



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 02:31 PM EDT

PDB ID : 1VY5 / pdb\_00001vy5  
Title : Crystal structure of the Thermus thermophilus 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptidyl-tRNA in the A site and deacylated tRNA in the P site.  
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.  
Deposited on : 2014-05-13  
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

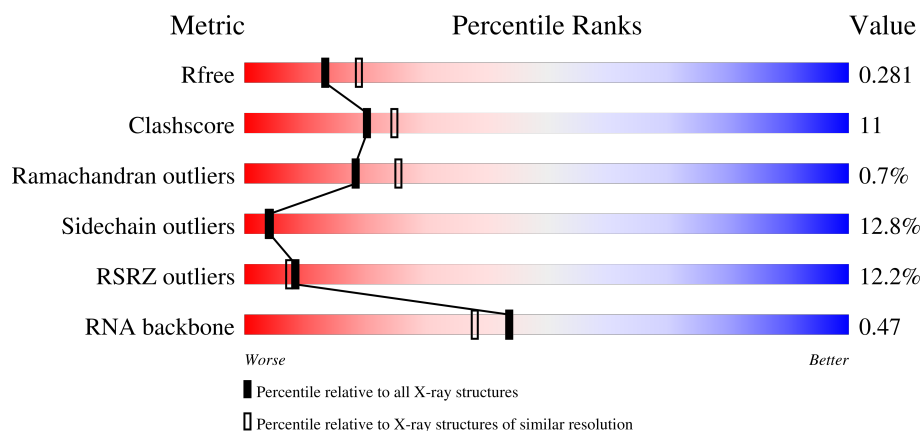
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1091 (2.54-2.54)                                      |
| Clashscore            | 190562                      | 1120 (2.54-2.54)                                      |
| Ramachandran outliers | 187476                      | 1106 (2.54-2.54)                                      |
| Sidechain outliers    | 187428                      | 1106 (2.54-2.54)                                      |
| RSRZ outliers         | 180081                      | 1091 (2.54-2.54)                                      |
| RNA backbone          | 3983                        | 1112 (2.80-2.28)                                      |

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

| Mol | Chain | Length | Quality of chain                                       |
|-----|-------|--------|--------------------------------------------------------|
| 1   | AA    | 1521   | <div> <div>5%</div> <div>51% 38% 9%</div> </div>       |
| 1   | CA    | 1521   | <div> <div>13%</div> <div>45% 43% 11%</div> </div>     |
| 2   | AB    | 256    | <div> <div>27%</div> <div>39% 41% 10% 10%</div> </div> |
| 2   | CB    | 256    | <div> <div>43%</div> <div>35% 41% 13% 10%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AC    | 239    |                  |
| 3   | CC    | 239    |                  |
| 4   | AD    | 209    |                  |
| 4   | CD    | 209    |                  |
| 5   | AE    | 162    |                  |
| 5   | CE    | 162    |                  |
| 6   | AF    | 101    |                  |
| 6   | CF    | 101    |                  |
| 7   | AG    | 156    |                  |
| 7   | CG    | 156    |                  |
| 8   | AH    | 138    |                  |
| 8   | CH    | 138    |                  |
| 9   | AI    | 128    |                  |
| 9   | CI    | 128    |                  |
| 10  | AJ    | 105    |                  |
| 10  | CJ    | 105    |                  |
| 11  | AK    | 129    |                  |
| 11  | CK    | 129    |                  |
| 12  | AL    | 132    |                  |
| 12  | CL    | 132    |                  |
| 13  | AM    | 126    |                  |
| 13  | CM    | 126    |                  |
| 14  | AN    | 61     |                  |
| 14  | CN    | 61     |                  |
| 15  | AO    | 89     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | CO    | 89     |                  |
| 16  | AP    | 88     |                  |
| 16  | CP    | 88     |                  |
| 17  | AQ    | 105    |                  |
| 17  | CQ    | 105    |                  |
| 18  | AR    | 88     |                  |
| 18  | CR    | 88     |                  |
| 19  | AS    | 93     |                  |
| 19  | CS    | 93     |                  |
| 20  | AT    | 106    |                  |
| 20  | CT    | 106    |                  |
| 21  | AU    | 27     |                  |
| 21  | CU    | 27     |                  |
| 22  | AV    | 24     |                  |
| 22  | CV    | 24     |                  |
| 23  | AW    | 76     |                  |
| 23  | CW    | 76     |                  |
| 24  | AX    | 77     |                  |
| 24  | CX    | 77     |                  |
| 25  | AY    | 76     |                  |
| 25  | CY    | 76     |                  |
| 26  | BA    | 2915   |                  |
| 26  | DA    | 2915   |                  |
| 27  | BB    | 121    |                  |
| 27  | DB    | 121    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BD    | 276    |                  |
| 28  | DD    | 276    |                  |
| 29  | BE    | 206    |                  |
| 29  | DE    | 206    |                  |
| 30  | BF    | 210    |                  |
| 30  | DF    | 210    |                  |
| 31  | BG    | 182    |                  |
| 31  | DG    | 182    |                  |
| 32  | BH    | 180    |                  |
| 32  | DH    | 180    |                  |
| 33  | BI    | 148    |                  |
| 33  | DI    | 148    |                  |
| 34  | BN    | 140    |                  |
| 34  | DN    | 140    |                  |
| 35  | BO    | 122    |                  |
| 35  | DO    | 122    |                  |
| 36  | BP    | 150    |                  |
| 36  | DP    | 150    |                  |
| 37  | BQ    | 141    |                  |
| 37  | DQ    | 141    |                  |
| 38  | BR    | 118    |                  |
| 38  | DR    | 118    |                  |
| 39  | BS    | 112    |                  |
| 39  | DS    | 112    |                  |
| 40  | BT    | 146    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | DT    | 146    |                  |
| 41  | BU    | 118    |                  |
| 41  | DU    | 118    |                  |
| 42  | BV    | 101    |                  |
| 42  | DV    | 101    |                  |
| 43  | BW    | 113    |                  |
| 43  | DW    | 113    |                  |
| 44  | BX    | 96     |                  |
| 44  | DX    | 96     |                  |
| 45  | BY    | 110    |                  |
| 45  | DY    | 110    |                  |
| 46  | BZ    | 206    |                  |
| 46  | DZ    | 206    |                  |
| 47  | B0    | 85     |                  |
| 47  | D0    | 85     |                  |
| 48  | B1    | 98     |                  |
| 48  | D1    | 98     |                  |
| 49  | B2    | 72     |                  |
| 49  | D2    | 72     |                  |
| 50  | B3    | 60     |                  |
| 50  | D3    | 60     |                  |
| 51  | B4    | 71     |                  |
| 51  | D4    | 71     |                  |
| 52  | B5    | 60     |                  |
| 52  | D5    | 60     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | B6    | 54     |                  |
| 53  | D6    | 54     |                  |
| 54  | B7    | 49     |                  |
| 54  | D7    | 49     |                  |
| 55  | B8    | 65     |                  |
| 55  | D8    | 65     |                  |
| 56  | B9    | 37     |                  |
| 56  | D9    | 37     |                  |

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297141 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 Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1498     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32205 | 14333 | 5970 | 10404 | 1498 |         |         |       |
| 1   | CA    | 1503     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32312 | 14381 | 5990 | 10438 | 1503 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1846  | 1179 | 331 | 331 | 5 |         |         |       |
| 2   | CB    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1167 | 326 | 327 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | AC    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 976 | 302 | 273 | 1 |         |         |       |
| 3   | CC    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1542  | 968 | 300 | 273 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1659  | 1040 | 326 | 286 | 7 |         |         |       |
| 4   | CD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1674  | 1050 | 333 | 284 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 213 | 198 | 4 |         |         |       |
| 5   | CE    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 511 | 143 | 149 | 3 |         |         |       |
| 6   | CF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1231  | 766 | 243 | 216 | 6 |         |         |       |
| 7   | CG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |
| 8   | CH    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 983   | 623 | 193 | 167 |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 978   | 619 | 190 | 169 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10  | AJ    | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 709   | 440 | 138 | 131 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 10  | CJ    | 96       | Total | C   | N   | O   |         |         |       |
|     |       |          | 714   | 445 | 138 | 131 | 0       | 0       | 0     |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 11  | AK    | 114      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 829   | 516 | 155 | 155 | 3       | 0       | 0     |
| 11  | CK    | 114      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 833   | 519 | 156 | 155 | 3       | 0       | 0     |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 12  | AL    | 122      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 930   | 585 | 185 | 159 | 1       | 0       | 0     |
| 12  | CL    | 122      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 930   | 585 | 185 | 159 | 1       | 0       | 0     |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 13  | AM    | 123      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 958   | 592 | 198 | 166 | 2       | 0       | 0     |
| 13  | CM    | 122      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 950   | 586 | 197 | 165 | 2       | 0       | 0     |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 728   | 456 | 144 | 126 | 2       | 0       | 0     |
| 15  | CO    | 88       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 728   | 456 | 144 | 126 | 2       | 0       | 0     |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 433 | 134 | 113 | 1 |         |         |       |
| 16  | CP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 677   | 430 | 133 | 113 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |
| 17  | CQ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AR    | 68       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |         |         |       |
| 18  | CR    | 68       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 652   | 417 | 120 | 113 | 2 |         |         |       |
| 19  | CS    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 646   | 412 | 119 | 113 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 446 | 156 | 124 | 2 |         |         |       |
| 20  | CT    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 446 | 155 | 124 | 2 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein Thx.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | AU    | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |
| 21  | CU    | 23       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |         |         |       |

- Molecule 22 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 22  | AV    | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 277   | 125 | 51 | 88 | 13 |         |         |       |
| 22  | CV    | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 252   | 115 | 46 | 80 | 11 |         |         |       |

- Molecule 23 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23  | AW    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1607  | 727 | 288 | 516 | 73 | 3 |         |         |       |
| 23  | CW    | 72       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1560  | 702 | 281 | 503 | 72 | 2 |         |         |       |

- Molecule 24 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 24  | AX    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1 |         |         |       |
| 24  | CX    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1 |         |         |       |

- Molecule 25 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 25  | AY    | 74       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1581  | 707 | 285 | 515 | 73 | 1 |         |         |       |
| 25  | CY    | 73       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1561  | 698 | 283 | 507 | 72 | 1 |         |         |       |

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26  | BA    | 2819     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60729 | 27026 | 11370 | 19515 | 2818 |         |         |       |

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| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 26  | DA    | 2800     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60311 | 26840 | 11284 | 19388 | 2799 |         |         |       |

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 27  | BB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |
| 27  | DB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28  | BD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |
| 28  | DD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |
| 29  | DE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30  | BF    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1584  | 1009 | 298 | 275 | 2 |         |         |       |
| 30  | DF    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1580  | 1007 | 297 | 274 | 2 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1425  | 914 | 256 | 251 | 4 |         |         |       |
| 31  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 911 | 258 | 251 | 4 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 32  | DH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1085  | 693 | 189 | 202 | 1 |         |         |       |
| 33  | DI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1061  | 680 | 186 | 194 | 1 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |
| 34  | DN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 35  | DO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BP    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |
| 36  | DP    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 37  | DQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 38  | DR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39  | BS    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |         |         |       |
| 39  | DS    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BT    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1091  | 680 | 225 | 185 | 1 |         |         |       |
| 40  | DT    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 675 | 224 | 183 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BU    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |
| 41  | DU    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | DV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BW    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |
| 43  | DW    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BX    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |
| 44  | DX    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |
| 45  | DY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BZ    | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1349  | 862 | 243 | 242 | 2 |         |         |       |
| 46  | DZ    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1360  | 870 | 243 | 245 | 2 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | B0    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 1 |         |         |       |
| 47  | D0    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 1 |         |         |       |



- Molecule 48 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | B1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |
| 48  | D1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | B2    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 49  | D2    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 50  | B3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 50  | D3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 464   | 296 | 90 | 78 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51  | B4    | 69       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 558   | 352 | 102 | 99 | 5 |         |         |       |
| 51  | D4    | 69       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 97  | 91 | 5 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |
| 52  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | B6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 53  | D6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 279 | 91 | 75 | 4 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | B7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 54  | D7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 55  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 511   | 328 | 99  | 82 | 2 |         |         |       |
| 55  | D8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 56  | B9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 56  | D9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | AA    | 214      | Total | Mg  | 0       | 0       |
|     |       |          | 214   | 214 |         |         |
| 57  | AE    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 57  | AF    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | AK    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | AM    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | AN    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | AW    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | AX    | 15       | Total<br>15  | Mg<br>15  | 0       | 0       |
| 57  | AY    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | BA    | 812      | Total<br>812 | Mg<br>812 | 0       | 0       |
| 57  | BB    | 20       | Total<br>20  | Mg<br>20  | 0       | 0       |
| 57  | BD    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 57  | BE    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 57  | BF    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 57  | BG    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | BN    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 57  | BO    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | BP    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | BQ    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | BR    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | BU    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 57  | BV    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | BW    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 57  | BX    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | BY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | BZ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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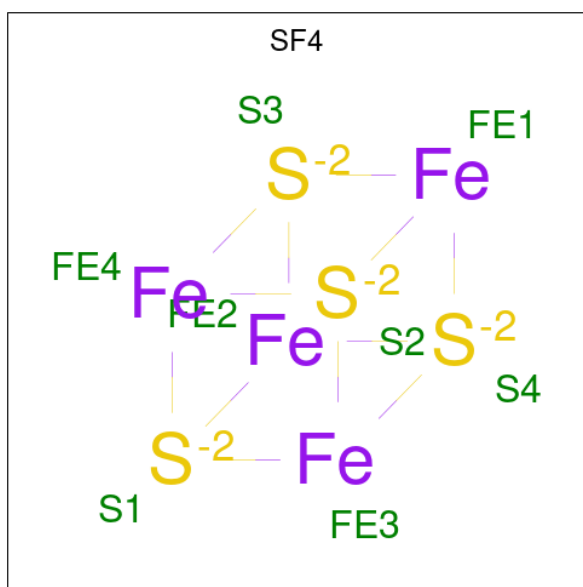
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57  | B0    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | B1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | B2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | B3    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | B4    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | B5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | B6    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 57  | B7    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 57  | B8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | B9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CA    | 170      | Total<br>170 | Mg<br>170 | 0       | 0       |
| 57  | CD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CK    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CV    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 57  | CX    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 57  | DA    | 677      | Total<br>677 | Mg<br>677 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 57  | DB    | 13       | Total<br>13 | Mg<br>13 | 0       | 0       |
| 57  | DD    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 57  | DE    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 57  | DF    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 57  | DG    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | DN    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | DO    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | DP    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 57  | DQ    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 57  | DR    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | DU    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 57  | DV    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 57  | DW    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 57  | DX    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | DY    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | D0    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | D3    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 57  | D8    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 58  | AD    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 58  | CD    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | AN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | BY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | B5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | B6    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | B9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | CN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | DY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | D4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 59  | D5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59  | D6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | D9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

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

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 60  | AX    | 1        | Total<br>1 | K<br>1 | 0       | 0       |
| 60  | CX    | 1        | Total<br>1 | K<br>1 | 0       | 0       |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61  | AA    | 227      | Total<br>227  | O<br>227  | 0       | 0       |
| 61  | AE    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | AJ    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | AL    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | AM    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | AU    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | AV    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | AW    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | AX    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 61  | AY    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | BA    | 1383     | Total<br>1383 | O<br>1383 | 0       | 0       |
| 61  | BB    | 36       | Total<br>36   | O<br>36   | 0       | 0       |
| 61  | BD    | 12       | Total<br>12   | O<br>12   | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 61  | BE    | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 61  | BF    | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 61  | BG    | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 61  | BI    | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 61  | BO    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 61  | BP    | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 61  | BQ    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 61  | BR    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 61  | BT    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 61  | BU    | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 61  | BV    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 61  | BW    | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 61  | BX    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 61  | BZ    | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 61  | B0    | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 61  | B1    | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 61  | B3    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 61  | B5    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 61  | B6    | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 61  | B7    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 61  | B8    | 8        | Total<br>8  | O<br>8  | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 61  | CA    | 185      | Total<br>185  | O<br>185  | 0       | 0       |
| 61  | CJ    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | CL    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | CT    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | CV    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | CW    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | DA    | 1025     | Total<br>1025 | O<br>1025 | 0       | 0       |
| 61  | DB    | 9        | Total<br>9    | O<br>9    | 0       | 0       |
| 61  | DD    | 19       | Total<br>19   | O<br>19   | 0       | 0       |
| 61  | DE    | 11       | Total<br>11   | O<br>11   | 0       | 0       |
| 61  | DF    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | DN    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | DO    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | DP    | 16       | Total<br>16   | O<br>16   | 0       | 0       |
| 61  | DR    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | DT    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | DU    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | DX    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | DY    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 61  | D0    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 61  | D1    | 1        | Total<br>1    | O<br>1    | 0       | 0       |

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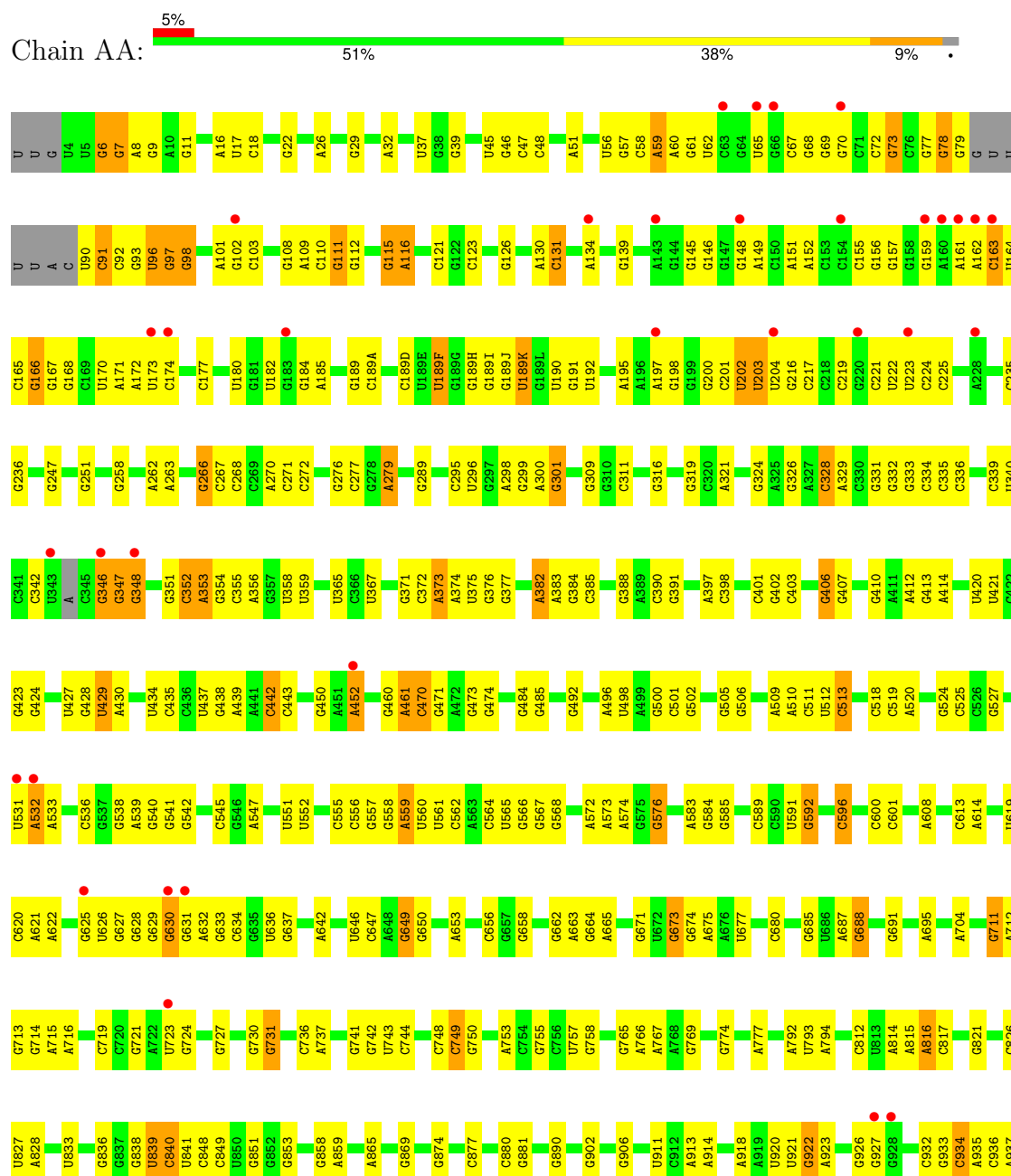
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 61  | D3    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 61  | D7    | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |
| 61  | D8    | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |

### 3 Residue-property plots

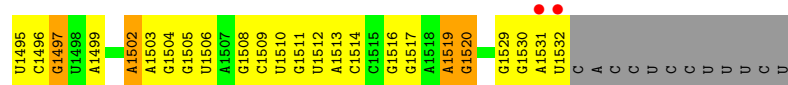
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S Ribosomal RNA

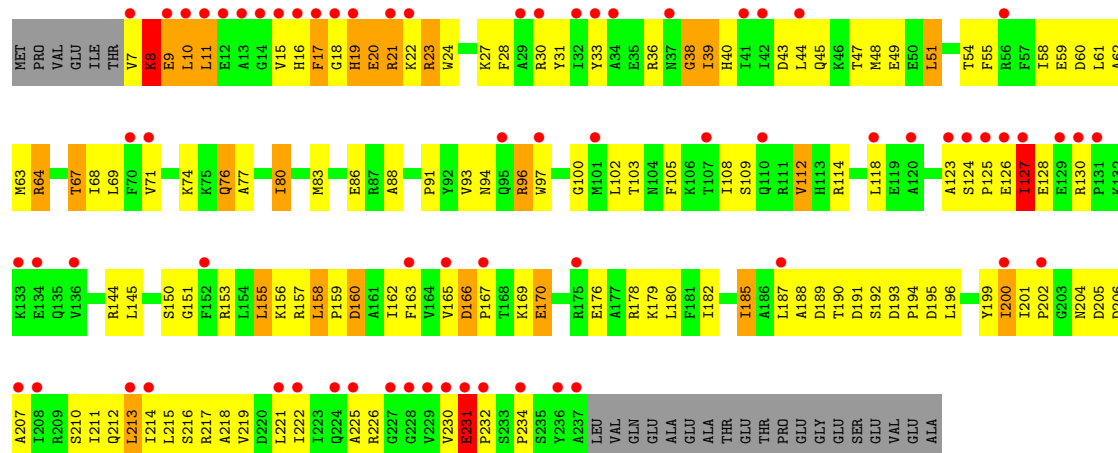




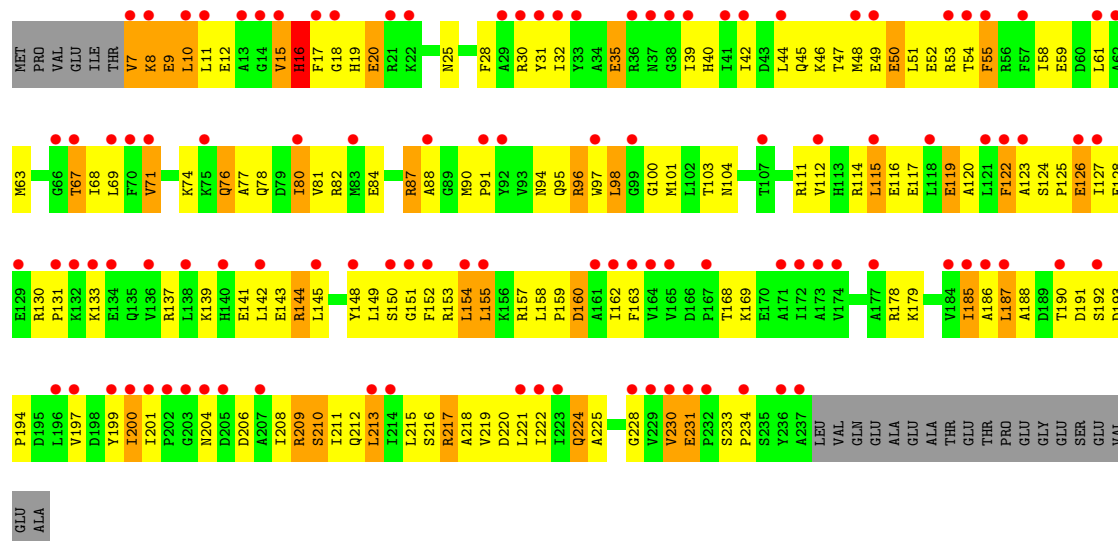
|        |       |       |       |       |       |        |      |      |      |      |      |      |
|--------|-------|-------|-------|-------|-------|--------|------|------|------|------|------|------|
| C1378  | U1315 | C1249 | A1179 | C1116 | G1050 | C995   | C932 | A828 | U646 | G542 | C447 | A373 |
| G1379  | G1316 | A1250 | A1180 | G1117 | C1051 | A996   | G933 | A996 | C647 | C543 | A448 | A374 |
| C1383  | C1317 | A1251 | G1181 | C1118 | U1052 | U997   | C934 | U833 | A649 | G544 | C449 | U375 |
| G1386  | A1318 | A1252 | G1182 | C1119 | G1053 | U998   | A935 | U834 | G650 | C545 | G649 | G376 |
| C1387  | C1319 | G1253 | A1183 | U1120 | C1054 | C999   | C936 | U838 | G651 | G546 | A451 | G377 |
| C1388  | C1320 | C1254 | G1184 | U1121 | U1055 | U1000  | A937 | U839 | A653 | A547 | A452 | A382 |
| U1391  | C1321 | A1256 | G1190 | U1122 | U1056 | A1001  | A938 | U841 | U651 | U551 | A453 | A383 |
| C1392  | C1322 | A1257 | A1191 | A1123 | G1057 | G1001A | C939 | U844 | C656 | U552 | C460 | G384 |
| U1393  | G1323 | C1258 | C1192 | G1124 | U1058 | G1002  | G942 | C848 | G657 | C556 | A461 | G388 |
| C1397  | A1324 | G1259 | U1196 | U1125 | C1060 | A1004  | A946 | G851 | G662 | A559 | C471 | A389 |
| A1398  | C1325 | A1260 | G1197 | U1126 | G1061 | A1005  | A947 | G852 | A663 | U560 | A472 | C390 |
| C1399  | C1326 | C1261 | U1198 | G1127 | U1062 | U1006  | C948 | G853 | G664 | C562 | C473 | G391 |
| C1402  | C1327 | C1262 | G1199 | C1128 | C1063 | C1007  | A949 | C857 | A665 | U561 | C474 | A393 |
| G1410  | G1331 | C1263 | C1200 | A1130 | G1064 | C1008  | U950 | G858 | U677 | C566 | C485 | G396 |
| C1411  | A1332 | A1269 | G1201 | G1131 | U1065 | G1009  | A951 | C859 | G673 | U565 | C486 | A397 |
| C1412  | C1333 | G1270 | A1201 | C1132 | C1066 | U951   | G951 | A859 | G674 | C567 | C488 | C398 |
| U1413  | A1334 | G1271 | G1202 | G1133 | A1067 | G1011  | U952 | A860 | G675 | A572 | C492 | C400 |
| G1419  | C1340 | C1272 | C1203 | G1134 | G1068 | U1012  | G953 | G861 | U757 | A573 | C496 | G406 |
| G1422  | C1341 | G1273 | A1204 | U1135 | C1069 | G1013  | G954 | C866 | U678 | C576 | A496 | G407 |
| C1423  | G1342 | G1274 | U1205 | C1070 | U1070 | A1014  | U955 | C867 | A766 | A577 | A498 | A408 |
| C1424  | A1343 | A1275 | G1206 | G1136 | C1071 | A1015  | U956 | G868 | A768 | A578 | A499 | A411 |
| C1429  | C1344 | G1276 | C1207 | C1137 | G1072 | A1016  | U957 | G869 | G769 | C579 | C501 | A412 |
| C1430  | G1345 | C1277 | G1208 | U1138 | U1073 | G1017  | A958 | G874 | C770 | U580 | C502 | C413 |
| U1435  | C1346 | U1278 | U1211 | U1139 | C1075 | C1018  | A959 | G875 | G771 | C581 | C503 | C414 |
| C1436  | U1351 | A1286 | U1212 | G1140 | C1076 | G1019  | U960 | C876 | G772 | C582 | C504 | A414 |
| U1442  | A1347 | A1287 | A1213 | G1141 | U1076 | U1020  | U961 | C877 | G773 | C583 | C505 | A415 |
| G1442  | C1352 | A1288 | C1214 | C1142 | G1081 | G1021  | G962 | C878 | G774 | C584 | C506 | C419 |
| G1442A | G1353 | G1289 | G1215 | G1143 | U1082 | G1022  | A964 | C879 | G775 | C585 | C507 | U420 |
| U1446  | C1354 | G1290 | C1216 | C1144 | G1083 | U1025  | G966 | C880 | G776 | C586 | C508 | U421 |
| C1452  | G1355 | G1291 | C1217 | U1145 | U1084 | U1026  | G967 | G885 | A777 | C587 | C509 | G422 |
| G1456  | A1357 | U1292 | C1218 | G1146 | U1085 | C1027  | A968 | G886 | G778 | C588 | C510 | G423 |
| G1457  | C1359 | G1293 | U1219 | U1147 | U1086 | G1028  | A969 | G887 | C779 | C589 | C511 | G424 |
| G1469  | U1360 | G1294 | C1220 | A1150 | G1087 | C1029  | G970 | C888 | A780 | C589 | C512 | G425 |
| C1479  | C1361 | C1297 | G1221 | C1151 | G1088 | U1030  | G971 | C889 | C784 | C590 | C513 | U426 |
| G1480  | C1362 | C1298 | G1222 | C1152 | G1089 | G1030A | C972 | G895 | C789 | C591 | C514 | U427 |
| G1486  | A1299 | C1299 | G1223 | G1153 | A1092 | C1030B | G973 | G898 | U789 | C592 | C518 | U428 |
| G1487  | G1300 | A1299 | U1232 | G1154 | A1093 | G1030C | A974 | A901 | C789 | C593 | C519 | U429 |
| C1490  | C1301 | U1300 | G1233 | C1155 | U1094 | A1030D | A975 | A914 | U804 | C594 | C520 | A430 |
| G1491  | U1301 | U1301 | C1234 | G1156 | G1095 | G1031  | A976 | A915 | C805 | C595 | C521 | A431 |
| A1492  | C1302 | U1302 | U1235 | C1157 | C1101 | C1032  | A977 | G916 | G712 | C596 | C522 | A432 |
| A1493  | C1303 | C1303 | U1236 | C1158 | A1101 | G1033  | A978 | U920 | G713 | C597 | C523 | C433 |
| G1494  | G1304 | G1304 | G1237 | U1159 | C1096 | U1040  | C979 | U921 | G714 | C598 | C524 | C434 |
|        | C1305 | G1305 | A1238 | A1169 | C1097 | A1041  | C980 | U922 | A715 | C599 | C525 | C435 |
|        | G1370 | U1308 | U1239 | A1170 | C1098 | U1042  | A981 | G922 | C719 | C600 | C526 | C436 |
|        | U1372 | G1309 | C1171 | G1171 | U1099 | C1043  | U982 | A815 | C720 | C601 | C527 | U437 |
|        | C1373 | G1310 | G1172 | C1172 | C1100 | G1044  | A983 | A816 | G721 | C602 | C528 | A438 |
|        | A1374 | G1311 | G1173 | A1110 | C1101 | A1044  | C984 | G924 | G722 | C603 | C529 | A439 |
|        | U1375 | G1312 | G1174 | C1113 | A1102 | C990   | C985 | G925 | A722 | C604 | C530 | A441 |
|        | C1376 | U1313 | G1175 | C1114 | C1103 | U1045  | C986 | G926 | U723 | C605 | C531 | C442 |
|        | A1377 | C1245 | A1176 | C1115 | U1046 | G1047  | U991 | G927 | G724 | C606 | C532 | C443 |
|        |       | C1246 | G1177 | C1116 | A1048 | U992   | U992 | C927 | U725 | C607 | C533 | C444 |
|        |       |       | G1178 | C1117 | U1049 | U993   | A994 | C931 | G727 | C608 | C534 | G445 |
|        |       |       |       |       |       |        |      |      |      |      | C535 | G446 |



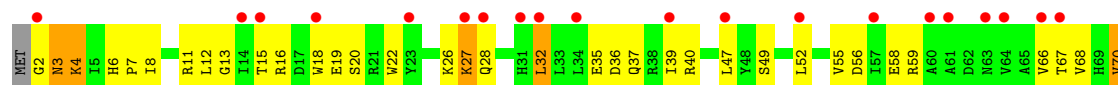
• Molecule 2: 30S ribosomal protein S2



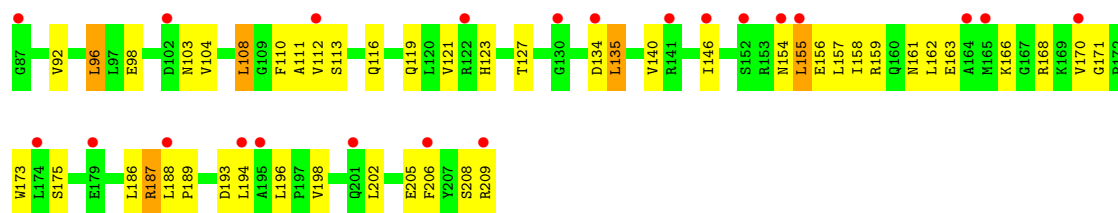
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3







• Molecule 5: 30S ribosomal protein S5



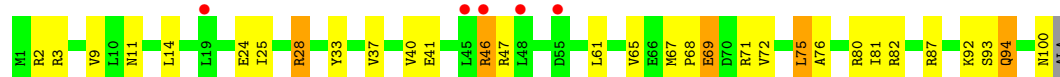
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



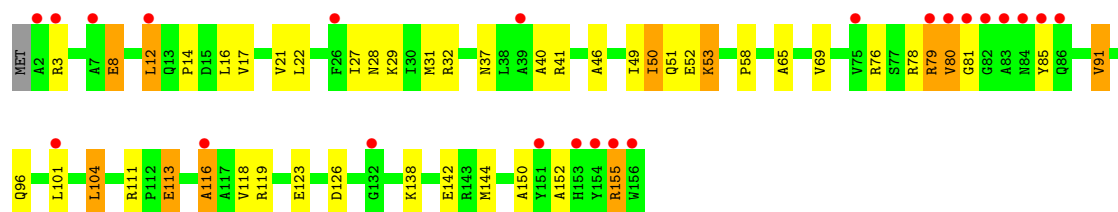
• Molecule 6: 30S ribosomal protein S6





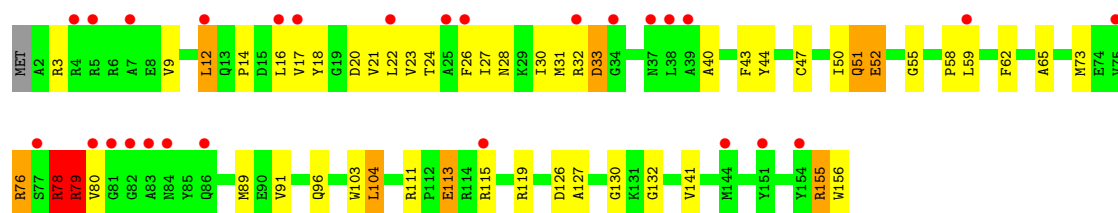
- Molecule 7: 30S ribosomal protein S7

Chain AG: 



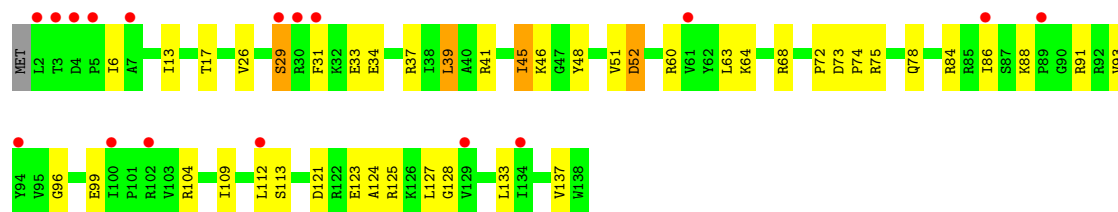
- Molecule 7: 30S ribosomal protein S7

Chain CG: 



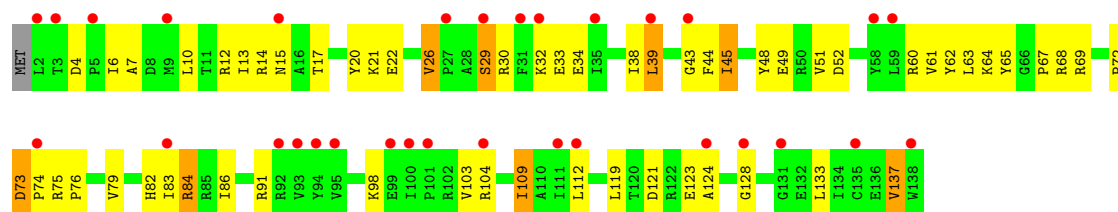
- Molecule 8: 30S ribosomal protein S8

Chain AH: 



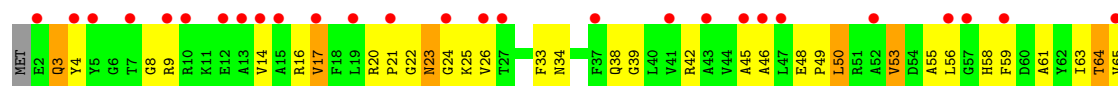
- Molecule 8: 30S ribosomal protein S8

Chain CH: 



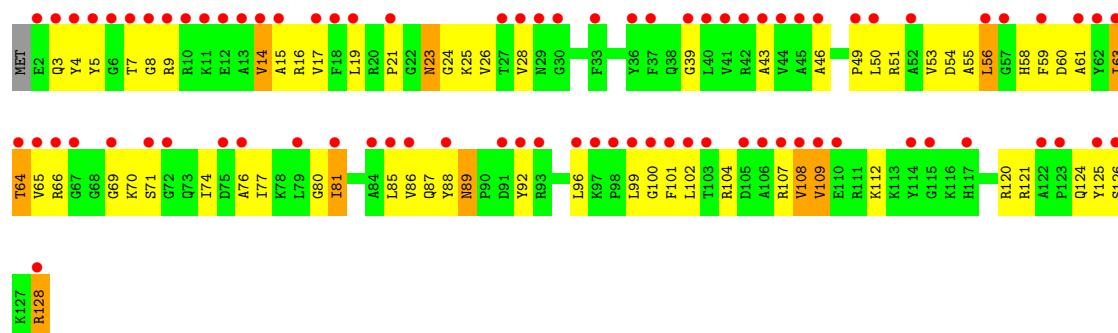
- Molecule 9: 30S ribosomal protein S9

Chain AI: 

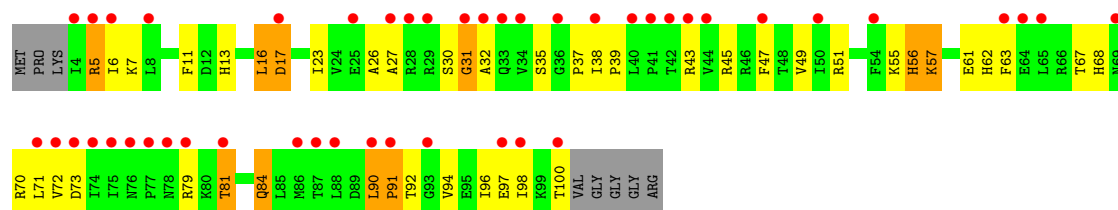




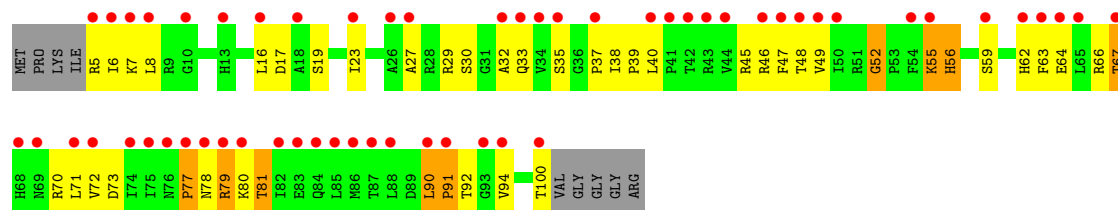
• Molecule 9: 30S ribosomal protein S9



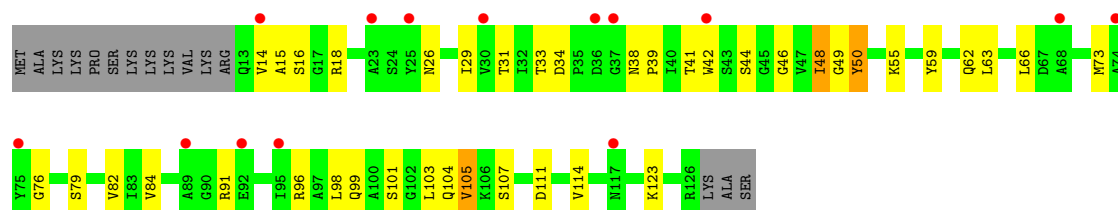
• Molecule 10: 30S ribosomal protein S10



