     |
| 54  | MG   | BB    | 202  | 1/1   | 0.87 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3446 | 1/1   | 0.87 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 2915 | 1/1   | 0.87 | 0.22 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 2947 | 1/1   | 0.87 | 0.23 | 26,26,26,26                 | 0     |
| 54  | MG   | DA    | 3164 | 1/1   | 0.87 | 0.29 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1678 | 1/1   | 0.87 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 2953 | 1/1   | 0.87 | 0.32 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1628 | 1/1   | 0.87 | 0.38 | 69,69,69,69                 | 0     |
| 54  | MG   | DU    | 206  | 1/1   | 0.87 | 0.12 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1774 | 1/1   | 0.87 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1810 | 1/1   | 0.87 | 0.11 | 75,75,75,75                 | 0     |
| 55  | ZN   | AA    | 2040 | 1/1   | 0.87 | 0.10 | 300,300,300,300             | 0     |
| 54  | MG   | DA    | 3461 | 1/1   | 0.87 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1677 | 1/1   | 0.88 | 0.24 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1620 | 1/1   | 0.88 | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3577 | 1/1   | 0.88 | 0.07 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1766 | 1/1   | 0.88 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3159 | 1/1   | 0.88 | 0.18 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1857 | 1/1   | 0.88 | 0.10 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1688 | 1/1   | 0.88 | 0.22 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3307 | 1/1   | 0.88 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | BU    | 202  | 1/1   | 0.88 | 0.06 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3114 | 1/1   | 0.88 | 0.16 | 67,67,67,67                 | 0     |
| 54  | MG   | B3    | 101  | 1/1   | 0.88 | 0.08 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 2909 | 1/1   | 0.88 | 0.24 | 25,25,25,25                 | 0     |
| 54  | MG   | BA    | 2979 | 1/1   | 0.88 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3748 | 1/1   | 0.88 | 0.17 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3453 | 1/1   | 0.88 | 0.28 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 2919 | 1/1   | 0.88 | 0.18 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3163 | 1/1   | 0.88 | 0.26 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 2930 | 1/1   | 0.88 | 0.19 | 31,31,31,31                 | 0     |
| 54  | MG   | DA    | 3758 | 1/1   | 0.88 | 0.13 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3167 | 1/1   | 0.88 | 0.22 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3054 | 1/1   | 0.88 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | B6    | 101  | 1/1   | 0.88 | 0.08 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3176 | 1/1   | 0.88 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 2952 | 1/1   | 0.88 | 0.25 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3184 | 1/1   | 0.88 | 0.25 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1793 | 1/1   | 0.88 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3186 | 1/1   | 0.88 | 0.09 | 23,23,23,23                 | 0     |
| 54  | MG   | BA    | 2903 | 1/1   | 0.88 | 0.08 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3579 | 1/1   | 0.88 | 0.12 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3337 | 1/1   | 0.88 | 0.23 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3775 | 1/1   | 0.88 | 0.16 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3339 | 1/1   | 0.88 | 0.20 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3189 | 1/1   | 0.88 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3347 | 1/1   | 0.88 | 0.32 | 98,98,98,98                 | 0     |
| 54  | MG   | AA    | 1657 | 1/1   | 0.88 | 0.26 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3122 | 1/1   | 0.88 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1795 | 1/1   | 0.88 | 0.19 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1755 | 1/1   | 0.88 | 0.23 | 62,62,62,62                 | 0     |
| 54  | MG   | AA    | 1967 | 1/1   | 0.88 | 0.07 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3635 | 1/1   | 0.88 | 0.10 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3640 | 1/1   | 0.88 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1628 | 1/1   | 0.88 | 0.27 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3463 | 1/1   | 0.88 | 0.15 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3391 | 1/1   | 0.88 | 0.19 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3251 | 1/1   | 0.88 | 0.12 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1887 | 1/1   | 0.88 | 0.09 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3253 | 1/1   | 0.88 | 0.21 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1719 | 1/1   | 0.88 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1912 | 1/1   | 0.88 | 0.14 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3532 | 1/1   | 0.88 | 0.18 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1896 | 1/1   | 0.88 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1616 | 1/1   | 0.88 | 0.12 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3503 | 1/1   | 0.88 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3664 | 1/1   | 0.88 | 0.08 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3224 | 1/1   | 0.88 | 0.13 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1807 | 1/1   | 0.88 | 0.09 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3191 | 1/1   | 0.88 | 0.29 | 79,79,79,79                 | 0     |
| 54  | MG   | DB    | 206  | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1726 | 1/1   | 0.88 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3257 | 1/1   | 0.88 | 0.09 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3054 | 1/1   | 0.88 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3332 | 1/1   | 0.88 | 0.18 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1729 | 1/1   | 0.88 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1907 | 1/1   | 0.88 | 0.11 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3258 | 1/1   | 0.88 | 0.13 | 100,100,100,100             | 0     |
| 54  | MG   | AA    | 1884 | 1/1   | 0.88 | 0.08 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1734 | 1/1   | 0.88 | 0.09 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3684 | 1/1   | 0.88 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3131 | 1/1   | 0.88 | 0.24 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 2916 | 1/1   | 0.88 | 0.20 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3251 | 1/1   | 0.88 | 0.26 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3014 | 1/1   | 0.88 | 0.29 | 49,49,49,49                 | 0     |
| 54  | MG   | BB    | 223  | 1/1   | 0.88 | 0.09 | 122,122,122,122             | 0     |
| 54  | MG   | DA    | 3531 | 1/1   | 0.88 | 0.22 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1825 | 1/1   | 0.88 | 0.06 | 106,106,106,106             | 0     |
| 54  | MG   | DA    | 3697 | 1/1   | 0.88 | 0.17 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3484 | 1/1   | 0.88 | 0.17 | 106,106,106,106             | 0     |
| 54  | MG   | BA    | 2918 | 1/1   | 0.88 | 0.24 | 46,46,46,46                 | 0     |
| 54  | MG   | CA    | 1921 | 1/1   | 0.88 | 0.22 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3096 | 1/1   | 0.88 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | AA    | 1731 | 1/1   | 0.88 | 0.28 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3548 | 1/1   | 0.88 | 0.13 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 2042 | 1/1   | 0.88 | 0.08 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3213 | 1/1   | 0.88 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1916 | 1/1   | 0.88 | 0.11 | 93,93,93,93                 | 0     |
| 54  | MG   | BA    | 3026 | 1/1   | 0.88 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3556 | 1/1   | 0.88 | 0.11 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 2937 | 1/1   | 0.88 | 0.20 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3424 | 1/1   | 0.88 | 0.15 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3425 | 1/1   | 0.88 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1769 | 1/1   | 0.88 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3220 | 1/1   | 0.88 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1641 | 1/1   | 0.88 | 0.14 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3566 | 1/1   | 0.88 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1788 | 1/1   | 0.88 | 0.08 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1760 | 1/1   | 0.88 | 0.09 | 118,118,118,118             | 0     |
| 54  | MG   | BA    | 3100 | 1/1   | 0.88 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | D6    | 101  | 1/1   | 0.88 | 0.37 | 98,98,98,98                 | 0     |
| 54  | MG   | D6    | 102  | 1/1   | 0.88 | 0.21 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1874 | 1/1   | 0.88 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3298 | 1/1   | 0.88 | 0.14 | 70,70,70,70                 | 0     |
| 54  | MG   | BB    | 214  | 1/1   | 0.89 | 0.14 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1793 | 1/1   | 0.89 | 0.17 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3734 | 1/1   | 0.89 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3582 | 1/1   | 0.89 | 0.09 | 116,116,116,116             | 0     |
| 54  | MG   | DA    | 3736 | 1/1   | 0.89 | 0.10 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3222 | 1/1   | 0.89 | 0.28 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3156 | 1/1   | 0.89 | 0.18 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 2936 | 1/1   | 0.89 | 0.24 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3149 | 1/1   | 0.89 | 0.21 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3590 | 1/1   | 0.89 | 0.09 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 2941 | 1/1   | 0.89 | 0.16 | 39,39,39,39                 | 0     |
| 54  | MG   | AA    | 1892 | 1/1   | 0.89 | 0.11 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3161 | 1/1   | 0.89 | 0.23 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3452 | 1/1   | 0.89 | 0.07 | 104,104,104,104             | 0     |
| 54  | MG   | AA    | 1673 | 1/1   | 0.89 | 0.07 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3454 | 1/1   | 0.89 | 0.22 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1642 | 1/1   | 0.89 | 0.16 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1717 | 1/1   | 0.89 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3755 | 1/1   | 0.89 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3756 | 1/1   | 0.89 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1645 | 1/1   | 0.89 | 0.28 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1684 | 1/1   | 0.89 | 0.16 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3606 | 1/1   | 0.89 | 0.16 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1973 | 1/1   | 0.89 | 0.13 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3120 | 1/1   | 0.89 | 0.20 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3182 | 1/1   | 0.89 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3170 | 1/1   | 0.89 | 0.21 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1732 | 1/1   | 0.89 | 0.27 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3614 | 1/1   | 0.89 | 0.14 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3616 | 1/1   | 0.89 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 2999 | 1/1   | 0.89 | 0.19 | 44,44,44,44                 | 0     |
| 54  | MG   | AA    | 1908 | 1/1   | 0.89 | 0.24 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3004 | 1/1   | 0.89 | 0.24 | 52,52,52,52                 | 0     |
| 54  | MG   | AA    | 1738 | 1/1   | 0.89 | 0.26 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3291 | 1/1   | 0.89 | 0.10 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3345 | 1/1   | 0.89 | 0.18 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3440 | 1/1   | 0.89 | 0.22 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1738 | 1/1   | 0.89 | 0.09 | 88,88,88,88                 | 0     |
| 54  | MG   | AA    | 1856 | 1/1   | 0.89 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3179 | 1/1   | 0.89 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 2997 | 1/1   | 0.89 | 0.25 | 60,60,60,60                 | 0     |
