



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:38 AM UTC

PDB ID : 4W2H / pdb\_00004w2h  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (co-crystallized), mRNA and deacylated tRNA in the P site  
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.  
Deposited on : 2014-09-12  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                           |   |                                                                  |
|---------------------------|---|------------------------------------------------------------------|
| MolProbity                | : | 4-5-2 with Phenix2.0                                             |
| Mogul                     | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)          | : | 2.0                                                              |
| EDS                       | : | 3.0                                                              |
| Buster-report             | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics     | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                      | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness           | : | 1.0.12                                                           |
| Ideal geometry (proteins) | : | Engh & Huber (2001)                                              |

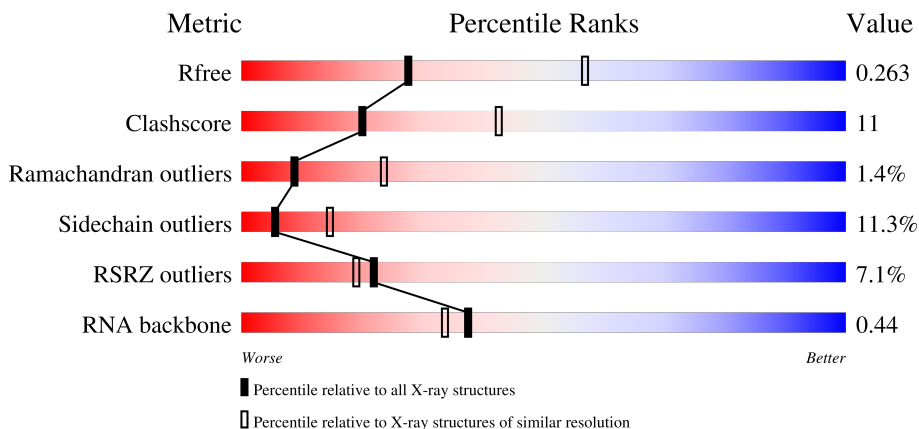
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |
| RNA backbone          | 3983                        | 1044 (2.90-2.50)                                      |

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>3%</div> <div>45%</div> <div>40%</div> <div>13%</div> <div>.</div> </div> |
| 1   | CA    | 1521   | <div> <div>7%</div> <div>44%</div> <div>40%</div> <div>15%</div> <div>.</div> </div> |

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | AB    | 256    |                  |
| 2   | CB    | 256    |                  |
| 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     |                  |

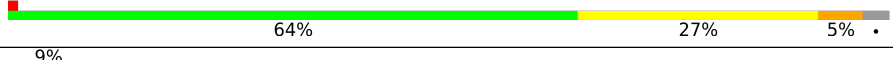
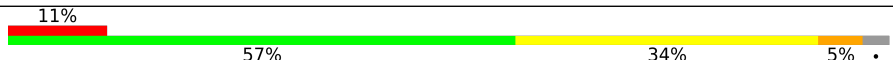
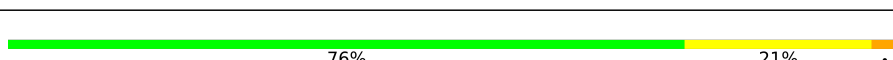
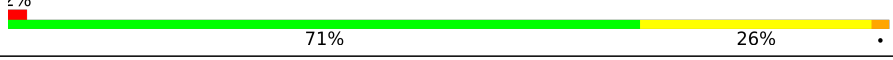
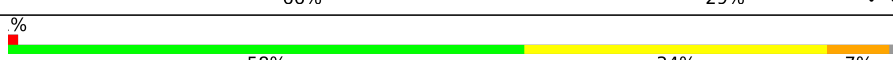
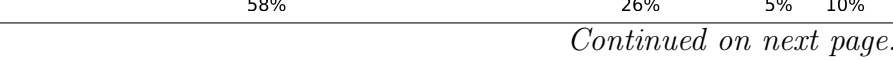
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14  | CN    | 61     |                  |
| 15  | AO    | 89     |                  |
| 15  | CO    | 89     |                  |
| 16  | AP    | 88     |                  |
| 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  | AX    | 77     |                  |
| 23  | CX    | 77     |                  |
| 24  | AY    | 76     |                  |
| 24  | CY    | 76     |                  |
| 25  | BA    | 2915   |                  |
| 25  | DA    | 2915   |                  |
| 26  | BB    | 121    |                  |
| 26  | DB    | 121    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 27  | BD    | 276    |    |
| 27  | DD    | 276    |    |
| 28  | BE    | 206    |    |
| 28  | DE    | 206    |    |
| 29  | BF    | 210    |    |
| 29  | DF    | 210    |    |
| 30  | BG    | 182    |    |
| 30  | DG    | 182    |    |
| 31  | BH    | 180    |    |
| 31  | DH    | 180    |    |
| 32  | BI    | 148    |   |
| 32  | DI    | 148    |  |
| 33  | BN    | 140    |  |
| 33  | DN    | 140    |  |
| 34  | BO    | 122    |  |
| 34  | DO    | 122    |  |
| 35  | BP    | 150    |  |
| 35  | DP    | 150    |  |
| 36  | BQ    | 141    |  |
| 36  | DQ    | 141    |  |
| 37  | BR    | 118    |  |
| 37  | DR    | 118    |  |
| 38  | BS    | 112    |  |
| 38  | DS    | 112    |  |
| 39  | BT    | 146    |  |

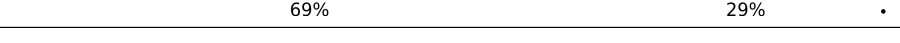
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | DT    | 146    |                  |
| 40  | BU    | 118    |                  |
| 40  | DU    | 118    |                  |
| 41  | BV    | 101    |                  |
| 41  | DV    | 101    |                  |
| 42  | BW    | 113    |                  |
| 42  | DW    | 113    |                  |
| 43  | BX    | 96     |                  |
| 43  | DX    | 96     |                  |
| 44  | BY    | 110    |                  |
| 44  | DY    | 110    |                  |
| 45  | BZ    | 206    |                  |
| 45  | DZ    | 206    |                  |
| 46  | B0    | 85     |                  |
| 46  | D0    | 85     |                  |
| 47  | B1    | 98     |                  |
| 47  | D1    | 98     |                  |
| 48  | B2    | 72     |                  |
| 48  | D2    | 72     |                  |
| 49  | B3    | 60     |                  |
| 49  | D3    | 60     |                  |
| 50  | B4    | 71     |                  |
| 50  | D4    | 71     |                  |
| 51  | B5    | 60     |                  |
| 51  | D5    | 60     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 52  | B6    | 54     |  |
| 52  | D6    | 54     |  |
| 53  | B7    | 49     |  |
| 53  | D7    | 49     |  |
| 54  | B8    | 65     |  |
| 54  | D8    | 65     |  |
| 55  | B9    | 37     |  |
| 55  | D9    | 37     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56  | MG   | CX    | 3002 | -         | -        | -       | X                |
| 56  | MG   | DA    | 3655 | -         | -        | -       | X                |

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 290807 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    | 1497     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32183 | 14323 | 5965 | 10398 | 1497 |         |         |       |
| 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    | 120      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 937   | 578 | 194 | 163 | 2       | 0       | 0     |
| 13  | CM    | 118      | Total | C   | N   | O   | S       |         |       |
|     |       |          | 920   | 566 | 191 | 161 | 2       | 0       | 0     |

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

| 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    | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 169   | 76 | 29 | 56 | 8 |         |         |       |
| 22  | CV    | 5        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 109   | 49 | 22 | 33 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 23  | AX    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1 |         |         |       |
| 23  | CX    | 76       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1625  | 725 | 294 | 529 | 76 | 1 |         |         |       |

- Molecule 24 is a RNA chain called E-site tRNA Acceptor Stem.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 24  | AY    | 18       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 385   | 171 | 71 | 125 | 18 |         |         |       |
| 24  | CY    | 5        | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 104   | 47  | 19 | 33  | 5  |         |         |       |

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25  | BA    | 2822     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60792 | 27054 | 11380 | 19537 | 2821 |         |         |       |
| 25  | DA    | 2800     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60311 | 26840 | 11284 | 19388 | 2799 |         |         |       |

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26  | BB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26  | DB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27  | BD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |
| 27  | DD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |
| 28  | DE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | BF    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1584  | 1009 | 298 | 275 | 2 |         |         |       |
| 29  | DF    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1580  | 1007 | 297 | 274 | 2 |         |         |       |

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1425  | 914 | 256 | 251 | 4 |         |         |       |
| 30  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 911 | 258 | 251 | 4 |         |         |       |

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 31  | DH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1085  | 693 | 189 | 202 | 1 |         |         |       |
| 32  | DI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1061  | 680 | 186 | 194 | 1 |         |         |       |

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |
| 33  | DN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 34  | DO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BP    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |
| 35  | DP    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 36  | DQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 37  | DR    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |   |         |         |       |
| 38  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |   |         |         |       |

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BT    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1091  | 680 | 225 | 185 | 1 |         |         |       |
| 39  | DT    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 675 | 224 | 183 | 1 |         |         |       |

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BU    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |
| 40  | DU    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |
| 41  | DV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BW    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | DW    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BX    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |
| 43  | DX    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |
| 44  | DY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 806   | 517 | 152 | 131 | 6 |         |         |       |

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BZ    | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1349  | 862 | 243 | 242 | 2 |         |         |       |
| 45  | DZ    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1360  | 870 | 243 | 245 | 2 |         |         |       |

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | B0    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 1 |         |         |       |
| 46  | D0    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 1 |         |         |       |

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | B1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |
| 47  | D1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 755   | 475 | 148 | 131 | 1 |         |         |       |

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | B2    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 48  | D2    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49  | B3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 49  | D3    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 464   | 296 | 90 | 78 |         |         |       |

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 50  | B4    | 69       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 558   | 352 | 102 | 99 | 5 |         |         |       |
| 50  | D4    | 69       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 97  | 91 | 5 |         |         |       |

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | B5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |
| 51  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 52  | D6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 279 | 91 | 75 | 4 |         |         |       |

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53  | B7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 53  | D7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | B8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 511   | 328 | 99  | 82 | 2 |         |         |       |
| 54  | D8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55  | B9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 55  | D9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56  | AA    | 190      | Total | Mg  | 0       | 0       |
|     |       |          | 190   | 190 |         |         |
| 56  | AD    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | AE    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 56  | AF    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | AM    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | AN    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | AQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 56  | AX    | 9        | Total | Mg  | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 56  | BA    | 814      | Total | Mg  | 0       | 0       |
|     |       |          | 814   | 814 |         |         |