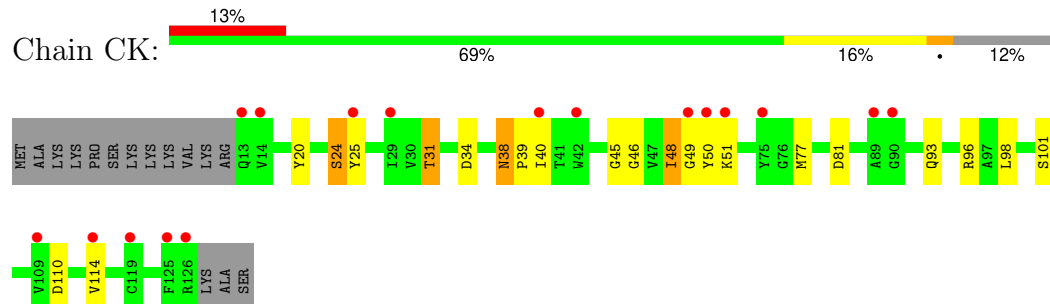
• Molecule 10: 30S ribosomal protein S10



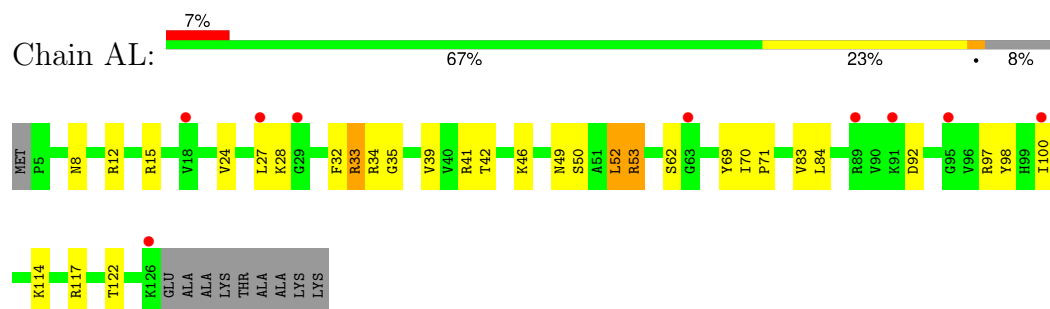
• Molecule 11: 30S ribosomal protein S11



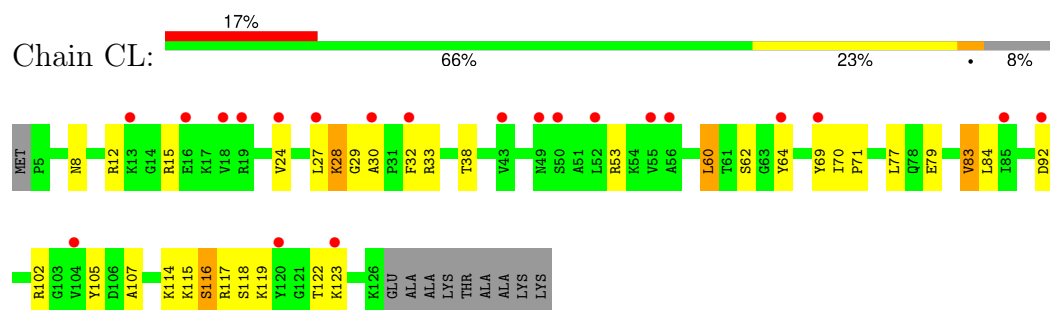
- Molecule 11: 30S ribosomal protein S11



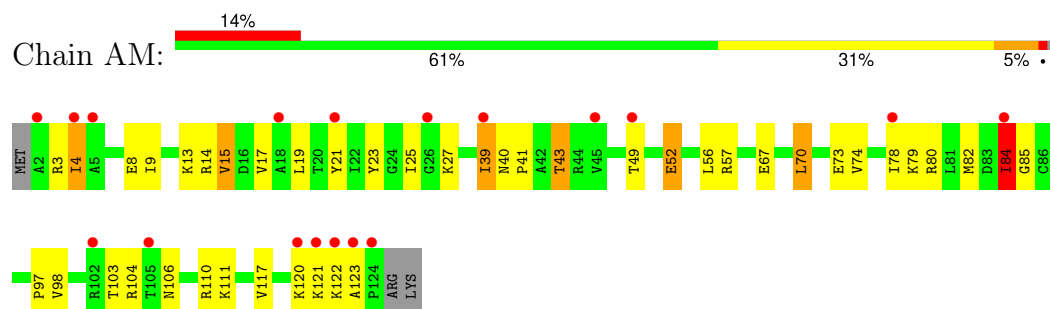
- Molecule 12: 30S ribosomal protein S12



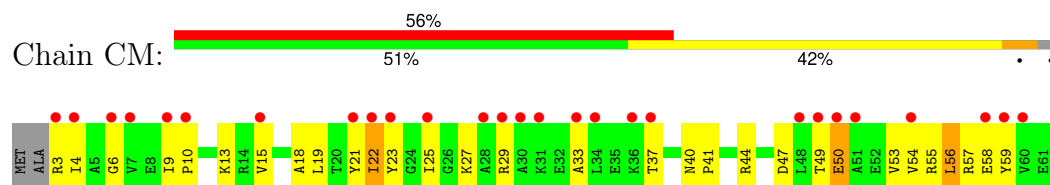
- Molecule 12: 30S ribosomal protein S12

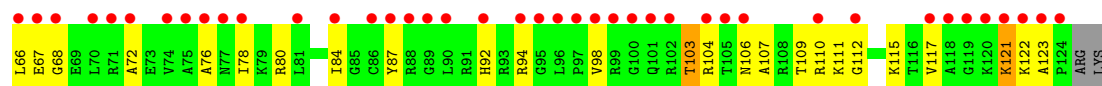


- Molecule 13: 30S ribosomal protein S13

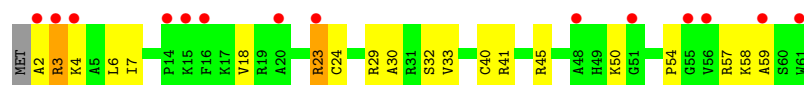


- Molecule 13: 30S ribosomal protein S13

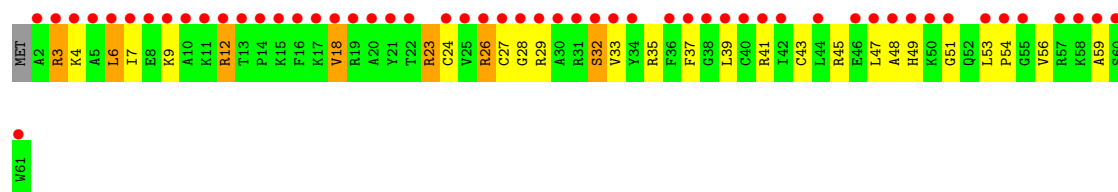
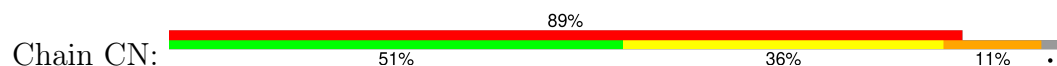




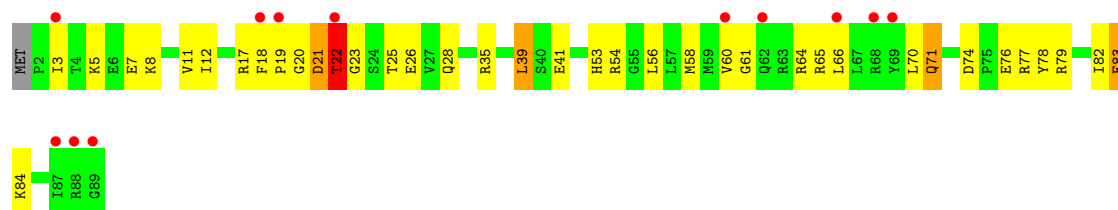
- Molecule 14: 30S ribosomal protein S14 type Z



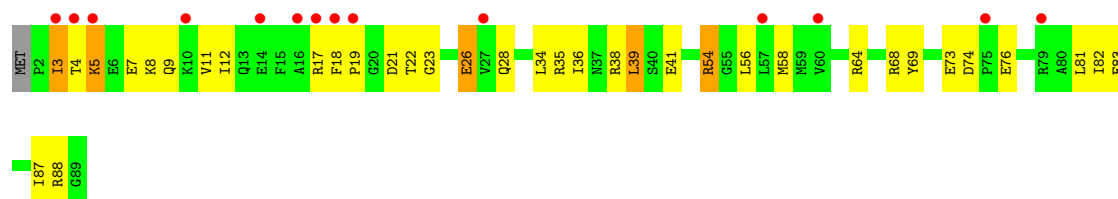
- Molecule 14: 30S ribosomal protein S14 type Z



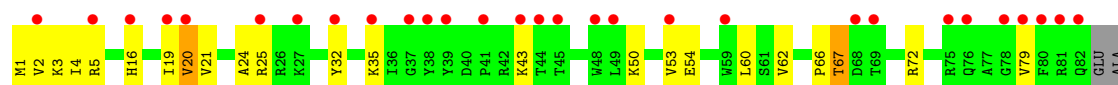
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

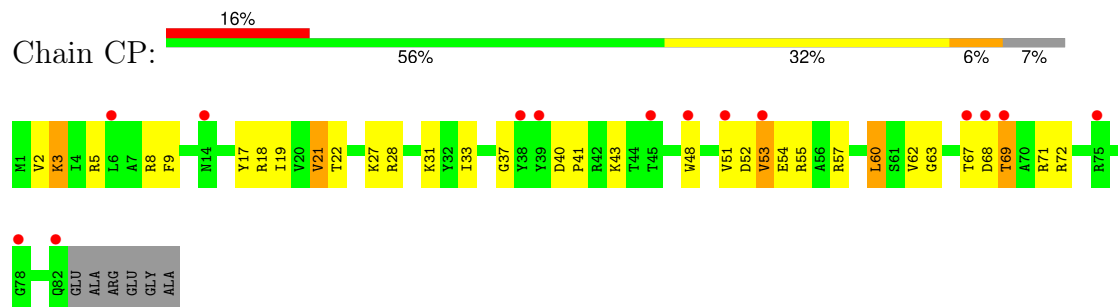


- Molecule 16: 30S ribosomal protein S16

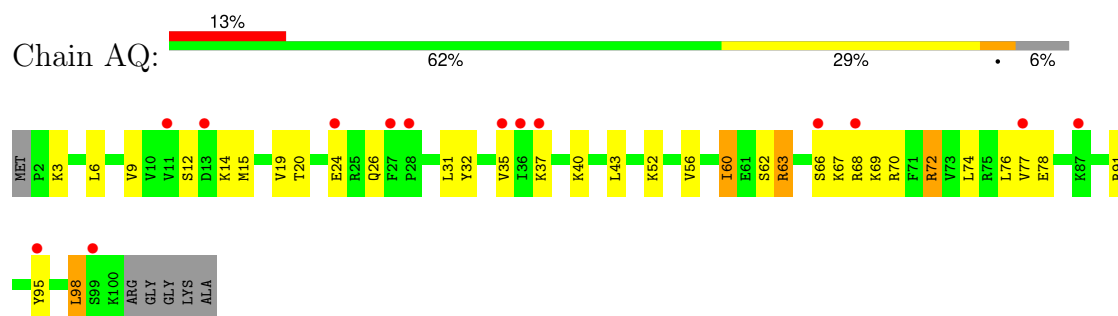


ARG  
GLU  
GLY  
ALA

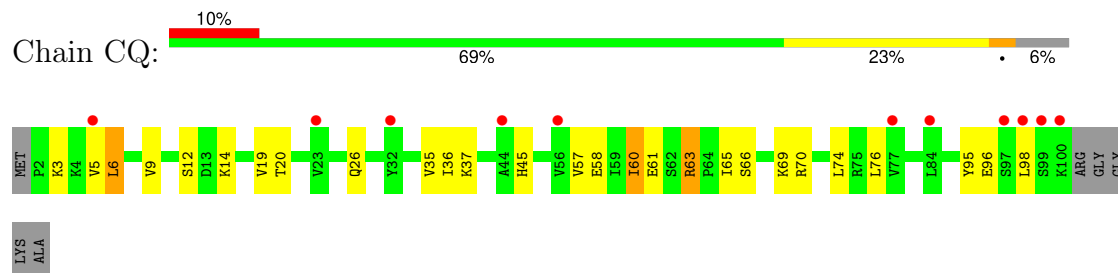
- Molecule 16: 30S ribosomal protein S16



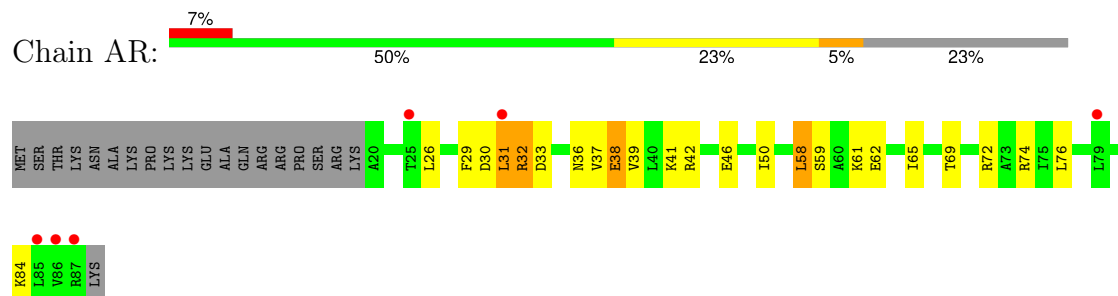
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

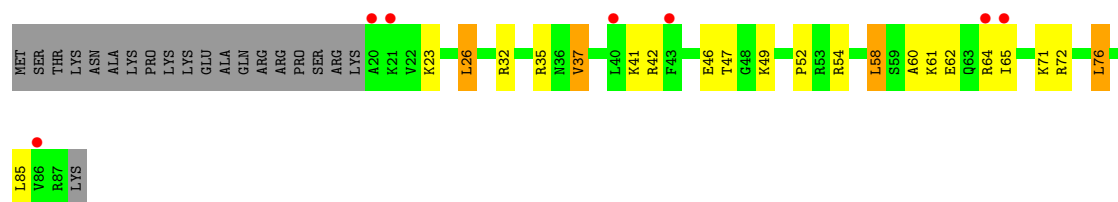


- Molecule 18: 30S ribosomal protein S18

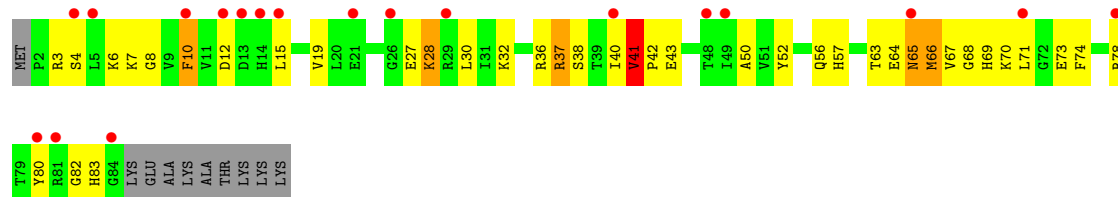


- Molecule 18: 30S ribosomal protein S18

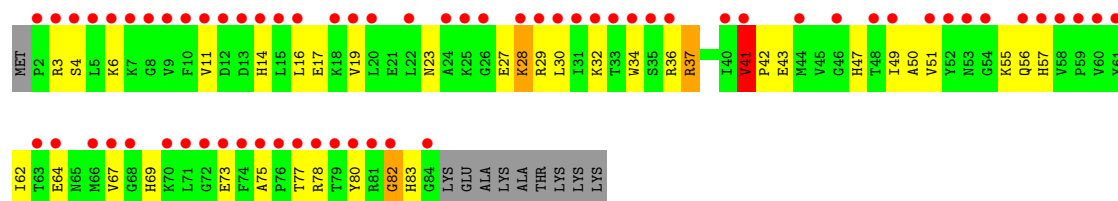
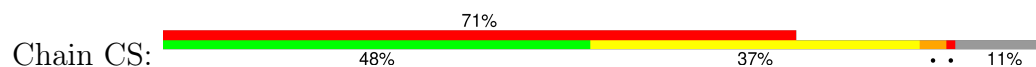




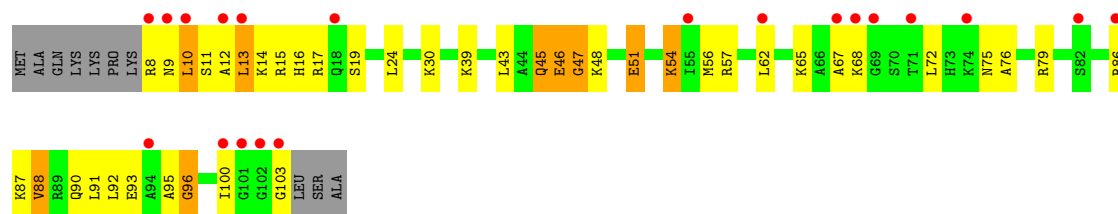
• Molecule 19: 30S ribosomal protein S19



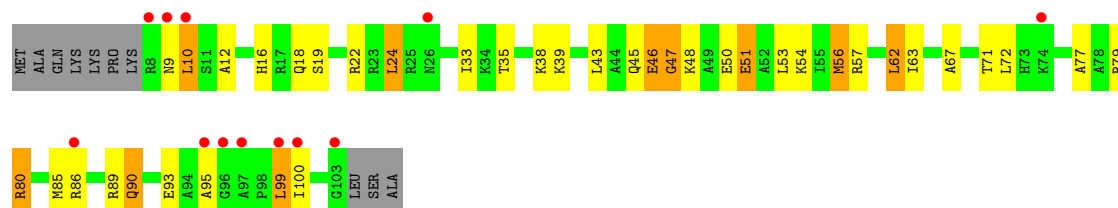
• Molecule 19: 30S ribosomal protein S19



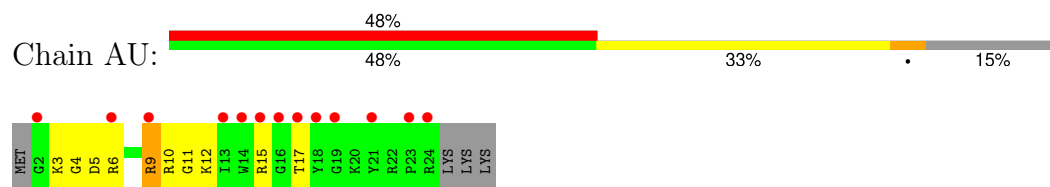
• Molecule 20: 30S ribosomal protein S20



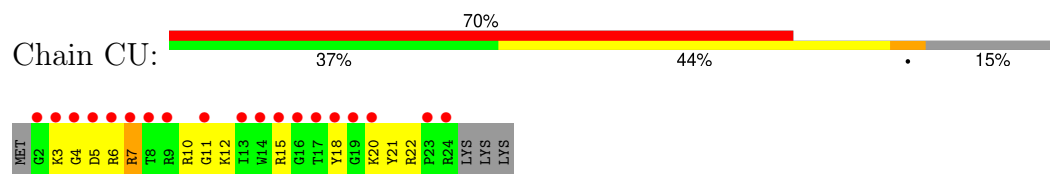
• Molecule 20: 30S ribosomal protein S20



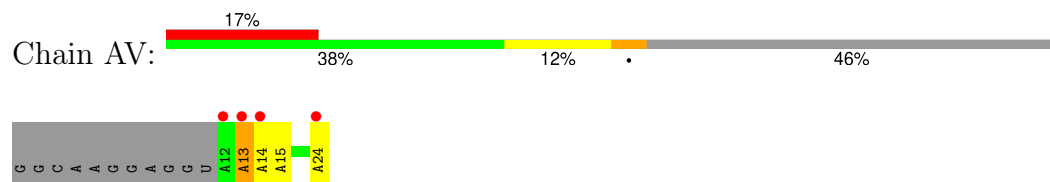
## • Molecule 21: 30S ribosomal protein Thx



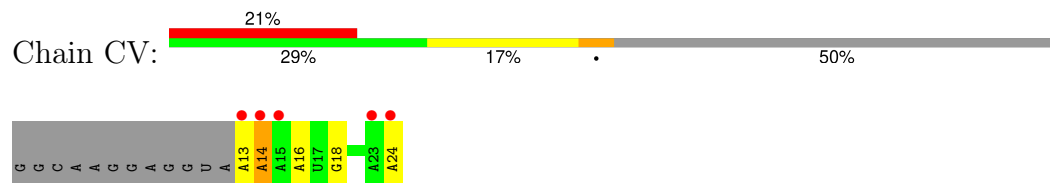
## • Molecule 21: 30S ribosomal protein Thx



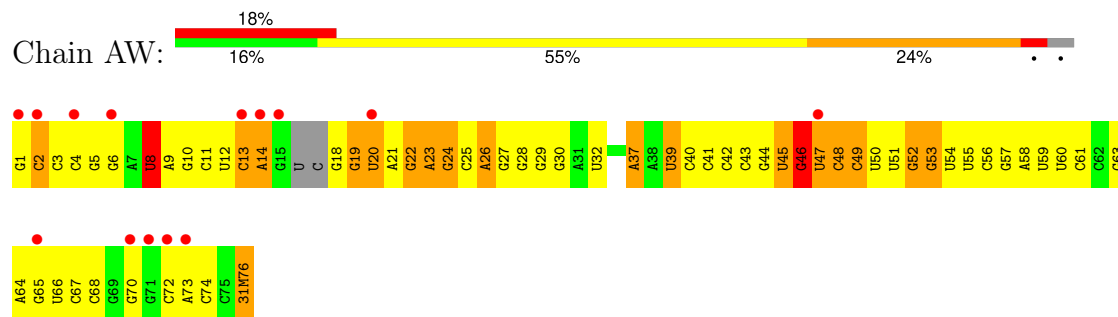
## • Molecule 22: mRNA



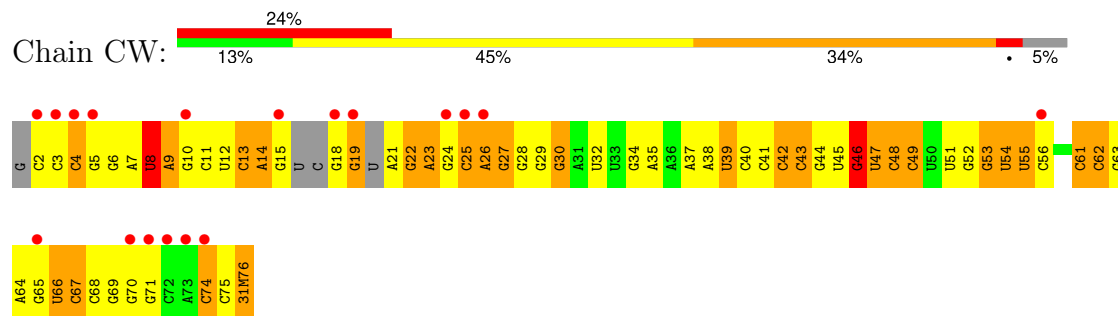
## • Molecule 22: mRNA



## • Molecule 23: A-site tRNA



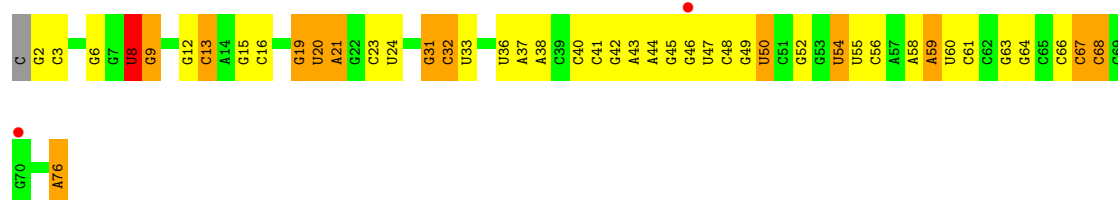
## • Molecule 23: A-site tRNA



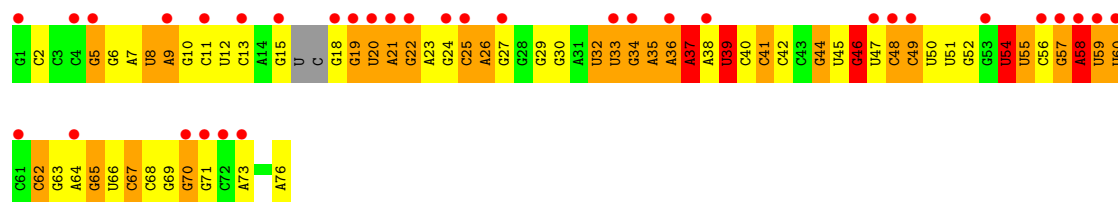
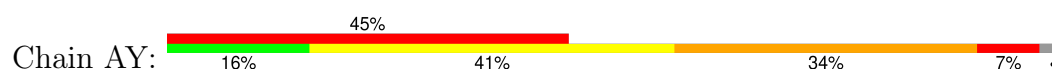
- Molecule 24: P-site tRNA