| 54  | MG   | CH    | 201  | 1/1   | 0.89 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3207 | 1/1   | 0.89 | 0.27 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3028 | 1/1   | 0.89 | 0.19 | 59,59,59,59                 | 0     |
| 54  | MG   | AC    | 105  | 1/1   | 0.89 | 0.13 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3563 | 1/1   | 0.89 | 0.20 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3037 | 1/1   | 0.89 | 0.24 | 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   | CA    | 1745 | 1/1   | 0.89 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3565 | 1/1   | 0.89 | 0.18 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 2929 | 1/1   | 0.89 | 0.26 | 32,32,32,32                 | 0     |
| 54  | MG   | CP    | 202  | 1/1   | 0.89 | 0.07 | 122,122,122,122             | 0     |
| 54  | MG   | AA    | 1625 | 1/1   | 0.89 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3372 | 1/1   | 0.89 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3310 | 1/1   | 0.89 | 0.09 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1858 | 1/1   | 0.89 | 0.06 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1605 | 1/1   | 0.89 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 2946 | 1/1   | 0.89 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3019 | 1/1   | 0.89 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3064 | 1/1   | 0.89 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3067 | 1/1   | 0.89 | 0.24 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 2948 | 1/1   | 0.89 | 0.16 | 29,29,29,29                 | 0     |
| 54  | MG   | CA    | 1839 | 1/1   | 0.89 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3075 | 1/1   | 0.89 | 0.12 | 43,43,43,43                 | 0     |
| 54  | MG   | CA    | 1756 | 1/1   | 0.89 | 0.05 | 57,57,57,57                 | 0     |
| 54  | MG   | AA    | 1705 | 1/1   | 0.89 | 0.11 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3392 | 1/1   | 0.89 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1776 | 1/1   | 0.89 | 0.23 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3261 | 1/1   | 0.89 | 0.15 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3031 | 1/1   | 0.89 | 0.08 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3090 | 1/1   | 0.89 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | DB    | 219  | 1/1   | 0.89 | 0.12 | 77,77,77,77                 | 0     |
| 54  | MG   | BW    | 101  | 1/1   | 0.89 | 0.12 | 65,65,65,65                 | 0     |
| 54  | MG   | CC    | 108  | 1/1   | 0.89 | 0.09 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1933 | 1/1   | 0.89 | 0.05 | 69,69,69,69                 | 0     |
| 54  | MG   | B4    | 101  | 1/1   | 0.89 | 0.17 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3267 | 1/1   | 0.89 | 0.31 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3406 | 1/1   | 0.89 | 0.11 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1635 | 1/1   | 0.89 | 0.16 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3034 | 1/1   | 0.89 | 0.17 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 2971 | 1/1   | 0.89 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | DE    | 302  | 1/1   | 0.89 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3095 | 1/1   | 0.89 | 0.10 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3105 | 1/1   | 0.89 | 0.28 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3529 | 1/1   | 0.89 | 0.14 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3530 | 1/1   | 0.89 | 0.13 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3554 | 1/1   | 0.89 | 0.18 | 72,72,72,72                 | 0     |
| 54  | MG   | D0    | 202  | 1/1   | 0.89 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3416 | 1/1   | 0.89 | 0.23 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1987 | 1/1   | 0.89 | 0.11 | 86,86,86,86                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3043 | 1/1   | 0.89 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3421 | 1/1   | 0.89 | 0.25 | 85,85,85,85                 | 0     |
| 54  | MG   | CA    | 1621 | 1/1   | 0.89 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3714 | 1/1   | 0.89 | 0.17 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3475 | 1/1   | 0.89 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3118 | 1/1   | 0.89 | 0.21 | 40,40,40,40                 | 0     |
| 54  | MG   | CA    | 1624 | 1/1   | 0.89 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | CA    | 1785 | 1/1   | 0.89 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1626 | 1/1   | 0.89 | 0.21 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1989 | 1/1   | 0.89 | 0.10 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3344 | 1/1   | 0.89 | 0.06 | 69,69,69,69                 | 0     |
| 54  | MG   | AA    | 1948 | 1/1   | 0.89 | 0.09 | 82,82,82,82                 | 0     |
| 54  | MG   | DZ    | 101  | 1/1   | 0.89 | 0.16 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3275 | 1/1   | 0.89 | 0.19 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1791 | 1/1   | 0.89 | 0.08 | 85,85,85,85                 | 0     |
| 54  | MG   | CD    | 125  | 1/1   | 0.89 | 0.09 | 83,83,83,83                 | 0     |
| 54  | MG   | CD    | 126  | 1/1   | 0.89 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3304 | 1/1   | 0.89 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1921 | 1/1   | 0.90 | 0.11 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3052 | 1/1   | 0.90 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3299 | 1/1   | 0.90 | 0.10 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3019 | 1/1   | 0.90 | 0.23 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3300 | 1/1   | 0.90 | 0.09 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3101 | 1/1   | 0.90 | 0.24 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3204 | 1/1   | 0.90 | 0.23 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3306 | 1/1   | 0.90 | 0.30 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1675 | 1/1   | 0.90 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3194 | 1/1   | 0.90 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3750 | 1/1   | 0.90 | 0.17 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3307 | 1/1   | 0.90 | 0.29 | 79,79,79,79                 | 0     |
| 54  | MG   | CA    | 1835 | 1/1   | 0.90 | 0.19 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3006 | 1/1   | 0.90 | 0.13 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3341 | 1/1   | 0.90 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3342 | 1/1   | 0.90 | 0.24 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1736 | 1/1   | 0.90 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3203 | 1/1   | 0.90 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3012 | 1/1   | 0.90 | 0.20 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1926 | 1/1   | 0.90 | 0.22 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3112 | 1/1   | 0.90 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 2964 | 1/1   | 0.90 | 0.21 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3353 | 1/1   | 0.90 | 0.07 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3519 | 1/1   | 0.90 | 0.09 | 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   | DA    | 3213 | 1/1   | 0.90 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3061 | 1/1   | 0.90 | 0.25 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1605 | 1/1   | 0.90 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | CA    | 1691 | 1/1   | 0.90 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3457 | 1/1   | 0.90 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 1716 | 1/1   | 0.90 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1763 | 1/1   | 0.90 | 0.30 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3065 | 1/1   | 0.90 | 0.19 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3636 | 1/1   | 0.90 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1619 | 1/1   | 0.90 | 0.32 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1669 | 1/1   | 0.90 | 0.23 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1779 | 1/1   | 0.90 | 0.11 | 104,104,104,104             | 0     |
| 54  | MG   | CA    | 1700 | 1/1   | 0.90 | 0.19 | 107,107,107,107             | 0     |
| 54  | MG   | CA    | 1945 | 1/1   | 0.90 | 0.10 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3231 | 1/1   | 0.90 | 0.34 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1619 | 1/1   | 0.90 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3651 | 1/1   | 0.90 | 0.20 | 98,98,98,98                 | 0     |
| 54  | MG   | CA    | 1620 | 1/1   | 0.90 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3653 | 1/1   | 0.90 | 0.14 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3396 | 1/1   | 0.90 | 0.19 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1782 | 1/1   | 0.90 | 0.18 | 106,106,106,106             | 0     |
| 54  | MG   | BA    | 3399 | 1/1   | 0.90 | 0.06 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3241 | 1/1   | 0.90 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3384 | 1/1   | 0.90 | 0.13 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3513 | 1/1   | 0.90 | 0.15 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1625 | 1/1   | 0.90 | 0.25 | 51,51,51,51                 | 0     |
| 54  | MG   | CA    | 1868 | 1/1   | 0.90 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3101 | 1/1   | 0.90 | 0.20 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3166 | 1/1   | 0.90 | 0.11 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1627 | 1/1   | 0.90 | 0.20 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 1670 | 1/1   | 0.90 | 0.11 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1944 | 1/1   | 0.90 | 0.10 | 111,111,111,111             | 0     |
| 54  | MG   | DB    | 207  | 1/1   | 0.90 | 0.11 | 99,99,99,99                 | 0     |
| 54  | MG   | AA    | 1615 | 1/1   | 0.90 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 3676 | 1/1   | 0.90 | 0.22 | 131,131,131,131             | 0     |
| 54  | MG   | BA    | 3277 | 1/1   | 0.90 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3264 | 1/1   | 0.90 | 0.24 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 2902 | 1/1   | 0.90 | 0.17 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3111 | 1/1   | 0.90 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1877 | 1/1   | 0.90 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | AA    | 1743 | 1/1   | 0.90 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3230 | 1/1   | 0.90 | 0.06 | 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   | AA    | 1601 | 1/1   | 0.90 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3537 | 1/1   | 0.90 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3274 | 1/1   | 0.90 | 0.19 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1606 | 1/1   | 0.90 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 2994 | 1/1   | 0.90 | 0.33 | 60,60,60,60                 | 0     |
| 54  | MG   | DB    | 223  | 1/1   | 0.90 | 0.06 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3485 | 1/1   | 0.90 | 0.25 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 2949 | 1/1   | 0.90 | 0.17 | 35,35,35,35                 | 0     |
| 54  | MG   | BA    | 3349 | 1/1   | 0.90 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3550 | 1/1   | 0.90 | 0.26 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3553 | 1/1   | 0.90 | 0.07 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3547 | 1/1   | 0.90 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3039 | 1/1   | 0.90 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3549 | 1/1   | 0.90 | 0.27 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3287 | 1/1   | 0.90 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3558 | 1/1   | 0.90 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3290 | 1/1   | 0.90 | 0.37 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 2962 | 1/1   | 0.90 | 0.15 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3183 | 1/1   | 0.90 | 0.09 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 2966 | 1/1   | 0.90 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | DA    | 2974 | 1/1   | 0.90 | 0.29 | 51,51,51,51                 | 0     |