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| Mol | Chain | Residues | Atoms       |          | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56  | BB    | 22       | Total<br>22 | Mg<br>22 | 0       | 0       |
| 56  | BD    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 56  | BE    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 56  | BF    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 56  | BG    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | BN    | 7        | Total<br>7  | Mg<br>7  | 0       | 0       |
| 56  | BO    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | BP    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 56  | BQ    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 56  | BR    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 56  | BU    | 9        | Total<br>9  | Mg<br>9  | 0       | 0       |
| 56  | BV    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 56  | BW    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |
| 56  | BX    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | BY    | 3        | Total<br>3  | Mg<br>3  | 0       | 0       |
| 56  | BZ    | 2        | Total<br>2  | Mg<br>2  | 0       | 0       |
| 56  | B0    | 5        | Total<br>5  | Mg<br>5  | 0       | 0       |
| 56  | B2    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | B3    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | B4    | 1        | Total<br>1  | Mg<br>1  | 0       | 0       |
| 56  | B5    | 4        | Total<br>4  | Mg<br>4  | 0       | 0       |

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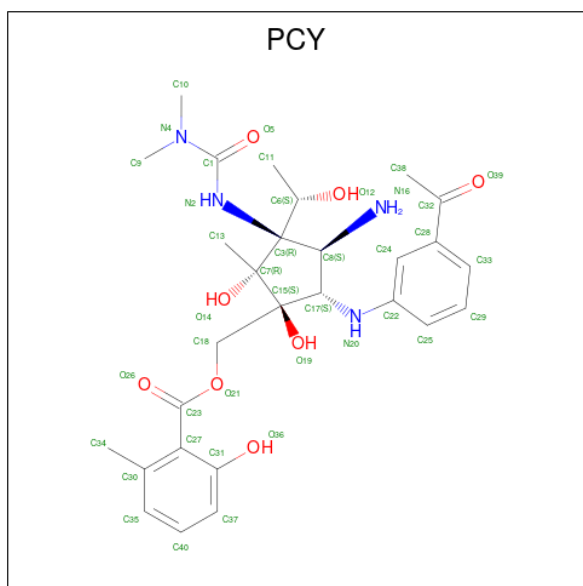
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56  | B6    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | B7    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | B8    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | B9    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | CA    | 175      | Total<br>175 | Mg<br>175 | 0       | 0       |
| 56  | CE    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | CF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | CJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | CT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | CX    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | DA    | 674      | Total<br>674 | Mg<br>674 | 0       | 0       |
| 56  | DB    | 10       | Total<br>10  | Mg<br>10  | 0       | 0       |
| 56  | DD    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 56  | DE    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | DF    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 56  | DG    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | DN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | DO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 56  | DP    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 56  | DQ    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 56  | DR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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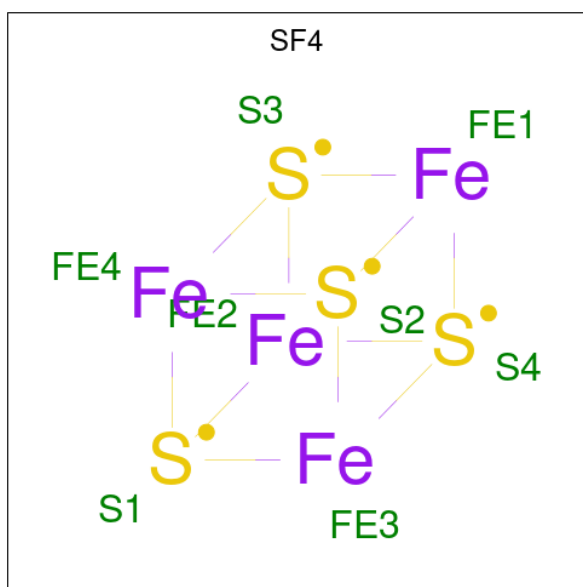
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | DU    | 4        | Total | Mg | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 56  | DV    | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 56  | DW    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | DY    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | D0    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 56  | D1    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | D3    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | D8    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 57 is Pactamycin (CCD ID: PCY) (formula:  $C_{28}H_{38}N_4O_8$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 57  | AA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 40    | 28 | 4 | 8 |         |         |
| 57  | CA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 40    | 28 | 4 | 8 |         |         |

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



| 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    | 175      | Total<br>175  | O<br>175  | 0       | 0       |
| 61  | AJ    | 2        | Total<br>2    | O<br>2    | 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  | AO    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | AV    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 61  | AX    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 61  | BA    | 1294     | Total<br>1294 | O<br>1294 | 0       | 0       |
| 61  | BB    | 34       | Total<br>34   | O<br>34   | 0       | 0       |
| 61  | BD    | 16       | Total<br>16   | O<br>16   | 0       | 0       |
| 61  | BE    | 12       | Total<br>12   | O<br>12   | 0       | 0       |
| 61  | BF    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 61  | BG    | 3        | Total<br>3    | O<br>3    | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | BI    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | BN    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | BO    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | BP    | 15       | Total<br>15  | O<br>15  | 0       | 0       |
| 61  | BQ    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | BR    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | BU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | BV    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | BW    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | BX    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | B0    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | B1    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | B3    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | B5    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 61  | B6    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | B7    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | B8    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 61  | CA    | 137      | Total<br>137 | O<br>137 | 0       | 0       |
| 61  | CD    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | CJ    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | CL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61  | CN    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | CT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | CX    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 61  | DA    | 924      | Total<br>924 | O<br>924 | 0       | 0       |
| 61  | DB    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 61  | DD    | 18       | Total<br>18  | O<br>18  | 0       | 0       |
| 61  | DE    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 61  | DF    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 61  | DN    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DO    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DP    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 61  | DR    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DU    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 61  | DV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DW    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DX    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | DY    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | D0    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 61  | D1    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 61  | D3    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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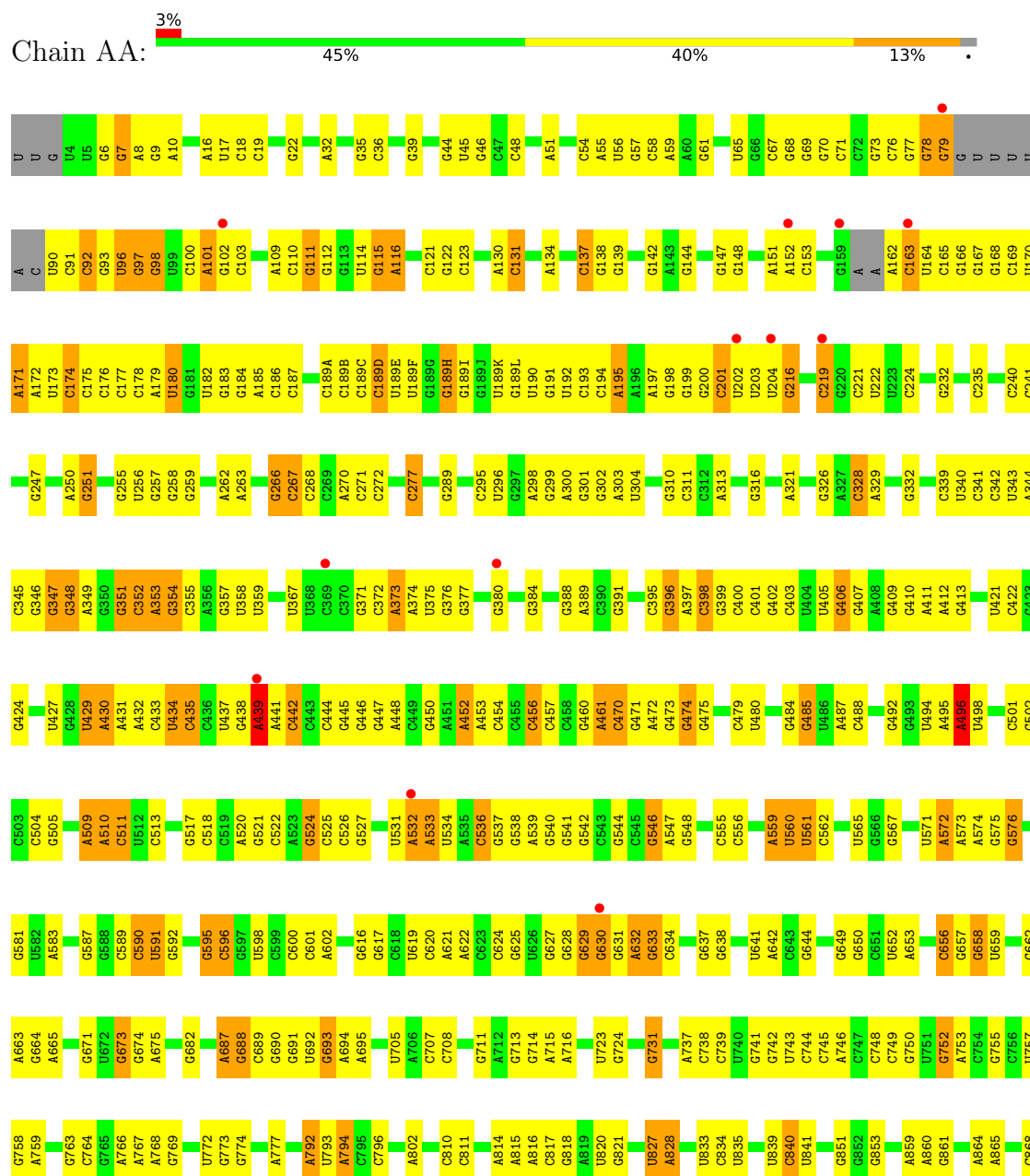
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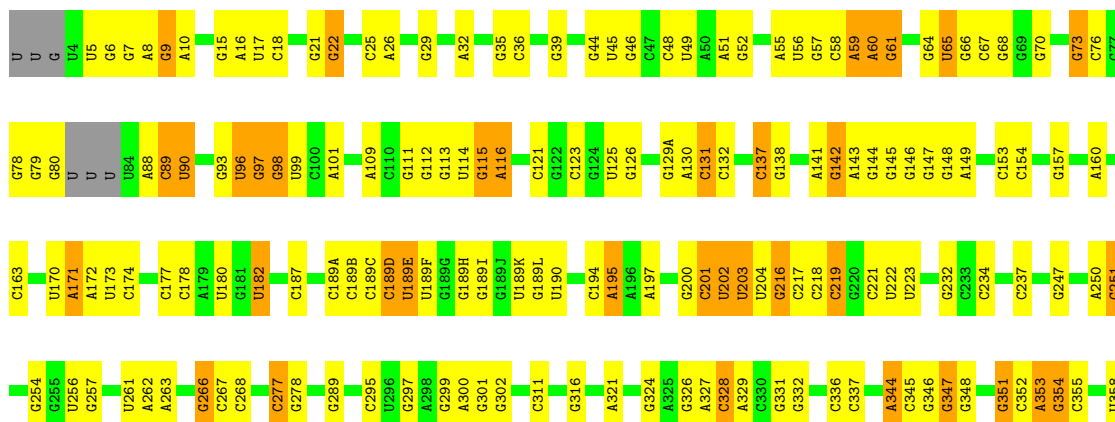
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 61  | D8    | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |