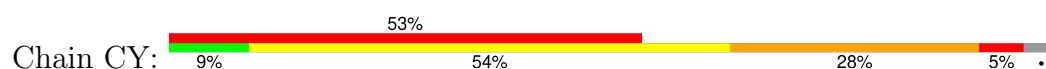
- Molecule 24: P-site tRNA



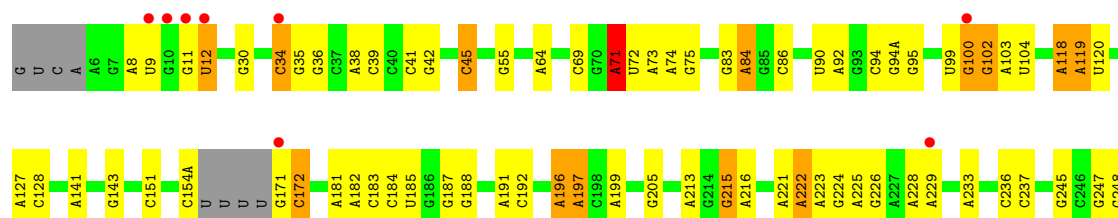
- Molecule 25: E-site tRNA



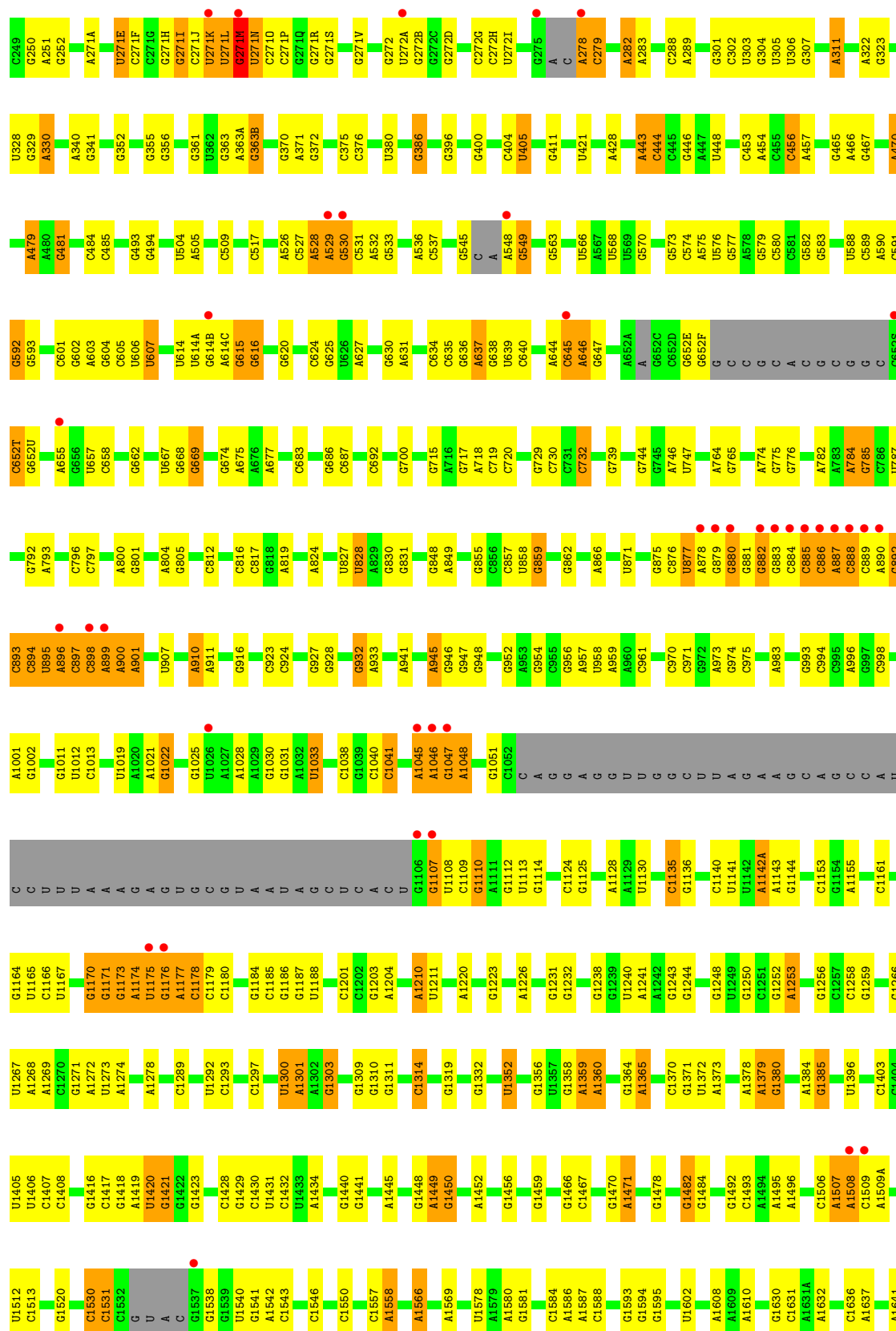
- Molecule 25: E-site tRNA

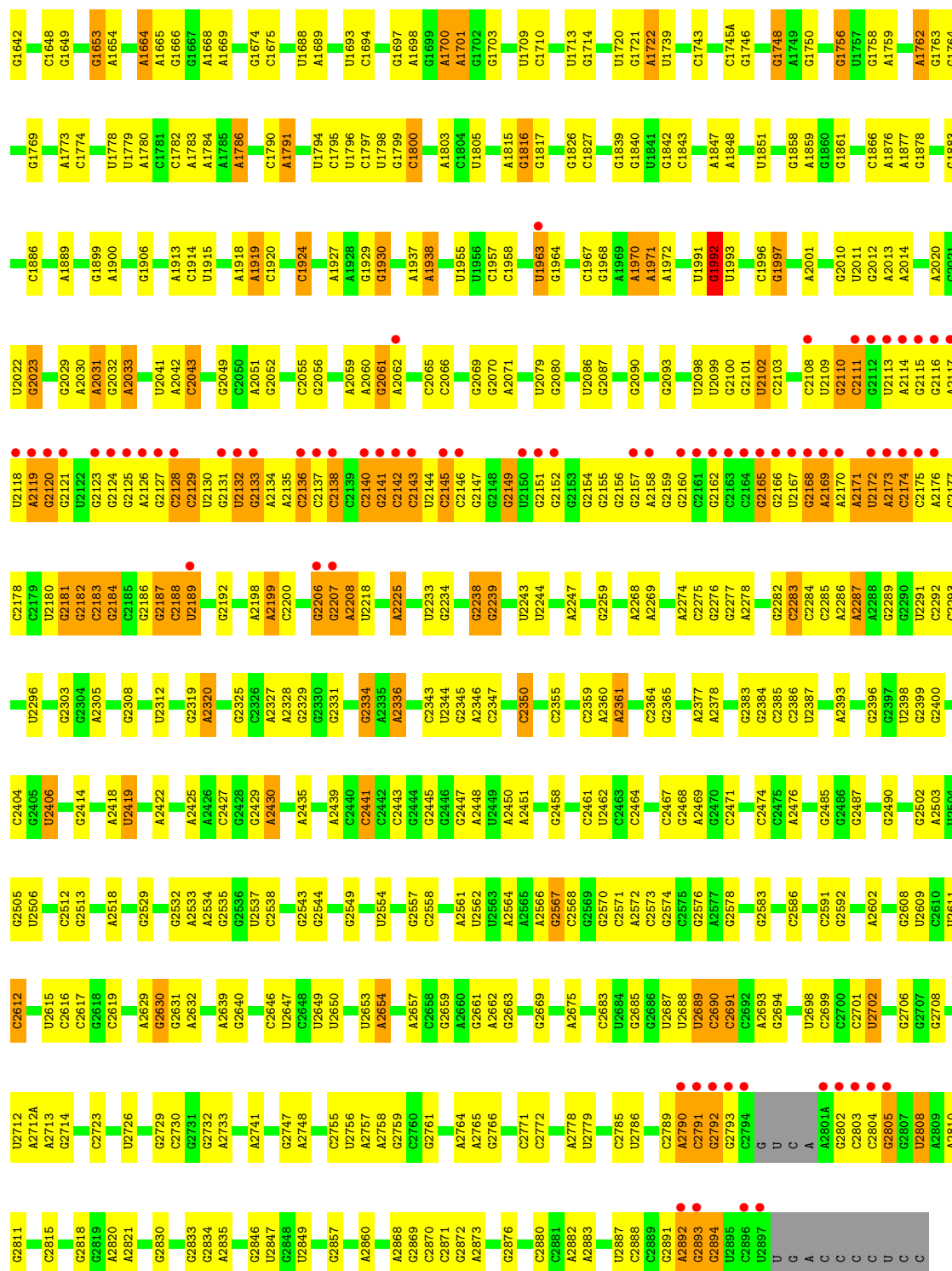


- Molecule 26: 23S Ribosomal RNA

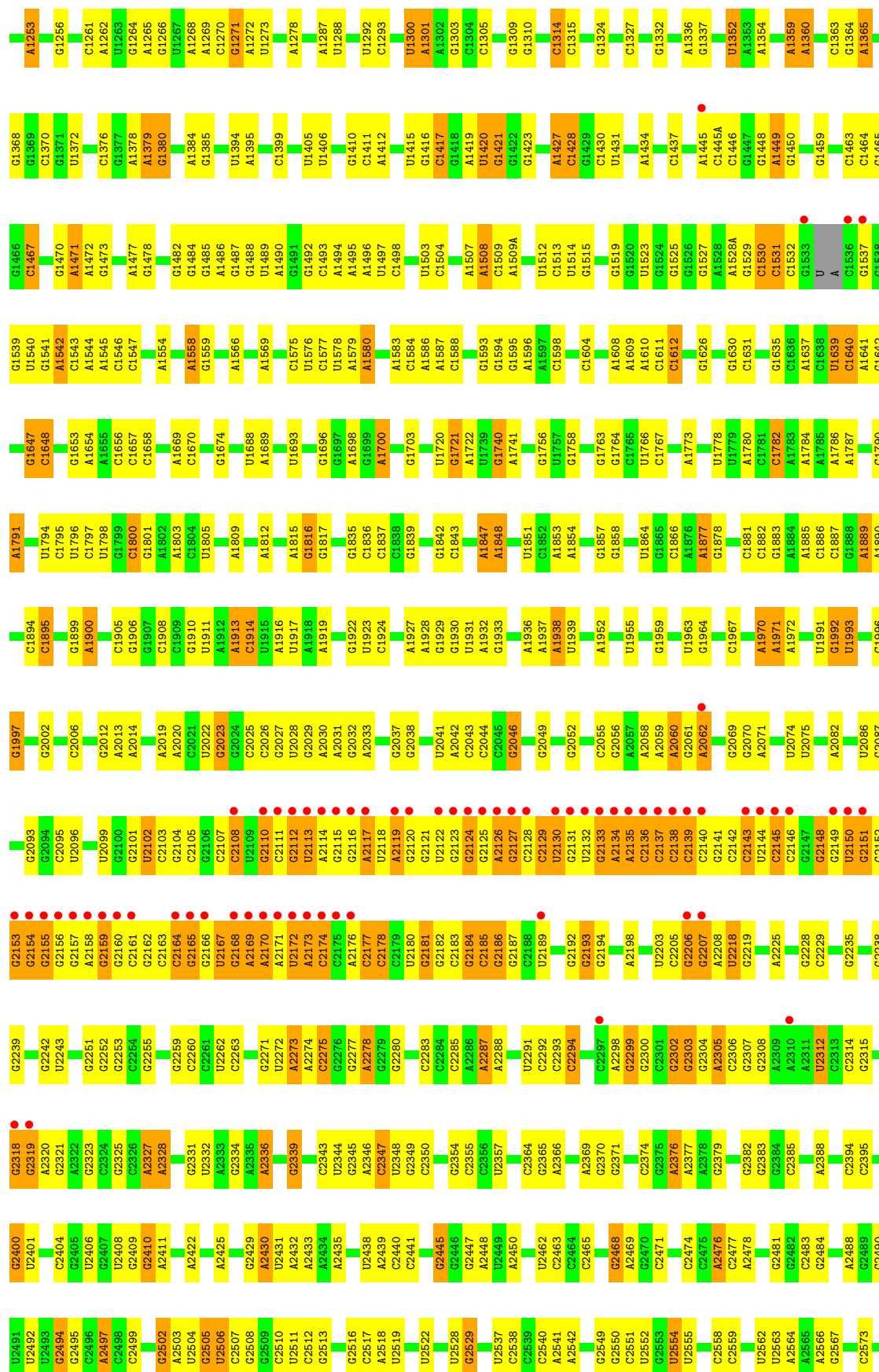


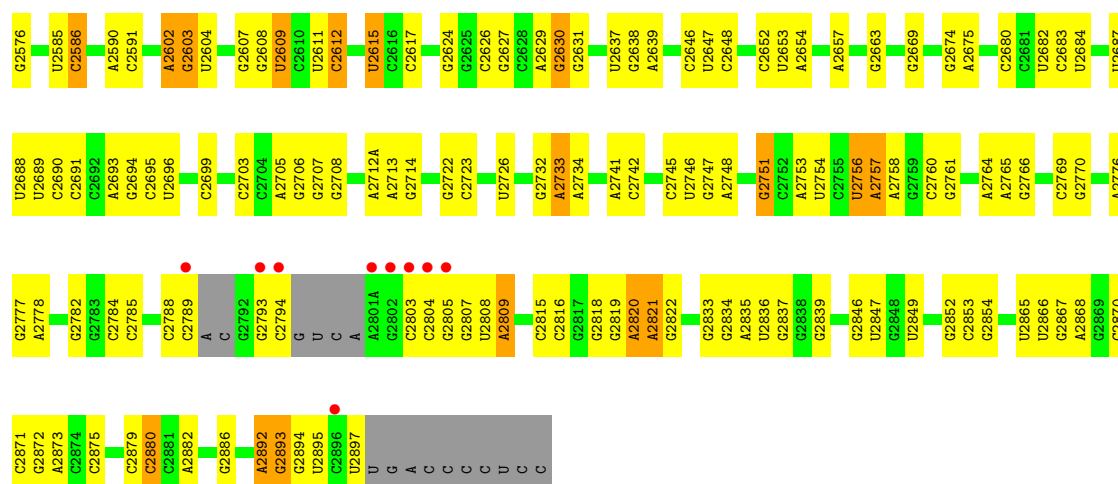




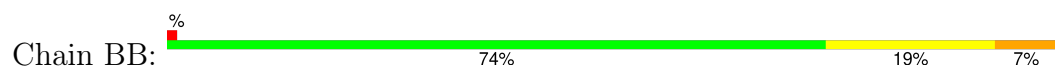


|       |       |       |       |      |      |       |      |      |       |      |      |      |       |       |       |
|-------|-------|-------|-------|------|------|-------|------|------|-------|------|------|------|-------|-------|-------|
| G1170 | G1171 | A1032 | A1033 | A953 | A954 | A878  | G796 | G698 | G623  | C535 | G446 | U839 | G271V | A196  | G89   |
| G     | U     | U1033 | U1034 | G954 | G954 | G879  | G796 | C698 | C624  | A536 | A447 | A340 | G271V | A197  | U90   |
| A     | A     | G1035 | G1036 | A957 | A957 | G880  | G797 | A699 | U625  | C537 | A448 | G341 | G271V | C198  | A92   |
| U     | U     | U1037 | U1038 | A959 | A959 | G882  | G798 | G700 | U626  | C540 | A449 | G352 | U272A | A199  | G94   |
| C     | A     | C1038 | C1039 | A960 | A960 | G883  | A802 | U709 | A627  | C541 | G452 | G363 | G272B | C203  | G94A  |
| C     | C     | G1039 | G1040 | C961 | C961 | C885  | U803 | G710 | G628  | C545 | C453 | C454 | G272C | G205  | G95   |
| U     | U     | G1042 | G1043 | C966 | C966 | C886  | A804 | G715 | A631  | C    | A454 | C364 | G272D | C208  | G100  |
| C     | C     | A     | A     | C967 | C967 | A887  | G805 | C721 | A637  | A    | C455 | C365 | G272E | C209  | G102  |
| C     | C     | G     | G     | A    | A    | C889  | G809 | U724 | U639  | G    | A456 | C366 | C272J | A103  | G109  |
| U     | U     | A     | A     | C971 | C971 | A890  | U810 | G725 | C640  | G    | A457 | C367 | G273  | G109  | G117  |
| G     | G     | A     | A     | G974 | G974 | G892  | C812 | G726 | C641  | G    | A458 | C368 | G274  | G118  | A118  |
| U     | U     | G     | G     | C975 | C975 | C894  | U813 | A727 | G642  | G    | G465 | G372 | G275  | G119  | A119  |
| C     | C     | C     | C     | A    | A    | U895  | C816 | G728 | A644  | G    | G466 | A371 | G276  | G120  | U120  |
| C     | C     | A     | A     | A983 | A983 | A896  | C817 | G729 | A646  | G    | G468 | G373 | A276  | G121  | U121  |
| C     | C     | A     | A     | A    | A    | C987  | C818 | G730 | A647  | G    | G469 | A374 | G277  | G122  | G125  |
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| C     | C     | A     | A     | A    | A    | C989  | C820 | A734 | G649  | G    | A478 | C376 | C285  | A127  | A127  |
| C     | C     | A     | A     | A    | A    | C990  | C821 | U740 | A652B | G    | A479 | C377 | C286  | G131  | G131  |
| C     | C     | A     | A     | A    | A    | A900  | C822 | G741 | G652C | G    | A480 | C378 | C287  | U230  | G140  |
| C     | C     | A     | A     | A    | A    | A901  | C823 | G744 | G652D | G    | A481 | C379 | C288  | G141  | A141  |
| C     | C     | A     | A     | A    | A    | C902  | C824 | A752 | G652E | G    | A482 | C380 | C289  | G142  | G143  |
| C     | C     | A     | A     | A    | A    | C903  | C825 | C753 | G     | G    | A483 | C381 | C290  | C143A | C143A |
| C     | C     | A     | A     | A    | A    | C904  | C826 | C754 | G     | G    | A484 | C382 | C291  | C144  | G145  |
| C     | C     | A     | A     | A    | A    | A910  | C827 | C755 | G     | G    | A485 | C383 | C292  | G149  | A149  |
| C     | C     | A     | A     | A    | A    | A911  | C828 | C756 | G     | G    | A486 | C384 | C293  | C154A | C154A |
| C     | C     | A     | A     | A    | A    | C912  | C829 | C757 | G     | G    | A487 | C385 | C294  | U157  | U157  |
| C     | C     | A     | A     | A    | A    | C913  | C830 | C758 | G     | G    | A488 | C386 | C295  | U     | U     |
| C     | C     | A     | A     | A    | A    | C914  | C831 | C759 | G     | G    | A489 | C387 | C296  | G171  | G171  |
| C     | C     | A     | A     | A    | A    | A917  | C832 | C760 | G     | G    | A490 | C388 | C297  | C172  | C172  |
| C     | C     | A     | A     | A    | A    | A918  | C833 | C761 | G     | G    | A491 | C389 | C298  | G173  | G173  |
| C     | C     | A     | A     | A    | A    | A919  | C834 | C762 | G     | G    | A492 | C390 | C299  | G178  | G178  |
| C     | C     | A     | A     | A    | A    | C920  | C835 | C763 | G     | G    | A493 | C391 | C300  | A181  | A181  |
| C     | C     | A     | A     | A    | A    | C921  | C836 | C764 | G     | G    | A494 | C392 | C301  | A182  | A182  |
| C     | C     | A     | A     | A    | A    | C922  | C837 | C765 | G     | G    | A495 | C393 | C302  | C183  | C183  |
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| C     | C     | A     | A     | A    | A    | C924  | C839 | C767 | G     | G    | A497 | C395 | C304  | U185  | U185  |
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| C     | C     | A     | A     | A    | A    | C926  | C841 | C769 | G     | G    | A499 | C397 | C306  | C192  | C192  |
| C     | C     | A     | A     | A    | A    | C927  | C842 | C770 | G     | G    | A500 | C398 | C307  | U193  | U193  |
| C     | C     | A     | A     | A    | A    | C928  | C843 | C771 | G     | G    | A501 | C399 | C308  | C194  | C194  |
| C     | C     | A     | A     | A    | A    | C929  | C844 | C772 | G     | G    | A502 | C400 | C309  | A195  | A195  |
| C     | C     | A     | A     | A    | A    | C930  | C845 | C773 | G     | G    | A503 | C401 | C310  |       |       |
| C     | C     | A     | A     | A    | A    | C931  | C846 | C774 | G     | G    | A504 | C402 | C311  |       |       |
| C     | C     | A     | A     | A    | A    | C932  | C847 | C775 | G     | G    | A505 | C403 | C312  |       |       |
| C     | C     | A     | A     | A    | A    | C933  | C848 | C776 | G     | G    | A506 | C404 | C313  |       |       |
| C     | C     | A     | A     | A    | A    | C934  | C849 | C777 | G     | G    | A507 | C405 | C314  |       |       |
| C     | C     | A     | A     | A    | A    | C935  | C850 | C778 | G     | G    | A508 | C406 | C315  |       |       |
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| C     | C     | A     | A     | A    | A    | C937  | C852 | C780 | G     | G    | A510 | C408 | C317  |       |       |
| C     | C     | A     | A     | A    | A    | C938  | C853 | C781 | G     | G    | A511 | C409 | C318  |       |       |
| C     | C     | A     | A     | A    | A    | C939  | C854 | C782 | G     | G    | A512 | C410 | C319  |       |       |
| C     | C     | A     | A     | A    | A    | C940  | C855 | C783 | G     | G    | A513 | C411 | C320  |       |       |
| C     | C     | A     | A     | A    | A    | C941  | C856 | C784 | G     | G    | A514 | C412 | C321  |       |       |
| C     | C     | A     | A     | A    | A    | C942  | C857 | C785 | G     | G    | A515 | C413 | C322  |       |       |
| C     | C     | A     | A     | A    | A    | C943  | C858 | C786 | G     | G    | A516 | C414 | C323  |       |       |
| C     | C     | A     | A     | A    | A    | C944  | C859 | C787 | G     | G    | A517 | C415 | C324  |       |       |
| C     | C     | A     | A     | A    | A    | C945  | C860 | C788 | G     | G    | A518 | C416 | C325  |       |       |
| C     | C     | A     | A     | A    | A    | C946  | C861 | C789 | G     | G    | A519 | C417 | C326  |       |       |
| C     | C     | A     | A     | A    | A    | C947  | C862 | C790 | G     | G    | A520 | C418 | C327  |       |       |
| C     | C     | A     | A     | A    | A    | C948  | C863 | C791 | G     | G    | A521 | C419 | C328  |       |       |
| C     | C     | A     | A     | A    | A    | C949  | C864 | C792 | G     | G    | A522 | C420 | C329  |       |       |
| C     | C     | A     | A     | A    | A    | C950  | C865 | C793 | G     | G    | A523 | C421 | C330  |       |       |
| C     | C     | A     | A     | A    | A    | C951  | C866 | C794 | G     | G    | A524 | C422 | C331  |       |       |
| C     | C     | A     | A     | A    | A    | C952  | C867 | C795 | G     | G    | A525 | C423 | C332  |       |       |
| C     | C     | A     | A     | A    | A    | C953  | C868 | C796 | G     | G    | A526 | C424 | C333  |       |       |
| C     | C     | A     | A     | A    | A    | C954  | C869 | C797 | G     | G    | A527 | C425 | C334  |       |       |
| C     | C     | A     | A     | A    | A    | C955  | C870 | C798 | G     | G    | A528 | C426 | C335  |       |       |
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| C     | C     | A     | A     | A    | A    | C957  | C872 | C800 | G     | G    | A530 | C428 | C337  |       |       |
| C     | C     | A     | A     | A    | A    | C958  | C873 | C801 | G     | G    | A531 | C429 | C338  |       |       |
| C     | C     | A     | A     | A    | A    | C959  | C874 | C802 | G     | G    | A532 | C430 | C339  |       |       |
| C     | C     | A     | A     | A    | A    | C960  | C875 | C803 | G     | G    | A533 | C431 | C340  |       |       |
| C     | C     | A     | A     | A    | A    | C961  | C876 | C804 | G     | G    | A534 | C432 | C341  |       |       |
| C     | C     | A     | A     | A    | A    | C962  | C877 | C805 | G     | G    | A535 | C433 | C342  |       |       |
| C     | C     | A     | A     | A    | A    | C963  | C878 | C806 | G     | G    | A536 | C434 | C343  |       |       |
| C     | C     | A     | A     | A    | A    | C964  | C879 | C807 | G     | G    | A537 | C435 | C344  |       |       |
| C     | C     | A     | A     | A    | A    | C965  | C880 | C808 | G     | G    | A538 | C436 | C345  |       |       |
| C     | C     | A     | A     | A    | A    | C966  | C881 | C809 | G     | G    | A539 | C437 | C346  |       |       |
| C     | C     | A     | A     | A    | A    | C967  | C882 | C810 | G     | G    | A540 | C438 | C347  |       |       |
| C     | C     | A     | A     | A    | A    | C968  | C883 | C811 | G     | G    | A541 | C439 | C348  |       |       |
| C     | C     | A     | A     | A    | A    | C969  | C884 | C812 | G     | G    | A542 | C440 | C349  |       |       |
| C     | C     | A     | A     | A    | A    | C970  | C885 | C813 | G     | G    | A543 | C441 | C350  |       |       |
| C     | C     | A     | A     | A    | A    | C971  | C886 | C814 | G     | G    | A544 | C442 | C351  |       |       |
| C     | C     | A     | A     | A    | A    | C972  | C887 | C815 | G     | G    | A545 | C443 | C352  |       |       |
| C     | C     | A     | A     | A    | A    | C973  | C888 | C816 | G     | G    | A546 | C444 | C353  |       |       |
| C     | C     | A     | A     | A    | A    | C974  | C889 | C817 | G     | G    | A547 | C445 | C354  |       |       |
| C     | C     | A     | A     | A    | A    | C975  | C890 | C818 | G     | G    | A548 | C446 | C355  |       |       |
| C     | C     | A     | A     | A    | A    | C976  | C891 | C819 | G     | G    | A549 | C447 | C356  |       |       |
| C     | C     | A     | A     | A    | A    | C977  | C892 | C820 | G     | G    | A550 | C448 | C357  |       |       |
| C     | C     | A     | A     | A    | A    | C978  | C893 | C821 | G     | G    | A551 | C449 | C358  |       |       |
| C     | C     | A     | A     | A    | A    | C979  | C894 | C822 | G     | G    | A552 | C450 | C359  |       |       |
| C     | C     | A     | A     | A    | A    | C980  | C895 | C823 | G     | G    | A553 | C451 | C360  |       |       |
| C     | C     | A     | A     | A    | A    | C981  | C896 | C824 | G     | G    | A554 | C452 | C361  |       |       |
| C     | C     | A     | A     | A    | A    | C982  | C897 | C825 | G     | G    | A555 | C453 | C362  |       |       |
| C     | C     | A     | A     | A    | A    | C983  | C898 | C826 | G     | G    | A556 | C454 | C363  |       |       |
| C     | C     | A     | A     | A    | A    | C984  | C899 | C827 | G     | G    | A557 | C455 | C364  |       |       |
| C     | C     | A     | A     | A    | A    | C985  | C900 | C828 | G     | G    | A558 | C456 | C365  |       |       |
| C     | C     | A     | A     | A    | A    | C986  | C901 | C829 | G     | G    | A559 | C457 | C366  |       |       |
| C     | C     | A     | A     | A    | A    | C987  | C902 | C830 | G     | G    | A560 | C458 | C367  |       |       |
| C     | C     | A     | A     | A    | A    | C988  | C903 | C831 | G     | G    | A561 | C459 | C368  |       |       |
| C     | C     | A     | A     | A    | A    | C989  | C904 | C832 | G     | G    | A562 | C460 | C369  |       |       |
| C     | C     | A     | A     | A    | A    | C990  | C905 | C833 | G     | G    | A563 | C461 | C370  |       |       |
| C     | C     | A     | A     | A    | A    | C991  | C906 | C834 | G     | G    | A564 | C462 | C371  |       |       |
| C     | C     | A     | A     | A    | A    | C992  | C907 | C835 | G     | G    | A565 | C463 | C372  |       |       |
| C     | C     | A     | A     | A    | A    | C993  | C908 | C836 | G     | G    | A566 | C464 | C373  |       |       |
| C     | C     | A     | A     | A    | A    | C994  | C909 | C837 | G     | G    | A567 | C465 | C374  |       |       |
| C     | C     | A     | A     | A    | A    | C995  | C910 | C838 | G     | G    | A568 | C466 | C375  |       |       |
| C     | C     | A     | A     | A    | A    | C996  | C911 | C839 | G     | G    | A569 | C467 | C376  |       |       |
| C     | C     | A     | A     | A    | A    | C997  | C912 | C840 | G     | G    | A570 | C468 | C377  |       |       |
| C     | C     | A     | A     | A    | A    | C998  | C913 | C841 | G     | G    | A571 | C469 | C378  |       |       |
| C     | C     | A     | A     | A    | A    | C999  | C914 | C842 | G     | G    | A572 | C470 | C379  |       |       |
| C     | C     | A     | A     | A    | A    | A1000 | C915 | C843 | G     | G    | A573 | C471 | C380  |       |       |
| C     | C     | A     | A     | A    | A    | A1001 | C916 | C844 | G     | G    | A574 | C472 | C381  |       |       |
| C     | C     | A     | A     | A    | A    | A1002 | C917 | C845 | G     | G    | A575 | C473 | C382  |       |       |
| C     | C     | A     | A     | A    | A</  |       |      |      |       |      |      |      |       |       |       |

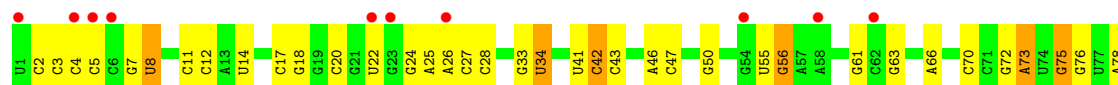




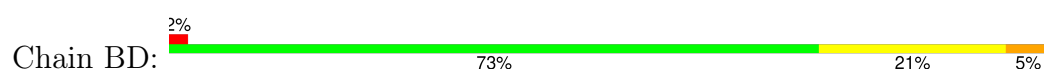
• Molecule 27: 5S Ribosomal RNA



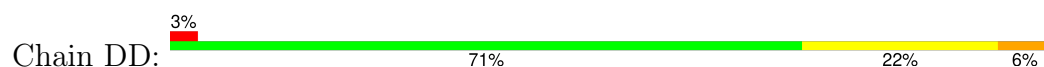
• Molecule 27: 5S Ribosomal RNA



• Molecule 28: 50S ribosomal protein L2

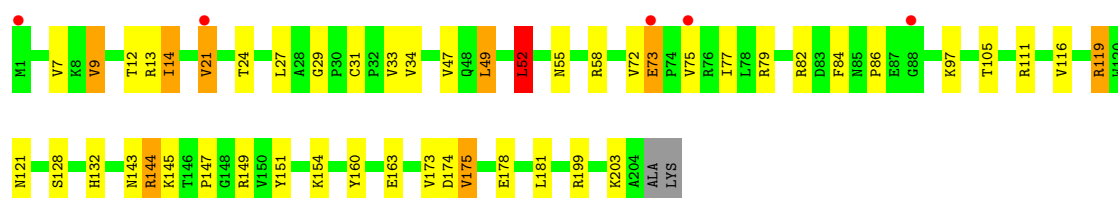
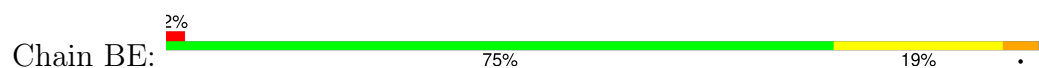


• Molecule 28: 50S ribosomal protein L2

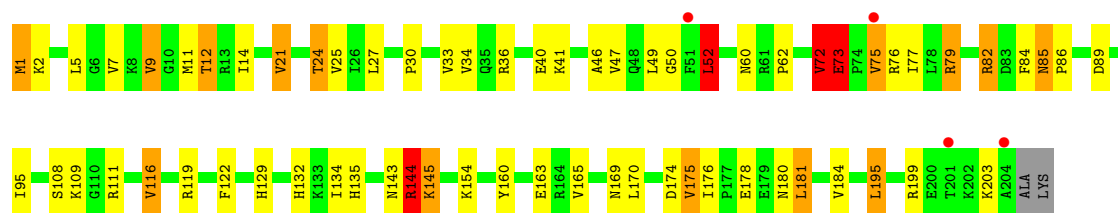




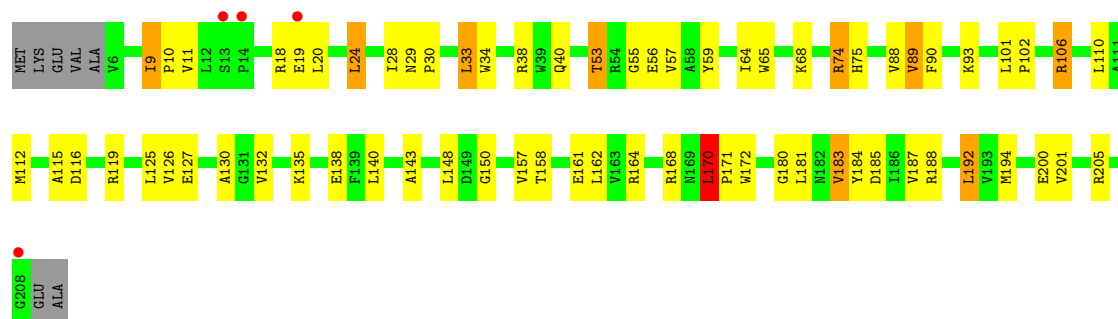
• Molecule 29: 50S ribosomal protein L3



• Molecule 29: 50S ribosomal protein L3

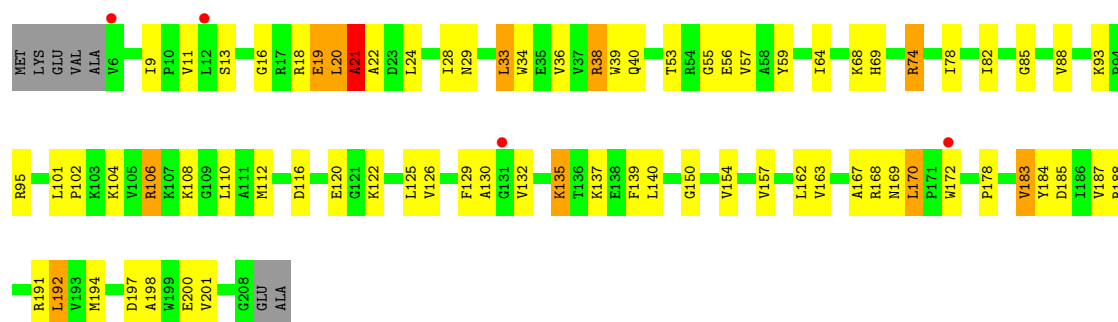


• Molecule 30: 50S ribosomal protein L4

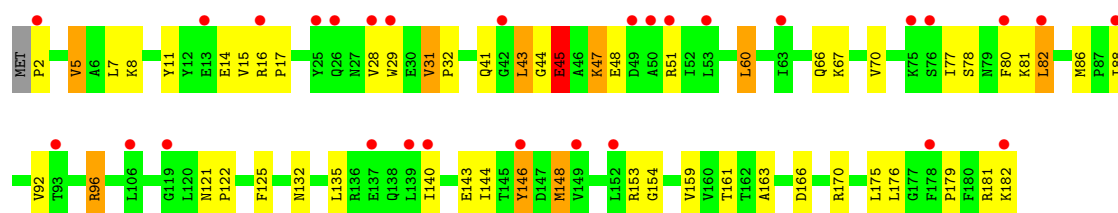


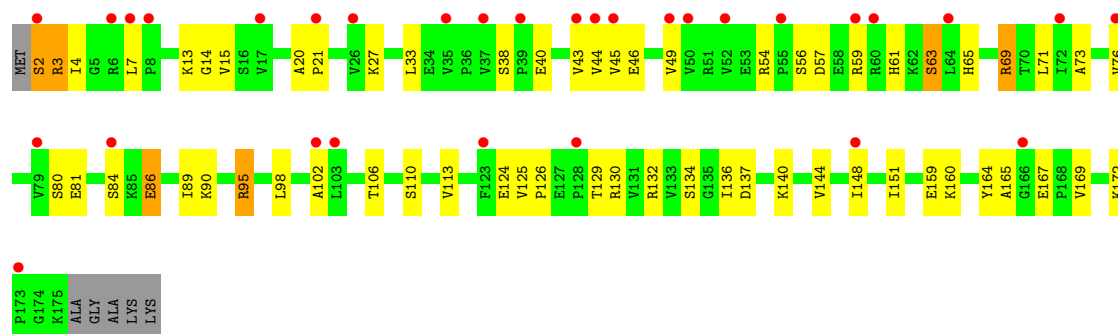
• Molecule 30: 50S ribosomal protein L4



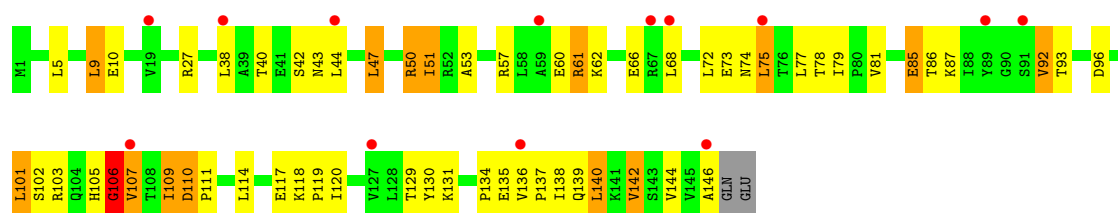


• Molecule 31: 50S ribosomal protein L5

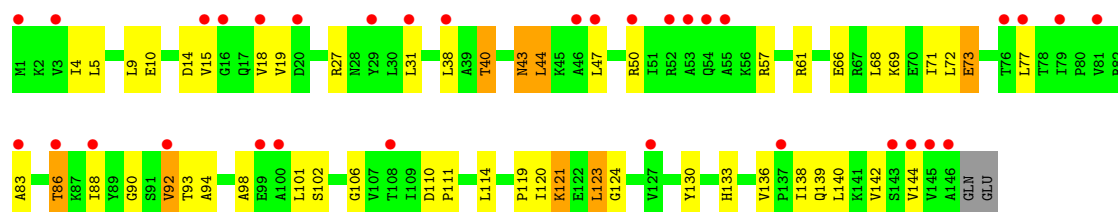




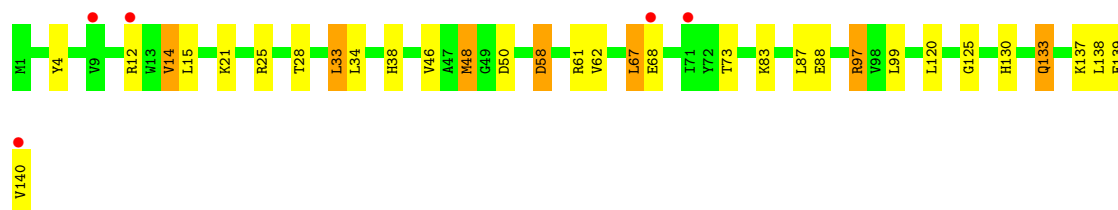
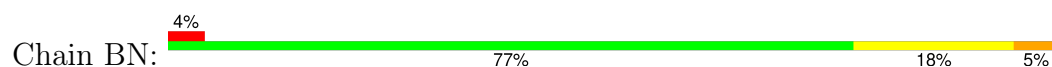
• Molecule 33: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L9



• Molecule 34: 50S ribosomal protein L13



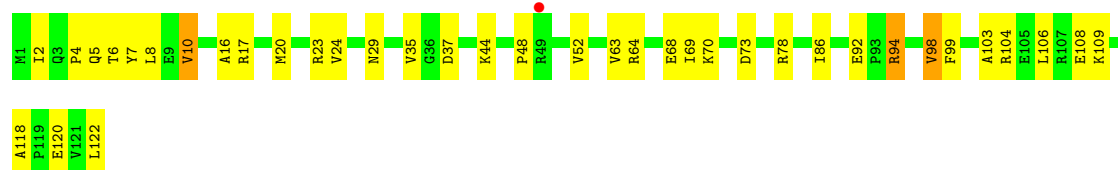
• Molecule 34: 50S ribosomal protein L13



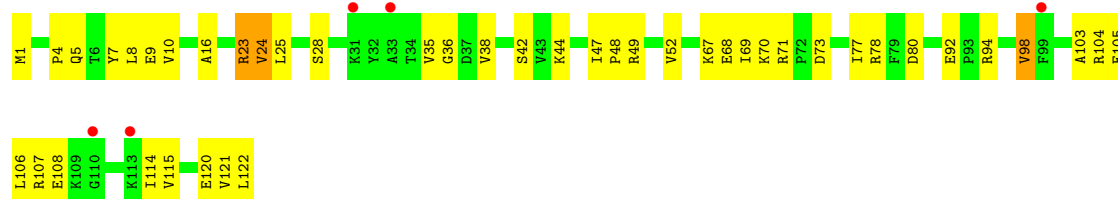




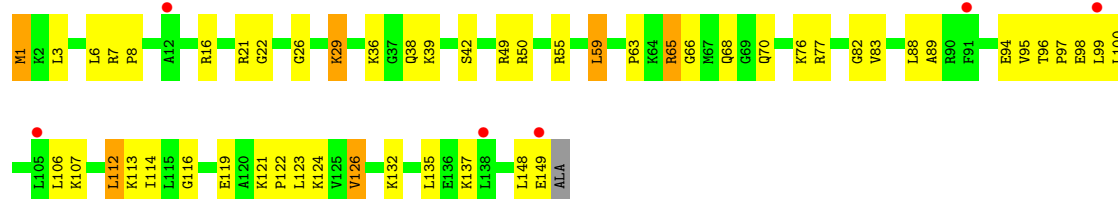
• Molecule 35: 50S ribosomal protein L14



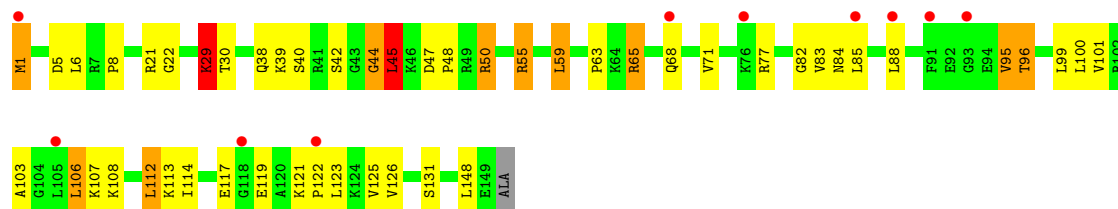
• Molecule 35: 50S ribosomal protein L14



• Molecule 36: 50S ribosomal protein L15

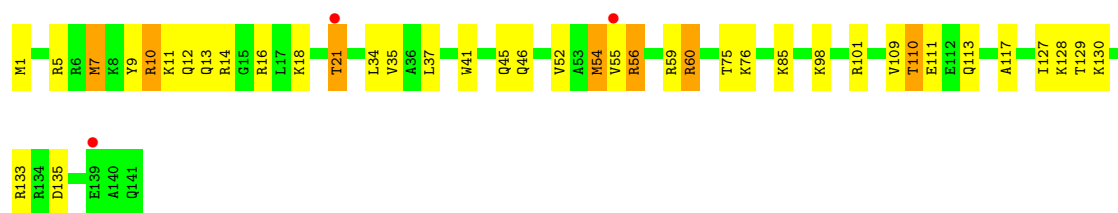


• Molecule 36: 50S ribosomal protein L15

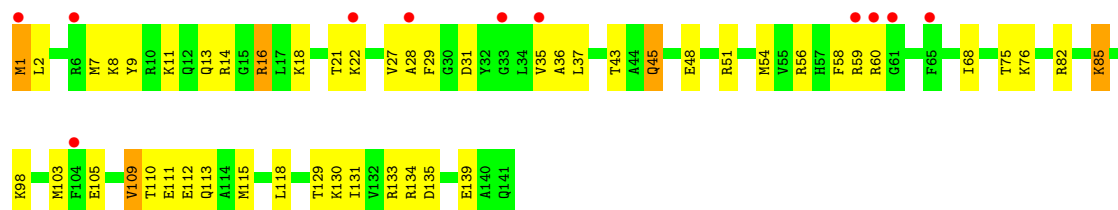


• Molecule 37: 50S ribosomal protein L16

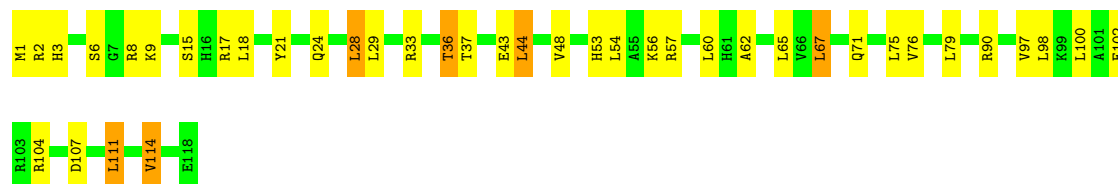




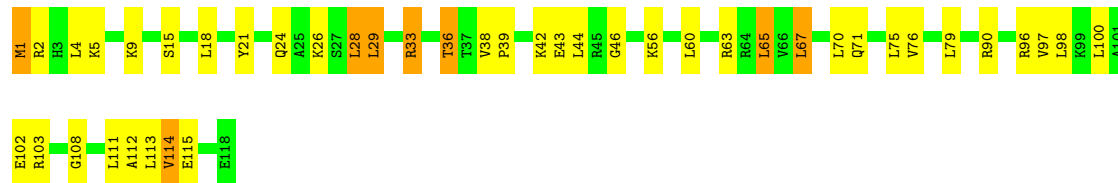
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

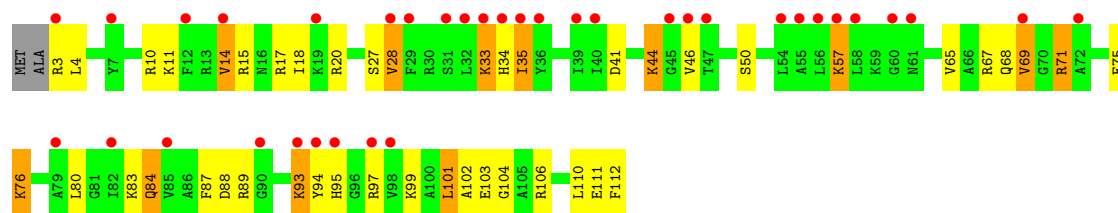


- Molecule 39: 50S ribosomal protein L18

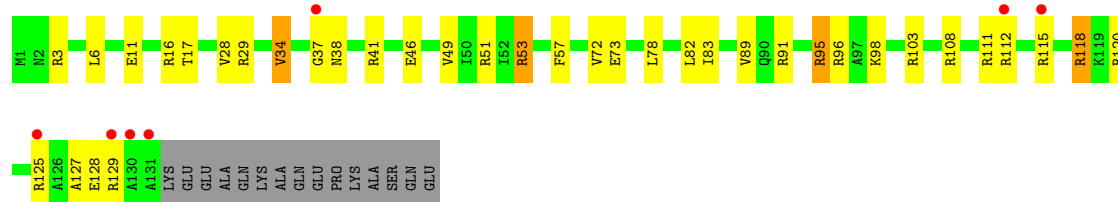


- Molecule 39: 50S ribosomal protein L18

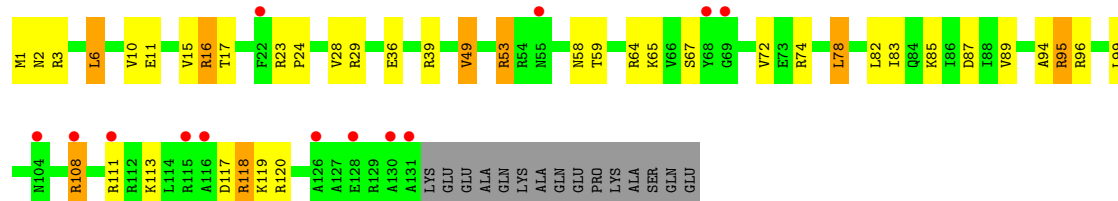




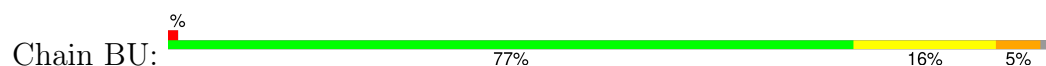
• Molecule 40: 50S ribosomal protein L19



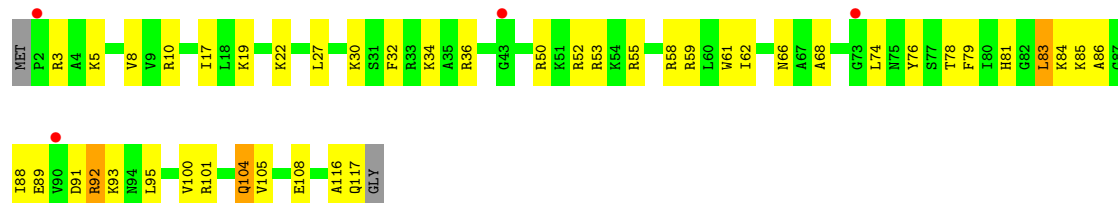
• Molecule 40: 50S ribosomal protein L19



• Molecule 41: 50S ribosomal protein L20

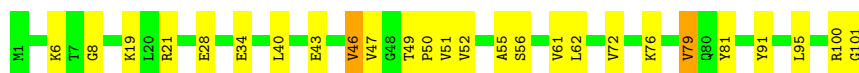


• Molecule 41: 50S ribosomal protein L20

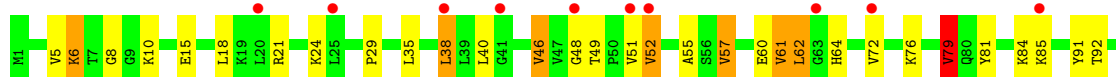


• Molecule 42: 50S ribosomal protein L21

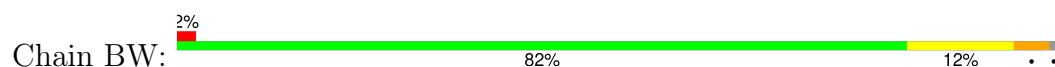




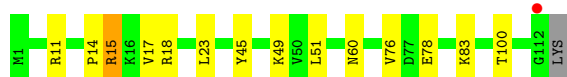
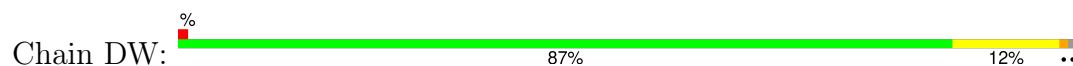
- Molecule 42: 50S ribosomal protein L21



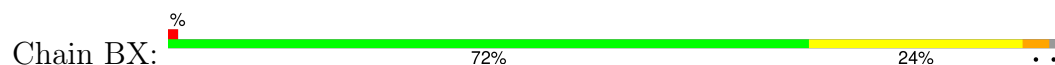
- Molecule 43: 50S ribosomal protein L22



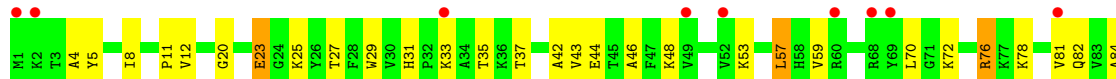
- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23

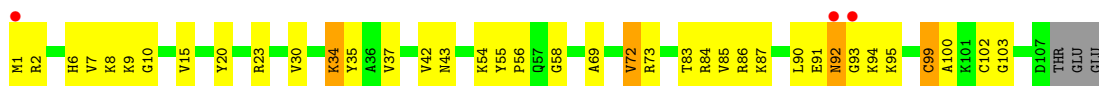


- Molecule 44: 50S ribosomal protein L23

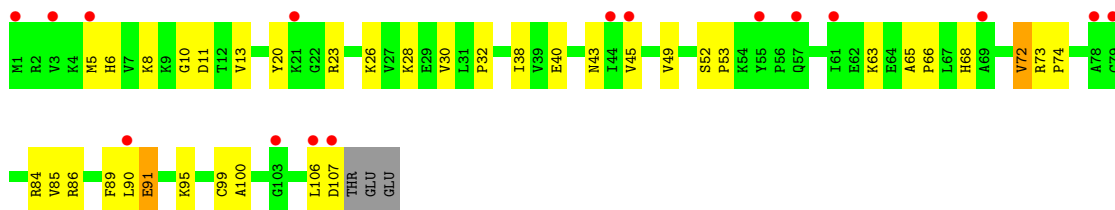


- Molecule 45: 50S ribosomal protein L24

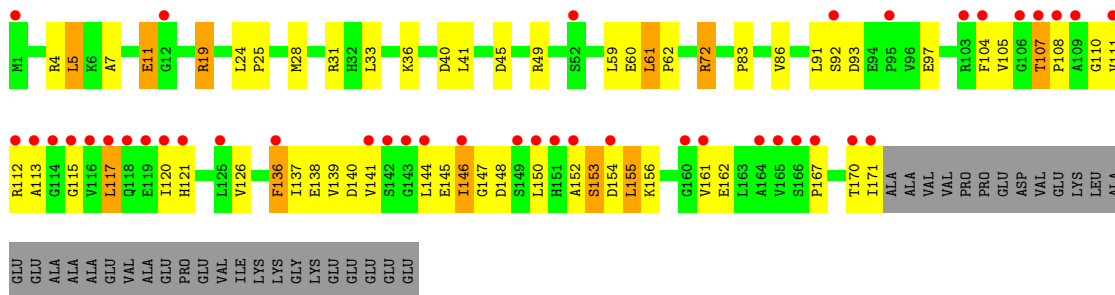




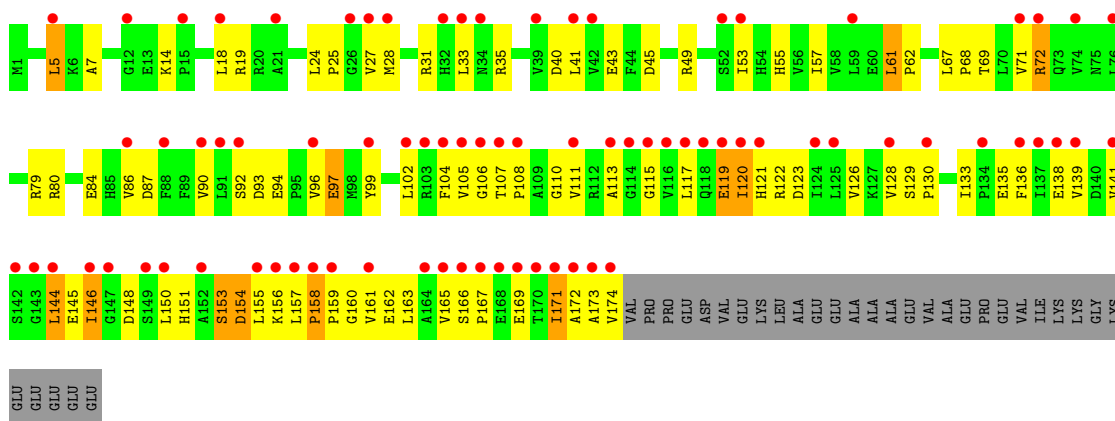
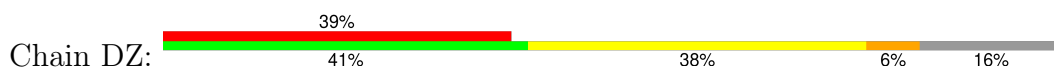
- Molecule 45: 50S ribosomal protein L24