| 54  | MG   | DR    | 201  | 1/1   | 0.90 | 0.09 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3551 | 1/1   | 0.90 | 0.06 | 98,98,98,98                 | 0     |
| 54  | MG   | BE    | 304  | 1/1   | 0.90 | 0.33 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3146 | 1/1   | 0.90 | 0.12 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3148 | 1/1   | 0.90 | 0.31 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1623 | 1/1   | 0.90 | 0.23 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3151 | 1/1   | 0.90 | 0.25 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 2906 | 1/1   | 0.90 | 0.08 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 2997 | 1/1   | 0.90 | 0.14 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 2951 | 1/1   | 0.90 | 0.15 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 3162 | 1/1   | 0.90 | 0.22 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3092 | 1/1   | 0.90 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3363 | 1/1   | 0.90 | 0.11 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 2998 | 1/1   | 0.90 | 0.06 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3366 | 1/1   | 0.90 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3435 | 1/1   | 0.90 | 0.16 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3139 | 1/1   | 0.90 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3178 | 1/1   | 0.90 | 0.20 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3737 | 1/1   | 0.90 | 0.17 | 88,88,88,88                 | 0     |
| 54  | MG   | BB    | 205  | 1/1   | 0.91 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3578 | 1/1   | 0.91 | 0.13 | 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   | BB    | 206  | 1/1   | 0.91 | 0.14 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1772 | 1/1   | 0.91 | 0.15 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1961 | 1/1   | 0.91 | 0.18 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1703 | 1/1   | 0.91 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3013 | 1/1   | 0.91 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 1969 | 1/1   | 0.91 | 0.06 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3145 | 1/1   | 0.91 | 0.27 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3470 | 1/1   | 0.91 | 0.11 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3406 | 1/1   | 0.91 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3188 | 1/1   | 0.91 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 2979 | 1/1   | 0.91 | 0.15 | 31,31,31,31                 | 0     |
| 54  | MG   | BA    | 3055 | 1/1   | 0.91 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3411 | 1/1   | 0.91 | 0.10 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3595 | 1/1   | 0.91 | 0.10 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3356 | 1/1   | 0.91 | 0.07 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3413 | 1/1   | 0.91 | 0.07 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 2993 | 1/1   | 0.91 | 0.28 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1717 | 1/1   | 0.91 | 0.19 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3165 | 1/1   | 0.91 | 0.18 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 2973 | 1/1   | 0.91 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3002 | 1/1   | 0.91 | 0.31 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3607 | 1/1   | 0.91 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | CA    | 1890 | 1/1   | 0.91 | 0.07 | 115,115,115,115             | 0     |
| 54  | MG   | DA    | 3460 | 1/1   | 0.91 | 0.16 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3102 | 1/1   | 0.91 | 0.06 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3196 | 1/1   | 0.91 | 0.36 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3250 | 1/1   | 0.91 | 0.27 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3769 | 1/1   | 0.91 | 0.16 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3419 | 1/1   | 0.91 | 0.07 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3361 | 1/1   | 0.91 | 0.06 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3011 | 1/1   | 0.91 | 0.14 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3329 | 1/1   | 0.91 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3620 | 1/1   | 0.91 | 0.12 | 98,98,98,98                 | 0     |
| 54  | MG   | DA    | 3012 | 1/1   | 0.91 | 0.20 | 35,35,35,35                 | 0     |
| 54  | MG   | AQ    | 101  | 1/1   | 0.91 | 0.08 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1723 | 1/1   | 0.91 | 0.12 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3062 | 1/1   | 0.91 | 0.13 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3338 | 1/1   | 0.91 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3191 | 1/1   | 0.91 | 0.27 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3147 | 1/1   | 0.91 | 0.28 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3020 | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 2924 | 1/1   | 0.91 | 0.18 | 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   | CA    | 1731 | 1/1   | 0.91 | 0.06 | 86,86,86,86                 | 0     |
| 54  | MG   | AA    | 1726 | 1/1   | 0.91 | 0.16 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3639 | 1/1   | 0.91 | 0.20 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3201 | 1/1   | 0.91 | 0.09 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3033 | 1/1   | 0.91 | 0.11 | 42,42,42,42                 | 0     |
| 54  | MG   | CP    | 203  | 1/1   | 0.91 | 0.09 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3643 | 1/1   | 0.91 | 0.08 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1859 | 1/1   | 0.91 | 0.08 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3354 | 1/1   | 0.91 | 0.16 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1652 | 1/1   | 0.91 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3801 | 1/1   | 0.91 | 0.11 | 101,101,101,101             | 0     |
| 54  | MG   | BA    | 3308 | 1/1   | 0.91 | 0.22 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3496 | 1/1   | 0.91 | 0.13 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3209 | 1/1   | 0.91 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3436 | 1/1   | 0.91 | 0.24 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1869 | 1/1   | 0.91 | 0.07 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3029 | 1/1   | 0.91 | 0.20 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3030 | 1/1   | 0.91 | 0.12 | 47,47,47,47                 | 0     |
| 54  | MG   | CA    | 1920 | 1/1   | 0.91 | 0.17 | 81,81,81,81                 | 0     |
| 54  | MG   | CX    | 102  | 1/1   | 0.91 | 0.06 | 104,104,104,104             | 0     |
| 54  | MG   | AA    | 2006 | 1/1   | 0.91 | 0.06 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3222 | 1/1   | 0.91 | 0.31 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3442 | 1/1   | 0.91 | 0.06 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3066 | 1/1   | 0.91 | 0.31 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1647 | 1/1   | 0.91 | 0.34 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1950 | 1/1   | 0.91 | 0.10 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3162 | 1/1   | 0.91 | 0.10 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3384 | 1/1   | 0.91 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1927 | 1/1   | 0.91 | 0.20 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3079 | 1/1   | 0.91 | 0.22 | 59,59,59,59                 | 0     |
| 54  | MG   | BU    | 203  | 1/1   | 0.91 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1668 | 1/1   | 0.91 | 0.27 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3449 | 1/1   | 0.91 | 0.16 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1670 | 1/1   | 0.91 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | BU    | 205  | 1/1   | 0.91 | 0.12 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3685 | 1/1   | 0.91 | 0.05 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1977 | 1/1   | 0.91 | 0.20 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3077 | 1/1   | 0.91 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | BA    | 2953 | 1/1   | 0.91 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3095 | 1/1   | 0.91 | 0.11 | 46,46,46,46                 | 0     |
| 54  | MG   | AA    | 1994 | 1/1   | 0.91 | 0.07 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 3578 | 1/1   | 0.91 | 0.16 | 98,98,98,98                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3399 | 1/1   | 0.91 | 0.24 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1939 | 1/1   | 0.91 | 0.05 | 87,87,87,87                 | 0     |
| 54  | MG   | CD    | 113  | 1/1   | 0.91 | 0.06 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1682 | 1/1   | 0.91 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3403 | 1/1   | 0.91 | 0.14 | 69,69,69,69                 | 0     |
| 54  | MG   | DH    | 202  | 1/1   | 0.91 | 0.13 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3128 | 1/1   | 0.91 | 0.25 | 72,72,72,72                 | 0     |
| 54  | MG   | DO    | 205  | 1/1   | 0.91 | 0.17 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1764 | 1/1   | 0.91 | 0.05 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3266 | 1/1   | 0.91 | 0.10 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3551 | 1/1   | 0.91 | 0.08 | 68,68,68,68                 | 0     |
| 54  | MG   | B8    | 101  | 1/1   | 0.91 | 0.14 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1686 | 1/1   | 0.91 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | CA    | 1603 | 1/1   | 0.91 | 0.30 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1770 | 1/1   | 0.91 | 0.11 | 85,85,85,85                 | 0     |
| 54  | MG   | D1    | 203  | 1/1   | 0.91 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1859 | 1/1   | 0.91 | 0.08 | 121,121,121,121             | 0     |
| 54  | MG   | BA    | 3041 | 1/1   | 0.91 | 0.08 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3115 | 1/1   | 0.91 | 0.22 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1767 | 1/1   | 0.91 | 0.21 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3340 | 1/1   | 0.91 | 0.13 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3461 | 1/1   | 0.91 | 0.12 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 2917 | 1/1   | 0.91 | 0.23 | 27,27,27,27                 | 0     |
| 54  | MG   | AA    | 1786 | 1/1   | 0.91 | 0.12 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3423 | 1/1   | 0.91 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 2920 | 1/1   | 0.91 | 0.19 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 2924 | 1/1   | 0.91 | 0.13 | 17,17,17,17                 | 0     |
| 54  | MG   | BA    | 2966 | 1/1   | 0.91 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3288 | 1/1   | 0.91 | 0.31 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1797 | 1/1   | 0.91 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1615 | 1/1   | 0.91 | 0.11 | 40,40,40,40                 | 0     |
| 54  | MG   | CW    | 201  | 1/1   | 0.92 | 0.30 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3584 | 1/1   | 0.92 | 0.09 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3586 | 1/1   | 0.92 | 0.25 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1609 | 1/1   | 0.92 | 0.30 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3408 | 1/1   | 0.92 | 0.08 | 75,75,75,75                 | 0     |
| 54  | MG   | CW    | 204  | 1/1   | 0.92 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1758 | 1/1   | 0.92 | 0.09 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1608 | 1/1   | 0.92 | 0.11 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3742 | 1/1   | 0.92 | 0.10 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3026 | 1/1   | 0.92 | 0.21 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 2974 | 1/1   | 0.92 | 0.25 | 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   | DA    | 3031 | 1/1   | 0.92 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3119 | 1/1   | 0.92 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3183 | 1/1   | 0.92 | 0.23 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1785 | 1/1   | 0.92 | 0.09 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1614 | 1/1   | 0.92 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 2930 | 1/1   | 0.92 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | CA    | 1931 | 1/1   | 0.92 | 0.08 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 2932 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | DA    | 3042 | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1766 | 1/1   | 0.92 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3172 | 1/1   | 0.92 | 0.22 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3759 | 1/1   | 0.92 | 0.10 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3331 | 1/1   | 0.92 | 0.11 | 70,70,70,70                 | 0     |