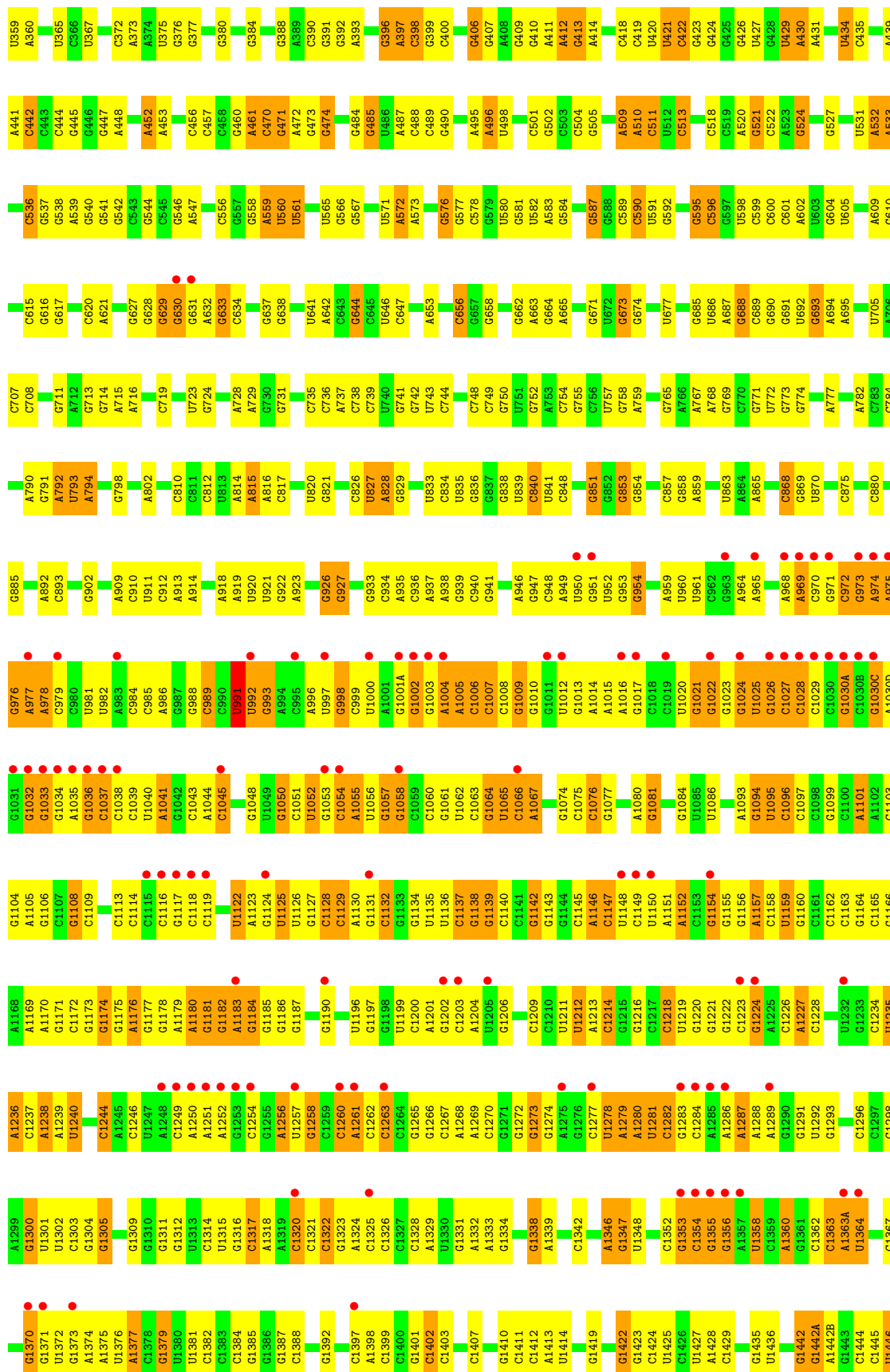
### 3 Residue-property plots

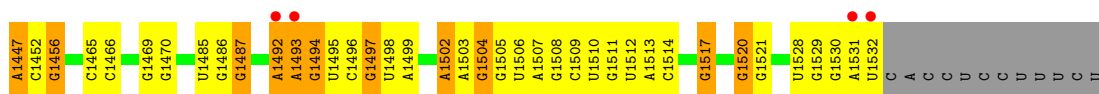
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