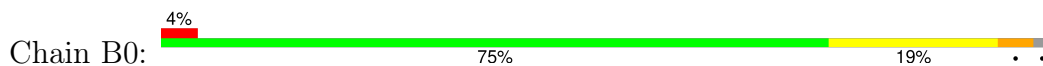
- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25

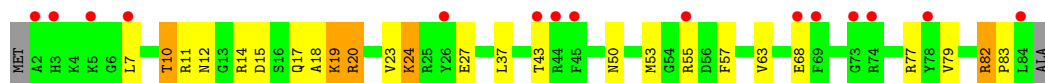


- Molecule 47: 50S ribosomal protein L27

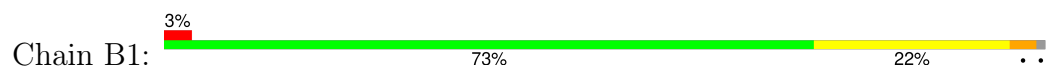




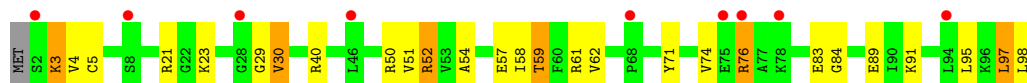
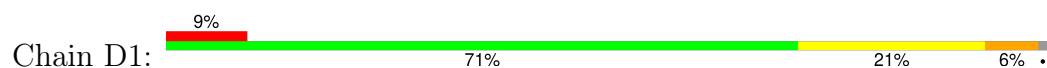
- Molecule 47: 50S ribosomal protein L27



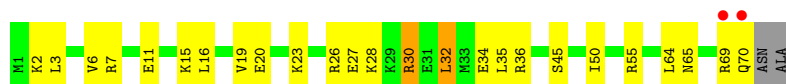
- Molecule 48: 50S ribosomal protein L28



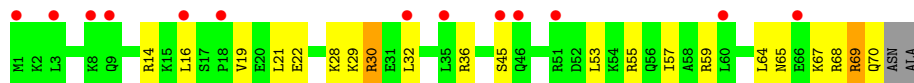
- Molecule 48: 50S ribosomal protein L28



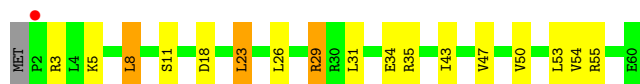
- Molecule 49: 50S ribosomal protein L29



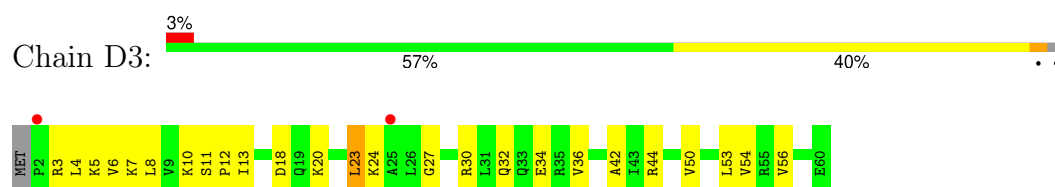
- Molecule 49: 50S ribosomal protein L29



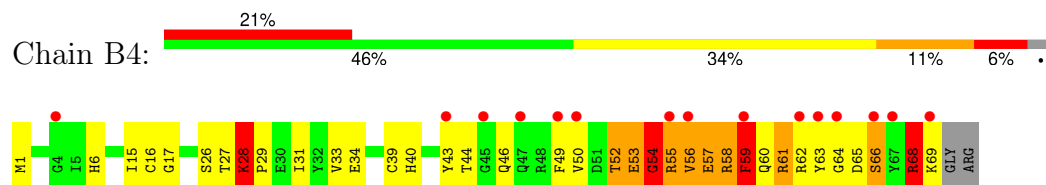
- Molecule 50: 50S ribosomal protein L30



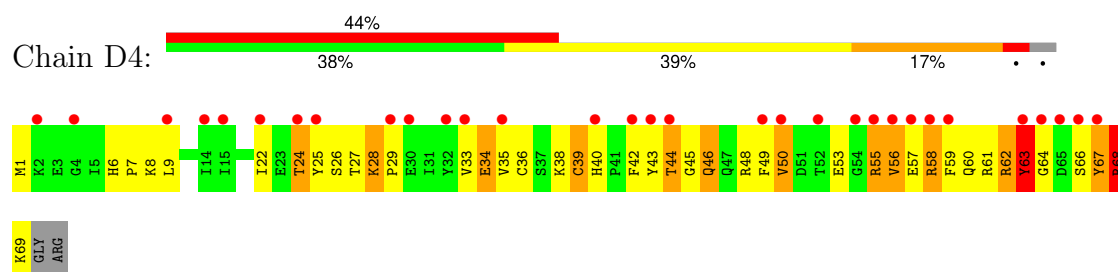
- Molecule 50: 50S ribosomal protein L30



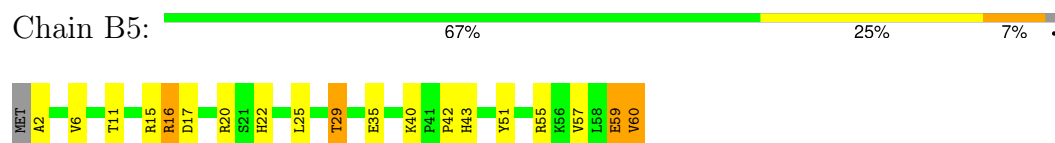
- Molecule 51: 50S ribosomal protein L31



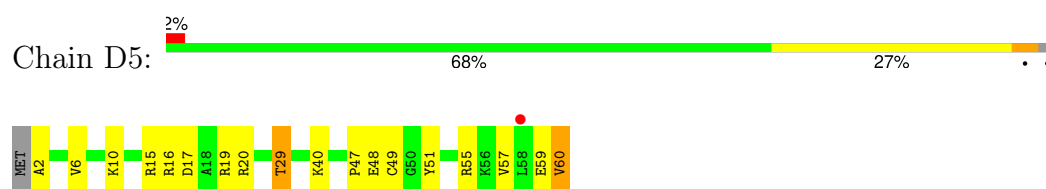
- Molecule 51: 50S ribosomal protein L31



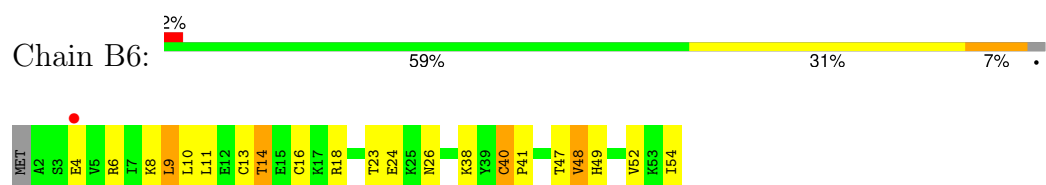
- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32

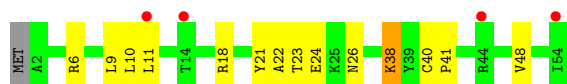


- Molecule 53: 50S ribosomal protein L33

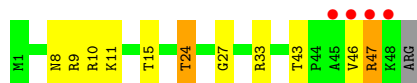
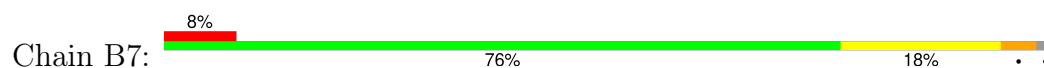


- Molecule 53: 50S ribosomal protein L33

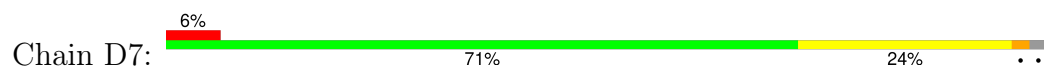




- Molecule 54: 50S ribosomal protein L34



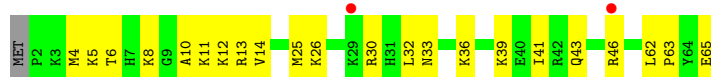
- Molecule 54: 50S ribosomal protein L34



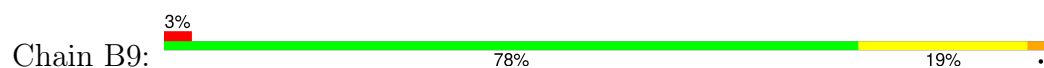
- Molecule 55: 50S ribosomal protein L35



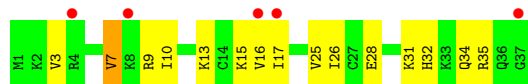
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.32Å 450.06Å 622.23Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 152.51 – 2.55<br>152.51 – 2.55                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.8 (152.51-2.55)<br>95.8 (152.51-2.55)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.28 (at 2.55Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.2_1309                                           | Depositor        |
| R, $R_{free}$                                                           | 0.233 , 0.280<br>0.235 , 0.281                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 90444 reflections (4.81%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 50.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.115                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 58.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 297141                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 5MU, SF4, K, 31M, MG, ZN, 5MC, PSU, 7MG, 4SU

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    | 0.21         | 0/36049     | 0.44        | 4/56261 (0.0%)  |
| 1   | CA    | 0.22         | 0/36170     | 0.47        | 11/56452 (0.0%) |
| 2   | AB    | 0.40         | 0/1881      | 1.01        | 11/2542 (0.4%)  |
| 2   | CB    | 0.44         | 0/1860      | 1.04        | 6/2518 (0.2%)   |
| 3   | AC    | 0.39         | 0/1576      | 0.87        | 1/2130 (0.0%)   |
| 3   | CC    | 0.43         | 0/1566      | 1.01        | 10/2119 (0.5%)  |
| 4   | AD    | 0.39         | 0/1689      | 0.90        | 2/2267 (0.1%)   |
| 4   | CD    | 0.38         | 0/1704      | 0.87        | 2/2284 (0.1%)   |
| 5   | AE    | 0.42         | 0/1145      | 0.92        | 1/1543 (0.1%)   |
| 5   | CE    | 0.43         | 0/1149      | 1.05        | 9/1548 (0.6%)   |
| 6   | AF    | 0.36         | 0/819       | 0.76        | 0/1111          |
| 6   | CF    | 0.38         | 0/829       | 0.81        | 0/1123          |
| 7   | AG    | 0.37         | 0/1250      | 0.87        | 1/1679 (0.1%)   |
| 7   | CG    | 0.37         | 0/1254      | 0.93        | 4/1683 (0.2%)   |
| 8   | AH    | 0.37         | 0/1108      | 0.85        | 0/1494          |
| 8   | CH    | 0.35         | 0/1108      | 0.89        | 2/1494 (0.1%)   |
| 9   | AI    | 0.40         | 0/1002      | 0.90        | 2/1346 (0.1%)   |
| 9   | CI    | 0.41         | 0/997       | 0.92        | 1/1343 (0.1%)   |
| 10  | AJ    | 0.40         | 0/722       | 0.99        | 4/982 (0.4%)    |
| 10  | CJ    | 0.44         | 0/727       | 1.01        | 5/988 (0.5%)    |
| 11  | AK    | 0.39         | 0/844       | 0.90        | 2/1145 (0.2%)   |
| 11  | CK    | 0.39         | 0/848       | 0.88        | 2/1149 (0.2%)   |
| 12  | AL    | 0.38         | 0/946       | 0.82        | 1/1274 (0.1%)   |
| 12  | CL    | 0.37         | 0/946       | 0.88        | 3/1274 (0.2%)   |
| 13  | AM    | 0.39         | 0/969       | 0.98        | 2/1302 (0.2%)   |
| 13  | CM    | 0.40         | 0/961       | 0.94        | 4/1291 (0.3%)   |
| 14  | AN    | 0.38         | 0/501       | 0.80        | 0/664           |
| 14  | CN    | 0.40         | 0/501       | 0.87        | 1/664 (0.2%)    |
| 15  | AO    | 0.38         | 0/739       | 0.88        | 2/985 (0.2%)    |
| 15  | CO    | 0.38         | 0/739       | 0.83        | 0/985           |
| 16  | AP    | 0.38         | 0/697       | 0.83        | 0/939           |
| 16  | CP    | 0.40         | 0/693       | 0.83        | 0/935           |

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 17  | AQ    | 0.36         | 0/836         | 0.80        | 0/1117          |
| 17  | CQ    | 0.33         | 0/836         | 0.79        | 0/1117          |
| 18  | AR    | 0.36         | 0/560         | 0.83        | 0/746           |
| 18  | CR    | 0.36         | 0/560         | 0.79        | 0/746           |
| 19  | AS    | 0.39         | 0/667         | 0.94        | 4/900 (0.4%)    |
| 19  | CS    | 0.45         | 0/661         | 1.05        | 3/893 (0.3%)    |
| 20  | AT    | 0.37         | 0/730         | 0.94        | 2/965 (0.2%)    |
| 20  | CT    | 0.38         | 0/729         | 0.82        | 0/965           |
| 21  | AU    | 0.33         | 0/203         | 0.80        | 0/266           |
| 21  | CU    | 0.38         | 0/203         | 0.91        | 0/266           |
| 22  | AV    | 0.21         | 0/310         | 0.37        | 0/480           |
| 22  | CV    | 0.25         | 0/282         | 0.48        | 0/437           |
| 23  | AW    | 0.28         | 0/1577        | 0.52        | 0/2454          |
| 23  | CW    | 0.35         | 0/1531        | 0.62        | 0/2379          |
| 24  | AX    | 0.27         | 0/1725        | 0.45        | 0/2689          |
| 24  | CX    | 0.24         | 0/1725        | 0.43        | 0/2689          |
| 25  | AY    | 0.35         | 1/1602 (0.1%) | 0.65        | 1/2493 (0.0%)   |
| 25  | CY    | 0.35         | 1/1579 (0.1%) | 0.61        | 0/2455          |
| 26  | BA    | 0.27         | 0/68013       | 0.46        | 4/106165 (0.0%) |
| 26  | DA    | 0.23         | 0/67542       | 0.45        | 0/105428        |
| 27  | BB    | 0.23         | 0/2878        | 0.43        | 0/4490          |
| 27  | DB    | 0.24         | 0/2878        | 0.46        | 0/4490          |
| 28  | BD    | 0.48         | 0/2186        | 0.92        | 6/2944 (0.2%)   |
| 28  | DD    | 0.43         | 0/2186        | 0.89        | 5/2944 (0.2%)   |
| 29  | BE    | 0.49         | 0/1592        | 0.90        | 2/2149 (0.1%)   |
| 29  | DE    | 0.45         | 0/1592        | 0.98        | 8/2149 (0.4%)   |
| 30  | BF    | 0.46         | 0/1619        | 0.85        | 4/2193 (0.2%)   |
| 30  | DF    | 0.41         | 0/1615        | 0.92        | 3/2188 (0.1%)   |
| 31  | BG    | 0.41         | 0/1450        | 0.90        | 5/1959 (0.3%)   |
| 31  | DG    | 0.42         | 0/1449        | 1.03        | 9/1958 (0.5%)   |
| 32  | BH    | 0.43         | 0/1356        | 0.86        | 1/1834 (0.1%)   |
| 32  | DH    | 0.41         | 0/1356        | 0.93        | 3/1834 (0.2%)   |
| 33  | BI    | 0.40         | 0/1100        | 0.95        | 7/1501 (0.5%)   |
| 33  | DI    | 0.40         | 0/1076        | 0.91        | 3/1471 (0.2%)   |
| 34  | BN    | 0.43         | 0/1144        | 0.89        | 2/1543 (0.1%)   |
| 34  | DN    | 0.39         | 0/1144        | 0.98        | 8/1543 (0.5%)   |
| 35  | BO    | 0.46         | 0/943         | 0.84        | 0/1269          |
| 35  | DO    | 0.41         | 0/943         | 0.82        | 0/1269          |
| 36  | BP    | 0.46         | 0/1152        | 0.85        | 2/1533 (0.1%)   |
| 36  | DP    | 0.39         | 0/1152        | 0.93        | 5/1533 (0.3%)   |
| 37  | BQ    | 0.44         | 0/1143        | 0.81        | 0/1527          |
| 37  | DQ    | 0.40         | 0/1143        | 0.84        | 0/1527          |
| 38  | BR    | 0.47         | 0/982         | 0.85        | 0/1312          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | DR    | 0.40         | 0/982           | 0.78        | 0/1312            |
| 39  | BS    | 0.40         | 0/887           | 0.87        | 1/1180 (0.1%)     |
| 39  | DS    | 0.39         | 0/880           | 0.96        | 1/1172 (0.1%)     |
| 40  | BT    | 0.41         | 0/1105          | 0.79        | 0/1477            |
| 40  | DT    | 0.38         | 0/1097          | 0.82        | 0/1468            |
| 41  | BU    | 0.51         | 0/977           | 0.82        | 0/1301            |
| 41  | DU    | 0.39         | 0/977           | 0.82        | 0/1301            |
| 42  | BV    | 0.49         | 0/782           | 0.83        | 1/1049 (0.1%)     |
| 42  | DV    | 0.39         | 0/782           | 0.83        | 0/1049            |
| 43  | BW    | 0.51         | 0/897           | 0.89        | 2/1205 (0.2%)     |
| 43  | DW    | 0.42         | 0/897           | 0.85        | 0/1205            |
| 44  | BX    | 0.47         | 0/764           | 0.86        | 0/1025            |
| 44  | DX    | 0.40         | 0/764           | 0.85        | 0/1025            |
| 45  | BY    | 0.42         | 0/819           | 0.90        | 1/1095 (0.1%)     |
| 45  | DY    | 0.37         | 0/819           | 0.87        | 1/1095 (0.1%)     |
| 46  | BZ    | 0.42         | 0/1379          | 0.98        | 5/1873 (0.3%)     |
| 46  | DZ    | 0.38         | 0/1390          | 0.98        | 12/1890 (0.6%)    |
| 47  | B0    | 0.43         | 0/662           | 0.85        | 2/881 (0.2%)      |
| 47  | D0    | 0.34         | 0/662           | 0.82        | 2/881 (0.2%)      |
| 48  | B1    | 0.46         | 0/762           | 0.87        | 0/1014            |
| 48  | D1    | 0.41         | 0/762           | 0.79        | 0/1014            |
| 49  | B2    | 0.42         | 0/590           | 0.86        | 0/781             |
| 49  | D2    | 0.35         | 0/590           | 0.74        | 0/781             |
| 50  | B3    | 0.46         | 0/474           | 0.88        | 2/635 (0.3%)      |
| 50  | D3    | 0.34         | 0/469           | 0.85        | 0/630             |
| 51  | B4    | 0.46         | 0/571           | 1.19        | 10/768 (1.3%)     |
| 51  | D4    | 0.49         | 0/545           | 1.24        | 8/737 (1.1%)      |
| 52  | B5    | 0.52         | 0/469           | 0.79        | 0/635             |
| 52  | D5    | 0.43         | 0/469           | 0.76        | 0/635             |
| 53  | B6    | 0.45         | 0/460           | 0.77        | 2/613 (0.3%)      |
| 53  | D6    | 0.37         | 0/456           | 0.72        | 0/608             |
| 54  | B7    | 0.51         | 0/426           | 0.82        | 1/561 (0.2%)      |
| 54  | D7    | 0.48         | 0/426           | 0.88        | 0/561             |
| 55  | B8    | 0.46         | 0/519           | 0.86        | 0/684             |
| 55  | D8    | 0.40         | 0/525           | 0.80        | 0/691             |
| 56  | B9    | 0.42         | 0/310           | 0.83        | 0/407             |
| 56  | D9    | 0.36         | 0/310           | 0.84        | 0/407             |
| All | All   | 0.30         | 2/316594 (0.0%) | 0.60        | 231/473970 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | AB    | 0                   | 4                   |
| 7   | AG    | 0                   | 2                   |
| 7   | CG    | 0                   | 1                   |
| 20  | CT    | 0                   | 1                   |
| 28  | BD    | 0                   | 1                   |
| 39  | BS    | 0                   | 1                   |
| 51  | B4    | 0                   | 2                   |
| 51  | D4    | 0                   | 1                   |
| All | All   | 0                   | 13                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 25  | AY    | 8   | 4SU  | O3'-P | 5.64 | 1.61        | 1.56     |
| 25  | CY    | 8   | 4SU  | O3'-P | 5.11 | 1.61        | 1.56     |

The worst 5 of 231 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 51  | B4    | 60  | GLN  | N-CA-C | -8.56 | 103.89      | 112.97   |
| 2   | AB    | 9   | GLU  | N-CA-C | 8.30  | 123.36      | 109.76   |
| 7   | CG    | 79  | ARG  | N-CA-C | 8.20  | 122.37      | 108.67   |
| 8   | CH    | 73  | ASP  | CA-C-N | 8.11  | 128.31      | 119.87   |
| 8   | CH    | 73  | ASP  | C-N-CA | 8.11  | 128.31      | 119.87   |

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | AB    | 18  | GLY  | Peptide |
| 2   | AB    | 231 | GLU  | Peptide |
| 2   | AB    | 8   | LYS  | Peptide |
| 2   | AB    | 9   | GLU  | Peptide |
| 7   | AG    | 78  | ARG  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32205 | 0        | 16254    | 503     | 0            |
| 1   | CA    | 32312 | 0        | 16307    | 665     | 0            |
| 2   | AB    | 1846  | 0        | 1867     | 97      | 0            |
| 2   | CB    | 1825  | 0        | 1828     | 105     | 0            |
| 3   | AC    | 1552  | 0        | 1546     | 55      | 0            |
| 3   | CC    | 1542  | 0        | 1517     | 82      | 0            |
| 4   | AD    | 1659  | 0        | 1676     | 73      | 0            |
| 4   | CD    | 1674  | 0        | 1714     | 63      | 0            |
| 5   | AE    | 1129  | 0        | 1185     | 34      | 0            |
| 5   | CE    | 1133  | 0        | 1191     | 34      | 0            |
| 6   | AF    | 806   | 0        | 793      | 26      | 0            |
| 6   | CF    | 816   | 0        | 808      | 20      | 0            |
| 7   | AG    | 1231  | 0        | 1238     | 30      | 0            |
| 7   | CG    | 1235  | 0        | 1249     | 37      | 0            |
| 8   | AH    | 1088  | 0        | 1126     | 27      | 0            |
| 8   | CH    | 1088  | 0        | 1126     | 41      | 0            |
| 9   | AI    | 983   | 0        | 986      | 47      | 0            |
| 9   | CI    | 978   | 0        | 966      | 48      | 0            |
| 10  | AJ    | 709   | 0        | 650      | 35      | 0            |
| 10  | CJ    | 714   | 0        | 672      | 36      | 0            |
| 11  | AK    | 829   | 0        | 825      | 20      | 0            |
| 11  | CK    | 833   | 0        | 836      | 17      | 0            |
| 12  | AL    | 930   | 0        | 980      | 24      | 0            |
| 12  | CL    | 930   | 0        | 980      | 27      | 0            |
| 13  | AM    | 958   | 0        | 1002     | 31      | 0            |
| 13  | CM    | 950   | 0        | 988      | 40      | 0            |
| 14  | AN    | 492   | 0        | 529      | 16      | 0            |
| 14  | CN    | 492   | 0        | 529      | 33      | 0            |
| 15  | AO    | 728   | 0        | 760      | 21      | 0            |
| 15  | CO    | 728   | 0        | 760      | 30      | 0            |
| 16  | AP    | 681   | 0        | 697      | 12      | 0            |
| 16  | CP    | 677   | 0        | 686      | 23      | 0            |
| 17  | AQ    | 823   | 0        | 891      | 22      | 0            |
| 17  | CQ    | 823   | 0        | 891      | 15      | 0            |
| 18  | AR    | 555   | 0        | 618      | 19      | 0            |
| 18  | CR    | 555   | 0        | 618      | 16      | 0            |
| 19  | AS    | 652   | 0        | 662      | 31      | 0            |
| 19  | CS    | 646   | 0        | 644      | 39      | 0            |
| 20  | AT    | 728   | 0        | 798      | 33      | 0            |
| 20  | CT    | 727   | 0        | 796      | 27      | 0            |
| 21  | AU    | 199   | 0        | 208      | 9       | 0            |
| 21  | CU    | 199   | 0        | 208      | 10      | 0            |
| 22  | AV    | 277   | 0        | 140      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | CV    | 252   | 0        | 130      | 7       | 0            |
| 23  | AW    | 1607  | 0        | 839      | 55      | 0            |
| 23  | CW    | 1560  | 0        | 803      | 56      | 0            |
| 24  | AX    | 1625  | 0        | 828      | 31      | 0            |
| 24  | CX    | 1625  | 0        | 828      | 30      | 0            |
| 25  | AY    | 1581  | 0        | 805      | 95      | 0            |
| 25  | CY    | 1561  | 0        | 796      | 79      | 0            |
| 26  | BA    | 60729 | 0        | 30621    | 675     | 0            |
| 26  | DA    | 60311 | 0        | 30409    | 889     | 0            |
| 27  | BB    | 2573  | 0        | 1306     | 21      | 0            |
| 27  | DB    | 2573  | 0        | 1306     | 50      | 0            |
| 28  | BD    | 2136  | 0        | 2218     | 53      | 0            |
| 28  | DD    | 2136  | 0        | 2218     | 63      | 0            |
| 29  | BE    | 1559  | 0        | 1618     | 30      | 0            |
| 29  | DE    | 1559  | 0        | 1618     | 47      | 0            |
| 30  | BF    | 1584  | 0        | 1625     | 51      | 0            |
| 30  | DF    | 1580  | 0        | 1619     | 53      | 0            |
| 31  | BG    | 1425  | 0        | 1443     | 39      | 0            |
| 31  | DG    | 1424  | 0        | 1434     | 68      | 0            |
| 32  | BH    | 1330  | 0        | 1407     | 28      | 0            |
| 32  | DH    | 1330  | 0        | 1407     | 30      | 0            |
| 33  | BI    | 1085  | 0        | 1114     | 43      | 0            |
| 33  | DI    | 1061  | 0        | 1080     | 26      | 0            |
| 34  | BN    | 1117  | 0        | 1183     | 16      | 0            |
| 34  | DN    | 1117  | 0        | 1184     | 29      | 0            |
| 35  | BO    | 933   | 0        | 996      | 22      | 0            |
| 35  | DO    | 933   | 0        | 996      | 28      | 0            |
| 36  | BP    | 1135  | 0        | 1212     | 39      | 0            |
| 36  | DP    | 1135  | 0        | 1212     | 43      | 0            |
| 37  | BQ    | 1122  | 0        | 1179     | 32      | 0            |
| 37  | DQ    | 1122  | 0        | 1179     | 36      | 0            |
| 38  | BR    | 968   | 0        | 1033     | 18      | 0            |
| 38  | DR    | 968   | 0        | 1033     | 29      | 0            |
| 39  | BS    | 877   | 0        | 938      | 23      | 0            |
| 39  | DS    | 870   | 0        | 923      | 34      | 0            |
| 40  | BT    | 1091  | 0        | 1151     | 28      | 0            |
| 40  | DT    | 1083  | 0        | 1136     | 31      | 0            |
| 41  | BU    | 959   | 0        | 1019     | 20      | 0            |
| 41  | DU    | 959   | 0        | 1019     | 38      | 0            |
| 42  | BV    | 771   | 0        | 830      | 13      | 0            |
| 42  | DV    | 771   | 0        | 830      | 25      | 0            |
| 43  | BW    | 886   | 0        | 939      | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | DW    | 886   | 0        | 940      | 10      | 0            |
| 44  | BX    | 750   | 0        | 814      | 17      | 0            |
| 44  | DX    | 750   | 0        | 814      | 23      | 0            |
| 45  | BY    | 806   | 0        | 881      | 23      | 0            |
| 45  | DY    | 806   | 0        | 881      | 27      | 0            |
| 46  | BZ    | 1349  | 0        | 1355     | 45      | 0            |
| 46  | DZ    | 1360  | 0        | 1363     | 63      | 0            |
| 47  | B0    | 653   | 0        | 674      | 14      | 0            |
| 47  | D0    | 653   | 0        | 674      | 20      | 0            |
| 48  | B1    | 755   | 0        | 826      | 20      | 0            |
| 48  | D1    | 755   | 0        | 826      | 18      | 0            |
| 49  | B2    | 588   | 0        | 643      | 12      | 0            |
| 49  | D2    | 588   | 0        | 643      | 12      | 0            |
| 50  | B3    | 469   | 0        | 518      | 9       | 0            |
| 50  | D3    | 464   | 0        | 514      | 13      | 0            |
| 51  | B4    | 558   | 0        | 544      | 24      | 0            |
| 51  | D4    | 532   | 0        | 503      | 34      | 0            |
| 52  | B5    | 455   | 0        | 465      | 12      | 0            |
| 52  | D5    | 455   | 0        | 465      | 12      | 0            |
| 53  | B6    | 453   | 0        | 473      | 12      | 0            |
| 53  | D6    | 449   | 0        | 469      | 8       | 0            |
| 54  | B7    | 418   | 0        | 467      | 9       | 0            |
| 54  | D7    | 418   | 0        | 467      | 10      | 0            |
| 55  | B8    | 511   | 0        | 571      | 23      | 0            |
| 55  | D8    | 517   | 0        | 582      | 13      | 0            |
| 56  | B9    | 307   | 0        | 335      | 7       | 0            |
| 56  | D9    | 307   | 0        | 335      | 13      | 0            |
| 57  | AA    | 214   | 0        | 0        | 0       | 0            |
| 57  | AE    | 3     | 0        | 0        | 0       | 0            |
| 57  | AF    | 1     | 0        | 0        | 0       | 0            |
| 57  | AK    | 1     | 0        | 0        | 0       | 0            |
| 57  | AM    | 1     | 0        | 0        | 0       | 0            |
| 57  | AN    | 2     | 0        | 0        | 0       | 0            |
| 57  | AW    | 4     | 0        | 0        | 0       | 0            |
| 57  | AX    | 15    | 0        | 0        | 0       | 0            |
| 57  | AY    | 3     | 0        | 0        | 0       | 0            |
| 57  | B0    | 3     | 0        | 0        | 0       | 0            |
| 57  | B1    | 1     | 0        | 0        | 0       | 0            |
| 57  | B2    | 1     | 0        | 0        | 0       | 0            |
| 57  | B3    | 2     | 0        | 0        | 0       | 0            |
| 57  | B4    | 1     | 0        | 0        | 0       | 0            |
| 57  | B5    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | B6    | 2     | 0        | 0        | 0       | 0            |
| 57  | B7    | 5     | 0        | 0        | 0       | 0            |
| 57  | B8    | 1     | 0        | 0        | 0       | 0            |
| 57  | B9    | 1     | 0        | 0        | 0       | 0            |
| 57  | BA    | 812   | 0        | 0        | 0       | 0            |
| 57  | BB    | 20    | 0        | 0        | 0       | 0            |
| 57  | BD    | 9     | 0        | 0        | 0       | 0            |
| 57  | BE    | 8     | 0        | 0        | 0       | 0            |
| 57  | BF    | 9     | 0        | 0        | 0       | 0            |
| 57  | BG    | 3     | 0        | 0        | 0       | 0            |
| 57  | BN    | 6     | 0        | 0        | 0       | 0            |
| 57  | BO    | 2     | 0        | 0        | 0       | 0            |
| 57  | BP    | 5     | 0        | 0        | 0       | 0            |
| 57  | BQ    | 5     | 0        | 0        | 0       | 0            |
| 57  | BR    | 2     | 0        | 0        | 0       | 0            |
| 57  | BU    | 8     | 0        | 0        | 0       | 0            |
| 57  | BV    | 5     | 0        | 0        | 0       | 0            |
| 57  | BW    | 4     | 0        | 0        | 0       | 0            |
| 57  | BX    | 3     | 0        | 0        | 0       | 0            |
| 57  | BY    | 1     | 0        | 0        | 0       | 0            |
| 57  | BZ    | 1     | 0        | 0        | 0       | 0            |
| 57  | CA    | 170   | 0        | 0        | 0       | 0            |
| 57  | CD    | 1     | 0        | 0        | 0       | 0            |
| 57  | CE    | 1     | 0        | 0        | 0       | 0            |
| 57  | CF    | 1     | 0        | 0        | 0       | 0            |
| 57  | CJ    | 1     | 0        | 0        | 0       | 0            |
| 57  | CK    | 1     | 0        | 0        | 0       | 0            |
| 57  | CT    | 1     | 0        | 0        | 0       | 0            |
| 57  | CV    | 1     | 0        | 0        | 0       | 0            |
| 57  | CW    | 1     | 0        | 0        | 0       | 0            |
| 57  | CX    | 3     | 0        | 0        | 1       | 0            |
| 57  | D0    | 1     | 0        | 0        | 0       | 0            |
| 57  | D3    | 1     | 0        | 0        | 0       | 0            |
| 57  | D8    | 1     | 0        | 0        | 0       | 0            |
| 57  | DA    | 677   | 0        | 0        | 0       | 0            |
| 57  | DB    | 13    | 0        | 0        | 0       | 0            |
| 57  | DD    | 9     | 0        | 0        | 0       | 0            |
| 57  | DE    | 4     | 0        | 0        | 0       | 0            |
| 57  | DF    | 4     | 0        | 0        | 0       | 0            |
| 57  | DG    | 1     | 0        | 0        | 0       | 0            |
| 57  | DN    | 1     | 0        | 0        | 0       | 0            |
| 57  | DO    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | DP    | 2     | 0        | 0        | 0       | 0            |
| 57  | DQ    | 4     | 0        | 0        | 0       | 0            |
| 57  | DR    | 1     | 0        | 0        | 0       | 0            |
| 57  | DU    | 2     | 0        | 0        | 0       | 0            |
| 57  | DV    | 3     | 0        | 0        | 0       | 0            |
| 57  | DW    | 4     | 0        | 0        | 0       | 0            |
| 57  | DX    | 1     | 0        | 0        | 0       | 0            |
| 57  | DY    | 1     | 0        | 0        | 0       | 0            |
| 58  | AD    | 8     | 0        | 0        | 0       | 0            |
| 58  | CD    | 8     | 0        | 0        | 0       | 0            |
| 59  | AN    | 1     | 0        | 0        | 0       | 0            |
| 59  | B4    | 1     | 0        | 0        | 0       | 0            |
| 59  | B5    | 1     | 0        | 0        | 0       | 0            |
| 59  | B6    | 1     | 0        | 0        | 0       | 0            |
| 59  | B9    | 1     | 0        | 0        | 0       | 0            |
| 59  | BY    | 1     | 0        | 0        | 0       | 0            |
| 59  | CN    | 1     | 0        | 0        | 0       | 0            |
| 59  | D4    | 1     | 0        | 0        | 0       | 0            |
| 59  | D5    | 1     | 0        | 0        | 0       | 0            |
| 59  | D6    | 1     | 0        | 0        | 0       | 0            |
| 59  | D9    | 1     | 0        | 0        | 0       | 0            |
| 59  | DY    | 1     | 0        | 0        | 0       | 0            |
| 60  | AX    | 1     | 0        | 0        | 0       | 0            |
| 60  | CX    | 1     | 0        | 0        | 0       | 0            |
| 61  | AA    | 227   | 0        | 0        | 17      | 0            |
| 61  | AE    | 2     | 0        | 0        | 0       | 0            |
| 61  | AJ    | 1     | 0        | 0        | 0       | 0            |
| 61  | AL    | 1     | 0        | 0        | 1       | 0            |
| 61  | AM    | 1     | 0        | 0        | 0       | 0            |
| 61  | AU    | 1     | 0        | 0        | 1       | 0            |
| 61  | AV    | 3     | 0        | 0        | 0       | 0            |
| 61  | AW    | 3     | 0        | 0        | 0       | 0            |
| 61  | AX    | 6     | 0        | 0        | 2       | 0            |
| 61  | AY    | 1     | 0        | 0        | 0       | 0            |
| 61  | B0    | 3     | 0        | 0        | 0       | 0            |
| 61  | B1    | 1     | 0        | 0        | 0       | 0            |
| 61  | B3    | 2     | 0        | 0        | 0       | 0            |
| 61  | B5    | 2     | 0        | 0        | 0       | 0            |
| 61  | B6    | 1     | 0        | 0        | 0       | 0            |
| 61  | B7    | 2     | 0        | 0        | 0       | 0            |
| 61  | B8    | 8     | 0        | 0        | 1       | 0            |
| 61  | BA    | 1383  | 0        | 0        | 61      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61  | BB    | 36     | 0        | 0        | 1       | 0            |
| 61  | BD    | 12     | 0        | 0        | 1       | 0            |
| 61  | BE    | 14     | 0        | 0        | 4       | 0            |
| 61  | BF    | 8      | 0        | 0        | 0       | 0            |
| 61  | BG    | 3      | 0        | 0        | 0       | 0            |
| 61  | BI    | 1      | 0        | 0        | 0       | 0            |
| 61  | BO    | 4      | 0        | 0        | 0       | 0            |
| 61  | BP    | 16     | 0        | 0        | 3       | 0            |
| 61  | BQ    | 4      | 0        | 0        | 0       | 0            |
| 61  | BR    | 2      | 0        | 0        | 0       | 0            |
| 61  | BT    | 2      | 0        | 0        | 0       | 0            |
| 61  | BU    | 3      | 0        | 0        | 0       | 0            |
| 61  | BV    | 2      | 0        | 0        | 0       | 0            |
| 61  | BW    | 1      | 0        | 0        | 0       | 0            |
| 61  | BX    | 4      | 0        | 0        | 0       | 0            |
| 61  | BZ    | 1      | 0        | 0        | 0       | 0            |
| 61  | CA    | 185    | 0        | 0        | 17      | 0            |
| 61  | CJ    | 2      | 0        | 0        | 1       | 0            |
| 61  | CL    | 1      | 0        | 0        | 0       | 0            |
| 61  | CT    | 1      | 0        | 0        | 0       | 0            |
| 61  | CV    | 1      | 0        | 0        | 0       | 0            |
| 61  | CW    | 2      | 0        | 0        | 0       | 0            |
| 61  | D0    | 3      | 0        | 0        | 0       | 0            |
| 61  | D1    | 1      | 0        | 0        | 0       | 0            |
| 61  | D3    | 1      | 0        | 0        | 1       | 0            |
| 61  | D7    | 3      | 0        | 0        | 0       | 0            |
| 61  | D8    | 4      | 0        | 0        | 0       | 0            |
| 61  | DA    | 1025   | 0        | 0        | 79      | 0            |
| 61  | DB    | 9      | 0        | 0        | 0       | 0            |
| 61  | DD    | 19     | 0        | 0        | 4       | 0            |
| 61  | DE    | 11     | 0        | 0        | 0       | 0            |
| 61  | DF    | 3      | 0        | 0        | 0       | 0            |
| 61  | DN    | 2      | 0        | 0        | 1       | 0            |
| 61  | DO    | 1      | 0        | 0        | 0       | 0            |
| 61  | DP    | 16     | 0        | 0        | 2       | 0            |
| 61  | DR    | 1      | 0        | 0        | 0       | 0            |
| 61  | DT    | 3      | 0        | 0        | 0       | 0            |
| 61  | DU    | 2      | 0        | 0        | 0       | 0            |
| 61  | DX    | 3      | 0        | 0        | 0       | 0            |
| 61  | DY    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 297141 | 0        | 196251   | 5318    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5318 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 25:CY:7:A:N6    | 25:CY:66:U:H3   | 1.37                     | 1.21              |
| 25:AY:49:C:N4   | 25:AY:65:G:H1   | 1.44                     | 1.16              |
| 26:DA:2139:C:N4 | 26:DA:2152:G:H1 | 1.42                     | 1.16              |
| 1:CA:1000:U:H3  | 1:CA:1041:A:N6  | 1.44                     | 1.15              |
| 1:CA:1002:G:H1  | 1:CA:1038:C:N4  | 1.48                     | 1.12              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2   | AB    | 229/256 (90%) | 208 (91%) | 14 (6%) | 7 (3%)   | 3           | 2   |
| 2   | CB    | 229/256 (90%) | 206 (90%) | 16 (7%) | 7 (3%)   | 3           | 2   |
| 3   | AC    | 204/239 (85%) | 195 (96%) | 8 (4%)  | 1 (0%)   | 24          | 34  |
| 3   | CC    | 204/239 (85%) | 189 (93%) | 15 (7%) | 0        | 100         | 100 |
| 4   | AD    | 206/209 (99%) | 197 (96%) | 7 (3%)  | 2 (1%)   | 12          | 17  |
| 4   | CD    | 206/209 (99%) | 196 (95%) | 9 (4%)  | 1 (0%)   | 24          | 34  |
| 5   | AE    | 146/162 (90%) | 142 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 5   | CE    | 146/162 (90%) | 140 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 6   | AF    | 98/101 (97%)  | 97 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 6   | CF    | 98/101 (97%)  | 97 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 7   | AG    | 153/156 (98%) | 144 (94%) | 5 (3%)  | 4 (3%)   | 4           | 3   |
| 7   | CG    | 153/156 (98%) | 144 (94%) | 8 (5%)  | 1 (1%)   | 18          | 25  |
| 8   | AH    | 135/138 (98%) | 134 (99%) | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 8   | CH    | 135/138 (98%) | 132 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 9   | AI    | 125/128 (98%) | 117 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 9   | CI    | 125/128 (98%) | 119 (95%) | 5 (4%)  | 1 (1%)   | 16          | 22  |
| 10  | AJ    | 95/105 (90%)  | 85 (90%)  | 6 (6%)  | 4 (4%)   | 2           | 1   |
| 10  | CJ    | 94/105 (90%)  | 85 (90%)  | 4 (4%)  | 5 (5%)   | 1           | 0   |
| 11  | AK    | 112/129 (87%) | 104 (93%) | 6 (5%)  | 2 (2%)   | 6           | 7   |
| 11  | CK    | 112/129 (87%) | 103 (92%) | 7 (6%)  | 2 (2%)   | 6           | 7   |
| 12  | AL    | 120/132 (91%) | 117 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 12  | CL    | 120/132 (91%) | 118 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 13  | AM    | 121/126 (96%) | 116 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 13  | CM    | 120/126 (95%) | 113 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 14  | AN    | 58/61 (95%)   | 56 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 14  | CN    | 58/61 (95%)   | 56 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 15  | AO    | 86/89 (97%)   | 82 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 15  | CO    | 86/89 (97%)   | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 16  | AP    | 80/88 (91%)   | 79 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 16  | CP    | 80/88 (91%)   | 78 (98%)  | 1 (1%)  | 1 (1%)   | 9           | 12  |
| 17  | AQ    | 97/105 (92%)  | 93 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 17  | CQ    | 97/105 (92%)  | 93 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 18  | AR    | 66/88 (75%)   | 65 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 18  | CR    | 66/88 (75%)   | 65 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 19  | AS    | 81/93 (87%)   | 73 (90%)  | 7 (9%)  | 1 (1%)   | 10          | 13  |
| 19  | CS    | 81/93 (87%)   | 72 (89%)  | 9 (11%) | 0        | 100         | 100 |
| 20  | AT    | 94/106 (89%)  | 87 (93%)  | 3 (3%)  | 4 (4%)   | 2           | 1   |
| 20  | CT    | 94/106 (89%)  | 88 (94%)  | 3 (3%)  | 3 (3%)   | 3           | 2   |
| 21  | AU    | 21/27 (78%)   | 20 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 21  | CU    | 21/27 (78%)   | 20 (95%)  | 1 (5%)  | 0        | 100         | 100 |
| 28  | BD    | 273/276 (99%) | 264 (97%) | 8 (3%)  | 1 (0%)   | 30          | 39  |
| 28  | DD    | 273/276 (99%) | 263 (96%) | 8 (3%)  | 2 (1%)   | 18          | 25  |
| 29  | BE    | 202/206 (98%) | 196 (97%) | 5 (2%)  | 1 (0%)   | 24          | 34  |
| 29  | DE    | 202/206 (98%) | 196 (97%) | 4 (2%)  | 2 (1%)   | 12          | 17  |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 30  | BF    | 201/210 (96%) | 200 (100%) | 0       | 1 (0%)   | 24          | 34  |
| 30  | DF    | 201/210 (96%) | 199 (99%)  | 0       | 2 (1%)   | 12          | 17  |
| 31  | BG    | 179/182 (98%) | 170 (95%)  | 8 (4%)  | 1 (1%)   | 21          | 29  |
| 31  | DG    | 179/182 (98%) | 171 (96%)  | 5 (3%)  | 3 (2%)   | 7           | 8   |
| 32  | BH    | 172/180 (96%) | 168 (98%)  | 3 (2%)  | 1 (1%)   | 21          | 29  |
| 32  | DH    | 172/180 (96%) | 166 (96%)  | 5 (3%)  | 1 (1%)   | 21          | 29  |
| 33  | BI    | 144/148 (97%) | 130 (90%)  | 11 (8%) | 3 (2%)   | 5           | 5   |
| 33  | DI    | 144/148 (97%) | 133 (92%)  | 10 (7%) | 1 (1%)   | 18          | 25  |
| 34  | BN    | 138/140 (99%) | 136 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 34  | DN    | 138/140 (99%) | 135 (98%)  | 2 (1%)  | 1 (1%)   | 18          | 25  |
| 35  | BO    | 120/122 (98%) | 114 (95%)  | 6 (5%)  | 0        | 100         | 100 |
| 35  | DO    | 120/122 (98%) | 116 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 36  | BP    | 147/150 (98%) | 140 (95%)  | 6 (4%)  | 1 (1%)   | 18          | 25  |
| 36  | DP    | 147/150 (98%) | 138 (94%)  | 7 (5%)  | 2 (1%)   | 9           | 11  |
| 37  | BQ    | 139/141 (99%) | 135 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 37  | DQ    | 139/141 (99%) | 134 (96%)  | 4 (3%)  | 1 (1%)   | 18          | 25  |
| 38  | BR    | 116/118 (98%) | 111 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 38  | DR    | 116/118 (98%) | 111 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 39  | BS    | 108/112 (96%) | 104 (96%)  | 3 (3%)  | 1 (1%)   | 14          | 20  |
| 39  | DS    | 108/112 (96%) | 105 (97%)  | 2 (2%)  | 1 (1%)   | 14          | 20  |
| 40  | BT    | 129/146 (88%) | 122 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 40  | DT    | 129/146 (88%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 41  | BU    | 114/118 (97%) | 114 (100%) | 0       | 0        | 100         | 100 |
| 41  | DU    | 114/118 (97%) | 114 (100%) | 0       | 0        | 100         | 100 |
| 42  | BV    | 99/101 (98%)  | 93 (94%)   | 6 (6%)  | 0        | 100         | 100 |
| 42  | DV    | 99/101 (98%)  | 95 (96%)   | 3 (3%)  | 1 (1%)   | 12          | 17  |
| 43  | BW    | 110/113 (97%) | 110 (100%) | 0       | 0        | 100         | 100 |
| 43  | DW    | 110/113 (97%) | 110 (100%) | 0       | 0        | 100         | 100 |
| 44  | BX    | 93/96 (97%)   | 89 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 44  | DX    | 93/96 (97%)   | 89 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 45  | BY    | 105/110 (96%) | 98 (93%)   | 7 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 45  | DY    | 105/110 (96%)     | 101 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 46  | BZ    | 169/206 (82%)     | 153 (90%)   | 15 (9%)  | 1 (1%)   | 21          | 29  |
| 46  | DZ    | 172/206 (84%)     | 161 (94%)   | 11 (6%)  | 0        | 100         | 100 |
| 47  | B0    | 81/85 (95%)       | 81 (100%)   | 0        | 0        | 100         | 100 |
| 47  | D0    | 81/85 (95%)       | 79 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 48  | B1    | 95/98 (97%)       | 94 (99%)    | 0        | 1 (1%)   | 11          | 15  |
| 48  | D1    | 95/98 (97%)       | 93 (98%)    | 1 (1%)   | 1 (1%)   | 11          | 15  |
| 49  | B2    | 68/72 (94%)       | 68 (100%)   | 0        | 0        | 100         | 100 |
| 49  | D2    | 68/72 (94%)       | 68 (100%)   | 0        | 0        | 100         | 100 |
| 50  | B3    | 57/60 (95%)       | 56 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 50  | D3    | 57/60 (95%)       | 55 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 51  | B4    | 67/71 (94%)       | 53 (79%)    | 11 (16%) | 3 (4%)   | 2           | 1   |
| 51  | D4    | 67/71 (94%)       | 53 (79%)    | 9 (13%)  | 5 (8%)   | 1           | 0   |
| 52  | B5    | 57/60 (95%)       | 53 (93%)    | 4 (7%)   | 0        | 100         | 100 |
| 52  | D5    | 57/60 (95%)       | 53 (93%)    | 4 (7%)   | 0        | 100         | 100 |
| 53  | B6    | 51/54 (94%)       | 49 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 53  | D6    | 51/54 (94%)       | 49 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 54  | B7    | 46/49 (94%)       | 46 (100%)   | 0        | 0        | 100         | 100 |
| 54  | D7    | 46/49 (94%)       | 45 (98%)    | 0        | 1 (2%)   | 5           | 5   |
| 55  | B8    | 62/65 (95%)       | 62 (100%)   | 0        | 0        | 100         | 100 |
| 55  | D8    | 62/65 (95%)       | 62 (100%)   | 0        | 0        | 100         | 100 |
| 56  | B9    | 35/37 (95%)       | 35 (100%)   | 0        | 0        | 100         | 100 |
| 56  | D9    | 35/37 (95%)       | 35 (100%)   | 0        | 0        | 100         | 100 |
| All | All   | 11409/12128 (94%) | 10908 (96%) | 416 (4%) | 85 (1%)  | 18          | 25  |