| 54  | MG   | CA    | 1851 | 1/1   | 0.92 | 0.18 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3073 | 1/1   | 0.92 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3055 | 1/1   | 0.92 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1848 | 1/1   | 0.92 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | AA    | 1873 | 1/1   | 0.92 | 0.06 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3058 | 1/1   | 0.92 | 0.26 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 2944 | 1/1   | 0.92 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 3060 | 1/1   | 0.92 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | BB    | 219  | 1/1   | 0.92 | 0.06 | 124,124,124,124             | 0     |
| 54  | MG   | DA    | 3206 | 1/1   | 0.92 | 0.20 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1702 | 1/1   | 0.92 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3180 | 1/1   | 0.92 | 0.23 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1692 | 1/1   | 0.92 | 0.13 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3182 | 1/1   | 0.92 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1630 | 1/1   | 0.92 | 0.22 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3215 | 1/1   | 0.92 | 0.23 | 58,58,58,58                 | 0     |
| 54  | MG   | AA    | 2008 | 1/1   | 0.92 | 0.12 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3632 | 1/1   | 0.92 | 0.07 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3074 | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 2949 | 1/1   | 0.92 | 0.28 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3638 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | CD    | 117  | 1/1   | 0.92 | 0.05 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 2950 | 1/1   | 0.92 | 0.13 | 29,29,29,29                 | 0     |
| 54  | MG   | AA    | 2010 | 1/1   | 0.92 | 0.16 | 83,83,83,83                 | 0     |
| 54  | MG   | BD    | 301  | 1/1   | 0.92 | 0.28 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3087 | 1/1   | 0.92 | 0.19 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3367 | 1/1   | 0.92 | 0.07 | 60,60,60,60                 | 0     |
| 54  | MG   | AA    | 1667 | 1/1   | 0.92 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1873 | 1/1   | 0.92 | 0.05 | 117,117,117,117             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3648 | 1/1   | 0.92 | 0.12 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3304 | 1/1   | 0.92 | 0.06 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3249 | 1/1   | 0.92 | 0.25 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1777 | 1/1   | 0.92 | 0.18 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3190 | 1/1   | 0.92 | 0.22 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1646 | 1/1   | 0.92 | 0.05 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3375 | 1/1   | 0.92 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | BF    | 301  | 1/1   | 0.92 | 0.15 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 2918 | 1/1   | 0.92 | 0.25 | 28,28,28,28                 | 0     |
| 54  | MG   | DA    | 3239 | 1/1   | 0.92 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3003 | 1/1   | 0.92 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3380 | 1/1   | 0.92 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1725 | 1/1   | 0.92 | 0.24 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3560 | 1/1   | 0.92 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3244 | 1/1   | 0.92 | 0.26 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1885 | 1/1   | 0.92 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3522 | 1/1   | 0.92 | 0.06 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 2935 | 1/1   | 0.92 | 0.14 | 33,33,33,33                 | 0     |
| 54  | MG   | CA    | 1802 | 1/1   | 0.92 | 0.15 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3004 | 1/1   | 0.92 | 0.10 | 30,30,30,30                 | 0     |
| 54  | MG   | DA    | 3108 | 1/1   | 0.92 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3258 | 1/1   | 0.92 | 0.06 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3395 | 1/1   | 0.92 | 0.12 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 2945 | 1/1   | 0.92 | 0.26 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3005 | 1/1   | 0.92 | 0.27 | 70,70,70,70                 | 0     |
| 54  | MG   | BO    | 201  | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3113 | 1/1   | 0.92 | 0.16 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3316 | 1/1   | 0.92 | 0.26 | 110,110,110,110             | 0     |
| 54  | MG   | CA    | 1891 | 1/1   | 0.92 | 0.05 | 113,113,113,113             | 0     |
| 54  | MG   | BA    | 3097 | 1/1   | 0.92 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3385 | 1/1   | 0.92 | 0.25 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3053 | 1/1   | 0.92 | 0.19 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 3695 | 1/1   | 0.92 | 0.06 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3545 | 1/1   | 0.92 | 0.26 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3547 | 1/1   | 0.92 | 0.13 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 2957 | 1/1   | 0.92 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3202 | 1/1   | 0.92 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3389 | 1/1   | 0.92 | 0.08 | 89,89,89,89                 | 0     |
| 54  | MG   | BA    | 3513 | 1/1   | 0.92 | 0.16 | 77,77,77,77                 | 0     |
| 54  | MG   | DO    | 202  | 1/1   | 0.92 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | CA    | 1816 | 1/1   | 0.92 | 0.20 | 65,65,65,65                 | 0     |
| 54  | MG   | DO    | 204  | 1/1   | 0.92 | 0.15 | 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   | DA    | 2982 | 1/1   | 0.92 | 0.20 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 2958 | 1/1   | 0.92 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 2988 | 1/1   | 0.92 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3322 | 1/1   | 0.92 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3103 | 1/1   | 0.92 | 0.18 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1877 | 1/1   | 0.92 | 0.19 | 80,80,80,80                 | 0     |
| 54  | MG   | AC    | 104  | 1/1   | 0.92 | 0.06 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 3058 | 1/1   | 0.92 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3289 | 1/1   | 0.92 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1672 | 1/1   | 0.92 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1659 | 1/1   | 0.92 | 0.10 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3215 | 1/1   | 0.92 | 0.19 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3428 | 1/1   | 0.92 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3005 | 1/1   | 0.92 | 0.32 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1673 | 1/1   | 0.92 | 0.18 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3296 | 1/1   | 0.92 | 0.30 | 82,82,82,82                 | 0     |
| 54  | MG   | BA    | 3157 | 1/1   | 0.92 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | D3    | 102  | 1/1   | 0.92 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3152 | 1/1   | 0.92 | 0.16 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3726 | 1/1   | 0.92 | 0.14 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3153 | 1/1   | 0.92 | 0.16 | 51,51,51,51                 | 0     |
| 54  | MG   | DW    | 101  | 1/1   | 0.92 | 0.15 | 75,75,75,75                 | 0     |
| 54  | MG   | DW    | 102  | 1/1   | 0.92 | 0.17 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1665 | 1/1   | 0.92 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3528 | 1/1   | 0.92 | 0.07 | 88,88,88,88                 | 0     |
| 54  | MG   | BB    | 203  | 1/1   | 0.92 | 0.07 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1697 | 1/1   | 0.92 | 0.08 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3029 | 1/1   | 0.93 | 0.16 | 34,34,34,34                 | 0     |
| 54  | MG   | DA    | 3030 | 1/1   | 0.93 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3078 | 1/1   | 0.93 | 0.23 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1780 | 1/1   | 0.93 | 0.13 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 2960 | 1/1   | 0.93 | 0.11 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3170 | 1/1   | 0.93 | 0.16 | 31,31,31,31                 | 0     |
| 54  | MG   | DA    | 3308 | 1/1   | 0.93 | 0.22 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3172 | 1/1   | 0.93 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3309 | 1/1   | 0.93 | 0.05 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3035 | 1/1   | 0.93 | 0.21 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1962 | 1/1   | 0.93 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1636 | 1/1   | 0.93 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1943 | 1/1   | 0.93 | 0.06 | 110,110,110,110             | 0     |
| 54  | MG   | BA    | 3371 | 1/1   | 0.93 | 0.08 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3311 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3048 | 1/1   | 0.93 | 0.04 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 2928 | 1/1   | 0.93 | 0.17 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3050 | 1/1   | 0.93 | 0.28 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1854 | 1/1   | 0.93 | 0.11 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3190 | 1/1   | 0.93 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3600 | 1/1   | 0.93 | 0.23 | 107,107,107,107             | 0     |
| 54  | MG   | AA    | 1700 | 1/1   | 0.93 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3174 | 1/1   | 0.93 | 0.26 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1721 | 1/1   | 0.93 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3330 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3564 | 1/1   | 0.93 | 0.09 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3608 | 1/1   | 0.93 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3175 | 1/1   | 0.93 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3333 | 1/1   | 0.93 | 0.09 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3088 | 1/1   | 0.93 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3200 | 1/1   | 0.93 | 0.23 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1650 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3443 | 1/1   | 0.93 | 0.04 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3444 | 1/1   | 0.93 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3065 | 1/1   | 0.93 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | BA    | 2970 | 1/1   | 0.93 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | CA    | 1881 | 1/1   | 0.93 | 0.06 | 105,105,105,105             | 0     |
| 54  | MG   | DA    | 3476 | 1/1   | 0.93 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3069 | 1/1   | 0.93 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3224 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 2907 | 1/1   | 0.93 | 0.18 | 23,23,23,23                 | 0     |
| 54  | MG   | BA    | 3323 | 1/1   | 0.93 | 0.05 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3782 | 1/1   | 0.93 | 0.13 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3483 | 1/1   | 0.93 | 0.13 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3484 | 1/1   | 0.93 | 0.19 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 2911 | 1/1   | 0.93 | 0.27 | 34,34,34,34                 | 0     |
| 54  | MG   | DA    | 3786 | 1/1   | 0.93 | 0.08 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3076 | 1/1   | 0.93 | 0.12 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3178 | 1/1   | 0.93 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3633 | 1/1   | 0.93 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | BU    | 201  | 1/1   | 0.93 | 0.34 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1981 | 1/1   | 0.93 | 0.05 | 115,115,115,115             | 0     |