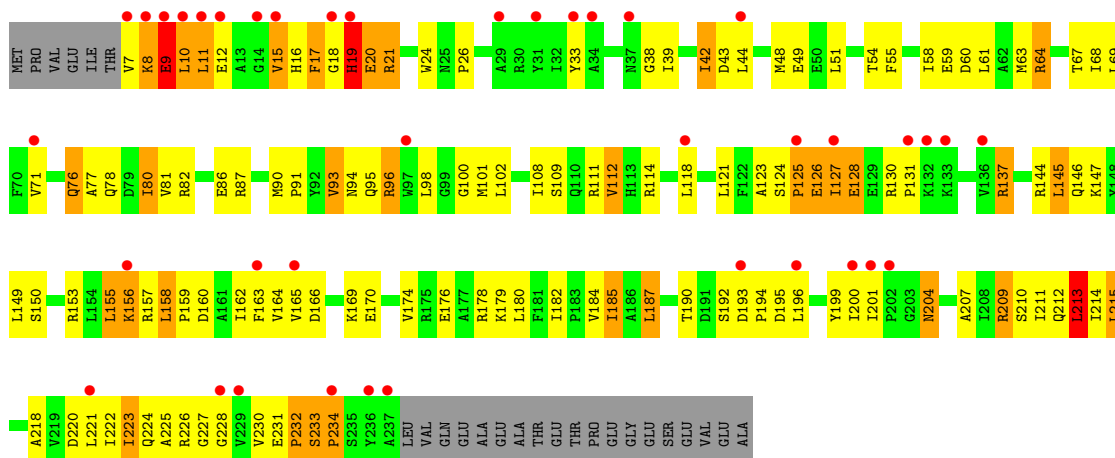




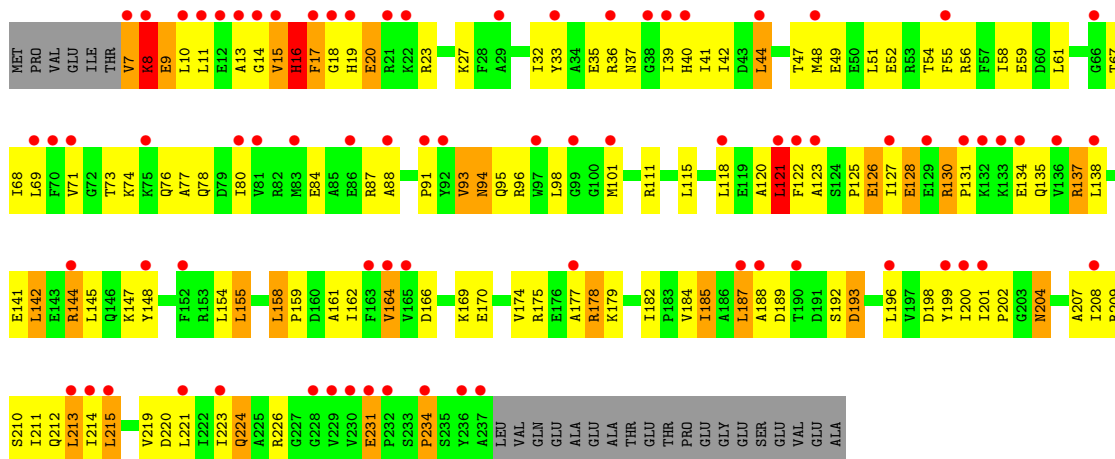




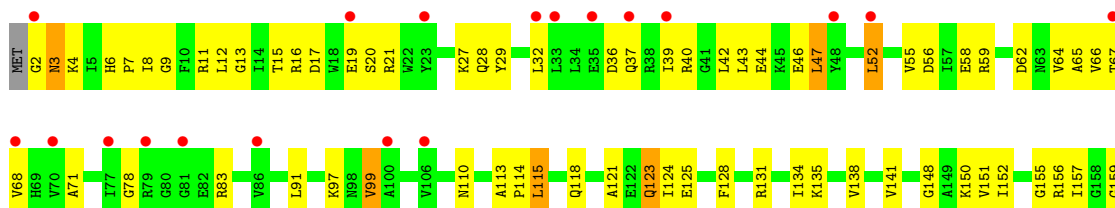
• Molecule 2: 30S Ribosomal Protein S2

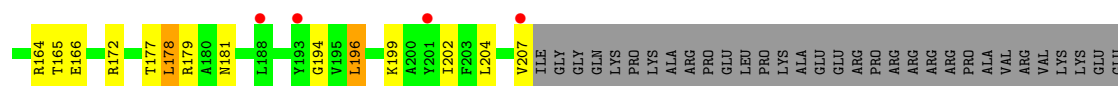


• Molecule 2: 30S Ribosomal Protein S2

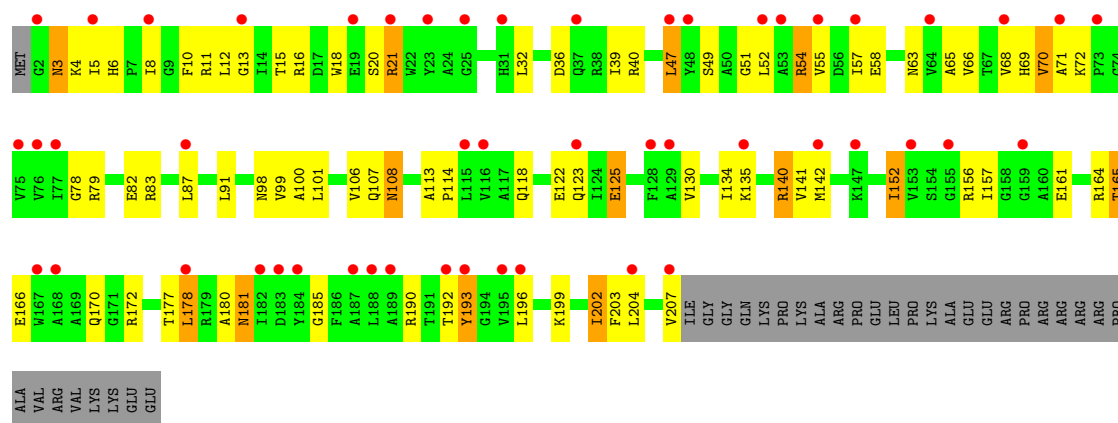


• Molecule 3: 30S Ribosomal Protein S3

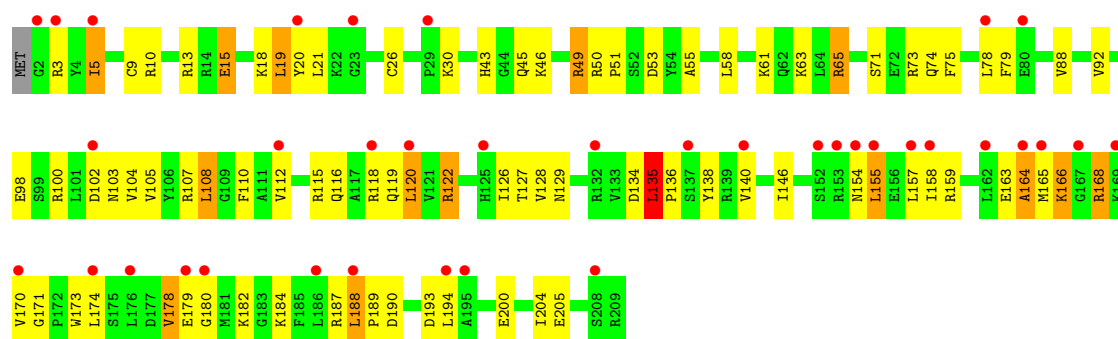




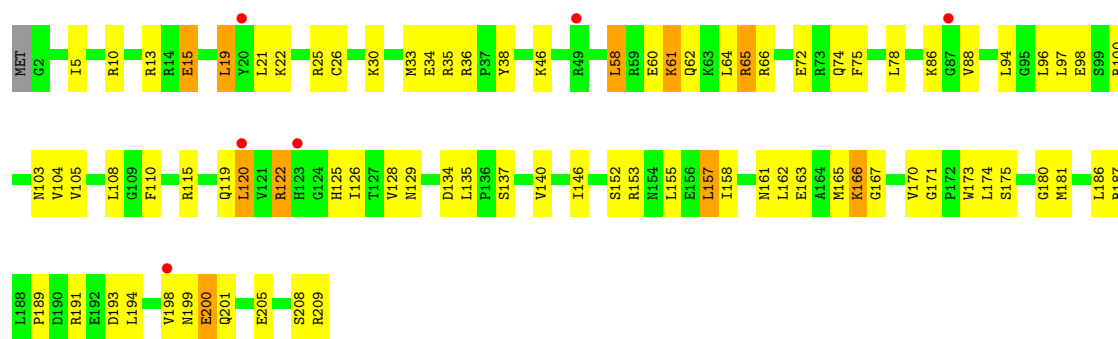
• Molecule 3: 30S Ribosomal Protein S3



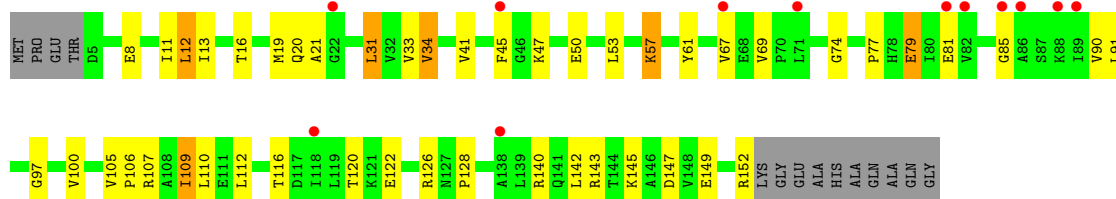
• Molecule 4: 30S Ribosomal Protein S4



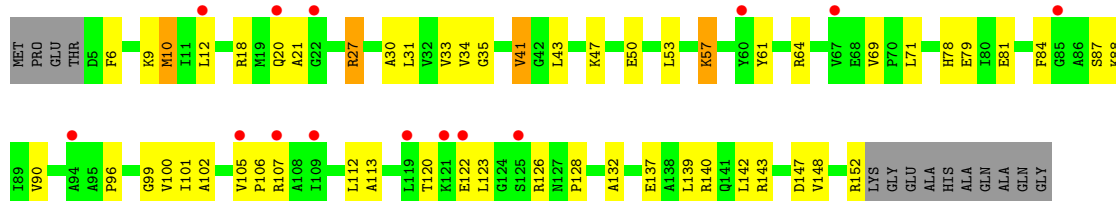
• Molecule 4: 30S Ribosomal Protein S4



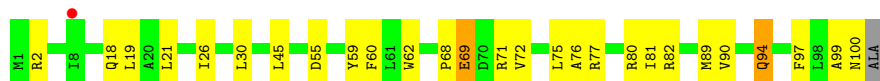
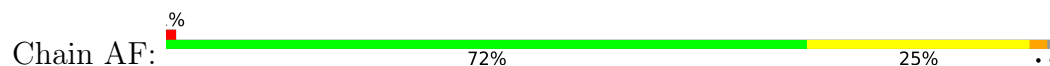
• Molecule 5: 30S Ribosomal Protein S5



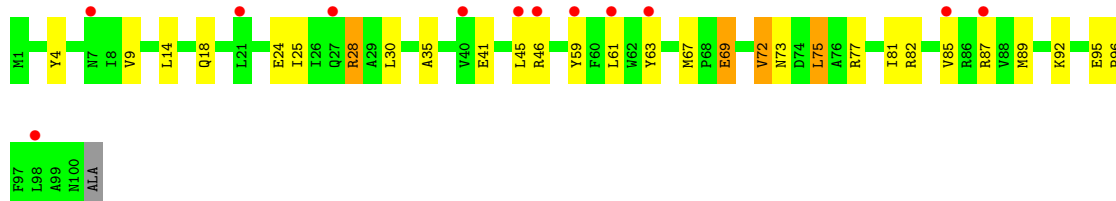
• Molecule 5: 30S Ribosomal Protein S5



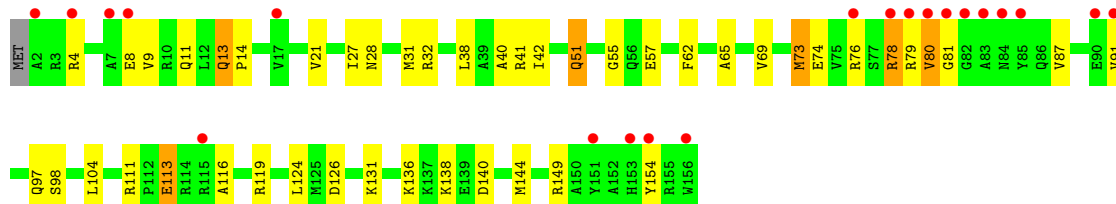
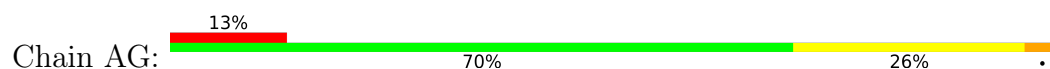
• Molecule 6: 30S Ribosomal Protein S6