5 of 85 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 126 | GLU  |
| 7   | AG    | 80  | VAL  |
| 20  | AT    | 10  | LEU  |
| 20  | AT    | 96  | GLY  |
| 28  | BD    | 275 | LYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | AB    | 192/220 (87%) | 153 (80%) | 39 (20%) | 1           | 1  |
| 2   | CB    | 187/220 (85%) | 148 (79%) | 39 (21%) | 1           | 1  |
| 3   | AC    | 143/188 (76%) | 116 (81%) | 27 (19%) | 1           | 1  |
| 3   | CC    | 140/188 (74%) | 119 (85%) | 21 (15%) | 3           | 2  |
| 4   | AD    | 170/181 (94%) | 149 (88%) | 21 (12%) | 4           | 4  |
| 4   | CD    | 173/181 (96%) | 153 (88%) | 20 (12%) | 5           | 6  |
| 5   | AE    | 113/123 (92%) | 104 (92%) | 9 (8%)   | 11          | 15 |
| 5   | CE    | 114/123 (93%) | 102 (90%) | 12 (10%) | 6           | 8  |
| 6   | AF    | 83/90 (92%)   | 72 (87%)  | 11 (13%) | 4           | 4  |
| 6   | CF    | 85/90 (94%)   | 77 (91%)  | 8 (9%)   | 8           | 10 |
| 7   | AG    | 119/127 (94%) | 106 (89%) | 13 (11%) | 6           | 7  |
| 7   | CG    | 120/127 (94%) | 107 (89%) | 13 (11%) | 6           | 7  |
| 8   | AH    | 114/119 (96%) | 101 (89%) | 13 (11%) | 5           | 6  |
| 8   | CH    | 114/119 (96%) | 99 (87%)  | 15 (13%) | 4           | 4  |
| 9   | AI    | 90/99 (91%)   | 72 (80%)  | 18 (20%) | 1           | 1  |
| 9   | CI    | 89/99 (90%)   | 75 (84%)  | 14 (16%) | 2           | 2  |
| 10  | AJ    | 66/92 (72%)   | 57 (86%)  | 9 (14%)  | 3           | 3  |
| 10  | CJ    | 69/92 (75%)   | 63 (91%)  | 6 (9%)   | 9           | 13 |
| 11  | AK    | 82/99 (83%)   | 75 (92%)  | 7 (8%)   | 10          | 13 |
| 11  | CK    | 83/99 (84%)   | 76 (92%)  | 7 (8%)   | 10          | 14 |
| 12  | AL    | 97/109 (89%)  | 92 (95%)  | 5 (5%)   | 21          | 32 |
| 12  | CL    | 97/109 (89%)  | 92 (95%)  | 5 (5%)   | 21          | 32 |
| 13  | AM    | 93/101 (92%)  | 79 (85%)  | 14 (15%) | 3           | 2  |
| 13  | CM    | 92/101 (91%)  | 77 (84%)  | 15 (16%) | 2           | 2  |
| 14  | AN    | 49/50 (98%)   | 42 (86%)  | 7 (14%)  | 3           | 3  |
| 14  | CN    | 49/50 (98%)   | 41 (84%)  | 8 (16%)  | 2           | 2  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15  | AO    | 78/80 (98%)    | 65 (83%)  | 13 (17%) | 2           | 2  |
| 15  | CO    | 78/80 (98%)    | 70 (90%)  | 8 (10%)  | 7           | 8  |
| 16  | AP    | 69/74 (93%)    | 59 (86%)  | 10 (14%) | 3           | 2  |
| 16  | CP    | 68/74 (92%)    | 60 (88%)  | 8 (12%)  | 5           | 5  |
| 17  | AQ    | 94/97 (97%)    | 81 (86%)  | 13 (14%) | 3           | 3  |
| 17  | CQ    | 94/97 (97%)    | 84 (89%)  | 10 (11%) | 6           | 7  |
| 18  | AR    | 59/77 (77%)    | 52 (88%)  | 7 (12%)  | 5           | 5  |
| 18  | CR    | 59/77 (77%)    | 51 (86%)  | 8 (14%)  | 3           | 3  |
| 19  | AS    | 69/80 (86%)    | 62 (90%)  | 7 (10%)  | 7           | 8  |
| 19  | CS    | 67/80 (84%)    | 61 (91%)  | 6 (9%)   | 9           | 11 |
| 20  | AT    | 70/82 (85%)    | 61 (87%)  | 9 (13%)  | 4           | 4  |
| 20  | CT    | 70/82 (85%)    | 58 (83%)  | 12 (17%) | 2           | 1  |
| 21  | AU    | 18/22 (82%)    | 16 (89%)  | 2 (11%)  | 6           | 6  |
| 21  | CU    | 18/22 (82%)    | 16 (89%)  | 2 (11%)  | 6           | 6  |
| 28  | BD    | 215/218 (99%)  | 193 (90%) | 22 (10%) | 7           | 8  |
| 28  | DD    | 215/218 (99%)  | 191 (89%) | 24 (11%) | 6           | 6  |
| 29  | BE    | 164/166 (99%)  | 142 (87%) | 22 (13%) | 4           | 3  |
| 29  | DE    | 164/166 (99%)  | 138 (84%) | 26 (16%) | 2           | 2  |
| 30  | BF    | 160/166 (96%)  | 140 (88%) | 20 (12%) | 4           | 4  |
| 30  | DF    | 159/166 (96%)  | 136 (86%) | 23 (14%) | 3           | 2  |
| 31  | BG    | 143/156 (92%)  | 128 (90%) | 15 (10%) | 6           | 8  |
| 31  | DG    | 142/156 (91%)  | 121 (85%) | 21 (15%) | 3           | 2  |
| 32  | BH    | 144/148 (97%)  | 125 (87%) | 19 (13%) | 4           | 4  |
| 32  | DH    | 144/148 (97%)  | 125 (87%) | 19 (13%) | 4           | 4  |
| 33  | BI    | 110/124 (89%)  | 87 (79%)  | 23 (21%) | 1           | 1  |
| 33  | DI    | 104/124 (84%)  | 87 (84%)  | 17 (16%) | 2           | 2  |
| 34  | BN    | 118/119 (99%)  | 99 (84%)  | 19 (16%) | 2           | 2  |
| 34  | DN    | 118/119 (99%)  | 102 (86%) | 16 (14%) | 3           | 3  |
| 35  | BO    | 100/100 (100%) | 91 (91%)  | 9 (9%)   | 9           | 11 |
| 35  | DO    | 100/100 (100%) | 90 (90%)  | 10 (10%) | 7           | 9  |
| 36  | BP    | 115/116 (99%)  | 99 (86%)  | 16 (14%) | 3           | 3  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 36  | DP    | 115/116 (99%)  | 100 (87%) | 15 (13%) | 4           | 4  |
| 37  | BQ    | 111/111 (100%) | 97 (87%)  | 14 (13%) | 4           | 4  |
| 37  | DQ    | 111/111 (100%) | 97 (87%)  | 14 (13%) | 4           | 4  |
| 38  | BR    | 101/101 (100%) | 80 (79%)  | 21 (21%) | 1           | 1  |
| 38  | DR    | 101/101 (100%) | 83 (82%)  | 18 (18%) | 2           | 1  |
| 39  | BS    | 87/88 (99%)    | 77 (88%)  | 10 (12%) | 5           | 6  |
| 39  | DS    | 85/88 (97%)    | 71 (84%)  | 14 (16%) | 2           | 2  |
| 40  | BT    | 115/127 (91%)  | 103 (90%) | 12 (10%) | 7           | 8  |
| 40  | DT    | 113/127 (89%)  | 100 (88%) | 13 (12%) | 5           | 6  |
| 41  | BU    | 93/94 (99%)    | 84 (90%)  | 9 (10%)  | 8           | 9  |
| 41  | DU    | 93/94 (99%)    | 84 (90%)  | 9 (10%)  | 8           | 9  |
| 42  | BV    | 80/82 (98%)    | 68 (85%)  | 12 (15%) | 3           | 2  |
| 42  | DV    | 80/82 (98%)    | 65 (81%)  | 15 (19%) | 1           | 1  |
| 43  | BW    | 90/92 (98%)    | 81 (90%)  | 9 (10%)  | 7           | 9  |
| 43  | DW    | 90/92 (98%)    | 84 (93%)  | 6 (7%)   | 15          | 21 |
| 44  | BX    | 77/78 (99%)    | 70 (91%)  | 7 (9%)   | 9           | 11 |
| 44  | DX    | 77/78 (99%)    | 69 (90%)  | 8 (10%)  | 7           | 8  |
| 45  | BY    | 85/91 (93%)    | 76 (89%)  | 9 (11%)  | 6           | 7  |
| 45  | DY    | 85/91 (93%)    | 78 (92%)  | 7 (8%)   | 10          | 14 |
| 46  | BZ    | 145/179 (81%)  | 128 (88%) | 17 (12%) | 5           | 6  |
| 46  | DZ    | 145/179 (81%)  | 123 (85%) | 22 (15%) | 3           | 2  |
| 47  | B0    | 65/67 (97%)    | 61 (94%)  | 4 (6%)   | 16          | 24 |
| 47  | D0    | 65/67 (97%)    | 61 (94%)  | 4 (6%)   | 16          | 24 |
| 48  | B1    | 80/83 (96%)    | 74 (92%)  | 6 (8%)   | 12          | 17 |
| 48  | D1    | 80/83 (96%)    | 68 (85%)  | 12 (15%) | 3           | 2  |
| 49  | B2    | 65/67 (97%)    | 56 (86%)  | 9 (14%)  | 3           | 3  |
| 49  | D2    | 65/67 (97%)    | 57 (88%)  | 8 (12%)  | 4           | 4  |
| 50  | B3    | 51/52 (98%)    | 45 (88%)  | 6 (12%)  | 5           | 5  |
| 50  | D3    | 50/52 (96%)    | 44 (88%)  | 6 (12%)  | 5           | 5  |
| 51  | B4    | 60/63 (95%)    | 47 (78%)  | 13 (22%) | 1           | 1  |
| 51  | D4    | 53/63 (84%)    | 43 (81%)  | 10 (19%) | 1           | 1  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 52  | B5    | 50/52 (96%)      | 43 (86%)   | 7 (14%)    | 3           | 3  |
| 52  | D5    | 50/52 (96%)      | 44 (88%)   | 6 (12%)    | 5           | 5  |
| 53  | B6    | 51/52 (98%)      | 45 (88%)   | 6 (12%)    | 5           | 5  |
| 53  | D6    | 50/52 (96%)      | 47 (94%)   | 3 (6%)     | 17          | 26 |
| 54  | B7    | 41/42 (98%)      | 38 (93%)   | 3 (7%)     | 13          | 18 |
| 54  | D7    | 41/42 (98%)      | 36 (88%)   | 5 (12%)    | 5           | 4  |
| 55  | B8    | 53/55 (96%)      | 47 (89%)   | 6 (11%)    | 5           | 6  |
| 55  | D8    | 54/55 (98%)      | 47 (87%)   | 7 (13%)    | 4           | 4  |
| 56  | B9    | 34/34 (100%)     | 33 (97%)   | 1 (3%)     | 37          | 55 |
| 56  | D9    | 34/34 (100%)     | 32 (94%)   | 2 (6%)     | 18          | 27 |
| All | All   | 9320/10066 (93%) | 8123 (87%) | 1197 (13%) | 4           | 4  |

5 of 1197 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | DG    | 140 | ILE  |
| 48  | D1    | 89  | GLU  |
| 33  | DI    | 40  | THR  |
| 31  | DG    | 136 | ARG  |
| 39  | DS    | 14  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DD    | 126 | GLN  |
| 44  | DX    | 82  | GLN  |
| 29  | DE    | 85  | ASN  |
| 35  | DO    | 89  | ASN  |
| 47  | D0    | 35  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1495/1521 (98%) | 307 (20%)         | 25 (1%)         |
| 1   | CA    | 1501/1521 (98%) | 317 (21%)         | 28 (1%)         |
| 22  | AV    | 12/24 (50%)     | 3 (25%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 22  | CV    | 11/24 (45%)     | 2 (18%)           | 0               |
| 23  | AW    | 71/76 (93%)     | 30 (42%)          | 2 (2%)          |
| 23  | CW    | 68/76 (89%)     | 32 (47%)          | 2 (2%)          |
| 24  | AX    | 75/77 (97%)     | 16 (21%)          | 0               |
| 24  | CX    | 75/77 (97%)     | 21 (28%)          | 0               |
| 25  | AY    | 72/76 (94%)     | 37 (51%)          | 4 (5%)          |
| 25  | CY    | 70/76 (92%)     | 33 (47%)          | 1 (1%)          |
| 26  | BA    | 2811/2915 (96%) | 450 (16%)         | 34 (1%)         |
| 26  | DA    | 2791/2915 (95%) | 553 (19%)         | 30 (1%)         |
| 27  | BB    | 119/121 (98%)   | 14 (11%)          | 0               |
| 27  | DB    | 119/121 (98%)   | 17 (14%)          | 0               |
| All | All   | 9290/9620 (96%) | 1832 (19%)        | 126 (1%)        |

5 of 1832 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 6   | G    |
| 1   | AA    | 7   | G    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 22  | G    |
| 1   | AA    | 29  | G    |

5 of 126 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 26  | BA    | 2181 | G    |
| 26  | DA    | 1427 | A    |
| 1   | CA    | 532  | A    |
| 26  | DA    | 1420 | U    |
| 26  | DA    | 2126 | A    |

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

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

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | MIA  | CY    | 37  | 25    | 21,24,32     | 1.65 | 4 (19%)  | 30,35,47    | 2.01 | 9 (30%)  |
| 25  | 5MU  | AY    | 54  | 25    | 19,22,23     | 1.49 | 5 (26%)  | 27,32,35    | 2.16 | 7 (25%)  |
| 23  | PSU  | CW    | 55  | 23    | 18,21,22     | 1.37 | 2 (11%)  | 21,30,33    | 2.11 | 3 (14%)  |
| 25  | PSU  | AY    | 39  | 25    | 18,21,22     | 1.57 | 4 (22%)  | 21,30,33    | 1.95 | 5 (23%)  |
| 23  | 5MU  | CW    | 54  | 23    | 19,22,23     | 1.34 | 4 (21%)  | 27,32,35    | 2.00 | 7 (25%)  |
| 25  | 4SU  | AY    | 8   | 25    | 18,21,22     | 1.87 | 5 (27%)  | 25,30,33    | 2.06 | 5 (20%)  |
| 23  | PSU  | CW    | 32  | 23    | 18,21,22     | 1.34 | 2 (11%)  | 21,30,33    | 1.99 | 3 (14%)  |
| 23  | 4SU  | CW    | 8   | 23    | 18,21,22     | 1.67 | 4 (22%)  | 25,30,33    | 2.41 | 5 (20%)  |
| 23  | 7MG  | CW    | 46  | 23    | 23,26,27     | 1.41 | 4 (17%)  | 27,39,42    | 2.51 | 6 (22%)  |
| 24  | 5MC  | CX    | 32  | 24    | 19,22,23     | 1.64 | 3 (15%)  | 26,32,35    | 1.17 | 3 (11%)  |
| 24  | 5MU  | AX    | 54  | 24,57 | 19,22,23     | 1.43 | 5 (26%)  | 27,32,35    | 1.96 | 5 (18%)  |
| 25  | MIA  | AY    | 37  | 25    | 21,24,32     | 1.63 | 4 (19%)  | 30,35,47    | 2.02 | 8 (26%)  |
| 24  | 4SU  | AX    | 8   | 24    | 18,21,22     | 2.28 | 5 (27%)  | 25,30,33    | 1.72 | 6 (24%)  |
| 23  | 31M  | AW    | 76  | 23    | 41,44,45     | 1.46 | 6 (14%)  | 50,61,64    | 1.72 | 11 (22%) |
| 23  | PSU  | AW    | 39  | 23    | 18,21,22     | 1.40 | 2 (11%)  | 21,30,33    | 1.85 | 4 (19%)  |
| 25  | 7MG  | CY    | 46  | 25    | 23,26,27     | 1.42 | 5 (21%)  | 27,39,42    | 2.67 | 9 (33%)  |
| 23  | PSU  | AW    | 32  | 23    | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 24  | 5MC  | AX    | 32  | 24    | 19,22,23     | 1.69 | 3 (15%)  | 26,32,35    | 1.28 | 3 (11%)  |
| 25  | PSU  | AY    | 55  | 25    | 18,21,22     | 1.37 | 3 (16%)  | 21,30,33    | 2.34 | 6 (28%)  |
| 23  | 5MU  | AW    | 54  | 23    | 19,22,23     | 1.39 | 5 (26%)  | 27,32,35    | 1.93 | 6 (22%)  |
| 23  | 4SU  | AW    | 8   | 23    | 18,21,22     | 1.80 | 4 (22%)  | 25,30,33    | 2.15 | 5 (20%)  |
| 25  | PSU  | CY    | 55  | 25    | 18,21,22     | 1.46 | 4 (22%)  | 21,30,33    | 2.45 | 6 (28%)  |
| 23  | PSU  | AW    | 55  | 23    | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 1.95 | 3 (14%)  |
| 25  | PSU  | AY    | 32  | 25    | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 2.01 | 4 (19%)  |
| 24  | PSU  | AX    | 55  | 24,57 | 18,21,22     | 1.33 | 2 (11%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 25  | 7MG  | AY    | 46  | 25    | 23,26,27     | 1.29 | 3 (13%)  | 27,39,42    | 2.94 | 7 (25%)  |
| 23  | 7MG  | AW    | 46  | 23    | 23,26,27     | 1.36 | 3 (13%)  | 27,39,42    | 2.63 | 7 (25%)  |
| 24  | PSU  | CX    | 55  | 24    | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 23  | 31M  | CW    | 76  | 23    | 41,44,45     | 1.38 | 5 (12%)  | 50,61,64    | 1.66 | 10 (20%) |
| 25  | 5MU  | CY    | 54  | 25    | 19,22,23     | 1.34 | 4 (21%)  | 27,32,35    | 2.19 | 6 (22%)  |
| 23  | PSU  | CW    | 39  | 23    | 18,21,22     | 1.35 | 2 (11%)  | 21,30,33    | 1.86 | 4 (19%)  |
| 24  | 5MU  | CX    | 54  | 24    | 19,22,23     | 1.39 | 5 (26%)  | 27,32,35    | 2.30 | 6 (22%)  |
| 23  | MIA  | CW    | 37  | 23    | 21,24,32     | 1.60 | 4 (19%)  | 30,35,47    | 2.04 | 7 (23%)  |
| 24  | 4SU  | CX    | 8   | 24    | 18,21,22     | 2.04 | 6 (33%)  | 25,30,33    | 1.37 | 4 (16%)  |
| 25  | PSU  | CY    | 39  | 25    | 18,21,22     | 1.44 | 3 (16%)  | 21,30,33    | 2.33 | 3 (14%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | 4SU  | CY    | 8   | 25   | 18,21,22     | 1.72 | 4 (22%)  | 25,30,33    | 3.08 | 6 (24%)  |
| 23  | MIA  | AW    | 37  | 23   | 28,31,32     | 2.30 | 7 (25%)  | 38,44,47    | 2.73 | 13 (34%) |
| 25  | PSU  | CY    | 32  | 25   | 18,21,22     | 1.38 | 2 (11%)  | 21,30,33    | 1.99 | 4 (19%)  |

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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|-------|---------|-------------|---------|
| 25  | MIA  | CY    | 37  | 25    | -       | 3/7/25/34   | 0/3/3/3 |
| 25  | 5MU  | AY    | 54  | 25    | -       | 2/7/25/26   | 0/2/2/2 |
| 23  | PSU  | CW    | 55  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | PSU  | AY    | 39  | 25    | -       | 2/7/25/26   | 0/2/2/2 |
| 23  | 5MU  | CW    | 54  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | 4SU  | AY    | 8   | 25    | -       | 1/7/25/26   | 0/2/2/2 |
| 23  | PSU  | CW    | 32  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 23  | 4SU  | CW    | 8   | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 23  | 7MG  | CW    | 46  | 23    | -       | 3/7/37/38   | 0/3/3/3 |
| 24  | 5MC  | CX    | 32  | 24    | -       | 0/7/25/26   | 0/2/2/2 |
| 24  | 5MU  | AX    | 54  | 24,57 | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | MIA  | AY    | 37  | 25    | -       | 2/7/25/34   | 0/3/3/3 |
| 24  | 4SU  | AX    | 8   | 24    | -       | 0/7/25/26   | 0/2/2/2 |
| 23  | 31M  | AW    | 76  | 23    | -       | 8/31/49/50  | 0/4/4/4 |
| 23  | PSU  | AW    | 39  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | 7MG  | CY    | 46  | 25    | -       | 4/7/37/38   | 0/3/3/3 |
| 23  | PSU  | AW    | 32  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 24  | 5MC  | AX    | 32  | 24    | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | PSU  | AY    | 55  | 25    | -       | 2/7/25/26   | 0/2/2/2 |
| 23  | 5MU  | AW    | 54  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 23  | 4SU  | AW    | 8   | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | PSU  | CY    | 55  | 25    | -       | 4/7/25/26   | 0/2/2/2 |
| 23  | PSU  | AW    | 55  | 23    | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | PSU  | AY    | 32  | 25    | -       | 1/7/25/26   | 0/2/2/2 |
| 24  | PSU  | AX    | 55  | 24,57 | -       | 0/7/25/26   | 0/2/2/2 |
| 25  | 7MG  | AY    | 46  | 25    | -       | 2/7/37/38   | 0/3/3/3 |
| 23  | 7MG  | AW    | 46  | 23    | -       | 3/7/37/38   | 0/3/3/3 |
| 24  | PSU  | CX    | 55  | 24    | -       | 1/7/25/26   | 0/2/2/2 |
| 23  | 31M  | CW    | 76  | 23    | -       | 11/31/49/50 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 25  | 5MU  | CY    | 54  | 25   | -       | 2/7/25/26  | 0/2/2/2 |
| 23  | PSU  | CW    | 39  | 23   | -       | 0/7/25/26  | 0/2/2/2 |
| 24  | 5MU  | CX    | 54  | 24   | -       | 0/7/25/26  | 0/2/2/2 |
| 23  | MIA  | CW    | 37  | 23   | -       | 0/7/25/34  | 0/3/3/3 |
| 24  | 4SU  | CX    | 8   | 24   | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | PSU  | CY    | 39  | 25   | -       | 2/7/25/26  | 0/2/2/2 |
| 25  | 4SU  | CY    | 8   | 25   | -       | 2/7/25/26  | 0/2/2/2 |
| 23  | MIA  | AW    | 37  | 23   | -       | 1/15/33/34 | 0/3/3/3 |
| 25  | PSU  | CY    | 32  | 25   | -       | 1/7/25/26  | 0/2/2/2 |

The worst 5 of 141 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 23  | AW    | 37  | MIA  | C13-C14 | 6.94  | 1.53        | 1.32     |
| 23  | AW    | 37  | MIA  | C2-S10  | -6.49 | 1.70        | 1.75     |
| 24  | AX    | 32  | 5MC  | C5-C4   | 6.12  | 1.48        | 1.44     |
| 24  | CX    | 32  | 5MC  | C5-C4   | 5.90  | 1.48        | 1.44     |
| 24  | AX    | 8   | 4SU  | C4-N3   | -5.37 | 1.32        | 1.37     |

The worst 5 of 218 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 25  | AY    | 46  | 7MG  | N9-C4-N3    | 10.29 | 140.54      | 125.46   |
| 23  | AW    | 37  | MIA  | C12-C13-C14 | -9.12 | 110.65      | 127.01   |
| 23  | AW    | 46  | 7MG  | N9-C4-N3    | 9.11  | 138.81      | 125.46   |
| 25  | CY    | 8   | 4SU  | C4-N3-C2    | -8.94 | 118.75      | 127.31   |
| 23  | CW    | 46  | 7MG  | N9-C4-N3    | 8.27  | 137.58      | 125.46   |

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | AW    | 37  | MIA  | C12-C13-C14-C16 |
| 23  | AW    | 76  | 31M  | NM-CAM-CTM-N    |
| 23  | AW    | 76  | 31M  | CBM-CAM-CTM-N   |
| 23  | AW    | 76  | 31M  | CBM-CAM-CTM-OTM |
| 25  | AY    | 46  | 7MG  | C4'-C5'-O5'-P   |

There are no ring outliers.