| 54  | MG   | DA    | 3637 | 1/1   | 0.93 | 0.12 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3083 | 1/1   | 0.93 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1721 | 1/1   | 0.93 | 0.29 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3796 | 1/1   | 0.93 | 0.11 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3494 | 1/1   | 0.93 | 0.06 | 110,110,110,110             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3221 | 1/1   | 0.93 | 0.16 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1966 | 1/1   | 0.93 | 0.10 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 2922 | 1/1   | 0.93 | 0.16 | 17,17,17,17                 | 0     |
| 54  | MG   | BA    | 2936 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3366 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 1790 | 1/1   | 0.93 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | CA    | 1812 | 1/1   | 0.93 | 0.15 | 86,86,86,86                 | 0     |
| 54  | MG   | BA    | 2942 | 1/1   | 0.93 | 0.27 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 2939 | 1/1   | 0.93 | 0.26 | 45,45,45,45                 | 0     |
| 54  | MG   | CA    | 1894 | 1/1   | 0.93 | 0.08 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3507 | 1/1   | 0.93 | 0.12 | 86,86,86,86                 | 0     |
| 54  | MG   | AW    | 202  | 1/1   | 0.93 | 0.11 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3339 | 1/1   | 0.93 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3511 | 1/1   | 0.93 | 0.14 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3658 | 1/1   | 0.93 | 0.31 | 88,88,88,88                 | 0     |
| 54  | MG   | DA    | 2948 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3099 | 1/1   | 0.93 | 0.29 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3662 | 1/1   | 0.93 | 0.11 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3100 | 1/1   | 0.93 | 0.06 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3282 | 1/1   | 0.93 | 0.10 | 103,103,103,103             | 0     |
| 54  | MG   | AA    | 1658 | 1/1   | 0.93 | 0.13 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1743 | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1979 | 1/1   | 0.93 | 0.06 | 104,104,104,104             | 0     |
| 54  | MG   | DA    | 3245 | 1/1   | 0.93 | 0.11 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3022 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | BA    | 3024 | 1/1   | 0.93 | 0.26 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3674 | 1/1   | 0.93 | 0.10 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3524 | 1/1   | 0.93 | 0.18 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1601 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 54  | MG   | CA    | 1823 | 1/1   | 0.93 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3680 | 1/1   | 0.93 | 0.07 | 75,75,75,75                 | 0     |
| 54  | MG   | DB    | 226  | 1/1   | 0.93 | 0.12 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 2970 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3257 | 1/1   | 0.93 | 0.22 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 2945 | 1/1   | 0.93 | 0.18 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3346 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 54  | MG   | DE    | 301  | 1/1   | 0.93 | 0.20 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 3533 | 1/1   | 0.93 | 0.07 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3404 | 1/1   | 0.93 | 0.06 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1752 | 1/1   | 0.93 | 0.16 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 2984 | 1/1   | 0.93 | 0.26 | 46,46,46,46                 | 0     |
| 54  | MG   | BA    | 3111 | 1/1   | 0.93 | 0.15 | 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   | BA    | 3243 | 1/1   | 0.93 | 0.05 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3351 | 1/1   | 0.93 | 0.04 | 69,69,69,69                 | 0     |
| 54  | MG   | CA    | 1611 | 1/1   | 0.93 | 0.22 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 2992 | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1613 | 1/1   | 0.93 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3353 | 1/1   | 0.93 | 0.16 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3354 | 1/1   | 0.93 | 0.06 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1838 | 1/1   | 0.93 | 0.22 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3113 | 1/1   | 0.93 | 0.16 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1739 | 1/1   | 0.93 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | CT    | 201  | 1/1   | 0.93 | 0.06 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1618 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | AA    | 1862 | 1/1   | 0.93 | 0.12 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1991 | 1/1   | 0.93 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3009 | 1/1   | 0.93 | 0.17 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 2952 | 1/1   | 0.93 | 0.17 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 3481 | 1/1   | 0.93 | 0.07 | 80,80,80,80                 | 0     |
| 54  | MG   | CA    | 1623 | 1/1   | 0.93 | 0.31 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3420 | 1/1   | 0.93 | 0.07 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3013 | 1/1   | 0.93 | 0.21 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3291 | 1/1   | 0.93 | 0.28 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3482 | 1/1   | 0.93 | 0.06 | 101,101,101,101             | 0     |
| 54  | MG   | AA    | 1796 | 1/1   | 0.93 | 0.16 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3420 | 1/1   | 0.93 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3155 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 54  | MG   | CC    | 104  | 1/1   | 0.93 | 0.11 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3571 | 1/1   | 0.93 | 0.16 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1889 | 1/1   | 0.93 | 0.11 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3487 | 1/1   | 0.93 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1807 | 1/1   | 0.93 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | AA    | 1688 | 1/1   | 0.93 | 0.14 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 2996 | 1/1   | 0.94 | 0.25 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3418 | 1/1   | 0.94 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1946 | 1/1   | 0.94 | 0.13 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 2998 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3410 | 1/1   | 0.94 | 0.13 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1630 | 1/1   | 0.94 | 0.30 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3131 | 1/1   | 0.94 | 0.21 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3538 | 1/1   | 0.94 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 2989 | 1/1   | 0.94 | 0.26 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1843 | 1/1   | 0.94 | 0.07 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1707 | 1/1   | 0.94 | 0.13 | 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   | BA    | 3259 | 1/1   | 0.94 | 0.07 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3432 | 1/1   | 0.94 | 0.19 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1751 | 1/1   | 0.94 | 0.17 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3138 | 1/1   | 0.94 | 0.26 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3083 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | AH    | 202  | 1/1   | 0.94 | 0.08 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3144 | 1/1   | 0.94 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 3744 | 1/1   | 0.94 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 2939 | 1/1   | 0.94 | 0.34 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 2965 | 1/1   | 0.94 | 0.05 | 30,30,30,30                 | 0     |
| 54  | MG   | BA    | 3313 | 1/1   | 0.94 | 0.08 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1837 | 1/1   | 0.94 | 0.06 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1777 | 1/1   | 0.94 | 0.24 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1632 | 1/1   | 0.94 | 0.22 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3269 | 1/1   | 0.94 | 0.06 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3154 | 1/1   | 0.94 | 0.25 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3753 | 1/1   | 0.94 | 0.22 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3225 | 1/1   | 0.94 | 0.06 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3427 | 1/1   | 0.94 | 0.11 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3599 | 1/1   | 0.94 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3157 | 1/1   | 0.94 | 0.10 | 51,51,51,51                 | 0     |
| 54  | MG   | CA    | 1783 | 1/1   | 0.94 | 0.15 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3155 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | CD    | 105  | 1/1   | 0.94 | 0.04 | 124,124,124,124             | 0     |
| 54  | MG   | DA    | 3763 | 1/1   | 0.94 | 0.09 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3187 | 1/1   | 0.94 | 0.03 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3431 | 1/1   | 0.94 | 0.09 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1639 | 1/1   | 0.94 | 0.12 | 42,42,42,42                 | 0     |
| 54  | MG   | CA    | 1865 | 1/1   | 0.94 | 0.08 | 85,85,85,85                 | 0     |
| 54  | MG   | BA    | 2915 | 1/1   | 0.94 | 0.14 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1867 | 1/1   | 0.94 | 0.22 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3036 | 1/1   | 0.94 | 0.22 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3374 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | AA    | 1988 | 1/1   | 0.94 | 0.07 | 93,93,93,93                 | 0     |
| 54  | MG   | DA    | 3177 | 1/1   | 0.94 | 0.19 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 3040 | 1/1   | 0.94 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 2917 | 1/1   | 0.94 | 0.21 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3231 | 1/1   | 0.94 | 0.08 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3621 | 1/1   | 0.94 | 0.05 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3325 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3498 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3045 | 1/1   | 0.94 | 0.27 | 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   | DA    | 3047 | 1/1   | 0.94 | 0.20 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3033 | 1/1   | 0.94 | 0.15 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3193 | 1/1   | 0.94 | 0.21 | 80,80,80,80                 | 0     |
| 54  | MG   | AA    | 2009 | 1/1   | 0.94 | 0.09 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3051 | 1/1   | 0.94 | 0.06 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 3327 | 1/1   | 0.94 | 0.10 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3479 | 1/1   | 0.94 | 0.06 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3334 | 1/1   | 0.94 | 0.16 | 45,45,45,45                 | 0     |
| 54  | MG   | CA    | 1799 | 1/1   | 0.94 | 0.16 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3192 | 1/1   | 0.94 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1618 | 1/1   | 0.94 | 0.22 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3331 | 1/1   | 0.94 | 0.28 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 2904 | 1/1   | 0.94 | 0.15 | 22,22,22,22                 | 0     |
| 54  | MG   | DA    | 2906 | 1/1   | 0.94 | 0.17 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 3197 | 1/1   | 0.94 | 0.20 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3198 | 1/1   | 0.94 | 0.06 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3199 | 1/1   | 0.94 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3333 | 1/1   | 0.94 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 2910 | 1/1   | 0.94 | 0.20 | 25,25,25,25                 | 0     |