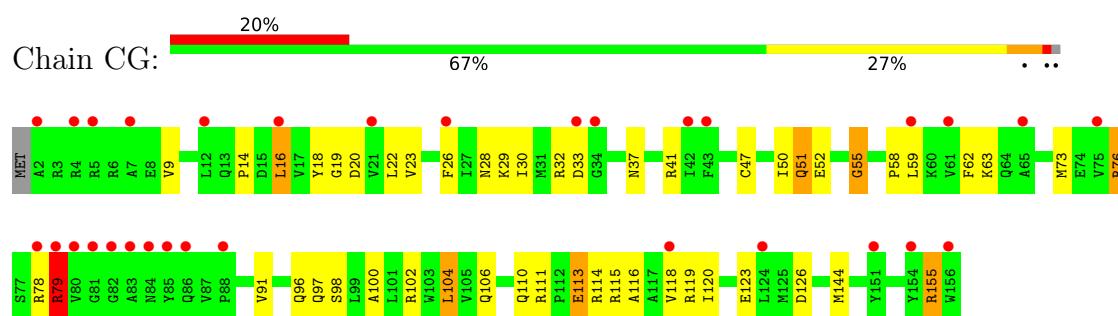
• Molecule 6: 30S Ribosomal Protein S6



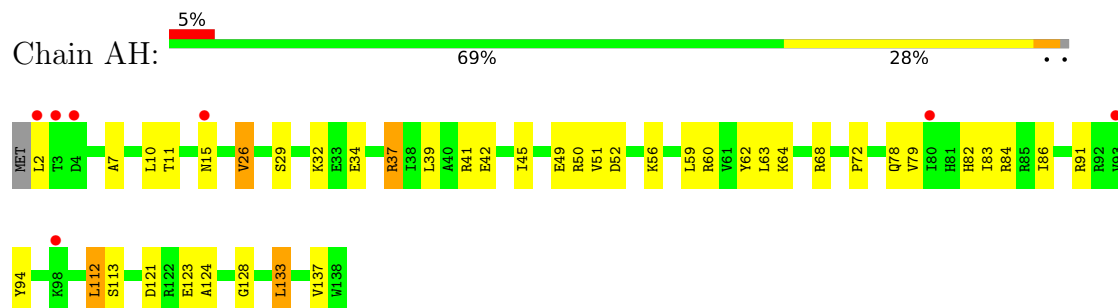
• Molecule 7: 30S Ribosomal Protein S7



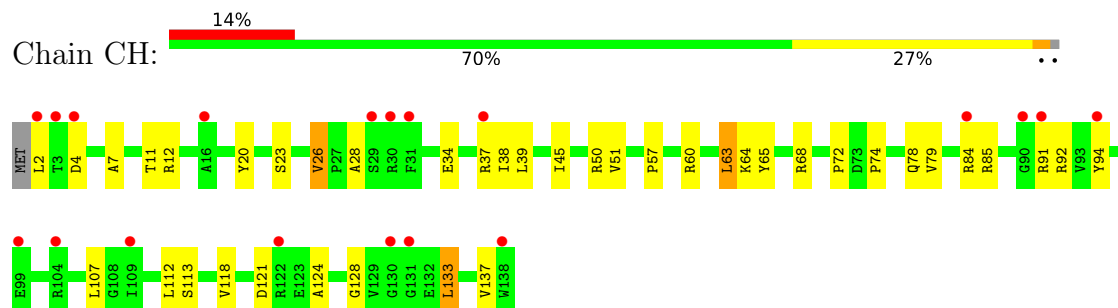
• Molecule 7: 30S Ribosomal Protein S7



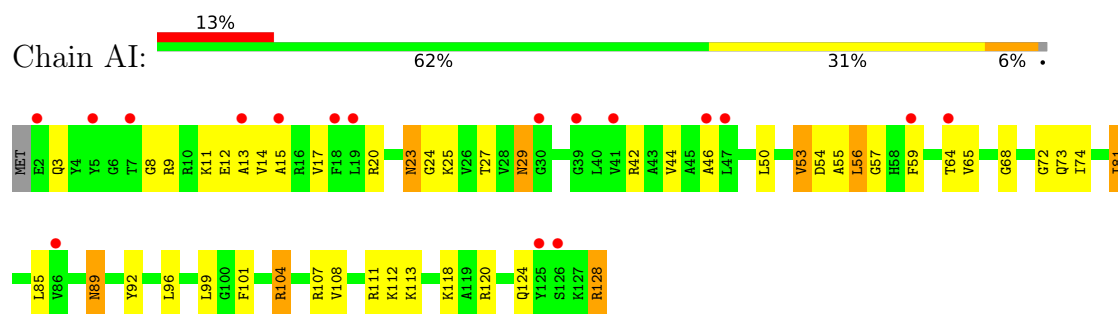
- Molecule 8: 30S Ribosomal Protein S8



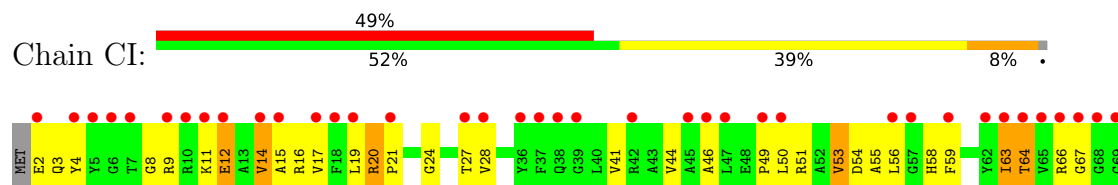
- Molecule 8: 30S Ribosomal Protein S8

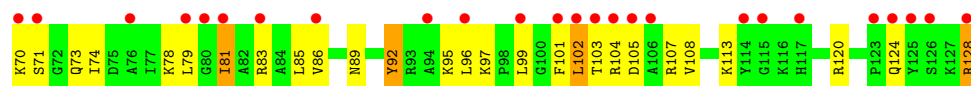


- Molecule 9: 30S Ribosomal Protein S9

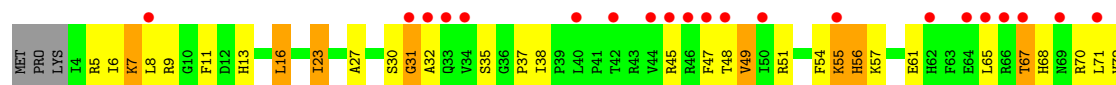


- Molecule 9: 30S Ribosomal Protein S9

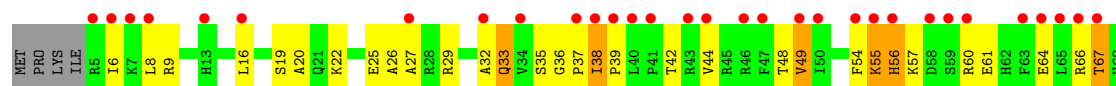
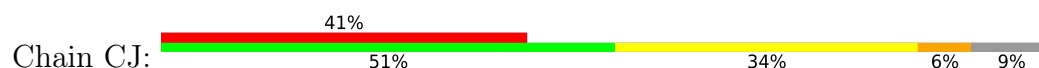




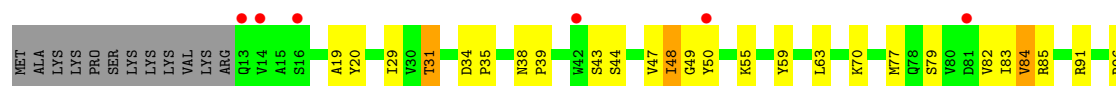
• Molecule 10: 30S Ribosomal Protein S10



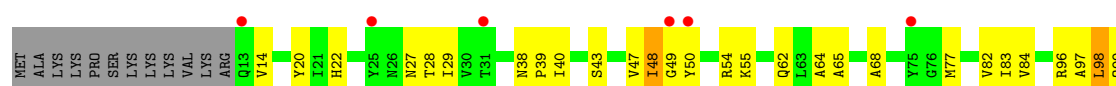
• Molecule 10: 30S Ribosomal Protein S10



• Molecule 11: 30S Ribosomal Protein S11

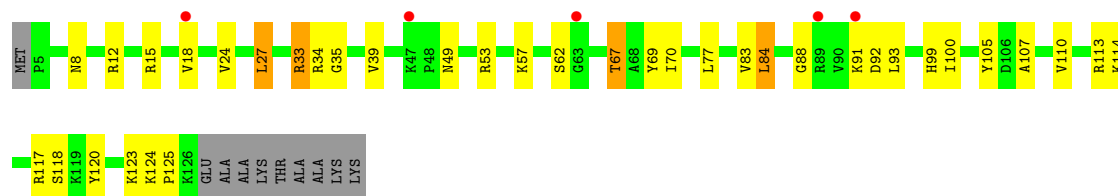


• Molecule 11: 30S Ribosomal Protein S11

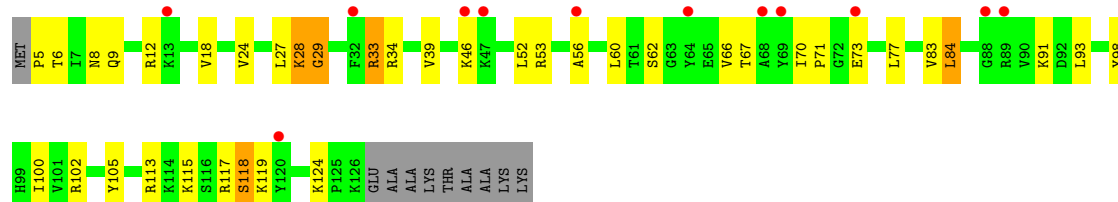


• Molecule 12: 30S Ribosomal Protein S12

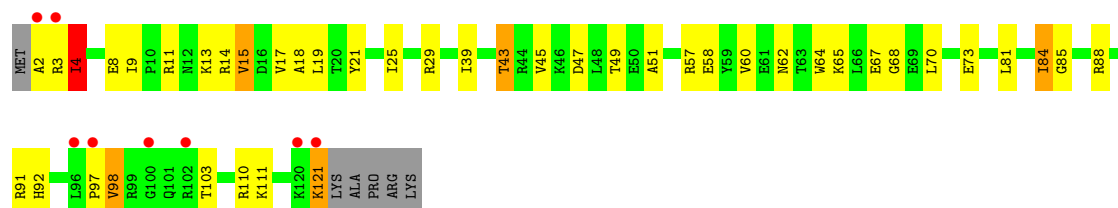




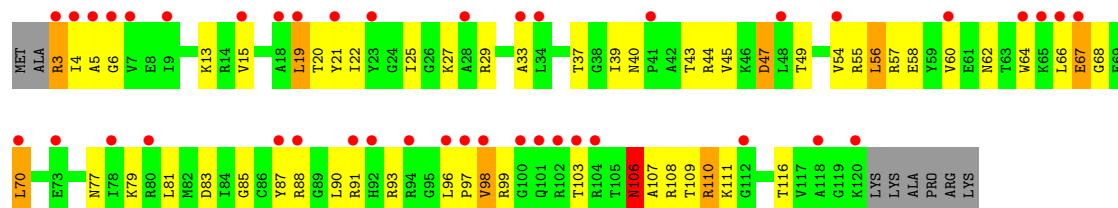
• Molecule 12: 30S Ribosomal Protein S12



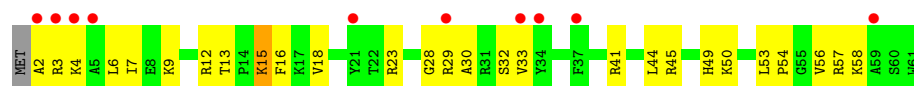
• Molecule 13: 30S Ribosomal Protein S13



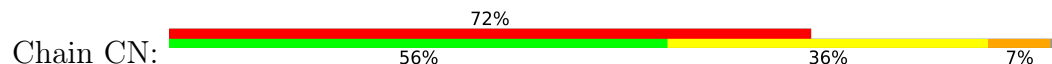
• Molecule 13: 30S Ribosomal Protein S13

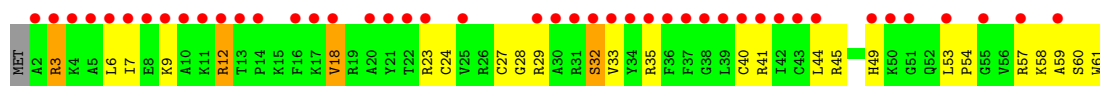


• Molecule 14: 30S Ribosomal Protein S14

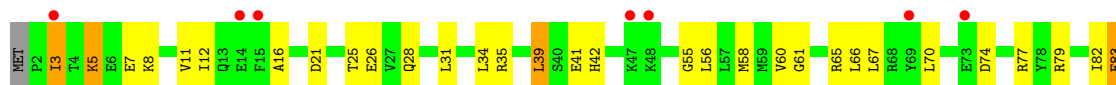


• Molecule 14: 30S Ribosomal Protein S14





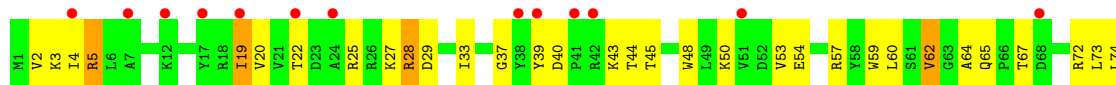
## ● Molecule 15: 30S Ribosomal Protein S15



## ● Molecule 15: 30S Ribosomal Protein S15



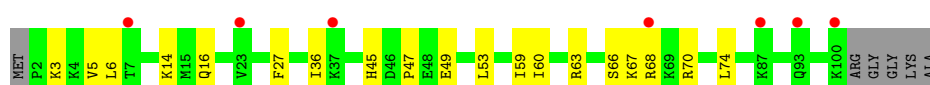
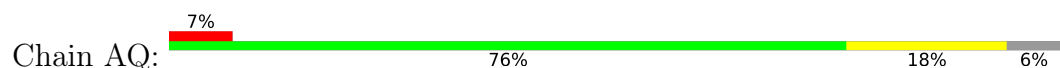
## ● Molecule 16: 30S Ribosomal Protein S16



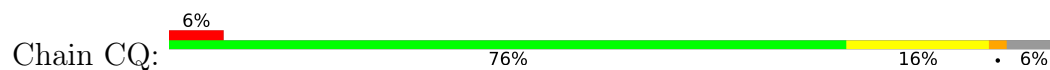
## ● Molecule 16: 30S Ribosomal Protein S16



## ● Molecule 17: 30S Ribosomal Protein S17



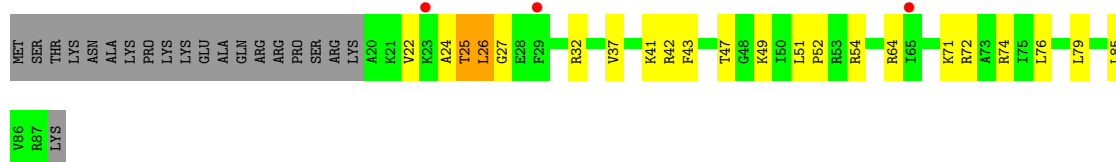
- Molecule 17: 30S Ribosomal Protein S17