28 monomers are involved in 63 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | CY    | 37  | MIA  | 2       | 0            |
| 25  | AY    | 54  | 5MU  | 1       | 0            |
| 23  | CW    | 55  | PSU  | 1       | 0            |
| 25  | AY    | 39  | PSU  | 4       | 0            |
| 23  | CW    | 54  | 5MU  | 1       | 0            |
| 25  | AY    | 8   | 4SU  | 1       | 0            |
| 23  | CW    | 8   | 4SU  | 2       | 0            |
| 23  | CW    | 46  | 7MG  | 1       | 0            |
| 24  | CX    | 32  | 5MC  | 1       | 0            |
| 25  | AY    | 37  | MIA  | 3       | 0            |
| 24  | AX    | 8   | 4SU  | 2       | 0            |
| 23  | AW    | 76  | 31M  | 5       | 0            |
| 23  | AW    | 39  | PSU  | 1       | 0            |
| 25  | CY    | 46  | 7MG  | 1       | 0            |
| 25  | AY    | 55  | PSU  | 4       | 0            |
| 23  | AW    | 8   | 4SU  | 1       | 0            |
| 25  | CY    | 55  | PSU  | 4       | 0            |
| 25  | AY    | 32  | PSU  | 2       | 0            |
| 24  | AX    | 55  | PSU  | 1       | 0            |
| 25  | AY    | 46  | 7MG  | 3       | 0            |
| 23  | AW    | 46  | 7MG  | 1       | 0            |
| 23  | CW    | 76  | 31M  | 7       | 0            |
| 23  | CW    | 39  | PSU  | 3       | 0            |
| 24  | CX    | 54  | 5MU  | 1       | 0            |
| 24  | CX    | 8   | 4SU  | 2       | 0            |
| 25  | CY    | 39  | PSU  | 4       | 0            |
| 25  | CY    | 8   | 4SU  | 5       | 0            |
| 23  | AW    | 37  | MIA  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2093 ligands modelled in this entry, 2091 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 58  | SF4  | CD    | 302 | 4    | 0,12,12      | -    | -           | -           |      |             |
| 58  | SF4  | AD    | 501 | 4    | 0,12,12      | -    | -           | -           |      |             |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 58  | SF4  | CD    | 302 | 4    | -       | -        | 0/6/5/5 |
| 58  | SF4  | AD    | 501 | 4    | -       | -        | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1498/1521 (98%) | 0.70   | 82 (5%) 30 30 | 42, 72, 93, 108       | 0     |
| 1   | CA    | 1503/1521 (98%) | 0.91   | 191 (12%) 8 7 | 44, 74, 94, 109       | 0     |
| 2   | AB    | 231/256 (90%)   | 1.68   | 69 (29%) 1 1  | 72, 82, 90, 94        | 0     |
| 2   | CB    | 231/256 (90%)   | 2.11   | 109 (47%) 0 0 | 73, 84, 90, 95        | 0     |
| 3   | AC    | 206/239 (86%)   | 1.55   | 50 (24%) 2 1  | 68, 79, 87, 94        | 0     |
| 3   | CC    | 206/239 (86%)   | 2.37   | 129 (62%) 0 0 | 71, 81, 89, 94        | 0     |
| 4   | AD    | 208/209 (99%)   | 1.50   | 50 (24%) 2 1  | 57, 72, 81, 90        | 0     |
| 4   | CD    | 208/209 (99%)   | 1.31   | 28 (13%) 7 5  | 58, 71, 80, 91        | 0     |
| 5   | AE    | 148/162 (91%)   | 1.27   | 18 (12%) 8 7  | 58, 71, 80, 85        | 0     |
| 5   | CE    | 148/162 (91%)   | 1.72   | 45 (30%) 1 0  | 60, 73, 81, 86        | 0     |
| 6   | AF    | 100/101 (99%)   | 1.17   | 8 (8%) 18 18  | 56, 69, 78, 82        | 0     |
| 6   | CF    | 100/101 (99%)   | 1.04   | 5 (5%) 34 33  | 57, 70, 78, 82        | 0     |
| 7   | AG    | 155/156 (99%)   | 1.33   | 23 (14%) 5 5  | 65, 75, 83, 91        | 0     |
| 7   | CG    | 155/156 (99%)   | 1.36   | 27 (17%) 4 3  | 66, 76, 84, 92        | 0     |
| 8   | AH    | 137/138 (99%)   | 1.24   | 17 (12%) 8 7  | 62, 72, 79, 87        | 0     |
| 8   | CH    | 137/138 (99%)   | 1.57   | 31 (22%) 2 2  | 64, 74, 80, 87        | 0     |
| 9   | AI    | 127/128 (99%)   | 1.79   | 50 (39%) 1 0  | 65, 80, 86, 89        | 0     |
| 9   | CI    | 127/128 (99%)   | 2.59   | 82 (64%) 0 0  | 68, 82, 88, 91        | 0     |
| 10  | AJ    | 97/105 (92%)    | 1.97   | 46 (47%) 0 0  | 64, 82, 90, 93        | 0     |
| 10  | CJ    | 96/105 (91%)    | 2.43   | 57 (59%) 0 0  | 67, 84, 91, 93        | 0     |
| 11  | AK    | 114/129 (88%)   | 1.11   | 14 (12%) 8 7  | 48, 70, 79, 84        | 0     |
| 11  | CK    | 114/129 (88%)   | 1.27   | 17 (14%) 5 5  | 51, 71, 79, 84        | 0     |
| 12  | AL    | 122/132 (92%)   | 0.94   | 9 (7%) 20 19  | 50, 65, 73, 78        | 0     |
| 12  | CL    | 122/132 (92%)   | 1.27   | 22 (18%) 3 3  | 53, 67, 75, 80        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|-------|
| 13  | AM    | 123/126 (97%)   | 1.28   | 18 (14%) | 6  | 5  | 55, 70, 81, 89        | 0     |
| 13  | CM    | 122/126 (96%)   | 2.45   | 70 (57%) | 0  | 0  | 70, 84, 91, 99        | 0     |
| 14  | AN    | 60/61 (98%)     | 1.69   | 14 (23%) | 2  | 1  | 67, 74, 83, 84        | 0     |
| 14  | CN    | 60/61 (98%)     | 3.17   | 54 (90%) | 0  | 0  | 69, 77, 84, 88        | 0     |
| 15  | AO    | 88/89 (98%)     | 1.23   | 12 (13%) | 7  | 5  | 56, 67, 80, 81        | 0     |
| 15  | CO    | 88/89 (98%)     | 1.28   | 14 (15%) | 5  | 4  | 59, 69, 80, 83        | 0     |
| 16  | AP    | 82/88 (93%)     | 1.78   | 29 (35%) | 1  | 0  | 57, 71, 80, 84        | 0     |
| 16  | CP    | 82/88 (93%)     | 1.36   | 14 (17%) | 4  | 3  | 58, 70, 80, 84        | 0     |
| 17  | AQ    | 99/105 (94%)    | 1.28   | 14 (14%) | 6  | 5  | 59, 71, 80, 84        | 0     |
| 17  | CQ    | 99/105 (94%)    | 1.13   | 11 (11%) | 10 | 9  | 61, 71, 81, 85        | 0     |
| 18  | AR    | 68/88 (77%)     | 0.97   | 6 (8%)   | 15 | 15 | 59, 68, 81, 83        | 0     |
| 18  | CR    | 68/88 (77%)     | 1.21   | 7 (10%)  | 12 | 11 | 61, 70, 80, 84        | 0     |
| 19  | AS    | 83/93 (89%)     | 1.62   | 19 (22%) | 2  | 2  | 71, 80, 86, 95        | 0     |
| 19  | CS    | 83/93 (89%)     | 2.82   | 66 (79%) | 0  | 0  | 74, 82, 89, 96        | 0     |
| 20  | AT    | 96/106 (90%)    | 1.43   | 20 (20%) | 2  | 2  | 57, 71, 81, 85        | 0     |
| 20  | CT    | 96/106 (90%)    | 1.24   | 12 (12%) | 8  | 7  | 58, 70, 82, 85        | 0     |
| 21  | AU    | 23/27 (85%)     | 2.13   | 13 (56%) | 0  | 0  | 67, 74, 77, 81        | 0     |
| 21  | CU    | 23/27 (85%)     | 2.66   | 19 (82%) | 0  | 0  | 70, 75, 80, 84        | 0     |
| 22  | AV    | 13/24 (54%)     | 1.45   | 4 (30%)  | 1  | 0  | 58, 81, 96, 99        | 0     |
| 22  | CV    | 12/24 (50%)     | 2.05   | 5 (41%)  | 0  | 0  | 63, 84, 93, 94        | 0     |
| 23  | AW    | 66/76 (86%)     | 1.47   | 14 (21%) | 2  | 2  | 68, 96, 103, 105      | 0     |
| 23  | CW    | 64/76 (84%)     | 1.75   | 18 (28%) | 1  | 1  | 73, 97, 103, 106      | 0     |
| 24  | AX    | 72/77 (93%)     | 0.45   | 2 (2%)   | 55 | 56 | 39, 68, 87, 91        | 0     |
| 24  | CX    | 72/77 (93%)     | 0.92   | 2 (2%)   | 55 | 56 | 53, 82, 93, 97        | 0     |
| 25  | AY    | 67/76 (88%)     | 2.05   | 34 (50%) | 0  | 0  | 44, 97, 102, 105      | 0     |
| 25  | CY    | 66/76 (86%)     | 2.26   | 40 (60%) | 0  | 0  | 47, 97, 102, 105      | 0     |
| 26  | BA    | 2819/2915 (96%) | -0.04  | 116 (4%) | 41 | 42 | 26, 45, 89, 104       | 0     |
| 26  | DA    | 2800/2915 (96%) | 0.05   | 100 (3%) | 46 | 47 | 30, 49, 90, 108       | 0     |
| 27  | BB    | 120/121 (99%)   | 0.46   | 1 (0%)   | 82 | 84 | 40, 64, 73, 86        | 0     |
| 27  | DB    | 120/121 (99%)   | 1.16   | 16 (13%) | 7  | 6  | 46, 69, 76, 90        | 0     |
| 28  | BD    | 275/276 (99%)   | 0.43   | 5 (1%)   | 67 | 68 | 27, 43, 58, 82        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | DD    | 275/276 (99%)  | 0.32   | 7 (2%) 58 59  | 29, 45, 61, 81        | 0     |
| 29  | BE    | 204/206 (99%)  | 0.45   | 5 (2%) 58 59  | 25, 48, 66, 80        | 0     |
| 29  | DE    | 204/206 (99%)  | 0.55   | 4 (1%) 65 65  | 29, 52, 67, 81        | 0     |
| 30  | BF    | 203/210 (96%)  | 0.55   | 4 (1%) 65 65  | 26, 53, 76, 87        | 0     |
| 30  | DF    | 203/210 (96%)  | 0.64   | 4 (1%) 65 65  | 30, 58, 77, 87        | 0     |
| 31  | BG    | 181/182 (99%)  | 1.34   | 29 (16%) 5 4  | 51, 69, 81, 88        | 0     |
| 31  | DG    | 181/182 (99%)  | 1.83   | 67 (37%) 1 0  | 56, 73, 82, 90        | 0     |
| 32  | BH    | 174/180 (96%)  | 1.10   | 13 (7%) 20 19 | 51, 65, 75, 88        | 0     |
| 32  | DH    | 174/180 (96%)  | 1.38   | 31 (17%) 4 3  | 55, 70, 78, 88        | 0     |
| 33  | BI    | 146/148 (98%)  | 1.13   | 13 (8%) 15 14 | 50, 74, 82, 87        | 0     |
| 33  | DI    | 146/148 (98%)  | 1.55   | 33 (22%) 2 2  | 52, 75, 82, 86        | 0     |
| 34  | BN    | 140/140 (100%) | 0.68   | 5 (3%) 46 47  | 32, 50, 67, 76        | 0     |
| 34  | DN    | 140/140 (100%) | 0.77   | 3 (2%) 63 64  | 36, 55, 70, 77        | 0     |
| 35  | BO    | 122/122 (100%) | 0.13   | 1 (0%) 82 84  | 30, 43, 59, 70        | 0     |
| 35  | DO    | 122/122 (100%) | 0.81   | 5 (4%) 41 42  | 45, 59, 73, 78        | 0     |
| 36  | BP    | 149/150 (99%)  | 0.79   | 6 (4%) 42 43  | 26, 55, 75, 83        | 0     |
| 36  | DP    | 149/150 (99%)  | 0.91   | 10 (6%) 24 23 | 30, 59, 77, 85        | 0     |
| 37  | BQ    | 141/141 (100%) | 0.63   | 3 (2%) 63 64  | 36, 52, 67, 80        | 0     |
| 37  | DQ    | 141/141 (100%) | 1.05   | 11 (7%) 19 18 | 41, 57, 70, 82        | 0     |
| 38  | BR    | 118/118 (100%) | -0.02  | 0 100 100     | 25, 36, 54, 59        | 0     |
| 38  | DR    | 118/118 (100%) | 0.45   | 0 100 100     | 40, 54, 65, 72        | 0     |
| 39  | BS    | 110/112 (98%)  | 0.35   | 0 100 100     | 38, 51, 65, 72        | 0     |
| 39  | DS    | 110/112 (98%)  | 1.75   | 36 (32%) 1 0  | 63, 77, 84, 92        | 0     |
| 40  | BT    | 131/146 (89%)  | 0.32   | 7 (5%) 32 31  | 32, 47, 69, 82        | 0     |
| 40  | DT    | 131/146 (89%)  | 0.95   | 13 (9%) 13 12 | 48, 63, 79, 85        | 0     |
| 41  | BU    | 116/118 (98%)  | -0.13  | 1 (0%) 81 83  | 18, 33, 49, 59        | 0     |
| 41  | DU    | 116/118 (98%)  | 0.88   | 4 (3%) 48 49  | 42, 61, 78, 84        | 0     |
| 42  | BV    | 101/101 (100%) | -0.04  | 0 100 100     | 21, 41, 58, 67        | 0     |
| 42  | DV    | 101/101 (100%) | 1.15   | 10 (9%) 13 12 | 41, 71, 83, 91        | 0     |
| 43  | BW    | 112/113 (99%)  | -0.05  | 2 (1%) 67 68  | 23, 34, 54, 79        | 0     |
| 43  | DW    | 112/113 (99%)  | 0.35   | 1 (0%) 81 83  | 39, 50, 67, 83        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | BX    | 95/96 (98%)       | 0.10   | 1 (1%) 78 79   | 23, 38, 61, 84        | 0     |
| 44  | DX    | 95/96 (98%)       | 1.01   | 14 (14%) 6 5   | 43, 60, 76, 79        | 0     |
| 45  | BY    | 107/110 (97%)     | 0.39   | 3 (2%) 55 56   | 32, 50, 69, 83        | 0     |
| 45  | DY    | 107/110 (97%)     | 1.32   | 16 (14%) 5 5   | 57, 71, 81, 88        | 0     |
| 46  | BZ    | 171/206 (83%)     | 1.21   | 42 (24%) 2 1   | 39, 64, 91, 95        | 0     |
| 46  | DZ    | 174/206 (84%)     | 2.12   | 80 (45%) 0 0   | 66, 84, 94, 101       | 0     |
| 47  | B0    | 83/85 (97%)       | 0.25   | 3 (3%) 46 47   | 27, 39, 61, 73        | 0     |
| 47  | D0    | 83/85 (97%)       | 1.33   | 15 (18%) 3 3   | 46, 66, 75, 82        | 0     |
| 48  | B1    | 97/98 (98%)       | 0.50   | 3 (3%) 51 52   | 30, 48, 70, 76        | 0     |
| 48  | D1    | 97/98 (98%)       | 0.79   | 9 (9%) 14 13   | 38, 58, 74, 83        | 0     |
| 49  | B2    | 70/72 (97%)       | 0.39   | 2 (2%) 53 55   | 34, 50, 64, 79        | 0     |
| 49  | D2    | 70/72 (97%)       | 1.25   | 13 (18%) 3 2   | 56, 70, 80, 86        | 0     |
| 50  | B3    | 59/60 (98%)       | 0.08   | 1 (1%) 69 69   | 24, 37, 63, 71        | 0     |
| 50  | D3    | 59/60 (98%)       | 0.74   | 2 (3%) 48 49   | 49, 64, 79, 85        | 0     |
| 51  | B4    | 69/71 (97%)       | 1.36   | 15 (21%) 2 2   | 54, 73, 87, 92        | 0     |
| 51  | D4    | 69/71 (97%)       | 2.08   | 31 (44%) 0 0   | 74, 88, 94, 99        | 0     |
| 52  | B5    | 59/60 (98%)       | -0.20  | 0 100 100      | 20, 33, 54, 67        | 0     |
| 52  | D5    | 59/60 (98%)       | 0.32   | 1 (1%) 69 69   | 36, 51, 67, 73        | 0     |
| 53  | B6    | 53/54 (98%)       | 0.14   | 1 (1%) 66 66   | 31, 44, 61, 68        | 0     |
| 53  | D6    | 53/54 (98%)       | 1.00   | 4 (7%) 20 19   | 52, 63, 76, 79        | 0     |
| 54  | B7    | 48/49 (97%)       | 0.12   | 4 (8%) 17 17   | 21, 30, 62, 76        | 0     |
| 54  | D7    | 48/49 (97%)       | 0.38   | 3 (6%) 26 25   | 33, 42, 61, 70        | 0     |
| 55  | B8    | 64/65 (98%)       | 0.15   | 1 (1%) 70 71   | 25, 36, 45, 60        | 0     |
| 55  | D8    | 64/65 (98%)       | 1.01   | 2 (3%) 51 52   | 46, 58, 66, 72        | 0     |
| 56  | B9    | 37/37 (100%)      | 0.40   | 1 (2%) 56 57   | 31, 49, 73, 74        | 0     |
| 56  | D9    | 37/37 (100%)      | 1.21   | 5 (13%) 7 5    | 46, 57, 73, 76        | 0     |
| All | All   | 20897/21748 (96%) | 0.77   | 2548 (12%) 8 7 | 18, 64, 89, 109       | 0     |