| 54  | MG   | BA    | 3508 | 1/1   | 0.94 | 0.04 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 2912 | 1/1   | 0.94 | 0.23 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 3352 | 1/1   | 0.94 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3067 | 1/1   | 0.94 | 0.18 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 2901 | 1/1   | 0.94 | 0.08 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1936 | 1/1   | 0.94 | 0.09 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3070 | 1/1   | 0.94 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3210 | 1/1   | 0.94 | 0.21 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3071 | 1/1   | 0.94 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3657 | 1/1   | 0.94 | 0.20 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3337 | 1/1   | 0.94 | 0.10 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1809 | 1/1   | 0.94 | 0.14 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3338 | 1/1   | 0.94 | 0.07 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1970 | 1/1   | 0.94 | 0.16 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 2926 | 1/1   | 0.94 | 0.10 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 2927 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3392 | 1/1   | 0.94 | 0.04 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3667 | 1/1   | 0.94 | 0.21 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3080 | 1/1   | 0.94 | 0.05 | 23,23,23,23                 | 0     |
| 54  | MG   | CA    | 1972 | 1/1   | 0.94 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3168 | 1/1   | 0.94 | 0.21 | 65,65,65,65                 | 0     |
| 54  | MG   | CA    | 1893 | 1/1   | 0.94 | 0.10 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3672 | 1/1   | 0.94 | 0.27 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 2940 | 1/1   | 0.94 | 0.19 | 25,25,25,25                 | 0     |
| 54  | MG   | BA    | 3203 | 1/1   | 0.94 | 0.26 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3225 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 2943 | 1/1   | 0.94 | 0.20 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 3395 | 1/1   | 0.94 | 0.07 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3678 | 1/1   | 0.94 | 0.08 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3134 | 1/1   | 0.94 | 0.24 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3397 | 1/1   | 0.94 | 0.22 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3011 | 1/1   | 0.94 | 0.14 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3460 | 1/1   | 0.94 | 0.06 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1671 | 1/1   | 0.94 | 0.10 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3383 | 1/1   | 0.94 | 0.07 | 32,32,32,32                 | 0     |
| 54  | MG   | BA    | 2927 | 1/1   | 0.94 | 0.23 | 32,32,32,32                 | 0     |
| 54  | MG   | DH    | 204  | 1/1   | 0.94 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | DO    | 201  | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1656 | 1/1   | 0.94 | 0.07 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 2959 | 1/1   | 0.94 | 0.14 | 26,26,26,26                 | 0     |
| 54  | MG   | DA    | 2960 | 1/1   | 0.94 | 0.18 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1905 | 1/1   | 0.94 | 0.04 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3390 | 1/1   | 0.94 | 0.24 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3102 | 1/1   | 0.94 | 0.18 | 49,49,49,49                 | 0     |
| 54  | MG   | CH    | 202  | 1/1   | 0.94 | 0.13 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3541 | 1/1   | 0.94 | 0.21 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3294 | 1/1   | 0.94 | 0.19 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3295 | 1/1   | 0.94 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3700 | 1/1   | 0.94 | 0.10 | 75,75,75,75                 | 0     |
| 54  | MG   | CA    | 1610 | 1/1   | 0.94 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3296 | 1/1   | 0.94 | 0.05 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 2980 | 1/1   | 0.94 | 0.27 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3549 | 1/1   | 0.94 | 0.37 | 70,70,70,70                 | 0     |
| 54  | MG   | DT    | 101  | 1/1   | 0.94 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3255 | 1/1   | 0.94 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | CA    | 1679 | 1/1   | 0.94 | 0.10 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 2002 | 1/1   | 0.94 | 0.07 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1681 | 1/1   | 0.94 | 0.17 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3260 | 1/1   | 0.94 | 0.05 | 53,53,53,53                 | 0     |
| 54  | MG   | D3    | 101  | 1/1   | 0.94 | 0.19 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3112 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1755 | 1/1   | 0.94 | 0.20 | 70,70,70,70                 | 0     |
| 54  | MG   | CQ    | 101  | 1/1   | 0.94 | 0.08 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3531 | 1/1   | 0.94 | 0.14 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3350 | 1/1   | 0.94 | 0.08 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3211 | 1/1   | 0.94 | 0.04 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 3119 | 1/1   | 0.94 | 0.30 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 2984 | 1/1   | 0.94 | 0.13 | 48,48,48,48                 | 0     |
| 54  | MG   | D7    | 101  | 1/1   | 0.94 | 0.24 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3121 | 1/1   | 0.94 | 0.05 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 2994 | 1/1   | 0.94 | 0.18 | 37,37,37,37                 | 0     |
| 54  | MG   | CA    | 1940 | 1/1   | 0.95 | 0.06 | 112,112,112,112             | 0     |
| 54  | MG   | DA    | 3777 | 1/1   | 0.95 | 0.06 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3104 | 1/1   | 0.95 | 0.19 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 2908 | 1/1   | 0.95 | 0.05 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 2920 | 1/1   | 0.95 | 0.19 | 36,36,36,36                 | 0     |
| 54  | MG   | BA    | 3107 | 1/1   | 0.95 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1836 | 1/1   | 0.95 | 0.22 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3469 | 1/1   | 0.95 | 0.13 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3015 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 3208 | 1/1   | 0.95 | 0.12 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3542 | 1/1   | 0.95 | 0.05 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3288 | 1/1   | 0.95 | 0.06 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3679 | 1/1   | 0.95 | 0.07 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1757 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3021 | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3023 | 1/1   | 0.95 | 0.13 | 28,28,28,28                 | 0     |
| 54  | MG   | AA    | 1745 | 1/1   | 0.95 | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | BA    | 3141 | 1/1   | 0.95 | 0.17 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 2938 | 1/1   | 0.95 | 0.15 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3585 | 1/1   | 0.95 | 0.06 | 114,114,114,114             | 0     |
| 54  | MG   | BA    | 3023 | 1/1   | 0.95 | 0.25 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3482 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1703 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3388 | 1/1   | 0.95 | 0.05 | 37,37,37,37                 | 0     |
| 54  | MG   | CA    | 1796 | 1/1   | 0.95 | 0.05 | 35,35,35,35                 | 0     |
| 54  | MG   | BA    | 2955 | 1/1   | 0.95 | 0.23 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 2976 | 1/1   | 0.95 | 0.13 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3028 | 1/1   | 0.95 | 0.12 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1602 | 1/1   | 0.95 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 2944 | 1/1   | 0.95 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | BA    | 2956 | 1/1   | 0.95 | 0.11 | 38,38,38,38                 | 0     |
| 54  | MG   | CC    | 106  | 1/1   | 0.95 | 0.04 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 2926 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3466 | 1/1   | 0.95 | 0.04 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3467 | 1/1   | 0.95 | 0.09 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3059 | 1/1   | 0.95 | 0.20 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3044 | 1/1   | 0.95 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3128 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3153 | 1/1   | 0.95 | 0.29 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3426 | 1/1   | 0.95 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 3408 | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 2957 | 1/1   | 0.95 | 0.18 | 20,20,20,20                 | 0     |
| 54  | MG   | BA    | 2980 | 1/1   | 0.95 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | CD    | 102  | 1/1   | 0.95 | 0.07 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3516 | 1/1   | 0.95 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 2964 | 1/1   | 0.95 | 0.09 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3305 | 1/1   | 0.95 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3429 | 1/1   | 0.95 | 0.09 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3324 | 1/1   | 0.95 | 0.12 | 34,34,34,34                 | 0     |
| 54  | MG   | DA    | 2968 | 1/1   | 0.95 | 0.14 | 20,20,20,20                 | 0     |
| 54  | MG   | DA    | 3619 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 2969 | 1/1   | 0.95 | 0.28 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 3143 | 1/1   | 0.95 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1836 | 1/1   | 0.95 | 0.07 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3234 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3729 | 1/1   | 0.95 | 0.12 | 73,73,73,73                 | 0     |
| 54  | MG   | DD    | 302  | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 2973 | 1/1   | 0.95 | 0.18 | 24,24,24,24                 | 0     |
| 54  | MG   | DA    | 3236 | 1/1   | 0.95 | 0.24 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3090 | 1/1   | 0.95 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 2039 | 1/1   | 0.95 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1617 | 1/1   | 0.95 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3271 | 1/1   | 0.95 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1768 | 1/1   | 0.95 | 0.15 | 52,52,52,52                 | 0     |
| 54  | MG   | DH    | 203  | 1/1   | 0.95 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3009 | 1/1   | 0.95 | 0.18 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 2985 | 1/1   | 0.95 | 0.14 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 3634 | 1/1   | 0.95 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3434 | 1/1   | 0.95 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | CA    | 1872 | 1/1   | 0.95 | 0.22 | 84,84,84,84                 | 0     |
| 54  | MG   | CA    | 1819 | 1/1   | 0.95 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3126 | 1/1   | 0.95 | 0.05 | 42,42,42,42                 | 0     |
| 54  | MG   | CD    | 118  | 1/1   | 0.95 | 0.05 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3250 | 1/1   | 0.95 | 0.15 | 44,44,44,44                 | 0     |
| 54  | MG   | D0    | 205  | 1/1   | 0.95 | 0.15 | 95,95,95,95                 | 0     |
| 54  | MG   | CA    | 1982 | 1/1   | 0.95 | 0.04 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3194 | 1/1   | 0.95 | 0.15 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1691 | 1/1   | 0.95 | 0.20 | 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   | DA    | 2995 | 1/1   | 0.95 | 0.21 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3355 | 1/1   | 0.95 | 0.13 | 64,64,64,64                 | 0     |
| 54  | MG   | D1    | 204  | 1/1   | 0.95 | 0.19 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 2986 | 1/1   | 0.95 | 0.16 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3546 | 1/1   | 0.95 | 0.24 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3649 | 1/1   | 0.95 | 0.12 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3038 | 1/1   | 0.95 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3163 | 1/1   | 0.95 | 0.05 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3000 | 1/1   | 0.95 | 0.16 | 31,31,31,31                 | 0     |
| 54  | MG   | DA    | 3086 | 1/1   | 0.95 | 0.12 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3760 | 1/1   | 0.95 | 0.06 | 206,206,206,206             | 0     |
| 54  | MG   | DA    | 3358 | 1/1   | 0.95 | 0.22 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 2901 | 1/1   | 0.95 | 0.18 | 28,28,28,28                 | 0     |