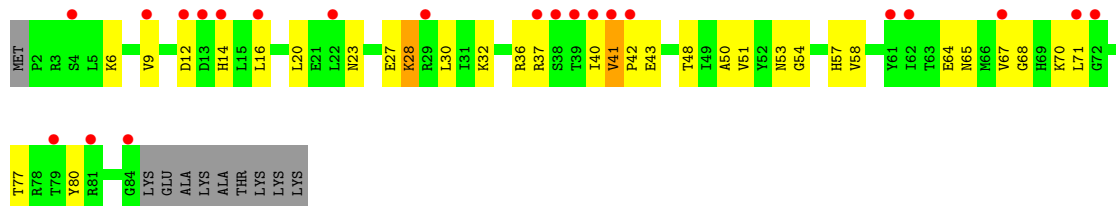
- Molecule 18: 30S Ribosomal Protein S18



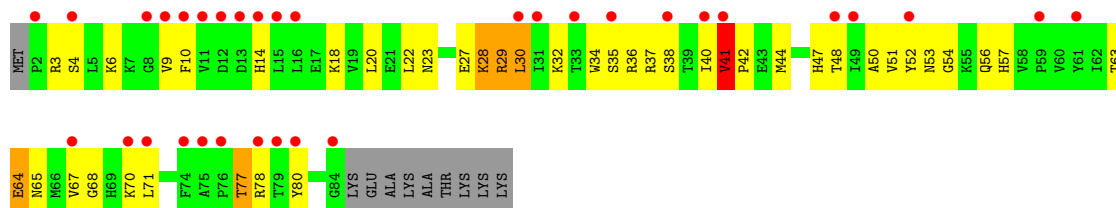
- Molecule 18: 30S Ribosomal Protein S18



- Molecule 19: 30S Ribosomal Protein S19

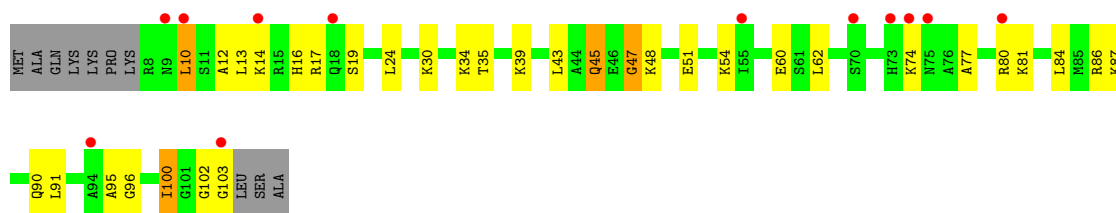


- Molecule 19: 30S Ribosomal Protein S19

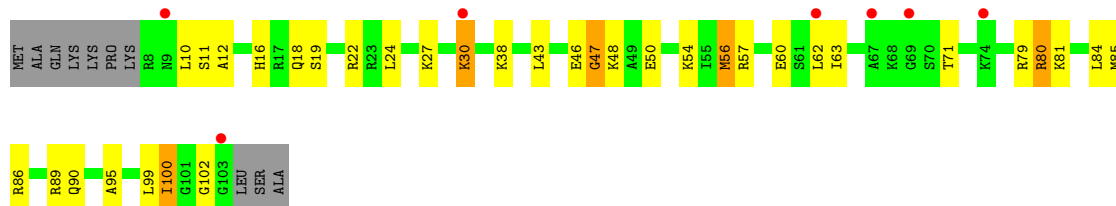


- Molecule 20: 30S Ribosomal Protein S20

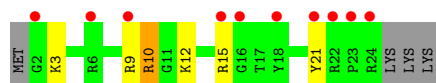




● Molecule 20: 30S Ribosomal Protein S20



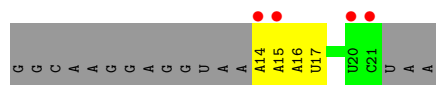
● Molecule 21: 30S Ribosomal Protein THX



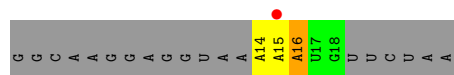
● Molecule 21: 30S Ribosomal Protein THX



● Molecule 22: mRNA

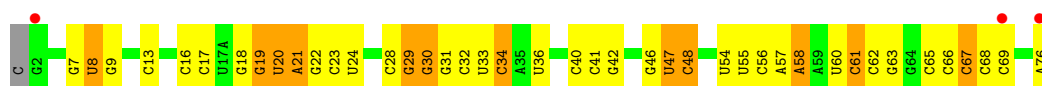


● Molecule 22: mRNA

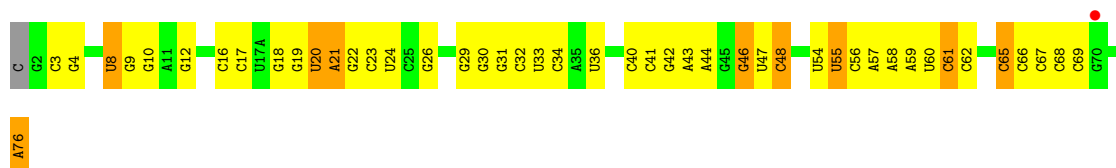


● Molecule 23: P-site tRNA

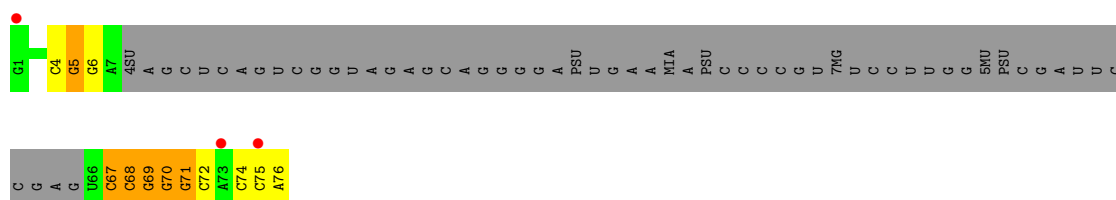




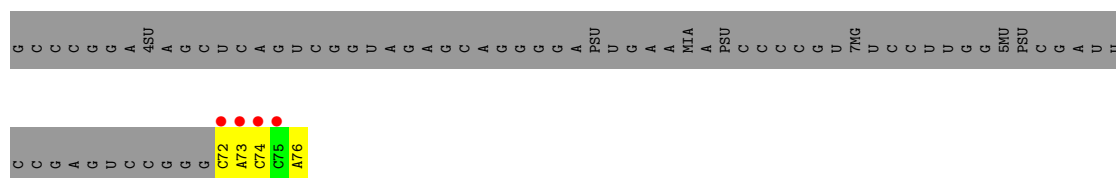
• Molecule 23: P-site tRNA



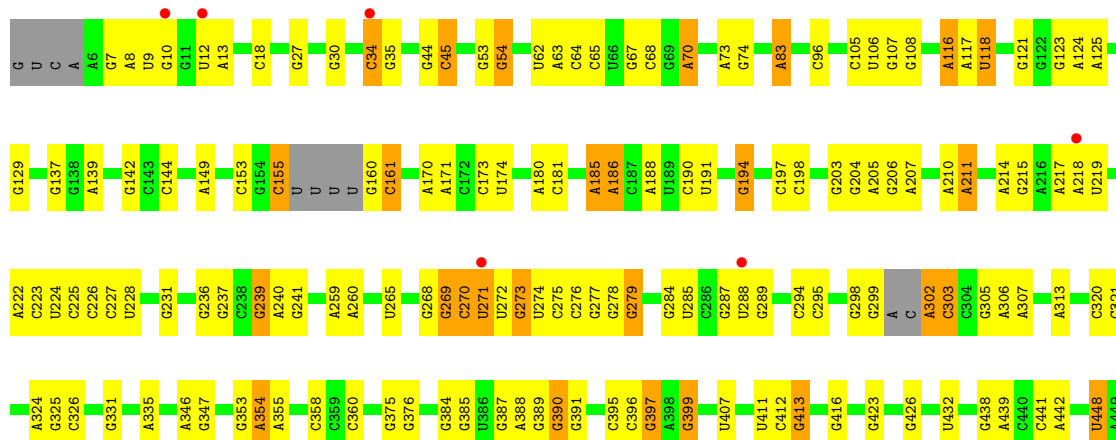
• Molecule 24: E-site tRNA Acceptor Stem



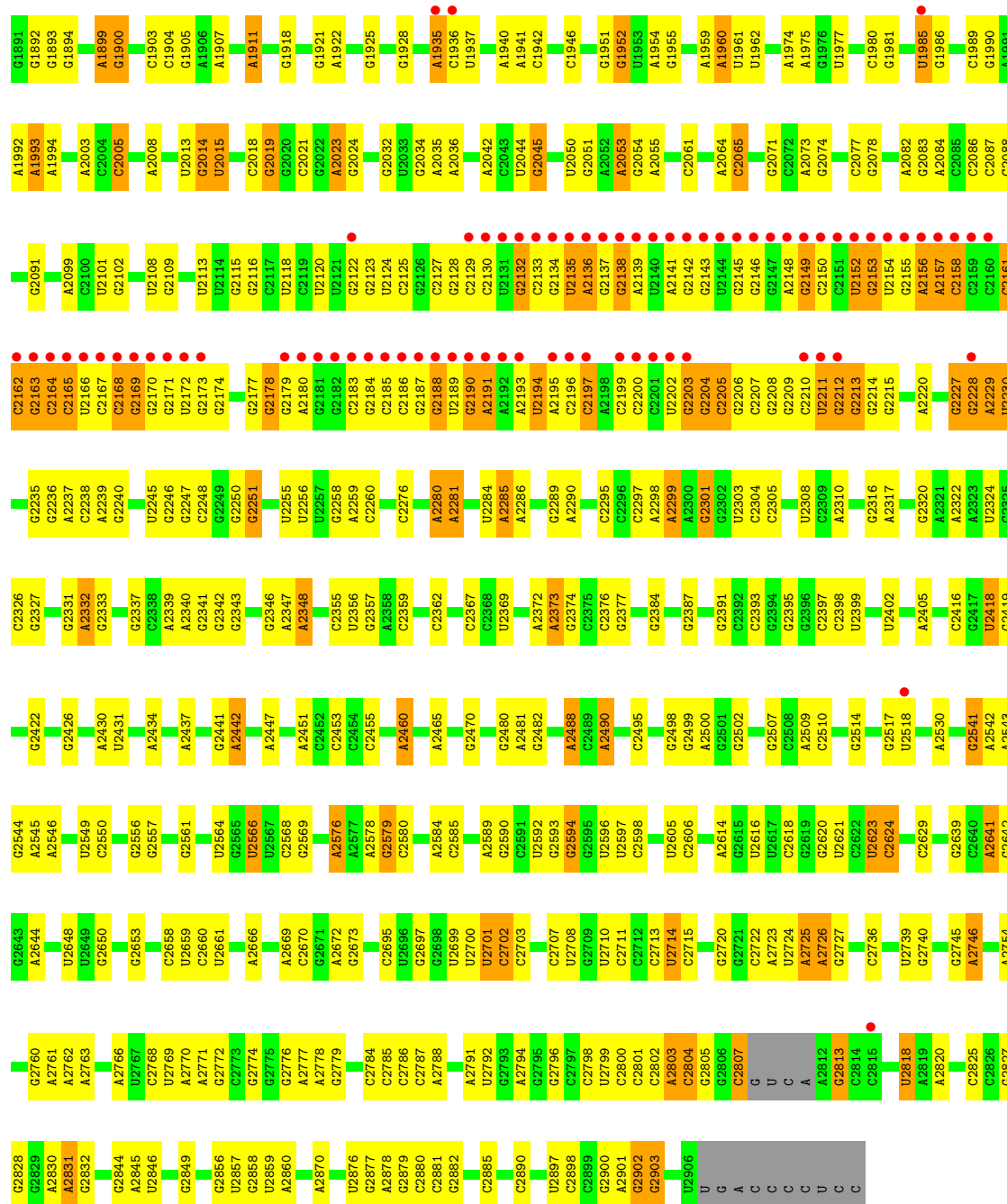
• Molecule 24: E-site tRNA Acceptor Stem