The worst 5 of 2548 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7   | AG    | 82  | GLY  | 8.4  |
| 14  | AN    | 2   | ALA  | 8.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13  | CM    | 123 | ALA  | 7.0  |
| 13  | CM    | 124 | PRO  | 7.0  |
| 28  | BD    | 276 | LYS  | 6.8  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 23  | 7MG  | AW    | 46  | 24/25 | 0.42 | 0.18 | 84,99,117,133              | 0     |
| 23  | 7MG  | CW    | 46  | 24/25 | 0.44 | 0.16 | 79,96,109,133              | 0     |
| 25  | 7MG  | CY    | 46  | 24/25 | 0.52 | 0.21 | 86,105,111,137             | 0     |
| 25  | MIA  | CY    | 37  | 22/30 | 0.54 | 0.18 | 72,95,113,138              | 0     |
| 23  | 4SU  | CW    | 8   | 20/21 | 0.59 | 0.15 | 81,98,120,127              | 0     |
| 25  | PSU  | CY    | 55  | 20/21 | 0.59 | 0.26 | 94,102,110,124             | 0     |
| 25  | 4SU  | CY    | 8   | 20/21 | 0.62 | 0.18 | 93,103,113,128             | 0     |
| 25  | PSU  | AY    | 55  | 20/21 | 0.64 | 0.17 | 93,101,108,122             | 0     |
| 25  | 5MU  | CY    | 54  | 21/22 | 0.67 | 0.25 | 78,94,109,140              | 0     |
| 25  | PSU  | CY    | 39  | 20/21 | 0.68 | 0.17 | 79,90,116,130              | 0     |
| 23  | 4SU  | AW    | 8   | 20/21 | 0.68 | 0.15 | 86,95,112,128              | 0     |
| 25  | 5MU  | AY    | 54  | 21/22 | 0.69 | 0.15 | 80,96,105,131              | 0     |
| 25  | 7MG  | AY    | 46  | 24/25 | 0.69 | 0.19 | 75,101,111,123             | 0     |
| 25  | PSU  | CY    | 32  | 20/21 | 0.71 | 0.15 | 80,92,101,107              | 0     |
| 25  | 4SU  | AY    | 8   | 20/21 | 0.71 | 0.14 | 82,96,103,118              | 0     |
| 25  | MIA  | AY    | 37  | 22/30 | 0.75 | 0.15 | 77,90,111,119              | 0     |
| 23  | PSU  | CW    | 55  | 20/21 | 0.75 | 0.13 | 79,89,99,104               | 0     |
| 25  | PSU  | AY    | 39  | 20/21 | 0.75 | 0.16 | 78,90,117,123              | 0     |
| 23  | 5MU  | CW    | 54  | 21/22 | 0.78 | 0.14 | 74,88,99,101               | 0     |
| 23  | MIA  | CW    | 37  | 22/30 | 0.80 | 0.13 | 75,85,92,100               | 0     |
| 23  | PSU  | AW    | 55  | 20/21 | 0.81 | 0.12 | 77,90,98,104               | 0     |
| 23  | 31M  | CW    | 76  | 41/42 | 0.83 | 0.24 | 50,63,73,88                | 20    |
| 23  | PSU  | CW    | 39  | 20/21 | 0.83 | 0.14 | 78,84,97,98                | 0     |
| 23  | PSU  | CW    | 32  | 20/21 | 0.84 | 0.15 | 81,87,94,103               | 0     |
| 25  | PSU  | AY    | 32  | 20/21 | 0.84 | 0.15 | 78,93,100,106              | 0     |
| 24  | 4SU  | CX    | 8   | 20/21 | 0.85 | 0.14 | 77,87,95,97                | 0     |
| 24  | 5MU  | CX    | 54  | 21/22 | 0.86 | 0.12 | 70,81,89,99                | 0     |
| 24  | PSU  | CX    | 55  | 20/21 | 0.86 | 0.12 | 70,80,91,96                | 0     |
| 23  | PSU  | AW    | 32  | 20/21 | 0.86 | 0.15 | 77,83,92,98                | 0     |
| 23  | 5MU  | AW    | 54  | 21/22 | 0.88 | 0.12 | 65,82,91,93                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 23  | PSU  | AW    | 39  | 20/21 | 0.89 | 0.12 | 73,82,95,97                 | 0     |
| 24  | 5MU  | AX    | 54  | 21/22 | 0.92 | 0.12 | 49,68,79,84                 | 0     |
| 23  | 31M  | AW    | 76  | 41/42 | 0.92 | 0.16 | 37,54,66,83                 | 9     |
| 24  | 5MC  | CX    | 32  | 21/22 | 0.92 | 0.14 | 63,76,86,88                 | 0     |
| 24  | 4SU  | AX    | 8   | 20/21 | 0.92 | 0.12 | 54,66,82,89                 | 0     |
| 24  | PSU  | AX    | 55  | 20/21 | 0.93 | 0.10 | 50,63,73,83                 | 0     |
| 23  | MIA  | AW    | 37  | 29/30 | 0.94 | 0.11 | 59,71,81,86                 | 0     |
| 24  | 5MC  | AX    | 32  | 21/22 | 0.95 | 0.11 | 43,53,62,78                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3448 | 1/1   | 0.54 | 0.40 | 70,70,70,70                 | 0     |
| 57  | MG   | BA    | 3670 | 1/1   | 0.60 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 3156 | 1/1   | 0.65 | 0.24 | 73,73,73,73                 | 0     |
| 57  | MG   | BA    | 3730 | 1/1   | 0.65 | 0.19 | 71,71,71,71                 | 0     |
| 57  | MG   | BA    | 3721 | 1/1   | 0.66 | 0.35 | 82,82,82,82                 | 0     |
| 57  | MG   | DA    | 3530 | 1/1   | 0.68 | 0.27 | 74,74,74,74                 | 0     |
| 57  | MG   | DA    | 3531 | 1/1   | 0.68 | 0.20 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3544 | 1/1   | 0.68 | 0.22 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3757 | 1/1   | 0.70 | 0.19 | 76,76,76,76                 | 0     |
| 57  | MG   | BA    | 3616 | 1/1   | 0.70 | 0.22 | 65,65,65,65                 | 0     |
| 57  | MG   | DB    | 3011 | 1/1   | 0.70 | 0.23 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3745 | 1/1   | 0.71 | 0.26 | 75,75,75,75                 | 0     |
| 57  | MG   | DR    | 5001 | 1/1   | 0.71 | 0.25 | 70,70,70,70                 | 0     |
| 57  | MG   | DA    | 3259 | 1/1   | 0.72 | 0.22 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3630 | 1/1   | 0.72 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3059 | 1/1   | 0.74 | 0.39 | 78,78,78,78                 | 0     |
| 57  | MG   | BA    | 3658 | 1/1   | 0.74 | 0.29 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3469 | 1/1   | 0.74 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3413 | 1/1   | 0.75 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3362 | 1/1   | 0.75 | 0.22 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3707 | 1/1   | 0.75 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3518 | 1/1   | 0.75 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3098 | 1/1   | 0.75 | 0.19 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3105 | 1/1   | 0.75 | 0.34 | 69,69,69,69                 | 0     |
| 57  | MG   | CV    | 101  | 1/1   | 0.75 | 0.28 | 72,72,72,72                 | 0     |
| 57  | MG   | AA    | 3199 | 1/1   | 0.75 | 0.26 | 73,73,73,73                 | 0     |
| 57  | MG   | DA    | 3673 | 1/1   | 0.75 | 0.25 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3262 | 1/1   | 0.75 | 0.23 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3320 | 1/1   | 0.75 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3728 | 1/1   | 0.76 | 0.24 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3724 | 1/1   | 0.76 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3521 | 1/1   | 0.76 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | DB    | 3001 | 1/1   | 0.76 | 0.25 | 64,64,64,64                 | 0     |
| 57  | MG   | BB    | 218  | 1/1   | 0.76 | 0.21 | 77,77,77,77                 | 0     |
| 57  | MG   | CA    | 3070 | 1/1   | 0.76 | 0.24 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3215 | 1/1   | 0.77 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3563 | 1/1   | 0.77 | 0.21 | 74,74,74,74                 | 0     |
| 57  | MG   | BA    | 3427 | 1/1   | 0.77 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3632 | 1/1   | 0.77 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3646 | 1/1   | 0.77 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3760 | 1/1   | 0.77 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3779 | 1/1   | 0.77 | 0.28 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3408 | 1/1   | 0.77 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3166 | 1/1   | 0.77 | 0.23 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3651 | 1/1   | 0.78 | 0.32 | 75,75,75,75                 | 0     |
| 57  | MG   | DA    | 3575 | 1/1   | 0.78 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3794 | 1/1   | 0.78 | 0.22 | 51,51,51,51                 | 0     |
| 57  | MG   | CA    | 3140 | 1/1   | 0.78 | 0.16 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3487 | 1/1   | 0.78 | 0.18 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3703 | 1/1   | 0.79 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3256 | 1/1   | 0.79 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3769 | 1/1   | 0.79 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3633 | 1/1   | 0.79 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3641 | 1/1   | 0.79 | 0.19 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3602 | 1/1   | 0.79 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3355 | 1/1   | 0.79 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3175 | 1/1   | 0.79 | 0.20 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3185 | 1/1   | 0.79 | 0.20 | 68,68,68,68                 | 0     |
| 57  | MG   | DD    | 303  | 1/1   | 0.79 | 0.20 | 87,87,87,87                 | 0     |
| 57  | MG   | DA    | 3415 | 1/1   | 0.79 | 0.24 | 68,68,68,68                 | 0     |
| 57  | MG   | DA    | 3313 | 1/1   | 0.80 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | CA    | 3102 | 1/1   | 0.80 | 0.14 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3128 | 1/1   | 0.80 | 0.23 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3607 | 1/1   | 0.80 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3626 | 1/1   | 0.80 | 0.13 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3583 | 1/1   | 0.80 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3771 | 1/1   | 0.80 | 0.23 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3020 | 1/1   | 0.80 | 0.20 | 76,76,76,76                 | 0     |
| 57  | MG   | DA    | 3140 | 1/1   | 0.80 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3683 | 1/1   | 0.80 | 0.26 | 73,73,73,73                 | 0     |
| 57  | MG   | BA    | 3434 | 1/1   | 0.80 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 3039 | 1/1   | 0.80 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3638 | 1/1   | 0.80 | 0.23 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3463 | 1/1   | 0.80 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3279 | 1/1   | 0.80 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | CA    | 3136 | 1/1   | 0.81 | 0.24 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3642 | 1/1   | 0.81 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3115 | 1/1   | 0.81 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3754 | 1/1   | 0.81 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3335 | 1/1   | 0.81 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3125 | 1/1   | 0.81 | 0.35 | 70,70,70,70                 | 0     |
| 57  | MG   | DB    | 3008 | 1/1   | 0.81 | 0.26 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3623 | 1/1   | 0.81 | 0.19 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3362 | 1/1   | 0.81 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3402 | 1/1   | 0.81 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | DV    | 3003 | 1/1   | 0.81 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3308 | 1/1   | 0.82 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3204 | 1/1   | 0.82 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3512 | 1/1   | 0.82 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3574 | 1/1   | 0.82 | 0.28 | 66,66,66,66                 | 0     |
| 57  | MG   | AX    | 3014 | 1/1   | 0.82 | 0.18 | 72,72,72,72                 | 0     |
| 57  | MG   | DA    | 3608 | 1/1   | 0.82 | 0.20 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3257 | 1/1   | 0.82 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3380 | 1/1   | 0.82 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3118 | 1/1   | 0.82 | 0.14 | 77,77,77,77                 | 0     |
| 57  | MG   | BA    | 3302 | 1/1   | 0.82 | 0.34 | 69,69,69,69                 | 0     |
| 57  | MG   | CA    | 3018 | 1/1   | 0.82 | 0.25 | 69,69,69,69                 | 0     |
| 57  | MG   | AA    | 3153 | 1/1   | 0.82 | 0.14 | 74,74,74,74                 | 0     |
| 57  | MG   | BA    | 3396 | 1/1   | 0.82 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3462 | 1/1   | 0.82 | 0.21 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 3083 | 1/1   | 0.82 | 0.19 | 79,79,79,79                 | 0     |
| 57  | MG   | DA    | 3484 | 1/1   | 0.82 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3193 | 1/1   | 0.82 | 0.14 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3654 | 1/1   | 0.82 | 0.15 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3274 | 1/1   | 0.82 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3127 | 1/1   | 0.82 | 0.14 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3550 | 1/1   | 0.83 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3399 | 1/1   | 0.83 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3196 | 1/1   | 0.83 | 0.13 | 74,74,74,74                 | 0     |
| 57  | MG   | BB    | 215  | 1/1   | 0.83 | 0.18 | 73,73,73,73                 | 0     |
| 57  | MG   | BA    | 3453 | 1/1   | 0.83 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | B4    | 502  | 1/1   | 0.83 | 0.13 | 71,71,71,71                 | 0     |
| 57  | MG   | DA    | 3421 | 1/1   | 0.83 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3430 | 1/1   | 0.83 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | AA    | 3002 | 1/1   | 0.83 | 0.26 | 71,71,71,71                 | 0     |
| 57  | MG   | CA    | 3027 | 1/1   | 0.83 | 0.26 | 64,64,64,64                 | 0     |
| 57  | MG   | CA    | 3152 | 1/1   | 0.83 | 0.28 | 76,76,76,76                 | 0     |
| 57  | MG   | BA    | 3335 | 1/1   | 0.83 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | CE    | 3001 | 1/1   | 0.83 | 0.11 | 79,79,79,79                 | 0     |
| 57  | MG   | CJ    | 5001 | 1/1   | 0.83 | 0.13 | 73,73,73,73                 | 0     |
| 57  | MG   | DA    | 3329 | 1/1   | 0.83 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3066 | 1/1   | 0.83 | 0.28 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3514 | 1/1   | 0.83 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3082 | 1/1   | 0.83 | 0.24 | 79,79,79,79                 | 0     |
| 57  | MG   | AA    | 3108 | 1/1   | 0.84 | 0.17 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3631 | 1/1   | 0.84 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3455 | 1/1   | 0.84 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3577 | 1/1   | 0.84 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | BB    | 206  | 1/1   | 0.84 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3117 | 1/1   | 0.84 | 0.14 | 79,79,79,79                 | 0     |
| 57  | MG   | DA    | 3614 | 1/1   | 0.84 | 0.10 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3057 | 1/1   | 0.84 | 0.27 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3417 | 1/1   | 0.84 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3741 | 1/1   | 0.84 | 0.18 | 64,64,64,64                 | 0     |
| 57  | MG   | AA    | 3026 | 1/1   | 0.84 | 0.23 | 70,70,70,70                 | 0     |
| 57  | MG   | AA    | 3054 | 1/1   | 0.84 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3641 | 1/1   | 0.84 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3301 | 1/1   | 0.84 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | CA    | 3153 | 1/1   | 0.84 | 0.28 | 70,70,70,70                 | 0     |
| 57  | MG   | AA    | 3172 | 1/1   | 0.84 | 0.15 | 72,72,72,72                 | 0     |
| 57  | MG   | CA    | 3049 | 1/1   | 0.84 | 0.27 | 63,63,63,63                 | 0     |
| 57  | MG   | CA    | 3059 | 1/1   | 0.84 | 0.18 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3225 | 1/1   | 0.84 | 0.30 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3524 | 1/1   | 0.84 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3093 | 1/1   | 0.84 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3443 | 1/1   | 0.84 | 0.17 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3669 | 1/1   | 0.85 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3470 | 1/1   | 0.85 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3478 | 1/1   | 0.85 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3070 | 1/1   | 0.85 | 0.32 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3681 | 1/1   | 0.85 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3128 | 1/1   | 0.85 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | AA    | 3187 | 1/1   | 0.85 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3028 | 1/1   | 0.85 | 0.39 | 76,76,76,76                 | 0     |
| 57  | MG   | BA    | 3540 | 1/1   | 0.85 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | AA    | 3170 | 1/1   | 0.85 | 0.13 | 75,75,75,75                 | 0     |
| 57  | MG   | DA    | 3541 | 1/1   | 0.85 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3316 | 1/1   | 0.85 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3554 | 1/1   | 0.85 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3197 | 1/1   | 0.85 | 0.16 | 70,70,70,70                 | 0     |
| 57  | MG   | DA    | 3317 | 1/1   | 0.85 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3590 | 1/1   | 0.85 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3598 | 1/1   | 0.85 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | AA    | 3004 | 1/1   | 0.85 | 0.11 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3339 | 1/1   | 0.85 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3618 | 1/1   | 0.85 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3388 | 1/1   | 0.85 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3146 | 1/1   | 0.85 | 0.27 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3619 | 1/1   | 0.85 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3623 | 1/1   | 0.85 | 0.20 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3111 | 1/1   | 0.85 | 0.17 | 79,79,79,79                 | 0     |
| 57  | MG   | AA    | 3209 | 1/1   | 0.85 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | AE    | 202  | 1/1   | 0.85 | 0.16 | 80,80,80,80                 | 0     |
| 57  | MG   | CT    | 3001 | 1/1   | 0.85 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3667 | 1/1   | 0.85 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3438 | 1/1   | 0.85 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3652 | 1/1   | 0.85 | 0.25 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3425 | 1/1   | 0.85 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3185 | 1/1   | 0.85 | 0.29 | 82,82,82,82                 | 0     |
| 57  | MG   | BA    | 3656 | 1/1   | 0.85 | 0.28 | 53,53,53,53                 | 0     |
| 57  | MG   | AX    | 3016 | 1/1   | 0.85 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3467 | 1/1   | 0.85 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3523 | 1/1   | 0.86 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3399 | 1/1   | 0.86 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3419 | 1/1   | 0.86 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3755 | 1/1   | 0.86 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3192 | 1/1   | 0.86 | 0.21 | 71,71,71,71                 | 0     |
| 57  | MG   | DA    | 3523 | 1/1   | 0.86 | 0.14 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3429 | 1/1   | 0.86 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3031 | 1/1   | 0.86 | 0.27 | 70,70,70,70                 | 0     |
| 57  | MG   | AA    | 3107 | 1/1   | 0.86 | 0.20 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3532 | 1/1   | 0.86 | 0.16 | 69,69,69,69                 | 0     |
| 57  | MG   | CA    | 3121 | 1/1   | 0.86 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3680 | 1/1   | 0.86 | 0.18 | 68,68,68,68                 | 0     |
| 57  | MG   | DA    | 3553 | 1/1   | 0.86 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3783 | 1/1   | 0.86 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3027 | 1/1   | 0.86 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3811 | 1/1   | 0.86 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | BB    | 202  | 1/1   | 0.86 | 0.27 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3591 | 1/1   | 0.86 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3353 | 1/1   | 0.86 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3160 | 1/1   | 0.86 | 0.21 | 59,59,59,59                 | 0     |
| 57  | MG   | CA    | 3159 | 1/1   | 0.86 | 0.25 | 70,70,70,70                 | 0     |
| 57  | MG   | AA    | 3200 | 1/1   | 0.86 | 0.19 | 73,73,73,73                 | 0     |
| 57  | MG   | DA    | 3403 | 1/1   | 0.86 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3406 | 1/1   | 0.86 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3470 | 1/1   | 0.86 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 3012 | 1/1   | 0.86 | 0.21 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3414 | 1/1   | 0.86 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3638 | 1/1   | 0.86 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3636 | 1/1   | 0.86 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3062 | 1/1   | 0.86 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3075 | 1/1   | 0.86 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3652 | 1/1   | 0.86 | 0.20 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3662 | 1/1   | 0.86 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 3021 | 1/1   | 0.86 | 0.24 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3391 | 1/1   | 0.86 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3447 | 1/1   | 0.86 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | CA    | 3037 | 1/1   | 0.86 | 0.33 | 73,73,73,73                 | 0     |
| 57  | MG   | AA    | 3069 | 1/1   | 0.86 | 0.14 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3740 | 1/1   | 0.86 | 0.18 | 28,28,28,28                 | 0     |
| 57  | MG   | CA    | 3055 | 1/1   | 0.86 | 0.21 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3230 | 1/1   | 0.86 | 0.17 | 73,73,73,73                 | 0     |
| 57  | MG   | DA    | 3433 | 1/1   | 0.87 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3076 | 1/1   | 0.87 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3079 | 1/1   | 0.87 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3548 | 1/1   | 0.87 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3750 | 1/1   | 0.87 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | AA    | 3184 | 1/1   | 0.87 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3066 | 1/1   | 0.87 | 0.10 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 3076 | 1/1   | 0.87 | 0.38 | 77,77,77,77                 | 0     |
| 57  | MG   | DA    | 3194 | 1/1   | 0.87 | 0.13 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3213 | 1/1   | 0.87 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3502 | 1/1   | 0.87 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3505 | 1/1   | 0.87 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3091 | 1/1   | 0.87 | 0.20 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3218 | 1/1   | 0.87 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3673 | 1/1   | 0.87 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3244 | 1/1   | 0.87 | 0.17 | 71,71,71,71                 | 0     |
| 57  | MG   | BA    | 3212 | 1/1   | 0.87 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3459 | 1/1   | 0.87 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3261 | 1/1   | 0.87 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3539 | 1/1   | 0.87 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3090 | 1/1   | 0.87 | 0.16 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3781 | 1/1   | 0.87 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3546 | 1/1   | 0.87 | 0.09 | 71,71,71,71                 | 0     |
| 57  | MG   | DA    | 3550 | 1/1   | 0.87 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3276 | 1/1   | 0.87 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3191 | 1/1   | 0.87 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3291 | 1/1   | 0.87 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 3112 | 1/1   | 0.87 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3686 | 1/1   | 0.87 | 0.23 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3586 | 1/1   | 0.87 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3466 | 1/1   | 0.87 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3124 | 1/1   | 0.87 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3318 | 1/1   | 0.87 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | CA    | 3126 | 1/1   | 0.87 | 0.18 | 67,67,67,67                 | 0     |
| 57  | MG   | AA    | 3100 | 1/1   | 0.87 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3620 | 1/1   | 0.87 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3486 | 1/1   | 0.87 | 0.15 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3411 | 1/1   | 0.87 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3628 | 1/1   | 0.87 | 0.19 | 76,76,76,76                 | 0     |
| 57  | MG   | AA    | 3047 | 1/1   | 0.87 | 0.28 | 63,63,63,63                 | 0     |
| 57  | MG   | CA    | 3149 | 1/1   | 0.87 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | BF    | 308  | 1/1   | 0.87 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3634 | 1/1   | 0.87 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3635 | 1/1   | 0.87 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3382 | 1/1   | 0.87 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3304 | 1/1   | 0.87 | 0.18 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3642 | 1/1   | 0.87 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | B6    | 102  | 1/1   | 0.87 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | CA    | 3157 | 1/1   | 0.87 | 0.11 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3006 | 1/1   | 0.87 | 0.26 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3732 | 1/1   | 0.87 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3409 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3735 | 1/1   | 0.87 | 0.31 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3530 | 1/1   | 0.87 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3024 | 1/1   | 0.87 | 0.29 | 74,74,74,74                 | 0     |
| 57  | MG   | CX    | 3003 | 1/1   | 0.87 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3049 | 1/1   | 0.87 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3073 | 1/1   | 0.87 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 3033 | 1/1   | 0.87 | 0.25 | 71,71,71,71                 | 0     |
| 57  | MG   | BA    | 3418 | 1/1   | 0.88 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3437 | 1/1   | 0.88 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3738 | 1/1   | 0.88 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3111 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 3051 | 1/1   | 0.88 | 0.18 | 81,81,81,81                 | 0     |
| 57  | MG   | AX    | 3009 | 1/1   | 0.88 | 0.22 | 64,64,64,64                 | 0     |
| 57  | MG   | CA    | 3057 | 1/1   | 0.88 | 0.18 | 76,76,76,76                 | 0     |
| 57  | MG   | DA    | 3141 | 1/1   | 0.88 | 0.19 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3181 | 1/1   | 0.88 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3058 | 1/1   | 0.88 | 0.21 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3615 | 1/1   | 0.88 | 0.29 | 68,68,68,68                 | 0     |
| 57  | MG   | DA    | 3495 | 1/1   | 0.88 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3424 | 1/1   | 0.88 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | CA    | 3069 | 1/1   | 0.88 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | AX    | 3011 | 1/1   | 0.88 | 0.21 | 78,78,78,78                 | 0     |
| 57  | MG   | BA    | 3231 | 1/1   | 0.88 | 0.31 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3238 | 1/1   | 0.88 | 0.25 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 3088 | 1/1   | 0.88 | 0.10 | 74,74,74,74                 | 0     |
| 57  | MG   | AA    | 3176 | 1/1   | 0.88 | 0.11 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3267 | 1/1   | 0.88 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3177 | 1/1   | 0.88 | 0.09 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3273 | 1/1   | 0.88 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | CA    | 3107 | 1/1   | 0.88 | 0.11 | 80,80,80,80                 | 0     |
| 57  | MG   | BA    | 3023 | 1/1   | 0.88 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3648 | 1/1   | 0.88 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3306 | 1/1   | 0.88 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3034 | 1/1   | 0.88 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3318 | 1/1   | 0.88 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3309 | 1/1   | 0.88 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3564 | 1/1   | 0.88 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3053 | 1/1   | 0.88 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3314 | 1/1   | 0.88 | 0.11 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3482 | 1/1   | 0.88 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3588 | 1/1   | 0.88 | 0.12 | 65,65,65,65                 | 0     |
| 57  | MG   | CA    | 3138 | 1/1   | 0.88 | 0.15 | 80,80,80,80                 | 0     |
| 57  | MG   | DA    | 3598 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3604 | 1/1   | 0.88 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3342 | 1/1   | 0.88 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | CA    | 3144 | 1/1   | 0.88 | 0.11 | 71,71,71,71                 | 0     |
| 57  | MG   | BB    | 207  | 1/1   | 0.88 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3037 | 1/1   | 0.88 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3340 | 1/1   | 0.88 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3036 | 1/1   | 0.88 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3356 | 1/1   | 0.88 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3627 | 1/1   | 0.88 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3360 | 1/1   | 0.88 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3387 | 1/1   | 0.88 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3109 | 1/1   | 0.88 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3117 | 1/1   | 0.88 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3383 | 1/1   | 0.88 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3388 | 1/1   | 0.88 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3398 | 1/1   | 0.88 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | CA    | 3004 | 1/1   | 0.88 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | CA    | 3168 | 1/1   | 0.88 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3545 | 1/1   | 0.88 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3649 | 1/1   | 0.88 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3138 | 1/1   | 0.88 | 0.22 | 71,71,71,71                 | 0     |
| 57  | MG   | BA    | 3709 | 1/1   | 0.88 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3655 | 1/1   | 0.88 | 0.09 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3661 | 1/1   | 0.88 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3129 | 1/1   | 0.88 | 0.22 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3401 | 1/1   | 0.88 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 3669 | 1/1   | 0.88 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3025 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3676 | 1/1   | 0.88 | 0.18 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3035 | 1/1   | 0.88 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3179 | 1/1   | 0.88 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3031 | 1/1   | 0.88 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3415 | 1/1   | 0.88 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | DP    | 201  | 1/1   | 0.88 | 0.21 | 70,70,70,70                 | 0     |
| 57  | MG   | DA    | 3426 | 1/1   | 0.88 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3594 | 1/1   | 0.88 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | DW    | 3003 | 1/1   | 0.88 | 0.13 | 72,72,72,72                 | 0     |
| 57  | MG   | DA    | 3440 | 1/1   | 0.89 | 0.11 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3046 | 1/1   | 0.89 | 0.17 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3103 | 1/1   | 0.89 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3451 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3593 | 1/1   | 0.89 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3117 | 1/1   | 0.89 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3300 | 1/1   | 0.89 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3596 | 1/1   | 0.89 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3397 | 1/1   | 0.89 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3482 | 1/1   | 0.89 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3206 | 1/1   | 0.89 | 0.20 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3608 | 1/1   | 0.89 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 3062 | 1/1   | 0.89 | 0.16 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3499 | 1/1   | 0.89 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3468 | 1/1   | 0.89 | 0.16 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 3067 | 1/1   | 0.89 | 0.28 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3160 | 1/1   | 0.89 | 0.25 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3473 | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | CA    | 3077 | 1/1   | 0.89 | 0.17 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3231 | 1/1   | 0.89 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3749 | 1/1   | 0.89 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3248 | 1/1   | 0.89 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3051 | 1/1   | 0.89 | 0.27 | 73,73,73,73                 | 0     |
| 57  | MG   | BA    | 3624 | 1/1   | 0.89 | 0.17 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3185 | 1/1   | 0.89 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3633 | 1/1   | 0.89 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3487 | 1/1   | 0.89 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3104 | 1/1   | 0.89 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3488 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3492 | 1/1   | 0.89 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3287 | 1/1   | 0.89 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3290 | 1/1   | 0.89 | 0.18 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3567 | 1/1   | 0.89 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3571 | 1/1   | 0.89 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3503 | 1/1   | 0.89 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3295 | 1/1   | 0.89 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 3145 | 1/1   | 0.89 | 0.19 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3319 | 1/1   | 0.89 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3515 | 1/1   | 0.89 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3796 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3799 | 1/1   | 0.89 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3520 | 1/1   | 0.89 | 0.19 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3423 | 1/1   | 0.89 | 0.13 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3668 | 1/1   | 0.89 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3615 | 1/1   | 0.89 | 0.16 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3072 | 1/1   | 0.89 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3331 | 1/1   | 0.89 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3535 | 1/1   | 0.89 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3625 | 1/1   | 0.89 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | CA    | 3150 | 1/1   | 0.89 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3671 | 1/1   | 0.89 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3095 | 1/1   | 0.89 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3679 | 1/1   | 0.89 | 0.16 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3631 | 1/1   | 0.89 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3022 | 1/1   | 0.89 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | CA    | 3158 | 1/1   | 0.89 | 0.17 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3243 | 1/1   | 0.89 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3167 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3385 | 1/1   | 0.89 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3554 | 1/1   | 0.89 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3700 | 1/1   | 0.89 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3572 | 1/1   | 0.89 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 3022 | 1/1   | 0.89 | 0.18 | 78,78,78,78                 | 0     |
| 57  | MG   | AX    | 3002 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3001 | 1/1   | 0.89 | 0.09 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3261 | 1/1   | 0.89 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3657 | 1/1   | 0.89 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3711 | 1/1   | 0.89 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3410 | 1/1   | 0.89 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3044 | 1/1   | 0.89 | 0.18 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3051 | 1/1   | 0.89 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3060 | 1/1   | 0.89 | 0.19 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3712 | 1/1   | 0.89 | 0.25 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3420 | 1/1   | 0.89 | 0.12 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3069 | 1/1   | 0.89 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 3036 | 1/1   | 0.89 | 0.21 | 66,66,66,66                 | 0     |
| 57  | MG   | DB    | 3013 | 1/1   | 0.89 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3718 | 1/1   | 0.89 | 0.12 | 71,71,71,71                 | 0     |
| 57  | MG   | DE    | 303  | 1/1   | 0.89 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3038 | 1/1   | 0.89 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3432 | 1/1   | 0.89 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | AA    | 3134 | 1/1   | 0.89 | 0.12 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3090 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | D3    | 3001 | 1/1   | 0.89 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | D8    | 5001 | 1/1   | 0.89 | 0.28 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 3156 | 1/1   | 0.90 | 0.27 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3471 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3077 | 1/1   | 0.90 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3622 | 1/1   | 0.90 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3081 | 1/1   | 0.90 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3375 | 1/1   | 0.90 | 0.14 | 68,68,68,68                 | 0     |
| 57  | MG   | AA    | 3046 | 1/1   | 0.90 | 0.20 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3161 | 1/1   | 0.90 | 0.26 | 65,65,65,65                 | 0     |
| 57  | MG   | CA    | 3060 | 1/1   | 0.90 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3017 | 1/1   | 0.90 | 0.26 | 71,71,71,71                 | 0     |
| 57  | MG   | DA    | 3452 | 1/1   | 0.90 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3634 | 1/1   | 0.90 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3213 | 1/1   | 0.90 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3005 | 1/1   | 0.90 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3759 | 1/1   | 0.90 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3147 | 1/1   | 0.90 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3481 | 1/1   | 0.90 | 0.24 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3149 | 1/1   | 0.90 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3640 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3761 | 1/1   | 0.90 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3492 | 1/1   | 0.90 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3764 | 1/1   | 0.90 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3498 | 1/1   | 0.90 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3205 | 1/1   | 0.90 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3206 | 1/1   | 0.90 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3207 | 1/1   | 0.90 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3516 | 1/1   | 0.90 | 0.10 | 67,67,67,67                 | 0     |
| 57  | MG   | CA    | 3087 | 1/1   | 0.90 | 0.19 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3501 | 1/1   | 0.90 | 0.11 | 71,71,71,71                 | 0     |
| 57  | MG   | AA    | 3136 | 1/1   | 0.90 | 0.17 | 70,70,70,70                 | 0     |
| 57  | MG   | DA    | 3219 | 1/1   | 0.90 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3222 | 1/1   | 0.90 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 3097 | 1/1   | 0.90 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3647 | 1/1   | 0.90 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3536 | 1/1   | 0.90 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3234 | 1/1   | 0.90 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3242 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3504 | 1/1   | 0.90 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3104 | 1/1   | 0.90 | 0.26 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3255 | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | AA    | 3139 | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | CA    | 3109 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3556 | 1/1   | 0.90 | 0.17 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3557 | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3558 | 1/1   | 0.90 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3405 | 1/1   | 0.90 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3409 | 1/1   | 0.90 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3268 | 1/1   | 0.90 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3569 | 1/1   | 0.90 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3117 | 1/1   | 0.90 | 0.25 | 71,71,71,71                 | 0     |
| 57  | MG   | CA    | 3118 | 1/1   | 0.90 | 0.31 | 68,68,68,68                 | 0     |
| 57  | MG   | CA    | 3120 | 1/1   | 0.90 | 0.26 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3052 | 1/1   | 0.90 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3812 | 1/1   | 0.90 | 0.22 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3202 | 1/1   | 0.90 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3593 | 1/1   | 0.90 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3594 | 1/1   | 0.90 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3008 | 1/1   | 0.90 | 0.32 | 73,73,73,73                 | 0     |
| 57  | MG   | CA    | 3133 | 1/1   | 0.90 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3300 | 1/1   | 0.90 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3294 | 1/1   | 0.90 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3609 | 1/1   | 0.90 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3541 | 1/1   | 0.90 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | AA    | 3205 | 1/1   | 0.90 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3311 | 1/1   | 0.90 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3146 | 1/1   | 0.90 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | BV    | 202  | 1/1   | 0.90 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3624 | 1/1   | 0.90 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | BX    | 3001 | 1/1   | 0.90 | 0.44 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3426 | 1/1   | 0.90 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | B5    | 101  | 1/1   | 0.90 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3321 | 1/1   | 0.90 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | AA    | 3147 | 1/1   | 0.90 | 0.16 | 70,70,70,70                 | 0     |
| 57  | MG   | BA    | 3684 | 1/1   | 0.90 | 0.13 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3555 | 1/1   | 0.90 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 3338 | 1/1   | 0.90 | 0.23 | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 3008 | 1/1   | 0.90 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | CA    | 3011 | 1/1   | 0.90 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3636 | 1/1   | 0.90 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3637 | 1/1   | 0.90 | 0.29 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3348 | 1/1   | 0.90 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 3354 | 1/1   | 0.90 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3693 | 1/1   | 0.90 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3643 | 1/1   | 0.90 | 0.12 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3102 | 1/1   | 0.90 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 3170 | 1/1   | 0.90 | 0.20 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3431 | 1/1   | 0.90 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3371 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3314 | 1/1   | 0.90 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3214 | 1/1   | 0.90 | 0.24 | 73,73,73,73                 | 0     |
| 57  | MG   | CA    | 3026 | 1/1   | 0.90 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | CX    | 3002 | 1/1   | 0.90 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | DA    | 3663 | 1/1   | 0.90 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3394 | 1/1   | 0.90 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3114 | 1/1   | 0.90 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3029 | 1/1   | 0.90 | 0.21 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3002 | 1/1   | 0.90 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3007 | 1/1   | 0.90 | 0.12 | 50,50,50,50                 | 0     |
| 57  | MG   | DB    | 3005 | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3010 | 1/1   | 0.90 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3121 | 1/1   | 0.90 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | BA    | 3121 | 1/1   | 0.90 | 0.33 | 64,64,64,64                 | 0     |
| 57  | MG   | AA    | 3155 | 1/1   | 0.90 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3601 | 1/1   | 0.90 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3351 | 1/1   | 0.90 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | AX    | 3008 | 1/1   | 0.90 | 0.18 | 70,70,70,70                 | 0     |
| 57  | MG   | CA    | 3041 | 1/1   | 0.90 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3071 | 1/1   | 0.90 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3359 | 1/1   | 0.90 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3422 | 1/1   | 0.90 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3717 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3431 | 1/1   | 0.91 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3013 | 1/1   | 0.91 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3591 | 1/1   | 0.91 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | AA    | 3092 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3725 | 1/1   | 0.91 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3432 | 1/1   | 0.91 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3078 | 1/1   | 0.91 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3450 | 1/1   | 0.91 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | CA    | 3052 | 1/1   | 0.91 | 0.14 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3731 | 1/1   | 0.91 | 0.27 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3454 | 1/1   | 0.91 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3083 | 1/1   | 0.91 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3465 | 1/1   | 0.91 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3123 | 1/1   | 0.91 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3468 | 1/1   | 0.91 | 0.15 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 3095 | 1/1   | 0.91 | 0.24 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3315 | 1/1   | 0.91 | 0.11 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3473 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3604 | 1/1   | 0.91 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | CA    | 3061 | 1/1   | 0.91 | 0.14 | 66,66,66,66                 | 0     |
| 57  | MG   | AA    | 3183 | 1/1   | 0.91 | 0.16 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3155 | 1/1   | 0.91 | 0.26 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3160 | 1/1   | 0.91 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3178 | 1/1   | 0.91 | 0.22 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3063 | 1/1   | 0.91 | 0.27 | 58,58,58,58                 | 0     |
| 57  | MG   | CA    | 3064 | 1/1   | 0.91 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3188 | 1/1   | 0.91 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3501 | 1/1   | 0.91 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3742 | 1/1   | 0.91 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3613 | 1/1   | 0.91 | 0.35 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3747 | 1/1   | 0.91 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3748 | 1/1   | 0.91 | 0.07 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 3520 | 1/1   | 0.91 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3208 | 1/1   | 0.91 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | CA    | 3071 | 1/1   | 0.91 | 0.21 | 68,68,68,68                 | 0     |
| 57  | MG   | AN    | 503  | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | AW    | 3001 | 1/1   | 0.91 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3465 | 1/1   | 0.91 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | AW    | 3003 | 1/1   | 0.91 | 0.17 | 72,72,72,72                 | 0     |
| 57  | MG   | DA    | 3534 | 1/1   | 0.91 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3223 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3120 | 1/1   | 0.91 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3097 | 1/1   | 0.91 | 0.38 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3626 | 1/1   | 0.91 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3239 | 1/1   | 0.91 | 0.33 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3126 | 1/1   | 0.91 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3552 | 1/1   | 0.91 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3355 | 1/1   | 0.91 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3127 | 1/1   | 0.91 | 0.25 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3251 | 1/1   | 0.91 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3023 | 1/1   | 0.91 | 0.10 | 74,74,74,74                 | 0     |
| 57  | MG   | CA    | 3108 | 1/1   | 0.91 | 0.14 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3365 | 1/1   | 0.91 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3639 | 1/1   | 0.91 | 0.28 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3566 | 1/1   | 0.91 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | CA    | 3113 | 1/1   | 0.91 | 0.11 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3782 | 1/1   | 0.91 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3271 | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3574 | 1/1   | 0.91 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3116 | 1/1   | 0.91 | 0.11 | 68,68,68,68                 | 0     |
| 57  | MG   | AA    | 3052 | 1/1   | 0.91 | 0.30 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3583 | 1/1   | 0.91 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3584 | 1/1   | 0.91 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3788 | 1/1   | 0.91 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3159 | 1/1   | 0.91 | 0.27 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3499 | 1/1   | 0.91 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3386 | 1/1   | 0.91 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3040 | 1/1   | 0.91 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3651 | 1/1   | 0.91 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3298 | 1/1   | 0.91 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3299 | 1/1   | 0.91 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3041 | 1/1   | 0.91 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3508 | 1/1   | 0.91 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3610 | 1/1   | 0.91 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3613 | 1/1   | 0.91 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3003 | 1/1   | 0.91 | 0.12 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3205 | 1/1   | 0.91 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3142 | 1/1   | 0.91 | 0.24 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3663 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3621 | 1/1   | 0.91 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | BD    | 302  | 1/1   | 0.91 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | BE    | 301  | 1/1   | 0.91 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | BE    | 308  | 1/1   | 0.91 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3001 | 1/1   | 0.91 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3064 | 1/1   | 0.91 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3327 | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3218 | 1/1   | 0.91 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3527 | 1/1   | 0.91 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3672 | 1/1   | 0.91 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3404 | 1/1   | 0.91 | 0.13 | 59,59,59,59                 | 0     |
| 57  | MG   | CA    | 3161 | 1/1   | 0.91 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | CA    | 3166 | 1/1   | 0.91 | 0.12 | 66,66,66,66                 | 0     |
| 57  | MG   | B7    | 101  | 1/1   | 0.91 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | B7    | 102  | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3018 | 1/1   | 0.91 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3406 | 1/1   | 0.91 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3065 | 1/1   | 0.91 | 0.24 | 63,63,63,63                 | 0     |
| 57  | MG   | CA    | 3009 | 1/1   | 0.91 | 0.14 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3644 | 1/1   | 0.91 | 0.08 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3010 | 1/1   | 0.91 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3374 | 1/1   | 0.91 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3033 | 1/1   | 0.91 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3048 | 1/1   | 0.91 | 0.26 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3653 | 1/1   | 0.91 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | CX    | 3004 | 1/1   | 0.91 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | CA    | 3014 | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3659 | 1/1   | 0.91 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3016 | 1/1   | 0.91 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 3017 | 1/1   | 0.91 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3244 | 1/1   | 0.91 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3017 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3024 | 1/1   | 0.91 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3078 | 1/1   | 0.91 | 0.31 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3695 | 1/1   | 0.91 | 0.13 | 67,67,67,67                 | 0     |
| 57  | MG   | AA    | 3173 | 1/1   | 0.91 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | DB    | 3004 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3048 | 1/1   | 0.91 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3411 | 1/1   | 0.91 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3264 | 1/1   | 0.91 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | DB    | 3012 | 1/1   | 0.91 | 0.26 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3057 | 1/1   | 0.91 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 3061 | 1/1   | 0.91 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3580 | 1/1   | 0.91 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | DF    | 3001 | 1/1   | 0.91 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3418 | 1/1   | 0.91 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3067 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 3030 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | AA    | 3174 | 1/1   | 0.91 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | D0    | 101  | 1/1   | 0.91 | 0.16 | 71,71,71,71                 | 0     |
| 57  | MG   | BA    | 3584 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3714 | 1/1   | 0.91 | 0.10 | 57,57,57,57                 | 0     |
| 59  | ZN   | D4    | 501  | 1/1   | 0.91 | 0.08 | 144,144,144,144             | 0     |
| 57  | MG   | DA    | 3429 | 1/1   | 0.92 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3526 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3087 | 1/1   | 0.92 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3364 | 1/1   | 0.92 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3145 | 1/1   | 0.92 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3436 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3095 | 1/1   | 0.92 | 0.28 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3532 | 1/1   | 0.92 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3110 | 1/1   | 0.92 | 0.14 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3372 | 1/1   | 0.92 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 3112 | 1/1   | 0.92 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3114 | 1/1   | 0.92 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3715 | 1/1   | 0.92 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3453 | 1/1   | 0.92 | 0.20 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3154 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3457 | 1/1   | 0.92 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3003 | 1/1   | 0.92 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3463 | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3720 | 1/1   | 0.92 | 0.16 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3132 | 1/1   | 0.92 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3133 | 1/1   | 0.92 | 0.24 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3139 | 1/1   | 0.92 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3198 | 1/1   | 0.92 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3723 | 1/1   | 0.92 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3474 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3476 | 1/1   | 0.92 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3177 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3012 | 1/1   | 0.92 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3389 | 1/1   | 0.92 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3180 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3485 | 1/1   | 0.92 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3165 | 1/1   | 0.92 | 0.24 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3566 | 1/1   | 0.92 | 0.17 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3180 | 1/1   | 0.92 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3497 | 1/1   | 0.92 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3570 | 1/1   | 0.92 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3184 | 1/1   | 0.92 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3038 | 1/1   | 0.92 | 0.32 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3186 | 1/1   | 0.92 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3503 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3576 | 1/1   | 0.92 | 0.07 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3513 | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3197 | 1/1   | 0.92 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3202 | 1/1   | 0.92 | 0.21 | 60,60,60,60                 | 0     |
| 57  | MG   | CA    | 3074 | 1/1   | 0.92 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3021 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3078 | 1/1   | 0.92 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3212 | 1/1   | 0.92 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3527 | 1/1   | 0.92 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | AA    | 3068 | 1/1   | 0.92 | 0.17 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3587 | 1/1   | 0.92 | 0.11 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3216 | 1/1   | 0.92 | 0.27 | 56,56,56,56                 | 0     |
| 57  | MG   | CA    | 3085 | 1/1   | 0.92 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3589 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | AA    | 3094 | 1/1   | 0.92 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3540 | 1/1   | 0.92 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | AA    | 3115 | 1/1   | 0.92 | 0.22 | 79,79,79,79                 | 0     |
| 57  | MG   | DA    | 3225 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3229 | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3592 | 1/1   | 0.92 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3408 | 1/1   | 0.92 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3224 | 1/1   | 0.92 | 0.28 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3154 | 1/1   | 0.92 | 0.16 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3229 | 1/1   | 0.92 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3243 | 1/1   | 0.92 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3599 | 1/1   | 0.92 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3417 | 1/1   | 0.92 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | CA    | 3110 | 1/1   | 0.92 | 0.10 | 65,65,65,65                 | 0     |
| 57  | MG   | AA    | 3178 | 1/1   | 0.92 | 0.21 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3180 | 1/1   | 0.92 | 0.13 | 73,73,73,73                 | 0     |
| 57  | MG   | BA    | 3421 | 1/1   | 0.92 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3064 | 1/1   | 0.92 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3573 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | AA    | 3058 | 1/1   | 0.92 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3044 | 1/1   | 0.92 | 0.25 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3258 | 1/1   | 0.92 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3578 | 1/1   | 0.92 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3793 | 1/1   | 0.92 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3260 | 1/1   | 0.92 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | CA    | 3125 | 1/1   | 0.92 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | AA    | 3157 | 1/1   | 0.92 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3283 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3592 | 1/1   | 0.92 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3073 | 1/1   | 0.92 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3288 | 1/1   | 0.92 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3289 | 1/1   | 0.92 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3602 | 1/1   | 0.92 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3800 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3605 | 1/1   | 0.92 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3075 | 1/1   | 0.92 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3629 | 1/1   | 0.92 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3630 | 1/1   | 0.92 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3275 | 1/1   | 0.92 | 0.12 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3612 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3278 | 1/1   | 0.92 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | BB    | 213  | 1/1   | 0.92 | 0.21 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3302 | 1/1   | 0.92 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | BA    | 3444 | 1/1   | 0.92 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3445 | 1/1   | 0.92 | 0.20 | 63,63,63,63                 | 0     |
| 57  | MG   | BB    | 219  | 1/1   | 0.92 | 0.17 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3446 | 1/1   | 0.92 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3285 | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3293 | 1/1   | 0.92 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3076 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | BG    | 202  | 1/1   | 0.92 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | BN    | 3004 | 1/1   | 0.92 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | BO    | 202  | 1/1   | 0.92 | 0.09 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3460 | 1/1   | 0.92 | 0.21 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3159 | 1/1   | 0.92 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3334 | 1/1   | 0.92 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | B2    | 3001 | 1/1   | 0.92 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3337 | 1/1   | 0.92 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | CD    | 301  | 1/1   | 0.92 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3301 | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3650 | 1/1   | 0.92 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | AA    | 3189 | 1/1   | 0.92 | 0.11 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3351 | 1/1   | 0.92 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3091 | 1/1   | 0.92 | 0.26 | 56,56,56,56                 | 0     |
| 57  | MG   | AW    | 3004 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | B7    | 104  | 1/1   | 0.92 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3358 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | B7    | 105  | 1/1   | 0.92 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3310 | 1/1   | 0.92 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3313 | 1/1   | 0.92 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3478 | 1/1   | 0.92 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3656 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3667 | 1/1   | 0.92 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3190 | 1/1   | 0.92 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3484 | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3012 | 1/1   | 0.92 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3113 | 1/1   | 0.92 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3037 | 1/1   | 0.92 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3668 | 1/1   | 0.92 | 0.20 | 60,60,60,60                 | 0     |
| 57  | MG   | AA    | 3101 | 1/1   | 0.92 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3672 | 1/1   | 0.92 | 0.29 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3400 | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3046 | 1/1   | 0.92 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3103 | 1/1   | 0.92 | 0.35 | 73,73,73,73                 | 0     |
| 57  | MG   | DB    | 3002 | 1/1   | 0.92 | 0.22 | 65,65,65,65                 | 0     |
| 57  | MG   | DB    | 3003 | 1/1   | 0.92 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3405 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3322 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3052 | 1/1   | 0.92 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3054 | 1/1   | 0.92 | 0.27 | 48,48,48,48                 | 0     |
| 57  | MG   | AX    | 3012 | 1/1   | 0.92 | 0.13 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3195 | 1/1   | 0.92 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3682 | 1/1   | 0.92 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3066 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3344 | 1/1   | 0.92 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | AA    | 3083 | 1/1   | 0.92 | 0.26 | 57,57,57,57                 | 0     |
| 57  | MG   | DQ    | 3004 | 1/1   | 0.92 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3685 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | AY    | 3002 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3089 | 1/1   | 0.92 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3002 | 1/1   | 0.92 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3361 | 1/1   | 0.92 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3143 | 1/1   | 0.92 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3427 | 1/1   | 0.92 | 0.10 | 45,45,45,45                 | 0     |
| 60  | K    | CX    | 3001 | 1/1   | 0.92 | 0.14 | 82,82,82,82                 | 0     |
| 57  | MG   | BA    | 3767 | 1/1   | 0.93 | 0.12 | 73,73,73,73                 | 0     |
| 57  | MG   | BA    | 3628 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3158 | 1/1   | 0.93 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3159 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3088 | 1/1   | 0.93 | 0.27 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3163 | 1/1   | 0.93 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3016 | 1/1   | 0.93 | 0.08 | 63,63,63,63                 | 0     |
| 57  | MG   | CA    | 3086 | 1/1   | 0.93 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3780 | 1/1   | 0.93 | 0.09 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3358 | 1/1   | 0.93 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3087 | 1/1   | 0.93 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | AY    | 3001 | 1/1   | 0.93 | 0.31 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3228 | 1/1   | 0.93 | 0.24 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3092 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | AA    | 3067 | 1/1   | 0.93 | 0.23 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3202 | 1/1   | 0.93 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3366 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3797 | 1/1   | 0.93 | 0.08 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3371 | 1/1   | 0.93 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3232 | 1/1   | 0.93 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3802 | 1/1   | 0.93 | 0.29 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3808 | 1/1   | 0.93 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3809 | 1/1   | 0.93 | 0.08 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3489 | 1/1   | 0.93 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3490 | 1/1   | 0.93 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3643 | 1/1   | 0.93 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3493 | 1/1   | 0.93 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3500 | 1/1   | 0.93 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | AY    | 3003 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3221 | 1/1   | 0.93 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3376 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3380 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | BB    | 209  | 1/1   | 0.93 | 0.33 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3506 | 1/1   | 0.93 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3032 | 1/1   | 0.93 | 0.10 | 67,67,67,67                 | 0     |
| 57  | MG   | CA    | 3127 | 1/1   | 0.93 | 0.16 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3511 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3236 | 1/1   | 0.93 | 0.24 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3519 | 1/1   | 0.93 | 0.11 | 63,63,63,63                 | 0     |
| 57  | MG   | AA    | 3150 | 1/1   | 0.93 | 0.15 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 3135 | 1/1   | 0.93 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3522 | 1/1   | 0.93 | 0.15 | 71,71,71,71                 | 0     |
| 57  | MG   | BB    | 220  | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3662 | 1/1   | 0.93 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3247 | 1/1   | 0.93 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3248 | 1/1   | 0.93 | 0.21 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3249 | 1/1   | 0.93 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | BE    | 305  | 1/1   | 0.93 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3254 | 1/1   | 0.93 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | AA    | 3179 | 1/1   | 0.93 | 0.14 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3538 | 1/1   | 0.93 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | BF    | 306  | 1/1   | 0.93 | 0.22 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3517 | 1/1   | 0.93 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3260 | 1/1   | 0.93 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3543 | 1/1   | 0.93 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | BG    | 201  | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3152 | 1/1   | 0.93 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3547 | 1/1   | 0.93 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3263 | 1/1   | 0.93 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3267 | 1/1   | 0.93 | 0.12 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 3109 | 1/1   | 0.93 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3394 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | BQ    | 3005 | 1/1   | 0.93 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3210 | 1/1   | 0.93 | 0.25 | 59,59,59,59                 | 0     |
| 57  | MG   | BV    | 204  | 1/1   | 0.93 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3160 | 1/1   | 0.93 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3263 | 1/1   | 0.93 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3163 | 1/1   | 0.93 | 0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | B0    | 103  | 1/1   | 0.93 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3398 | 1/1   | 0.93 | 0.09 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3125 | 1/1   | 0.93 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3537 | 1/1   | 0.93 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3293 | 1/1   | 0.93 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3538 | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3296 | 1/1   | 0.93 | 0.07 | 28,28,28,28                 | 0     |
| 57  | MG   | AA    | 3093 | 1/1   | 0.93 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3271 | 1/1   | 0.93 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3543 | 1/1   | 0.93 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | AA    | 3006 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | CW    | 3001 | 1/1   | 0.93 | 0.16 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3590 | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3305 | 1/1   | 0.93 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3003 | 1/1   | 0.93 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | AA    | 3070 | 1/1   | 0.93 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3694 | 1/1   | 0.93 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3279 | 1/1   | 0.93 | 0.21 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3696 | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3316 | 1/1   | 0.93 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3552 | 1/1   | 0.93 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 3009 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3033 | 1/1   | 0.93 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3015 | 1/1   | 0.93 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3288 | 1/1   | 0.93 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3611 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3019 | 1/1   | 0.93 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3560 | 1/1   | 0.93 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3562 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3032 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3616 | 1/1   | 0.93 | 0.09 | 71,71,71,71                 | 0     |
| 57  | MG   | BA    | 3413 | 1/1   | 0.93 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3568 | 1/1   | 0.93 | 0.07 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3038 | 1/1   | 0.93 | 0.15 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3131 | 1/1   | 0.93 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3342 | 1/1   | 0.93 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | AA    | 3118 | 1/1   | 0.93 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3298 | 1/1   | 0.93 | 0.20 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3352 | 1/1   | 0.93 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | AA    | 3119 | 1/1   | 0.93 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3153 | 1/1   | 0.93 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3722 | 1/1   | 0.93 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3056 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | AA    | 3072 | 1/1   | 0.93 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3303 | 1/1   | 0.93 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3364 | 1/1   | 0.93 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3366 | 1/1   | 0.93 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3367 | 1/1   | 0.93 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3368 | 1/1   | 0.93 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3001 | 1/1   | 0.93 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | CA    | 3034 | 1/1   | 0.93 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3376 | 1/1   | 0.93 | 0.19 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3061 | 1/1   | 0.93 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3165 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3070 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3384 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3311 | 1/1   | 0.93 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3168 | 1/1   | 0.93 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3654 | 1/1   | 0.93 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3734 | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3172 | 1/1   | 0.93 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | CA    | 3048 | 1/1   | 0.93 | 0.15 | 67,67,67,67                 | 0     |
| 57  | MG   | DA    | 3658 | 1/1   | 0.93 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3078 | 1/1   | 0.93 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | AX    | 3004 | 1/1   | 0.93 | 0.16 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3065 | 1/1   | 0.93 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3082 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3083 | 1/1   | 0.93 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | AX    | 3007 | 1/1   | 0.93 | 0.10 | 67,67,67,67                 | 0     |
| 57  | MG   | CA    | 3054 | 1/1   | 0.93 | 0.31 | 69,69,69,69                 | 0     |
| 57  | MG   | AA    | 3131 | 1/1   | 0.93 | 0.16 | 71,71,71,71                 | 0     |
| 57  | MG   | AA    | 3061 | 1/1   | 0.93 | 0.30 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3098 | 1/1   | 0.93 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3325 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3416 | 1/1   | 0.93 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3200 | 1/1   | 0.93 | 0.31 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3456 | 1/1   | 0.93 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3337 | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | DB    | 3007 | 1/1   | 0.93 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3751 | 1/1   | 0.93 | 0.09 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3753 | 1/1   | 0.93 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3424 | 1/1   | 0.93 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | AX    | 3010 | 1/1   | 0.93 | 0.16 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3461 | 1/1   | 0.93 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3124 | 1/1   | 0.93 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3462 | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3126 | 1/1   | 0.93 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | DQ    | 3002 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3130 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3343 | 1/1   | 0.93 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3102 | 1/1   | 0.93 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3349 | 1/1   | 0.93 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | DW    | 3004 | 1/1   | 0.93 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | DY    | 502  | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3021 | 1/1   | 0.93 | 0.20 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3439 | 1/1   | 0.93 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 3075 | 1/1   | 0.93 | 0.18 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3443 | 1/1   | 0.93 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3766 | 1/1   | 0.93 | 0.09 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 3096 | 1/1   | 0.94 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3317 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | AX    | 3015 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3106 | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3108 | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3423 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3053 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3448 | 1/1   | 0.94 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3182 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3320 | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3321 | 1/1   | 0.94 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3457 | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 3122 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3183 | 1/1   | 0.94 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3603 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3435 | 1/1   | 0.94 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3024 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3607 | 1/1   | 0.94 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3128 | 1/1   | 0.94 | 0.20 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 3025 | 1/1   | 0.94 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3018 | 1/1   | 0.94 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3080 | 1/1   | 0.94 | 0.23 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3136 | 1/1   | 0.94 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3138 | 1/1   | 0.94 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3765 | 1/1   | 0.94 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | AA    | 3079 | 1/1   | 0.94 | 0.17 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3207 | 1/1   | 0.94 | 0.23 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3073 | 1/1   | 0.94 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3148 | 1/1   | 0.94 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3768 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3151 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3153 | 1/1   | 0.94 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3621 | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3157 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | CA    | 3076 | 1/1   | 0.94 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3770 | 1/1   | 0.94 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3472 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3347 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 3079 | 1/1   | 0.94 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3164 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3776 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3169 | 1/1   | 0.94 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3170 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3778 | 1/1   | 0.94 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3469 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3486 | 1/1   | 0.94 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3348 | 1/1   | 0.94 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 3213 | 1/1   | 0.94 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3188 | 1/1   | 0.94 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3475 | 1/1   | 0.94 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3192 | 1/1   | 0.94 | 0.12 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3494 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | CA    | 3095 | 1/1   | 0.94 | 0.23 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3496 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3787 | 1/1   | 0.94 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3198 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3200 | 1/1   | 0.94 | 0.11 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3477 | 1/1   | 0.94 | 0.18 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3203 | 1/1   | 0.94 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3062 | 1/1   | 0.94 | 0.27 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3093 | 1/1   | 0.94 | 0.22 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3106 | 1/1   | 0.94 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | AF    | 3001 | 1/1   | 0.94 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3209 | 1/1   | 0.94 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3210 | 1/1   | 0.94 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3211 | 1/1   | 0.94 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3635 | 1/1   | 0.94 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3101 | 1/1   | 0.94 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3214 | 1/1   | 0.94 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3007 | 1/1   | 0.94 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 3111 | 1/1   | 0.94 | 0.08 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3801 | 1/1   | 0.94 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3106 | 1/1   | 0.94 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3803 | 1/1   | 0.94 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | AM    | 201  | 1/1   | 0.94 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3493 | 1/1   | 0.94 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3494 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3228 | 1/1   | 0.94 | 0.22 | 38,38,38,38                 | 0     |
| 57  | MG   | CA    | 3119 | 1/1   | 0.94 | 0.08 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3237 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3644 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 3122 | 1/1   | 0.94 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | BB    | 205  | 1/1   | 0.94 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3017 | 1/1   | 0.94 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3548 | 1/1   | 0.94 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3549 | 1/1   | 0.94 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3239 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3649 | 1/1   | 0.94 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | BB    | 210  | 1/1   | 0.94 | 0.07 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3245 | 1/1   | 0.94 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3129 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | CA    | 3132 | 1/1   | 0.94 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3502 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3561 | 1/1   | 0.94 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3250 | 1/1   | 0.94 | 0.13 | 69,69,69,69                 | 0     |
| 57  | MG   | CA    | 3134 | 1/1   | 0.94 | 0.17 | 69,69,69,69                 | 0     |
| 57  | MG   | DA    | 3565 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | BB    | 214  | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3135 | 1/1   | 0.94 | 0.24 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3116 | 1/1   | 0.94 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | CA    | 3139 | 1/1   | 0.94 | 0.24 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3505 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3084 | 1/1   | 0.94 | 0.26 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3143 | 1/1   | 0.94 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3118 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3265 | 1/1   | 0.94 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3582 | 1/1   | 0.94 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | BD    | 304  | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | CA    | 3147 | 1/1   | 0.94 | 0.20 | 64,64,64,64                 | 0     |
| 57  | MG   | DA    | 3585 | 1/1   | 0.94 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | CA    | 3148 | 1/1   | 0.94 | 0.16 | 70,70,70,70                 | 0     |
| 57  | MG   | DA    | 3272 | 1/1   | 0.94 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3659 | 1/1   | 0.94 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | BE    | 303  | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | AA    | 3137 | 1/1   | 0.94 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | BE    | 307  | 1/1   | 0.94 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3005 | 1/1   | 0.94 | 0.18 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3284 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | BF    | 304  | 1/1   | 0.94 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3665 | 1/1   | 0.94 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3122 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3024 | 1/1   | 0.94 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3516 | 1/1   | 0.94 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | AA    | 3009 | 1/1   | 0.94 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | BN    | 3006 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | AX    | 3003 | 1/1   | 0.94 | 0.10 | 71,71,71,71                 | 0     |
| 57  | MG   | BQ    | 3004 | 1/1   | 0.94 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3393 | 1/1   | 0.94 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | BR    | 201  | 1/1   | 0.94 | 0.22 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3268 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3674 | 1/1   | 0.94 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3269 | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3307 | 1/1   | 0.94 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | BZ    | 3001 | 1/1   | 0.94 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | B0    | 102  | 1/1   | 0.94 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3035 | 1/1   | 0.94 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3531 | 1/1   | 0.94 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3273 | 1/1   | 0.94 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3039 | 1/1   | 0.94 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3047 | 1/1   | 0.94 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3005 | 1/1   | 0.94 | 0.28 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3006 | 1/1   | 0.94 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3403 | 1/1   | 0.94 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3134 | 1/1   | 0.94 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3328 | 1/1   | 0.94 | 0.09 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3138 | 1/1   | 0.94 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3139 | 1/1   | 0.94 | 0.26 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3332 | 1/1   | 0.94 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3289 | 1/1   | 0.94 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3018 | 1/1   | 0.94 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3290 | 1/1   | 0.94 | 0.21 | 40,40,40,40                 | 0     |
| 57  | MG   | AA    | 3066 | 1/1   | 0.94 | 0.29 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3551 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3645 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3030 | 1/1   | 0.94 | 0.06 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3704 | 1/1   | 0.94 | 0.09 | 77,77,77,77                 | 0     |
| 57  | MG   | DA    | 3650 | 1/1   | 0.94 | 0.09 | 67,67,67,67                 | 0     |
| 57  | MG   | AX    | 3006 | 1/1   | 0.94 | 0.08 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3296 | 1/1   | 0.94 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3022 | 1/1   | 0.94 | 0.17 | 71,71,71,71                 | 0     |
| 57  | MG   | CA    | 3013 | 1/1   | 0.94 | 0.20 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3058 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3156 | 1/1   | 0.94 | 0.24 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3564 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3359 | 1/1   | 0.94 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3007 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3660 | 1/1   | 0.94 | 0.20 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3361 | 1/1   | 0.94 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 3019 | 1/1   | 0.94 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | CA    | 3020 | 1/1   | 0.94 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | AA    | 3112 | 1/1   | 0.94 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3161 | 1/1   | 0.94 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3162 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | CA    | 3025 | 1/1   | 0.94 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3372 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3675 | 1/1   | 0.94 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3573 | 1/1   | 0.94 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3068 | 1/1   | 0.94 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3378 | 1/1   | 0.94 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3379 | 1/1   | 0.94 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3307 | 1/1   | 0.94 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3308 | 1/1   | 0.94 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3579 | 1/1   | 0.94 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3072 | 1/1   | 0.94 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3163 | 1/1   | 0.94 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3391 | 1/1   | 0.94 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3729 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3396 | 1/1   | 0.94 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | DD    | 307  | 1/1   | 0.94 | 0.26 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3581 | 1/1   | 0.94 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3582 | 1/1   | 0.94 | 0.17 | 74,74,74,74                 | 0     |
| 57  | MG   | DF    | 3002 | 1/1   | 0.94 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | DN    | 5001 | 1/1   | 0.94 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | AA    | 3056 | 1/1   | 0.94 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3201 | 1/1   | 0.94 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | DQ    | 3003 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3585 | 1/1   | 0.94 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | AA    | 3045 | 1/1   | 0.94 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | DU    | 3001 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | DU    | 3002 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3442 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | DW    | 3001 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3085 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3047 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3088 | 1/1   | 0.94 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3071 | 1/1   | 0.94 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3091 | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3092 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 3096 | 1/1   | 0.94 | 0.34 | 63,63,63,63                 | 0     |
| 57  | MG   | CA    | 3050 | 1/1   | 0.94 | 0.32 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3173 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3175 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3369 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3370 | 1/1   | 0.95 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3657 | 1/1   | 0.95 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3509 | 1/1   | 0.95 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | AX    | 3005 | 1/1   | 0.95 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3041 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3189 | 1/1   | 0.95 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3513 | 1/1   | 0.95 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3664 | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3196 | 1/1   | 0.95 | 0.21 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3130 | 1/1   | 0.95 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3242 | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3666 | 1/1   | 0.95 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3466 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3201 | 1/1   | 0.95 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3011 | 1/1   | 0.95 | 0.26 | 57,57,57,57                 | 0     |
| 57  | MG   | AA    | 3039 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3382 | 1/1   | 0.95 | 0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3518 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3383 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3163 | 1/1   | 0.95 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3251 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | BG    | 203  | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3479 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3252 | 1/1   | 0.95 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | CA    | 3145 | 1/1   | 0.95 | 0.09 | 66,66,66,66                 | 0     |
| 57  | MG   | BN    | 3005 | 1/1   | 0.95 | 0.04 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3675 | 1/1   | 0.95 | 0.08 | 67,67,67,67                 | 0     |
| 57  | MG   | BA    | 3676 | 1/1   | 0.95 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3529 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3488 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3217 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3055 | 1/1   | 0.95 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 3132 | 1/1   | 0.95 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3220 | 1/1   | 0.95 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | BU    | 204  | 1/1   | 0.95 | 0.17 | 35,35,35,35                 | 0     |
| 57  | MG   | CA    | 3154 | 1/1   | 0.95 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3130 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3224 | 1/1   | 0.95 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3087 | 1/1   | 0.95 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | AA    | 3029 | 1/1   | 0.95 | 0.25 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3062 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3266 | 1/1   | 0.95 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | AA    | 3034 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3233 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3508 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3510 | 1/1   | 0.95 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3511 | 1/1   | 0.95 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3162 | 1/1   | 0.95 | 0.09 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3514 | 1/1   | 0.95 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | AA    | 3071 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3238 | 1/1   | 0.95 | 0.28 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 3164 | 1/1   | 0.95 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | CA    | 3165 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 3035 | 1/1   | 0.95 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3546 | 1/1   | 0.95 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3697 | 1/1   | 0.95 | 0.11 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3246 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3147 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3528 | 1/1   | 0.95 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3529 | 1/1   | 0.95 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3701 | 1/1   | 0.95 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3549 | 1/1   | 0.95 | 0.19 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3272 | 1/1   | 0.95 | 0.36 | 48,48,48,48                 | 0     |
| 57  | MG   | CK    | 3001 | 1/1   | 0.95 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3252 | 1/1   | 0.95 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | B9    | 502  | 1/1   | 0.95 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3001 | 1/1   | 0.95 | 0.14 | 75,75,75,75                 | 0     |
| 57  | MG   | BA    | 3149 | 1/1   | 0.95 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3708 | 1/1   | 0.95 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3274 | 1/1   | 0.95 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3007 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3545 | 1/1   | 0.95 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3151 | 1/1   | 0.95 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3068 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | AA    | 3073 | 1/1   | 0.95 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3412 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3716 | 1/1   | 0.95 | 0.09 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3551 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3269 | 1/1   | 0.95 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3282 | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | AA    | 3141 | 1/1   | 0.95 | 0.18 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3555 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3015 | 1/1   | 0.95 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3567 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | AA    | 3208 | 1/1   | 0.95 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3559 | 1/1   | 0.95 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3277 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3562 | 1/1   | 0.95 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | AA    | 3143 | 1/1   | 0.95 | 0.08 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3281 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3021 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3022 | 1/1   | 0.95 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | AA    | 3030 | 1/1   | 0.95 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3292 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3570 | 1/1   | 0.95 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3026 | 1/1   | 0.95 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3211 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3077 | 1/1   | 0.95 | 0.25 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3292 | 1/1   | 0.95 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3033 | 1/1   | 0.95 | 0.08 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3294 | 1/1   | 0.95 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3579 | 1/1   | 0.95 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3164 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | AA    | 3181 | 1/1   | 0.95 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3297 | 1/1   | 0.95 | 0.05 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3428 | 1/1   | 0.95 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3081 | 1/1   | 0.95 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3587 | 1/1   | 0.95 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3430 | 1/1   | 0.95 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3047 | 1/1   | 0.95 | 0.19 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3169 | 1/1   | 0.95 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3303 | 1/1   | 0.95 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3049 | 1/1   | 0.95 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3170 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3595 | 1/1   | 0.95 | 0.08 | 59,59,59,59                 | 0     |
| 57  | MG   | CA    | 3032 | 1/1   | 0.95 | 0.29 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3600 | 1/1   | 0.95 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | BA    | 3006 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3310 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3173 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3606 | 1/1   | 0.95 | 0.14 | 71,71,71,71                 | 0     |
| 57  | MG   | DA    | 3059 | 1/1   | 0.95 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | CA    | 3035 | 1/1   | 0.95 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3439 | 1/1   | 0.95 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3743 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3063 | 1/1   | 0.95 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3305 | 1/1   | 0.95 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3746 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3326 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3175 | 1/1   | 0.95 | 0.08 | 20,20,20,20                 | 0     |
| 57  | MG   | CA    | 3042 | 1/1   | 0.95 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3113 | 1/1   | 0.95 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3619 | 1/1   | 0.95 | 0.08 | 69,69,69,69                 | 0     |
| 57  | MG   | BA    | 3089 | 1/1   | 0.95 | 0.05 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3595 | 1/1   | 0.95 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3622 | 1/1   | 0.95 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | AA    | 3149 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3016 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3450 | 1/1   | 0.95 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | AA    | 3055 | 1/1   | 0.95 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | AN    | 502  | 1/1   | 0.95 | 0.34 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3098 | 1/1   | 0.95 | 0.13 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3341 | 1/1   | 0.95 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3080 | 1/1   | 0.95 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3346 | 1/1   | 0.95 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3191 | 1/1   | 0.95 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3606 | 1/1   | 0.95 | 0.11 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3763 | 1/1   | 0.95 | 0.09 | 24,24,24,24                 | 0     |
| 57  | MG   | DA    | 3353 | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3193 | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3196 | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3640 | 1/1   | 0.95 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3610 | 1/1   | 0.95 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3100 | 1/1   | 0.95 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3614 | 1/1   | 0.95 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3201 | 1/1   | 0.95 | 0.30 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3019 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3618 | 1/1   | 0.95 | 0.11 | 65,65,65,65                 | 0     |
| 57  | MG   | CA    | 3068 | 1/1   | 0.95 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3773 | 1/1   | 0.95 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3100 | 1/1   | 0.95 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3775 | 1/1   | 0.95 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3370 | 1/1   | 0.95 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3203 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | CA    | 3072 | 1/1   | 0.95 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3204 | 1/1   | 0.95 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3326 | 1/1   | 0.95 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3329 | 1/1   | 0.95 | 0.12 | 60,60,60,60                 | 0     |
| 57  | MG   | AA    | 3019 | 1/1   | 0.95 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3116 | 1/1   | 0.95 | 0.25 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3206 | 1/1   | 0.95 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3627 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3119 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3385 | 1/1   | 0.95 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3120 | 1/1   | 0.95 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3098 | 1/1   | 0.95 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3392 | 1/1   | 0.95 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | CA    | 3081 | 1/1   | 0.95 | 0.05 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3395 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3208 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3789 | 1/1   | 0.95 | 0.07 | 12,12,12,12                 | 0     |
| 57  | MG   | BA    | 3790 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3792 | 1/1   | 0.95 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3129 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3209 | 1/1   | 0.95 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3131 | 1/1   | 0.95 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3345 | 1/1   | 0.95 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | DB    | 3009 | 1/1   | 0.95 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3480 | 1/1   | 0.95 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 3134 | 1/1   | 0.95 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | CA    | 3093 | 1/1   | 0.95 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | DD    | 301  | 1/1   | 0.95 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3137 | 1/1   | 0.95 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | DD    | 304  | 1/1   | 0.95 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | DD    | 306  | 1/1   | 0.95 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3211 | 1/1   | 0.95 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | DD    | 309  | 1/1   | 0.95 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3107 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | DE    | 304  | 1/1   | 0.95 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3485 | 1/1   | 0.95 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | AA    | 3099 | 1/1   | 0.95 | 0.24 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3145 | 1/1   | 0.95 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3215 | 1/1   | 0.95 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 3120 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3805 | 1/1   | 0.95 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3354 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3152 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3027 | 1/1   | 0.95 | 0.06 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3115 | 1/1   | 0.95 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3227 | 1/1   | 0.95 | 0.25 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3645 | 1/1   | 0.95 | 0.05 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3428 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | BB    | 204  | 1/1   | 0.95 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3030 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | AA    | 3080 | 1/1   | 0.95 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | AA    | 3122 | 1/1   | 0.95 | 0.08 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3119 | 1/1   | 0.95 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 3123 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3368 | 1/1   | 0.95 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3464 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3050 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3762 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3233 | 1/1   | 0.96 | 0.25 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3004 | 1/1   | 0.96 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3236 | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3226 | 1/1   | 0.96 | 0.26 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3051 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3528 | 1/1   | 0.96 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3008 | 1/1   | 0.96 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 3130 | 1/1   | 0.96 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3232 | 1/1   | 0.96 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3646 | 1/1   | 0.96 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3013 | 1/1   | 0.96 | 0.04 | 40,40,40,40                 | 0     |
| 57  | MG   | AA    | 3010 | 1/1   | 0.96 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3483 | 1/1   | 0.96 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3237 | 1/1   | 0.96 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3240 | 1/1   | 0.96 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3060 | 1/1   | 0.96 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3240 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3241 | 1/1   | 0.96 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3772 | 1/1   | 0.96 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3324 | 1/1   | 0.96 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3774 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3536 | 1/1   | 0.96 | 0.22 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3108 | 1/1   | 0.96 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 3133 | 1/1   | 0.96 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3027 | 1/1   | 0.96 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3028 | 1/1   | 0.96 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3029 | 1/1   | 0.96 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3328 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3031 | 1/1   | 0.96 | 0.25 | 43,43,43,43                 | 0     |
| 57  | MG   | AA    | 3081 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3330 | 1/1   | 0.96 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3331 | 1/1   | 0.96 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3507 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3257 | 1/1   | 0.96 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3509 | 1/1   | 0.96 | 0.08 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3036 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3044 | 1/1   | 0.96 | 0.23 | 62,62,62,62                 | 0     |
| 57  | MG   | CA    | 3045 | 1/1   | 0.96 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3043 | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3515 | 1/1   | 0.96 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3332 | 1/1   | 0.96 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3785 | 1/1   | 0.96 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3786 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3249 | 1/1   | 0.96 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3336 | 1/1   | 0.96 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | BA    | 3437 | 1/1   | 0.96 | 0.10 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3250 | 1/1   | 0.96 | 0.38 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3171 | 1/1   | 0.96 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3526 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3008 | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3275 | 1/1   | 0.96 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3256 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3556 | 1/1   | 0.96 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3278 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3557 | 1/1   | 0.96 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3533 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3280 | 1/1   | 0.96 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3798 | 1/1   | 0.96 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 3282 | 1/1   | 0.96 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | AA    | 3015 | 1/1   | 0.96 | 0.11 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3064 | 1/1   | 0.96 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3065 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3346 | 1/1   | 0.96 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3174 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3063 | 1/1   | 0.96 | 0.25 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3203 | 1/1   | 0.96 | 0.06 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3804 | 1/1   | 0.96 | 0.32 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3451 | 1/1   | 0.96 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3350 | 1/1   | 0.96 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3262 | 1/1   | 0.96 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3352 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3178 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | AA    | 3075 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3578 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | AA    | 3085 | 1/1   | 0.96 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3687 | 1/1   | 0.96 | 0.09 | 22,22,22,22                 | 0     |
| 57  | MG   | BA    | 3690 | 1/1   | 0.96 | 0.22 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3691 | 1/1   | 0.96 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3053 | 1/1   | 0.96 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | DA    | 3306 | 1/1   | 0.96 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3207 | 1/1   | 0.96 | 0.11 | 65,65,65,65                 | 0     |
| 57  | MG   | CA    | 3080 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3063 | 1/1   | 0.96 | 0.04 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 3089 | 1/1   | 0.96 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3464 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3312 | 1/1   | 0.96 | 0.06 | 54,54,54,54                 | 0     |
| 57  | MG   | BB    | 216  | 1/1   | 0.96 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | CA    | 3084 | 1/1   | 0.96 | 0.12 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | AA    | 3140 | 1/1   | 0.96 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3190 | 1/1   | 0.96 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | AA    | 3043 | 1/1   | 0.96 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3702 | 1/1   | 0.96 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3576 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 57  | MG   | BD    | 303  | 1/1   | 0.96 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3322 | 1/1   | 0.96 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3323 | 1/1   | 0.96 | 0.06 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3101 | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3091 | 1/1   | 0.96 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 3092 | 1/1   | 0.96 | 0.05 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3107 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3330 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3074 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3109 | 1/1   | 0.96 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3333 | 1/1   | 0.96 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | BD    | 305  | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | BD    | 309  | 1/1   | 0.96 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3026 | 1/1   | 0.96 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3113 | 1/1   | 0.96 | 0.24 | 60,60,60,60                 | 0     |
| 57  | MG   | CA    | 3101 | 1/1   | 0.96 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3596 | 1/1   | 0.96 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3276 | 1/1   | 0.96 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | BE    | 304  | 1/1   | 0.96 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3601 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | CA    | 3105 | 1/1   | 0.96 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3343 | 1/1   | 0.96 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3345 | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3472 | 1/1   | 0.96 | 0.04 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3199 | 1/1   | 0.96 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3350 | 1/1   | 0.96 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3710 | 1/1   | 0.96 | 0.09 | 57,57,57,57                 | 0     |
| 57  | MG   | BF    | 301  | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | BF    | 302  | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | BF    | 303  | 1/1   | 0.96 | 0.33 | 49,49,49,49                 | 0     |
| 57  | MG   | AA    | 3142 | 1/1   | 0.96 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3476 | 1/1   | 0.96 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 3114 | 1/1   | 0.96 | 0.06 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3713 | 1/1   | 0.96 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | BF    | 309  | 1/1   | 0.96 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3077 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3374 | 1/1   | 0.96 | 0.12 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3363 | 1/1   | 0.96 | 0.06 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3479 | 1/1   | 0.96 | 0.06 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3135 | 1/1   | 0.96 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | BN    | 3001 | 1/1   | 0.96 | 0.22 | 53,53,53,53                 | 0     |
| 57  | MG   | BN    | 3002 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 57  | MG   | BN    | 3003 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | CA    | 3123 | 1/1   | 0.96 | 0.07 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3600 | 1/1   | 0.96 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3284 | 1/1   | 0.96 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3375 | 1/1   | 0.96 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3142 | 1/1   | 0.96 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3029 | 1/1   | 0.96 | 0.43 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3146 | 1/1   | 0.96 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3132 | 1/1   | 0.96 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | BP    | 201  | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3381 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3150 | 1/1   | 0.96 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | BA    | 3133 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | AA    | 3169 | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3389 | 1/1   | 0.96 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | BU    | 201  | 1/1   | 0.96 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | BU    | 202  | 1/1   | 0.96 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3135 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | BU    | 207  | 1/1   | 0.96 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3647 | 1/1   | 0.96 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3648 | 1/1   | 0.96 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | CA    | 3137 | 1/1   | 0.96 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3397 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 57  | MG   | BV    | 201  | 1/1   | 0.96 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3162 | 1/1   | 0.96 | 0.21 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3727 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3401 | 1/1   | 0.96 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3031 | 1/1   | 0.96 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | BW    | 202  | 1/1   | 0.96 | 0.19 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3404 | 1/1   | 0.96 | 0.06 | 48,48,48,48                 | 0     |
| 57  | MG   | AA    | 3124 | 1/1   | 0.96 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | BX    | 3002 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3171 | 1/1   | 0.96 | 0.08 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3172 | 1/1   | 0.96 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3142 | 1/1   | 0.96 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | AE    | 201  | 1/1   | 0.96 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3664 | 1/1   | 0.96 | 0.13 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3666 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 3412 | 1/1   | 0.96 | 0.21 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3176 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3088 | 1/1   | 0.96 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3671 | 1/1   | 0.96 | 0.21 | 74,74,74,74                 | 0     |
| 57  | MG   | DA    | 3179 | 1/1   | 0.96 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | B1    | 101  | 1/1   | 0.96 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3674 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3733 | 1/1   | 0.96 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3392 | 1/1   | 0.96 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3677 | 1/1   | 0.96 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | CA    | 3151 | 1/1   | 0.96 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3186 | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | AA    | 3171 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | B6    | 101  | 1/1   | 0.96 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3736 | 1/1   | 0.96 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3193 | 1/1   | 0.96 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3620 | 1/1   | 0.96 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3739 | 1/1   | 0.96 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | DB    | 3010 | 1/1   | 0.96 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | B7    | 103  | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3090 | 1/1   | 0.96 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3395 | 1/1   | 0.96 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3217 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3036 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3222 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3434 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | AA    | 3126 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | CA    | 3005 | 1/1   | 0.96 | 0.05 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3510 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3438 | 1/1   | 0.96 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3090 | 1/1   | 0.96 | 0.24 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3402 | 1/1   | 0.96 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | DF    | 3003 | 1/1   | 0.96 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3441 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | CA    | 3169 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3445 | 1/1   | 0.96 | 0.06 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 3446 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3226 | 1/1   | 0.96 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3155 | 1/1   | 0.96 | 0.22 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3094 | 1/1   | 0.96 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3312 | 1/1   | 0.96 | 0.12 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DV    | 3001 | 1/1   | 0.96 | 0.09 | 70,70,70,70                 | 0     |
| 57  | MG   | DV    | 3002 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3043 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3756 | 1/1   | 0.96 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3637 | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3455 | 1/1   | 0.96 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | DX    | 101  | 1/1   | 0.96 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3456 | 1/1   | 0.96 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3758 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3458 | 1/1   | 0.96 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3461 | 1/1   | 0.96 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | AA    | 3128 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 60  | K    | AX    | 3001 | 1/1   | 0.96 | 0.08 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3519 | 1/1   | 0.96 | 0.06 | 55,55,55,55                 | 0     |
| 57  | MG   | CA    | 3096 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3390 | 1/1   | 0.97 | 0.11 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3123 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | CA    | 3099 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3230 | 1/1   | 0.97 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3512 | 1/1   | 0.97 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3617 | 1/1   | 0.97 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | CA    | 3103 | 1/1   | 0.97 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3056 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | BO    | 201  | 1/1   | 0.97 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3158 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3104 | 1/1   | 0.97 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3105 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3004 | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3304 | 1/1   | 0.97 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | BP    | 204  | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | BP    | 205  | 1/1   | 0.97 | 0.10 | 65,65,65,65                 | 0     |
| 57  | MG   | DA    | 3525 | 1/1   | 0.97 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | BQ    | 3001 | 1/1   | 0.97 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | BQ    | 3002 | 1/1   | 0.97 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | BQ    | 3003 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3309 | 1/1   | 0.97 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | AA    | 3116 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3186 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3115 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3176 | 1/1   | 0.97 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3625 | 1/1   | 0.97 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3535 | 1/1   | 0.97 | 0.06 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BU    | 203  | 1/1   | 0.97 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3537 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 3125 | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3319 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | AA    | 3014 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 3121 | 1/1   | 0.97 | 0.04 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3542 | 1/1   | 0.97 | 0.06 | 24,24,24,24                 | 0     |
| 57  | MG   | BA    | 3241 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 3162 | 1/1   | 0.97 | 0.06 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3324 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | DA    | 3325 | 1/1   | 0.97 | 0.06 | 35,35,35,35                 | 0     |
| 57  | MG   | BV    | 203  | 1/1   | 0.97 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3097 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | BV    | 205  | 1/1   | 0.97 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | BW    | 201  | 1/1   | 0.97 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3181 | 1/1   | 0.97 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | BW    | 204  | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3632 | 1/1   | 0.97 | 0.05 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3407 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | CA    | 3131 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | BX    | 3003 | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 3336 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | BY    | 502  | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3246 | 1/1   | 0.97 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | B0    | 101  | 1/1   | 0.97 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 3110 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3410 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3038 | 1/1   | 0.97 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3136 | 1/1   | 0.97 | 0.05 | 30,30,30,30                 | 0     |
| 57  | MG   | DA    | 3344 | 1/1   | 0.97 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | B3    | 3002 | 1/1   | 0.97 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | DA    | 3568 | 1/1   | 0.97 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | CA    | 3141 | 1/1   | 0.97 | 0.09 | 92,92,92,92                 | 0     |
| 57  | MG   | BA    | 3323 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | AA    | 3164 | 1/1   | 0.97 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3187 | 1/1   | 0.97 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | BA    | 3253 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3254 | 1/1   | 0.97 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3420 | 1/1   | 0.97 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3255 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3422 | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3189 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3581 | 1/1   | 0.97 | 0.08 | 57,57,57,57                 | 0     |
| 57  | MG   | B8    | 101  | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3534 | 1/1   | 0.97 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | AA    | 3165 | 1/1   | 0.97 | 0.08 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3002 | 1/1   | 0.97 | 0.08 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3161 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3140 | 1/1   | 0.97 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3365 | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3333 | 1/1   | 0.97 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3334 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3653 | 1/1   | 0.97 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3369 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 3166 | 1/1   | 0.97 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3167 | 1/1   | 0.97 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3168 | 1/1   | 0.97 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3539 | 1/1   | 0.97 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3655 | 1/1   | 0.97 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3192 | 1/1   | 0.97 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3141 | 1/1   | 0.97 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3777 | 1/1   | 0.97 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3194 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3340 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3177 | 1/1   | 0.97 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3661 | 1/1   | 0.97 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3433 | 1/1   | 0.97 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3547 | 1/1   | 0.97 | 0.17 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3341 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3182 | 1/1   | 0.97 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3435 | 1/1   | 0.97 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3393 | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3436 | 1/1   | 0.97 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3104 | 1/1   | 0.97 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3617 | 1/1   | 0.97 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | DA    | 3187 | 1/1   | 0.97 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3105 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3265 | 1/1   | 0.97 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3190 | 1/1   | 0.97 | 0.27 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3023 | 1/1   | 0.97 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3144 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | AA    | 3082 | 1/1   | 0.97 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3044 | 1/1   | 0.97 | 0.12 | 20,20,20,20                 | 0     |
| 57  | MG   | BA    | 3558 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | CA    | 3028 | 1/1   | 0.97 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3199 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3629 | 1/1   | 0.97 | 0.09 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3148 | 1/1   | 0.97 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3561 | 1/1   | 0.97 | 0.05 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3046 | 1/1   | 0.97 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3677 | 1/1   | 0.97 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | BA    | 3678 | 1/1   | 0.97 | 0.05 | 65,65,65,65                 | 0     |
| 57  | MG   | BA    | 3563 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3150 | 1/1   | 0.97 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3020 | 1/1   | 0.97 | 0.26 | 53,53,53,53                 | 0     |
| 57  | MG   | DA    | 3011 | 1/1   | 0.97 | 0.05 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3639 | 1/1   | 0.97 | 0.22 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3012 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3110 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | DA    | 3419 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 3014 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3452 | 1/1   | 0.97 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3111 | 1/1   | 0.97 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | CA    | 3040 | 1/1   | 0.97 | 0.05 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3571 | 1/1   | 0.97 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | DA    | 3020 | 1/1   | 0.97 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3810 | 1/1   | 0.97 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | CA    | 3043 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3454 | 1/1   | 0.97 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3112 | 1/1   | 0.97 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | BB    | 201  | 1/1   | 0.97 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3689 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | BB    | 203  | 1/1   | 0.97 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3277 | 1/1   | 0.97 | 0.35 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3575 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3356 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3210 | 1/1   | 0.97 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | BB    | 208  | 1/1   | 0.97 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3048 | 1/1   | 0.97 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3360 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | CA    | 3056 | 1/1   | 0.97 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | BB    | 211  | 1/1   | 0.97 | 0.04 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3665 | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3235 | 1/1   | 0.97 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3444 | 1/1   | 0.97 | 0.05 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3039 | 1/1   | 0.97 | 0.05 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3041 | 1/1   | 0.97 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3670 | 1/1   | 0.97 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | BB    | 212  | 1/1   | 0.97 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | BA    | 3281 | 1/1   | 0.97 | 0.29 | 60,60,60,60                 | 0     |
| 57  | MG   | DA    | 3045 | 1/1   | 0.97 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3698 | 1/1   | 0.97 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3157 | 1/1   | 0.97 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3283 | 1/1   | 0.97 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | BB    | 217  | 1/1   | 0.97 | 0.05 | 29,29,29,29                 | 0     |
| 57  | MG   | AA    | 3194 | 1/1   | 0.97 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | CA    | 3065 | 1/1   | 0.97 | 0.25 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3053 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | AA    | 3168 | 1/1   | 0.97 | 0.06 | 59,59,59,59                 | 0     |
| 57  | MG   | DA    | 3055 | 1/1   | 0.97 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | DB    | 3006 | 1/1   | 0.97 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3367 | 1/1   | 0.97 | 0.13 | 29,29,29,29                 | 0     |
| 57  | MG   | DA    | 3057 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3058 | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | BD    | 301  | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3706 | 1/1   | 0.97 | 0.05 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3286 | 1/1   | 0.97 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3287 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3258 | 1/1   | 0.97 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3216 | 1/1   | 0.97 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | BD    | 306  | 1/1   | 0.97 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | BD    | 308  | 1/1   | 0.97 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3079 | 1/1   | 0.97 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3475 | 1/1   | 0.97 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | DE    | 301  | 1/1   | 0.97 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | DE    | 302  | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | AA    | 3148 | 1/1   | 0.97 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3264 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | BE    | 302  | 1/1   | 0.97 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3219 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3220 | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 57  | MG   | DG    | 3001 | 1/1   | 0.97 | 0.04 | 55,55,55,55                 | 0     |
| 57  | MG   | AA    | 3129 | 1/1   | 0.97 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | DO    | 5001 | 1/1   | 0.97 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3378 | 1/1   | 0.97 | 0.04 | 28,28,28,28                 | 0     |
| 57  | MG   | DP    | 202  | 1/1   | 0.97 | 0.06 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3295 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3074 | 1/1   | 0.97 | 0.08 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3223 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3481 | 1/1   | 0.97 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3297 | 1/1   | 0.97 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3082 | 1/1   | 0.97 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3491 | 1/1   | 0.97 | 0.06 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3299 | 1/1   | 0.97 | 0.04 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3054 | 1/1   | 0.97 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | CA    | 3089 | 1/1   | 0.97 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | BA    | 3167 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3084 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3084 | 1/1   | 0.97 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3490 | 1/1   | 0.97 | 0.06 | 54,54,54,54                 | 0     |
| 57  | MG   | DA    | 3286 | 1/1   | 0.97 | 0.06 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3500 | 1/1   | 0.97 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | DA    | 3086 | 1/1   | 0.97 | 0.04 | 43,43,43,43                 | 0     |
| 59  | ZN   | CN    | 501  | 1/1   | 0.97 | 0.07 | 93,93,93,93                 | 0     |
| 59  | ZN   | DY    | 501  | 1/1   | 0.97 | 0.06 | 96,96,96,96                 | 0     |
| 57  | MG   | BA    | 3612 | 1/1   | 0.97 | 0.05 | 21,21,21,21                 | 0     |
| 57  | MG   | CA    | 3094 | 1/1   | 0.97 | 0.19 | 70,70,70,70                 | 0     |
| 57  | MG   | AA    | 3212 | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3569 | 1/1   | 0.98 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3025 | 1/1   | 0.98 | 0.05 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3137 | 1/1   | 0.98 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3442 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3589 | 1/1   | 0.98 | 0.06 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3049 | 1/1   | 0.98 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3744 | 1/1   | 0.98 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | BD    | 307  | 1/1   | 0.98 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3489 | 1/1   | 0.98 | 0.04 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3259 | 1/1   | 0.98 | 0.10 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 3183 | 1/1   | 0.98 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3449 | 1/1   | 0.98 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3491 | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3599 | 1/1   | 0.98 | 0.04 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3214 | 1/1   | 0.98 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3660 | 1/1   | 0.98 | 0.06 | 61,61,61,61                 | 0     |
| 57  | MG   | BA    | 3577 | 1/1   | 0.98 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | AA    | 3151 | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |
| 57  | MG   | BE    | 306  | 1/1   | 0.98 | 0.10 | 26,26,26,26                 | 0     |
| 57  | MG   | BA    | 3752 | 1/1   | 0.98 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 3191 | 1/1   | 0.98 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3009 | 1/1   | 0.98 | 0.06 | 28,28,28,28                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | DA    | 3460 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3425 | 1/1   | 0.98 | 0.04 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3028 | 1/1   | 0.98 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3195 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3010 | 1/1   | 0.98 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3011 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 57  | MG   | AA    | 3050 | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | BF    | 307  | 1/1   | 0.98 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3221 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3586 | 1/1   | 0.98 | 0.04 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3032 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3471 | 1/1   | 0.98 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3146 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3204 | 1/1   | 0.98 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3373 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3270 | 1/1   | 0.98 | 0.05 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3013 | 1/1   | 0.98 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3085 | 1/1   | 0.98 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3377 | 1/1   | 0.98 | 0.06 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3480 | 1/1   | 0.98 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3184 | 1/1   | 0.98 | 0.22 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3379 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3440 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 57  | MG   | CA    | 3155 | 1/1   | 0.98 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | BA    | 3441 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3086 | 1/1   | 0.98 | 0.07 | 22,22,22,22                 | 0     |
| 57  | MG   | BP    | 202  | 1/1   | 0.98 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | BP    | 203  | 1/1   | 0.98 | 0.07 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3014 | 1/1   | 0.98 | 0.23 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3347 | 1/1   | 0.98 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3059 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | DA    | 3349 | 1/1   | 0.98 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3094 | 1/1   | 0.98 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | BA    | 3188 | 1/1   | 0.98 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3521 | 1/1   | 0.98 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | DA    | 3097 | 1/1   | 0.98 | 0.04 | 33,33,33,33                 | 0     |
| 57  | MG   | BA    | 3605 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3099 | 1/1   | 0.98 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3522 | 1/1   | 0.98 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | DA    | 3357 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3227 | 1/1   | 0.98 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3384 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3525 | 1/1   | 0.98 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 3504 | 1/1   | 0.98 | 0.04 | 47,47,47,47                 | 0     |
| 57  | MG   | BR    | 202  | 1/1   | 0.98 | 0.07 | 31,31,31,31                 | 0     |
| 57  | MG   | DA    | 3506 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3692 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3447 | 1/1   | 0.98 | 0.07 | 72,72,72,72                 | 0     |
| 57  | MG   | BA    | 3611 | 1/1   | 0.98 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3784 | 1/1   | 0.98 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | CF    | 3001 | 1/1   | 0.98 | 0.05 | 46,46,46,46                 | 0     |
| 57  | MG   | BU    | 205  | 1/1   | 0.98 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | BU    | 206  | 1/1   | 0.98 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3152 | 1/1   | 0.98 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | BU    | 208  | 1/1   | 0.98 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3449 | 1/1   | 0.98 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | AA    | 3114 | 1/1   | 0.98 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3280 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 57  | MG   | BA    | 3699 | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 57  | MG   | AA    | 3042 | 1/1   | 0.98 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | DA    | 3377 | 1/1   | 0.98 | 0.06 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3791 | 1/1   | 0.98 | 0.07 | 28,28,28,28                 | 0     |
| 57  | MG   | DA    | 3003 | 1/1   | 0.98 | 0.09 | 27,27,27,27                 | 0     |
| 57  | MG   | BA    | 3234 | 1/1   | 0.98 | 0.03 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3381 | 1/1   | 0.98 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | BW    | 203  | 1/1   | 0.98 | 0.05 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3235 | 1/1   | 0.98 | 0.05 | 42,42,42,42                 | 0     |
| 57  | MG   | AW    | 3002 | 1/1   | 0.98 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | AA    | 3144 | 1/1   | 0.98 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3705 | 1/1   | 0.98 | 0.08 | 62,62,62,62                 | 0     |
| 57  | MG   | DA    | 3253 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3390 | 1/1   | 0.98 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3127 | 1/1   | 0.98 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3124 | 1/1   | 0.98 | 0.07 | 19,19,19,19                 | 0     |
| 57  | MG   | BA    | 3195 | 1/1   | 0.98 | 0.06 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3338 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3339 | 1/1   | 0.98 | 0.05 | 23,23,23,23                 | 0     |
| 57  | MG   | BA    | 3158 | 1/1   | 0.98 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3542 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | BA    | 3197 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | B3    | 3001 | 1/1   | 0.98 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | BA    | 3544 | 1/1   | 0.98 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3807 | 1/1   | 0.98 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | DD    | 302  | 1/1   | 0.98 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3040 | 1/1   | 0.98 | 0.24 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3400 | 1/1   | 0.98 | 0.05 | 33,33,33,33                 | 0     |
| 57  | MG   | DD    | 305  | 1/1   | 0.98 | 0.04 | 36,36,36,36                 | 0     |
| 57  | MG   | DA    | 3023 | 1/1   | 0.98 | 0.29 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3291 | 1/1   | 0.98 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | DD    | 308  | 1/1   | 0.98 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | DA    | 3270 | 1/1   | 0.98 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | DA    | 3407 | 1/1   | 0.98 | 0.03 | 66,66,66,66                 | 0     |
| 57  | MG   | BA    | 3467 | 1/1   | 0.98 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | AA    | 3106 | 1/1   | 0.98 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3719 | 1/1   | 0.98 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | CA    | 3100 | 1/1   | 0.98 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | BA    | 3067 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3245 | 1/1   | 0.98 | 0.16 | 34,34,34,34                 | 0     |
| 57  | MG   | DF    | 3004 | 1/1   | 0.98 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3096 | 1/1   | 0.98 | 0.23 | 54,54,54,54                 | 0     |
| 57  | MG   | BA    | 3553 | 1/1   | 0.98 | 0.04 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3247 | 1/1   | 0.98 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 3560 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 57  | MG   | DA    | 3034 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | DQ    | 3001 | 1/1   | 0.98 | 0.04 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3154 | 1/1   | 0.98 | 0.26 | 48,48,48,48                 | 0     |
| 57  | MG   | BA    | 3042 | 1/1   | 0.98 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3726 | 1/1   | 0.98 | 0.14 | 63,63,63,63                 | 0     |
| 57  | MG   | BA    | 3474 | 1/1   | 0.98 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | DA    | 3285 | 1/1   | 0.98 | 0.06 | 32,32,32,32                 | 0     |
| 57  | MG   | BA    | 3069 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | AE    | 203  | 1/1   | 0.98 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | DA    | 3040 | 1/1   | 0.98 | 0.05 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3559 | 1/1   | 0.98 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3042 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | DW    | 3002 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | DA    | 3572 | 1/1   | 0.98 | 0.05 | 62,62,62,62                 | 0     |
| 57  | MG   | BA    | 3166 | 1/1   | 0.98 | 0.04 | 38,38,38,38                 | 0     |
| 57  | MG   | AX    | 3013 | 1/1   | 0.98 | 0.06 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3045 | 1/1   | 0.98 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | AA    | 3182 | 1/1   | 0.98 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3414 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 57  | MG   | AK    | 3001 | 1/1   | 0.98 | 0.13 | 44,44,44,44                 | 0     |
| 58  | SF4  | AD    | 501  | 8/8   | 0.98 | 0.06 | 62,68,73,86                 | 0     |
| 58  | SF4  | CD    | 302  | 8/8   | 0.98 | 0.06 | 60,68,83,86                 | 0     |
| 59  | ZN   | B4    | 501  | 1/1   | 0.98 | 0.04 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | BA    | 3737 | 1/1   | 0.98 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | DA    | 3050 | 1/1   | 0.98 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | BA    | 3416 | 1/1   | 0.98 | 0.07 | 21,21,21,21                 | 0     |
| 59  | ZN   | D9    | 501  | 1/1   | 0.98 | 0.05 | 68,68,68,68                 | 0     |
| 57  | MG   | BA    | 3357 | 1/1   | 0.98 | 0.09 | 25,25,25,25                 | 0     |
| 57  | MG   | DA    | 3174 | 1/1   | 0.98 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | BA    | 3037 | 1/1   | 0.99 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | DA    | 3386 | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |
| 57  | MG   | DA    | 3459 | 1/1   | 0.99 | 0.05 | 47,47,47,47                 | 0     |
| 57  | MG   | DA    | 3387 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 57  | MG   | DA    | 3102 | 1/1   | 0.99 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3565 | 1/1   | 0.99 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | BA    | 3495 | 1/1   | 0.99 | 0.06 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3580 | 1/1   | 0.99 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3496 | 1/1   | 0.99 | 0.08 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3498 | 1/1   | 0.99 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | BA    | 3609 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 57  | MG   | BA    | 3588 | 1/1   | 0.99 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | BA    | 3483 | 1/1   | 0.99 | 0.06 | 28,28,28,28                 | 0     |
| 57  | MG   | BA    | 3533 | 1/1   | 0.99 | 0.04 | 59,59,59,59                 | 0     |
| 57  | MG   | AA    | 3167 | 1/1   | 0.99 | 0.05 | 57,57,57,57                 | 0     |
| 57  | MG   | BA    | 3795 | 1/1   | 0.99 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | BA    | 3198 | 1/1   | 0.99 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | DA    | 3266 | 1/1   | 0.99 | 0.04 | 57,57,57,57                 | 0     |
| 57  | MG   | AA    | 3074 | 1/1   | 0.99 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3143 | 1/1   | 0.99 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3144 | 1/1   | 0.99 | 0.05 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3477 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 57  | MG   | BA    | 3363 | 1/1   | 0.99 | 0.04 | 22,22,22,22                 | 0     |
| 57  | MG   | DA    | 3517 | 1/1   | 0.99 | 0.04 | 51,51,51,51                 | 0     |
| 57  | MG   | DA    | 3597 | 1/1   | 0.99 | 0.03 | 51,51,51,51                 | 0     |
| 57  | MG   | BA    | 3103 | 1/1   | 0.99 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3060 | 1/1   | 0.99 | 0.09 | 30,30,30,30                 | 0     |
| 57  | MG   | BA    | 3597 | 1/1   | 0.99 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | BA    | 3015 | 1/1   | 0.99 | 0.05 | 32,32,32,32                 | 0     |
| 57  | MG   | DA    | 3373 | 1/1   | 0.99 | 0.07 | 44,44,44,44                 | 0     |
| 57  | MG   | DA    | 3603 | 1/1   | 0.99 | 0.05 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3507 | 1/1   | 0.99 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | BF    | 305  | 1/1   | 0.99 | 0.03 | 49,49,49,49                 | 0     |
| 57  | MG   | BA    | 3688 | 1/1   | 0.99 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | BA    | 3524 | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 59  | ZN   | AN    | 501  | 1/1   | 0.99 | 0.05 | 69,69,69,69                 | 0     |