| 54  | MG   | BA    | 3165 | 1/1   | 0.95 | 0.05 | 46,46,46,46                 | 0     |
| 54  | MG   | D3    | 103  | 1/1   | 0.95 | 0.05 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3362 | 1/1   | 0.95 | 0.15 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 2903 | 1/1   | 0.95 | 0.23 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 2963 | 1/1   | 0.95 | 0.13 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3181 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 2905 | 1/1   | 0.95 | 0.21 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3663 | 1/1   | 0.95 | 0.08 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3459 | 1/1   | 0.95 | 0.05 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1984 | 1/1   | 0.95 | 0.06 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3272 | 1/1   | 0.95 | 0.21 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 2931 | 1/1   | 0.95 | 0.09 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 2902 | 1/1   | 0.96 | 0.09 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3039 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 2925 | 1/1   | 0.96 | 0.13 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 2950 | 1/1   | 0.96 | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1837 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3427 | 1/1   | 0.96 | 0.11 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 2993 | 1/1   | 0.96 | 0.21 | 52,52,52,52                 | 0     |
| 54  | MG   | AA    | 1683 | 1/1   | 0.96 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 2955 | 1/1   | 0.96 | 0.19 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3341 | 1/1   | 0.96 | 0.05 | 119,119,119,119             | 0     |
| 54  | MG   | BA    | 3164 | 1/1   | 0.96 | 0.10 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3229 | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3045 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 54  | MG   | BA    | 3197 | 1/1   | 0.96 | 0.09 | 103,103,103,103             | 0     |
| 54  | MG   | BA    | 3046 | 1/1   | 0.96 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 2963 | 1/1   | 0.96 | 0.22 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 2941 | 1/1   | 0.96 | 0.13 | 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   | BA    | 3075 | 1/1   | 0.96 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | BE    | 302  | 1/1   | 0.96 | 0.09 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3787 | 1/1   | 0.96 | 0.08 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1909 | 1/1   | 0.96 | 0.06 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1803 | 1/1   | 0.96 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | BE    | 305  | 1/1   | 0.96 | 0.09 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3566 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3344 | 1/1   | 0.96 | 0.10 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3242 | 1/1   | 0.96 | 0.09 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3346 | 1/1   | 0.96 | 0.06 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3561 | 1/1   | 0.96 | 0.22 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1737 | 1/1   | 0.96 | 0.04 | 132,132,132,132             | 0     |
| 54  | MG   | DA    | 3348 | 1/1   | 0.96 | 0.16 | 58,58,58,58                 | 0     |
| 54  | MG   | AC    | 108  | 1/1   | 0.96 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | CD    | 114  | 1/1   | 0.96 | 0.04 | 109,109,109,109             | 0     |
| 54  | MG   | BA    | 3140 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3239 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3068 | 1/1   | 0.96 | 0.21 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 2977 | 1/1   | 0.96 | 0.09 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3079 | 1/1   | 0.96 | 0.14 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3252 | 1/1   | 0.96 | 0.22 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3574 | 1/1   | 0.96 | 0.08 | 74,74,74,74                 | 0     |
| 54  | MG   | DB    | 202  | 1/1   | 0.96 | 0.06 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3253 | 1/1   | 0.96 | 0.19 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3158 | 1/1   | 0.96 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3025 | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3360 | 1/1   | 0.96 | 0.06 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3692 | 1/1   | 0.96 | 0.08 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3693 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3480 | 1/1   | 0.96 | 0.05 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1980 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 1791 | 1/1   | 0.96 | 0.04 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 2959 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | BA    | 3439 | 1/1   | 0.96 | 0.15 | 73,73,73,73                 | 0     |
| 54  | MG   | AA    | 1718 | 1/1   | 0.96 | 0.05 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3246 | 1/1   | 0.96 | 0.05 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3701 | 1/1   | 0.96 | 0.13 | 92,92,92,92                 | 0     |
| 54  | MG   | BA    | 3486 | 1/1   | 0.96 | 0.12 | 90,90,90,90                 | 0     |
| 54  | MG   | BA    | 3247 | 1/1   | 0.96 | 0.14 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3082 | 1/1   | 0.96 | 0.36 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3173 | 1/1   | 0.96 | 0.06 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3707 | 1/1   | 0.96 | 0.10 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3475 | 1/1   | 0.96 | 0.08 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3174 | 1/1   | 0.96 | 0.10 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3175 | 1/1   | 0.96 | 0.18 | 34,34,34,34                 | 0     |
| 54  | MG   | AA    | 1686 | 1/1   | 0.96 | 0.17 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3084 | 1/1   | 0.96 | 0.19 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3401 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | BA    | 2947 | 1/1   | 0.96 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | BA    | 2983 | 1/1   | 0.96 | 0.17 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 3277 | 1/1   | 0.96 | 0.20 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 2908 | 1/1   | 0.96 | 0.16 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3486 | 1/1   | 0.96 | 0.06 | 90,90,90,90                 | 0     |
| 54  | MG   | AA    | 1690 | 1/1   | 0.96 | 0.05 | 91,91,91,91                 | 0     |
| 54  | MG   | CA    | 1643 | 1/1   | 0.96 | 0.18 | 66,66,66,66                 | 0     |
| 54  | MG   | DG    | 202  | 1/1   | 0.96 | 0.10 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3721 | 1/1   | 0.96 | 0.06 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3282 | 1/1   | 0.96 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3364 | 1/1   | 0.96 | 0.06 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3010 | 1/1   | 0.96 | 0.18 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3093 | 1/1   | 0.96 | 0.23 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 2933 | 1/1   | 0.96 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3330 | 1/1   | 0.96 | 0.04 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3035 | 1/1   | 0.96 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3369 | 1/1   | 0.96 | 0.04 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3391 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 54  | MG   | B5    | 101  | 1/1   | 0.96 | 0.15 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3615 | 1/1   | 0.96 | 0.06 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3393 | 1/1   | 0.96 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 2922 | 1/1   | 0.96 | 0.19 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 2923 | 1/1   | 0.96 | 0.08 | 18,18,18,18                 | 0     |
| 54  | MG   | CA    | 1710 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3016 | 1/1   | 0.96 | 0.13 | 23,23,23,23                 | 0     |
| 54  | MG   | CA    | 1767 | 1/1   | 0.96 | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | CA    | 1884 | 1/1   | 0.96 | 0.06 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 2928 | 1/1   | 0.96 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | AA    | 1681 | 1/1   | 0.96 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 2932 | 1/1   | 0.96 | 0.15 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3022 | 1/1   | 0.96 | 0.20 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 2933 | 1/1   | 0.96 | 0.28 | 31,31,31,31                 | 0     |
| 54  | MG   | DT    | 102  | 1/1   | 0.96 | 0.21 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3372 | 1/1   | 0.96 | 0.19 | 53,53,53,53                 | 0     |
| 54  | MG   | CA    | 1654 | 1/1   | 0.96 | 0.07 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 2938 | 1/1   | 0.96 | 0.07 | 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   | DU    | 204  | 1/1   | 0.96 | 0.06 | 99,99,99,99                 | 0     |
| 54  | MG   | BA    | 3458 | 1/1   | 0.96 | 0.06 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3208 | 1/1   | 0.96 | 0.16 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3096 | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | CC    | 101  | 1/1   | 0.96 | 0.05 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 2942 | 1/1   | 0.96 | 0.15 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 3523 | 1/1   | 0.96 | 0.04 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 2969 | 1/1   | 0.96 | 0.24 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3525 | 1/1   | 0.96 | 0.15 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3552 | 1/1   | 0.96 | 0.18 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3260 | 1/1   | 0.96 | 0.31 | 77,77,77,77                 | 0     |
| 54  | MG   | D5    | 101  | 1/1   | 0.96 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 2946 | 1/1   | 0.96 | 0.23 | 40,40,40,40                 | 0     |
| 54  | MG   | BB    | 218  | 1/1   | 0.96 | 0.03 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3530 | 1/1   | 0.96 | 0.21 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3123 | 1/1   | 0.96 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3320 | 1/1   | 0.96 | 0.10 | 131,131,131,131             | 0     |
| 54  | MG   | DA    | 2958 | 1/1   | 0.97 | 0.08 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3025 | 1/1   | 0.97 | 0.12 | 25,25,25,25                 | 0     |
| 54  | MG   | DA    | 3312 | 1/1   | 0.97 | 0.06 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3289 | 1/1   | 0.97 | 0.26 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3027 | 1/1   | 0.97 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3001 | 1/1   | 0.97 | 0.13 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3504 | 1/1   | 0.97 | 0.04 | 115,115,115,115             | 0     |
| 54  | MG   | BA    | 2919 | 1/1   | 0.97 | 0.13 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 3085 | 1/1   | 0.97 | 0.04 | 40,40,40,40                 | 0     |
| 54  | MG   | AA    | 1778 | 1/1   | 0.97 | 0.04 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1712 | 1/1   | 0.97 | 0.06 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 2967 | 1/1   | 0.97 | 0.12 | 39,39,39,39                 | 0     |
| 54  | MG   | DB    | 210  | 1/1   | 0.97 | 0.06 | 114,114,114,114             | 0     |
| 54  | MG   | AA    | 1811 | 1/1   | 0.97 | 0.04 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1787 | 1/1   | 0.97 | 0.05 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3731 | 1/1   | 0.97 | 0.06 | 67,67,67,67                 | 0     |
| 54  | MG   | CA    | 1685 | 1/1   | 0.97 | 0.04 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3248 | 1/1   | 0.97 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 2971 | 1/1   | 0.97 | 0.22 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 2972 | 1/1   | 0.97 | 0.26 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 2913 | 1/1   | 0.97 | 0.22 | 30,30,30,30                 | 0     |
| 54  | MG   | DA    | 2914 | 1/1   | 0.97 | 0.13 | 19,19,19,19                 | 0     |
| 54  | MG   | DA    | 2975 | 1/1   | 0.97 | 0.09 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 2978 | 1/1   | 0.97 | 0.11 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3110 | 1/1   | 0.97 | 0.11 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1687 | 1/1   | 0.97 | 0.06 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3046 | 1/1   | 0.97 | 0.09 | 19,19,19,19                 | 0     |