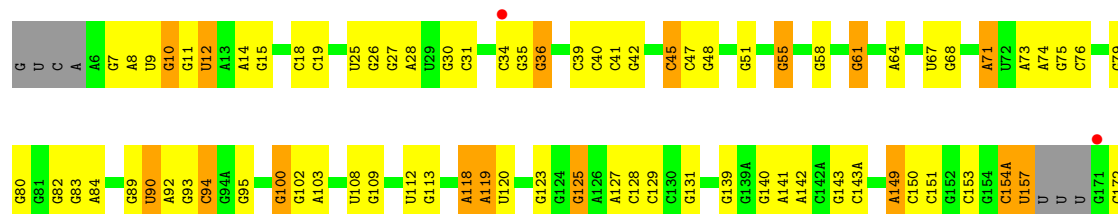
• Molecule 25: 23S Ribosomal RNA



|       |       |       |       |       |       |       |      |      |      |      |      |
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| U1788 | C1685 | C1564 | A1314 | G1200 | A1056 | A957  | U875 | C768 | C663 | C556 | A450 |
| G1789 | U1686 | G1565 | A1315 | Al201 | G1057 | C981  | A876 | A769 | A557 | A557 | A455 |
| A1790 | C1453 | G1567 | C1316 | U1211 | C1058 | G982  | G877 | G776 | G558 | G558 | A469 |
| A1793 | A1688 | C1454 | G1317 | C1212 | C1059 | A963  | C885 | C777 | C560 | C560 | A470 |
| G1795 | G1689 |       | U1319 | U1213 | U1065 | A964  | U886 | A782 | A561 | A561 | C471 |
| G1796 | G1694 | G1462 | A1320 | G1214 | A1066 | G965  | C887 | A782 | C562 | C562 | C472 |
| C1695 | C1695 | C1463 | U1338 | G1215 | A1067 | G973  | U894 | U787 | G569 | G569 | A473 |
| G1698 | G1698 | U1466 | C1339 | G1217 | G1068 | G974  | G895 | G789 | C    | C    | U474 |
| U1799 | U1797 | U1467 | C1343 | G1218 | G1071 | G977  | A896 | G789 | A572 | A572 | C477 |
| G1800 | G1700 | G1468 | A1344 | U1220 | A1073 | A978  | C897 | U794 | G573 | G573 | C478 |
| A1804 | A1701 | C1474 | U1346 | G1221 | A1074 | A986  | U898 | G795 | U577 | U577 | C479 |
| U1809 | C1710 | C1475 | A1347 | A1222 | A1075 | G989  | G902 | G795 | U577 | U577 | A480 |
| U1810 | A1711 | C1476 | A1348 | C1223 | A1076 | A990  | C903 | C801 | G586 | G586 | C481 |
| A1811 | A1811 | A1480 | G1349 | C1224 | A1077 | A991  | C904 | C802 | G591 | G591 | C482 |
| C1812 | G1714 | A1480 | C1360 | G1225 | A1078 | G992  | U905 | C805 | U591 | U591 | A483 |
| C1813 | A1715 | A1491 | C1361 | C1226 | G1086 | G993  | G906 | C805 | G596 | G596 | C484 |
| A1814 | A1716 | G1495 | C1366 | G1232 | U1081 | G997  | U907 | A808 | C597 | C597 | G495 |
| A1815 | C1717 | A1496 | C1366 | U1233 | G1082 | A998  | A908 | A808 | A598 | A598 | A496 |
| A1816 | G1721 | G1497 | G1370 | C1246 | G1083 | G999  | A910 | G812 | U599 | U599 | A497 |
| A1817 | G1722 | C1595 | C1373 | A1249 | G1084 | G1000 | A913 | G812 | G600 | G600 | G502 |
| A1820 | A1723 | C1597 | C1373 | A1249 | C1086 | C1000 | A913 | G812 | A601 | A601 | A503 |
| A1821 | U1735 | U1501 | G1378 | A1255 | C1087 | A1001 | U918 | A821 | G602 | G602 | A504 |
| G1823 | A1736 | G1503 | G1378 | U1256 | G1087 | U1003 | U918 | G822 | C603 | C603 | A505 |
| U1827 | U1740 | C1604 | U1387 | G1257 | G1090 | A1004 | G922 | G823 | A609 | A609 | A506 |
| C1828 | G1741 | A1605 | G1388 | A1258 | A1091 | A1005 | U924 | A829 | C610 | C610 | G510 |
| U1829 | G1742 | G1513 | G1389 | C1263 | G1092 | C1006 | G927 | A830 | U611 | U611 | C511 |
| C1830 | G1743 | C1514 | G1390 | U1265 | G1093 | C1006 | G928 | A830 | C624 | C624 | G515 |
| G1831 | G1744 | A1614 | C1391 | A1265 | A1094 | C1006 | G929 | C837 | G625 | G625 | G516 |
| G1832 | A1745 | G1517 | U1398 | G1269 | G1097 | U1014 | G930 | C837 | A626 | A626 | A517 |
| A1833 | G1746 | A1518 | A1405 | G1272 | C1098 | C1015 | C931 | G839 | G627 | G627 | G518 |
| A1834 | A1747 | G1525 | A1406 | A1272 | C1098 | C1015 | C932 | C842 | U629 | U629 | G519 |
| A1841 | A1748 | G1529 | A1411 | U1280 | C1098 | C1015 | C933 | C843 | U630 | U630 | G525 |
| G1842 | G1750 | G1535 | A1416 | U1284 | C1098 | C1015 | C934 | C844 | G636 | G636 | A526 |
| G1845 | C1757 | U1536 | C1416 | G1285 | C1098 | C1015 | C935 | C844 | A527 | A527 | A528 |
| A1846 | C1757 | A1536 | G1417 | U1286 | C1098 | C1015 | C936 | A847 | U529 | U529 | U529 |
| G1847 | C1758 | C1631 | U1418 | A1287 | C1098 | C1015 | G937 | G846 | A530 | A530 | A530 |
| G1848 | C1759 | A1632 | U1418 | U1287 | C1098 | C1015 | G938 | A849 | G641 | G641 | G533 |
| G1857 | U1765 | A1634 | A1425 | G1290 | C1098 | C1015 | C939 | A849 | G642 | G642 | C534 |
| C1858 | G1766 | A1542 | G1426 | A1293 | C1098 | C1015 | C940 | G852 | G645 | G645 | C537 |
| G1859 | A1767 | U1549 | A1430 | A1296 | C1098 | C1015 | C941 | G856 | A646 | A646 | G537 |
| C1874 | U1768 | C1550 | C1431 | G1296 | C1098 | C1015 | C942 | U857 | A652 | A652 | C542 |
| A1878 | G1776 | C1551 | C1432 | A1299 | C1098 | C1015 | C943 | U858 | A656 | A656 | U544 |
| A1879 | A1654 | C1552 | C1433 | A1300 | C1098 | C1015 | C944 | C859 | G659 | G659 | C552 |
| G1880 | A1655 | A1553 | C1433 | U1301 | C1098 | C1015 | A945 | C859 | C660 | C660 | A553 |
| G1881 | G1781 | C1554 | U1440 | G1302 | C1098 | C1015 | A946 | C859 | G661 | G661 | A554 |
| U1882 | C1785 | A1556 | A1441 | U1302 | C1098 | C1015 | A946 | C859 | A662 | A662 | G555 |
| A1890 | A1786 | G1676 | U1442 | G1312 | C1098 | C1015 | C950 | C865 |      |      |      |
|       | G1787 | C1677 | U1443 | U1313 | C1098 | C1015 | U951 | A866 |      |      |      |
|       |       |       | U1444 | U1313 | C1098 | C1015 | G952 | A866 |      |      |      |
|       |       |       | C1444 | U1313 | C1098 | C1015 | U953 | C872 |      |      |      |
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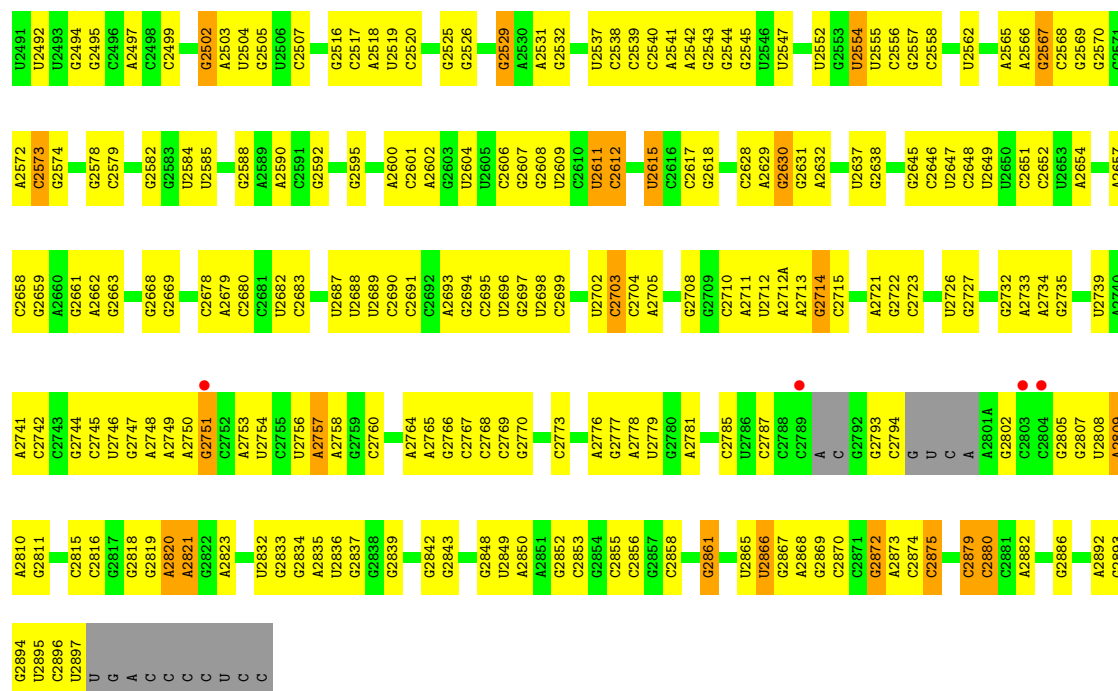