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*Continued from previous page...*

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | ZN   | BY    | 501  | 1/1   | 0.99 | 0.03 | 58,58,58,58                 | 0     |
| 57  | MG   | BA    | 3806 | 1/1   | 0.99 | 0.08 | 30,30,30,30                 | 0     |
| 59  | ZN   | B5    | 102  | 1/1   | 0.99 | 0.05 | 48,48,48,48                 | 0     |
| 59  | ZN   | B6    | 103  | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 59  | ZN   | B9    | 501  | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 57  | MG   | DA    | 3016 | 1/1   | 0.99 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | DA    | 3156 | 1/1   | 0.99 | 0.04 | 51,51,51,51                 | 0     |
| 57  | MG   | AA    | 3086 | 1/1   | 0.99 | 0.08 | 57,57,57,57                 | 0     |
| 59  | ZN   | D5    | 501  | 1/1   | 0.99 | 0.04 | 58,58,58,58                 | 0     |
| 59  | ZN   | D6    | 501  | 1/1   | 0.99 | 0.04 | 71,71,71,71                 | 0     |
| 57  | MG   | DA    | 3315 | 1/1   | 0.99 | 0.03 | 42,42,42,42                 | 0     |
| 57  | MG   | BA    | 3458 | 1/1   | 0.99 | 0.05 | 18,18,18,18                 | 0     |
| 57  | MG   | BA    | 3099 | 1/1   | 0.99 | 0.04 | 41,41,41,41                 | 0     |
| 57  | MG   | BA    | 3327 | 1/1   | 1.00 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | BA    | 3497 | 1/1   | 1.00 | 0.06 | 28,28,28,28                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.