| 54  | MG   | DA    | 3259 | 1/1   | 0.97 | 0.27 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3060 | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | BA    | 3047 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 3149 | 1/1   | 0.97 | 0.26 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 2921 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3340 | 1/1   | 0.97 | 0.08 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3252 | 1/1   | 0.97 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 3497 | 1/1   | 0.97 | 0.04 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3052 | 1/1   | 0.97 | 0.04 | 42,42,42,42                 | 0     |
| 54  | MG   | CA    | 1692 | 1/1   | 0.97 | 0.08 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3500 | 1/1   | 0.97 | 0.04 | 60,60,60,60                 | 0     |
| 54  | MG   | CD    | 101  | 1/1   | 0.97 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 2990 | 1/1   | 0.97 | 0.10 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 2925 | 1/1   | 0.97 | 0.25 | 38,38,38,38                 | 0     |
| 54  | MG   | CA    | 1853 | 1/1   | 0.97 | 0.08 | 101,101,101,101             | 0     |
| 54  | MG   | CA    | 1693 | 1/1   | 0.97 | 0.04 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3576 | 1/1   | 0.97 | 0.04 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3273 | 1/1   | 0.97 | 0.03 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 2929 | 1/1   | 0.97 | 0.15 | 24,24,24,24                 | 0     |
| 54  | MG   | DA    | 3129 | 1/1   | 0.97 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3510 | 1/1   | 0.97 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | CA    | 1773 | 1/1   | 0.97 | 0.04 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3431 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 2931 | 1/1   | 0.97 | 0.20 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3329 | 1/1   | 0.97 | 0.05 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3007 | 1/1   | 0.97 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 2934 | 1/1   | 0.97 | 0.10 | 22,22,22,22                 | 0     |
| 54  | MG   | CA    | 1902 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3602 | 1/1   | 0.97 | 0.06 | 116,116,116,116             | 0     |
| 54  | MG   | BA    | 3381 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 2937 | 1/1   | 0.97 | 0.15 | 25,25,25,25                 | 0     |
| 54  | MG   | BA    | 2985 | 1/1   | 0.97 | 0.04 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3286 | 1/1   | 0.97 | 0.24 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3779 | 1/1   | 0.97 | 0.07 | 72,72,72,72                 | 0     |
| 54  | MG   | CD    | 111  | 1/1   | 0.97 | 0.04 | 87,87,87,87                 | 0     |
| 54  | MG   | AA    | 1880 | 1/1   | 0.97 | 0.04 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3210 | 1/1   | 0.97 | 0.05 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3522 | 1/1   | 0.97 | 0.08 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3171 | 1/1   | 0.97 | 0.04 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3234 | 1/1   | 0.97 | 0.04 | 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   | DA    | 3147 | 1/1   | 0.97 | 0.08 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3212 | 1/1   | 0.97 | 0.13 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 2909 | 1/1   | 0.97 | 0.06 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3150 | 1/1   | 0.97 | 0.22 | 54,54,54,54                 | 0     |
| 54  | MG   | CD    | 119  | 1/1   | 0.97 | 0.05 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3527 | 1/1   | 0.97 | 0.06 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3098 | 1/1   | 0.97 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3300 | 1/1   | 0.97 | 0.06 | 28,28,28,28                 | 0     |
| 54  | MG   | AA    | 1626 | 1/1   | 0.97 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1709 | 1/1   | 0.97 | 0.09 | 58,58,58,58                 | 0     |
| 54  | MG   | CA    | 1640 | 1/1   | 0.97 | 0.05 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 2999 | 1/1   | 0.97 | 0.11 | 27,27,27,27                 | 0     |
| 54  | MG   | BA    | 3418 | 1/1   | 0.97 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | CA    | 1713 | 1/1   | 0.97 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3543 | 1/1   | 0.97 | 0.04 | 96,96,96,96                 | 0     |
| 54  | MG   | CA    | 1714 | 1/1   | 0.97 | 0.06 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3233 | 1/1   | 0.97 | 0.18 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3072 | 1/1   | 0.98 | 0.03 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1968 | 1/1   | 0.98 | 0.03 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3280 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3757 | 1/1   | 0.98 | 0.05 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3564 | 1/1   | 0.98 | 0.09 | 49,49,49,49                 | 0     |
| 54  | MG   | BE    | 303  | 1/1   | 0.98 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | AA    | 1660 | 1/1   | 0.98 | 0.06 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 2983 | 1/1   | 0.98 | 0.29 | 34,34,34,34                 | 0     |
| 54  | MG   | DA    | 3077 | 1/1   | 0.98 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1778 | 1/1   | 0.98 | 0.03 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3148 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 2968 | 1/1   | 0.98 | 0.05 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 3572 | 1/1   | 0.98 | 0.05 | 60,60,60,60                 | 0     |
| 54  | MG   | C1    | 101  | 1/1   | 0.98 | 0.05 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3452 | 1/1   | 0.98 | 0.03 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3017 | 1/1   | 0.98 | 0.20 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1856 | 1/1   | 0.98 | 0.03 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1677 | 1/1   | 0.98 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | DE    | 303  | 1/1   | 0.98 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | DA    | 3458 | 1/1   | 0.98 | 0.05 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1820 | 1/1   | 0.98 | 0.04 | 98,98,98,98                 | 0     |
| 54  | MG   | BA    | 3262 | 1/1   | 0.98 | 0.04 | 58,58,58,58                 | 0     |
| 54  | MG   | DA    | 3776 | 1/1   | 0.98 | 0.06 | 71,71,71,71                 | 0     |
| 54  | MG   | AA    | 1784 | 1/1   | 0.98 | 0.05 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1952 | 1/1   | 0.98 | 0.03 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3646 | 1/1   | 0.98 | 0.07 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3521 | 1/1   | 0.98 | 0.04 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3265 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3407 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3139 | 1/1   | 0.98 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3140 | 1/1   | 0.98 | 0.04 | 26,26,26,26                 | 0     |
| 54  | MG   | BA    | 3021 | 1/1   | 0.98 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | D0    | 201  | 1/1   | 0.98 | 0.11 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3040 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 54  | MG   | CA    | 1827 | 1/1   | 0.98 | 0.04 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3001 | 1/1   | 0.98 | 0.19 | 46,46,46,46                 | 0     |
| 54  | MG   | BA    | 2934 | 1/1   | 0.98 | 0.27 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3042 | 1/1   | 0.98 | 0.04 | 28,28,28,28                 | 0     |
| 54  | MG   | BA    | 3108 | 1/1   | 0.98 | 0.05 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 2916 | 1/1   | 0.98 | 0.16 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 3254 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3133 | 1/1   | 0.98 | 0.18 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 2914 | 1/1   | 0.98 | 0.12 | 17,17,17,17                 | 0     |
| 54  | MG   | DA    | 2961 | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | D1    | 206  | 1/1   | 0.98 | 0.06 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3303 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1815 | 1/1   | 0.98 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 2990 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 2975 | 1/1   | 0.98 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3604 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 3426 | 1/1   | 0.98 | 0.09 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3209 | 1/1   | 0.98 | 0.06 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3485 | 1/1   | 0.98 | 0.04 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1914 | 1/1   | 0.98 | 0.06 | 36,36,36,36                 | 0     |
| 54  | MG   | AA    | 1974 | 1/1   | 0.98 | 0.12 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 2962 | 1/1   | 0.98 | 0.09 | 20,20,20,20                 | 0     |
| 54  | MG   | DA    | 3062 | 1/1   | 0.98 | 0.18 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3160 | 1/1   | 0.98 | 0.03 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3219 | 1/1   | 0.98 | 0.04 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3192 | 1/1   | 0.98 | 0.04 | 54,54,54,54                 | 0     |
| 54  | MG   | AA    | 1943 | 1/1   | 0.98 | 0.06 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3312 | 1/1   | 0.98 | 0.05 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3091 | 1/1   | 0.98 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 2025 | 1/1   | 0.98 | 0.33 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3093 | 1/1   | 0.98 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 2976 | 1/1   | 0.98 | 0.19 | 31,31,31,31                 | 0     |
| 54  | MG   | BA    | 2940 | 1/1   | 0.98 | 0.19 | 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   | DA    | 3687 | 1/1   | 0.98 | 0.06 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3171 | 1/1   | 0.98 | 0.10 | 45,45,45,45                 | 0     |
| 55  | ZN   | AG    | 301  | 1/1   | 0.98 | 0.16 | 82,82,82,82                 | 0     |
| 55  | ZN   | CQ    | 104  | 1/1   | 0.98 | 0.03 | 142,142,142,142             | 0     |
| 54  | MG   | DA    | 3623 | 1/1   | 0.99 | 0.02 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3000 | 1/1   | 0.99 | 0.07 | 25,25,25,25                 | 0     |
| 54  | MG   | DA    | 3659 | 1/1   | 0.99 | 0.04 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 2986 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3053 | 1/1   | 0.99 | 0.04 | 28,28,28,28                 | 0     |
| 54  | MG   | DA    | 3180 | 1/1   | 0.99 | 0.03 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3425 | 1/1   | 0.99 | 0.02 | 98,98,98,98                 | 0     |
| 54  | MG   | DD    | 303  | 1/1   | 0.99 | 0.13 | 43,43,43,43                 | 0     |
| 54  | MG   | DA    | 2977 | 1/1   | 0.99 | 0.02 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3309 | 1/1   | 0.99 | 0.04 | 20,20,20,20                 | 0     |
| 54  | MG   | DA    | 3702 | 1/1   | 0.99 | 0.04 | 22,22,22,22                 | 0     |
| 54  | MG   | AA    | 1961 | 1/1   | 0.99 | 0.04 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3117 | 1/1   | 0.99 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3552 | 1/1   | 0.99 | 0.04 | 130,130,130,130             | 0     |
| 54  | MG   | CA    | 1900 | 1/1   | 0.99 | 0.03 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 2000 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3099 | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 2954 | 1/1   | 0.99 | 0.03 | 16,16,16,16                 | 0     |
| 54  | MG   | DA    | 3767 | 1/1   | 0.99 | 0.04 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3326 | 1/1   | 0.99 | 0.04 | 54,54,54,54                 | 0     |
| 55  | ZN   | AQ    | 102  | 1/1   | 0.99 | 0.04 | 142,142,142,142             | 0     |
| 55  | ZN   | CG    | 302  | 1/1   | 0.99 | 0.14 | 94,94,94,94                 | 0     |
| 54  | MG   | BA    | 3236 | 1/1   | 0.99 | 0.09 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3166 | 1/1   | 1.00 | 0.02 | 25,25,25,25                 | 0     |

## 5.5 Other polymers ⓘ

There are no such residues in this entry.