• Molecule 25: 23S Ribosomal RNA



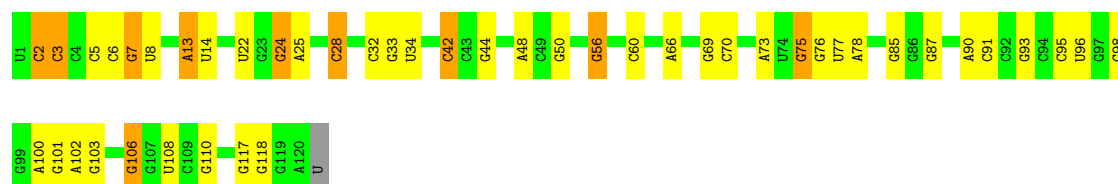


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| C2402 | A2320 | G2239 | G2153 | G2010 | A1916 | A1809 | A1698 | C1600 | G1435  | U1357 | G1264 |
| U2406 | A2321 | G2240 | G2154 | U2011 | U1917 | A1810 | G1699 | C1601 | G1436  | G1358 | A1265 |
| G2407 | A2322 | A2241 | G2155 | G2012 | U1918 | G1811 | A1700 | U1602 | C1437  | A1359 | G1266 |
| U2408 | G2323 | C2248 | G2156 | A2013 | A1919 | A1812 | A1701 | G1607 | A1445  | A1360 | U1267 |
| G2409 | G2324 | C2248 | G2157 | G2014 | U1922 | G1813 | G1702 | C1607 | A1445  | U1268 | A1268 |
| G2410 | G2325 | G2285 | A2158 | A2019 | U1923 | A1814 | G1703 | A1608 | C1445A | A1269 | A1269 |
| A2411 | A2327 | G2256 | G2159 | A2020 | G1927 | A1815 | G1704 | A1609 | C1446  | C1270 | G1270 |
| G2415 | A2328 | G2257 | G2160 | A2021 | A1927 | G1822 | G1705 | A1610 | G1447  | A1365 | G1271 |
| G2416 | G2329 | C2258 | G2161 | U2022 | A1928 | G1823 | C1711 | A1616 | G1448  | A1272 | A1272 |
| C2417 | G2330 | C2261 | G2162 | G2023 | G1929 | G1823 | C1711 | C1615 | A1449  | U1273 | U1273 |
| A2418 | G2331 | U2262 | G2163 | G2024 | G1930 | G1823 | C1711 | C1617 | G1369  | A1278 | A1278 |
| U2419 | U2332 | U2262 | G2164 | C2025 | U1931 | G1826 | G1721 | C1617 | A1452  | G1370 | G1279 |
| G2420 | C2335 | C2263 | G2166 | C2026 | U1932 | C1827 | A1722 | C1618 | U1453  | G1371 | U1282 |
| G2421 | A2336 | C2264 | G2167 | G2027 | G1933 | G1828 | U1739 | A1618 | G1455  | A1372 | G1283 |
| A2422 | G2337 | A2268 | G2168 | G2028 | A1936 | G1835 | G1740 | G1626 | G1459  | G1376 | G1288 |
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| C2440 | C2364 | A2288 | G2184 | G2046 | A1971 | G1878 | U1779 | C1658 | G1492  | U1406 | A1317 |
| C2442 | G2365 | U2291 | G2185 | A2051 | A1972 | C1879 | A1780 | C1660 | C1493  | G1318 | C1318 |
| G2445 | C2369 | C2292 | G2186 | A2052 | A1973 | G1883 | A1783 | U1659 | C1494  | G1319 | C1319 |
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| U2455 | G2371 | C2294 | G2188 | A2054 | G1979 | A1889 | A1785 | A1665 | A1496  | A1412 | A1321 |
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| C2456 | G2373 | U2296 | A2198 | A2056 | C1982 | A1890 | A1786 | G1667 | C1498  | U1326 | U1326 |
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| A2469 | C2384 | A2304 | G2219 | A2061 | U1993 | U1898 | G1792 | C1674 | A1507  | A1419 | A1419 |
| G2470 | C2385 | A2305 | G2224 | C2065 | U1993 | A1899 | G1792 | G1674 | A1508  | G1421 | G1337 |
| U2473 | C2386 | G2308 | A2225 | C2066 | C1996 | A1900 | U1796 | C1686 | G1422  | G1338 | G1338 |
| C2474 | A2387 | A2309 | G2226 | G2069 | C1997 | A1900 | C1797 | C1687 | C1589  | U1341 | U1341 |
| C2475 | A2388 | A2310 | G2227 | G2070 | G1998 | G1906 | U1798 | G1688 | A1509  | G1423 | A1342 |
| A2476 | C2394 | U2312 | G2228 | U2074 | G1998 | G1907 | G1799 | U1688 | A1509B | G1343 | G1343 |
| U2476 | C2395 | G2313 | G2229 | U2075 | G2000 | C1908 | A1689 | A1689 | G1510  | A1427 | G1344 |
| C2483 | G2396 | C2314 | G2234 | A2001 | A2001 | C1908 | G1801 | U1682 | U1514  | G1428 | U1352 |
| G2484 | G2397 | G2315 | G2235 | G2002 | G2002 | A1912 | A1802 | U1693 | G1515  | G1429 | A1353 |
| G2490 | C2400 | G2318 | G2237 | C2006 | C2006 | A1913 | A1803 | C1696 | U1431  | A1430 | A1354 |
|       |       |       |       |       |       | C1914 | U1805 |       |        | G1355 | G1355 |



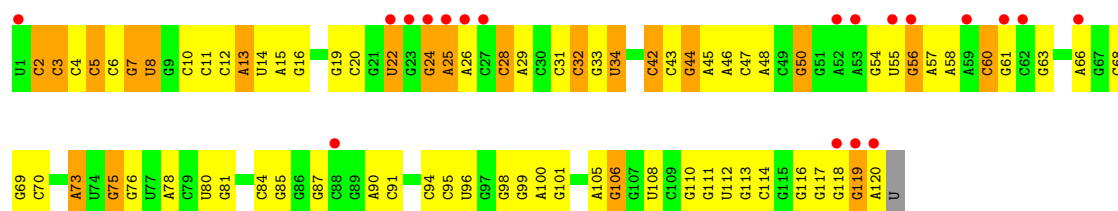
### • Molecule 26: 5S Ribosomal RNA

Chain BB: 61% 30% 8% .



### • Molecule 26: 5S Ribosomal RNA

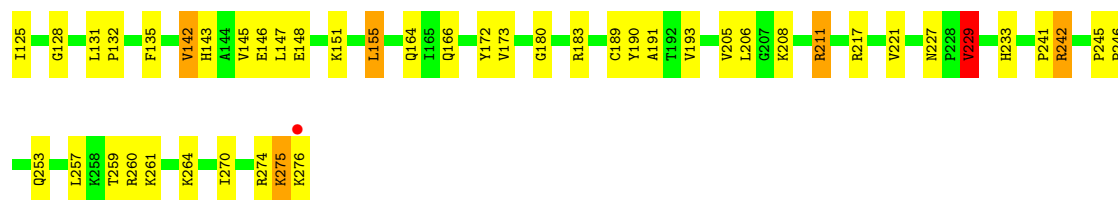
Chain DB: 16% 36% 46% 17% .



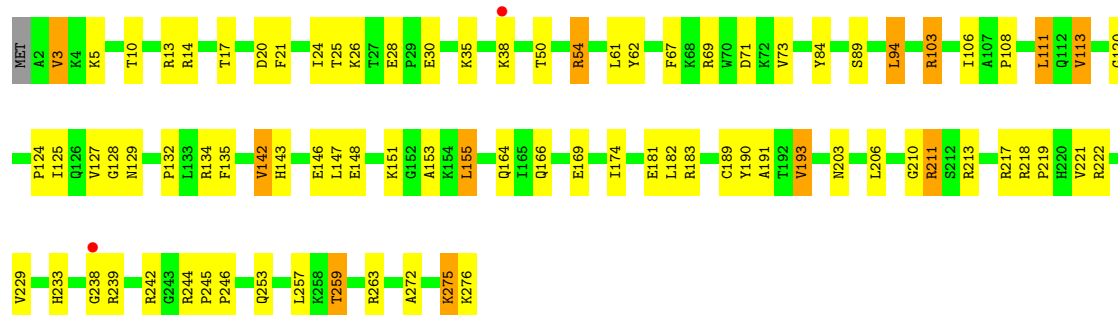
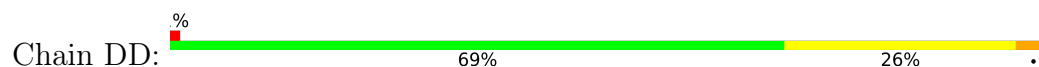
### • Molecule 27: 50S Ribosomal Protein L2

Chain BD: 70% 25% .

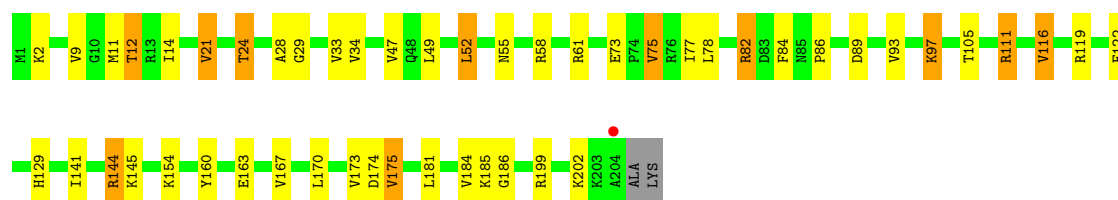
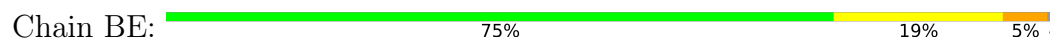




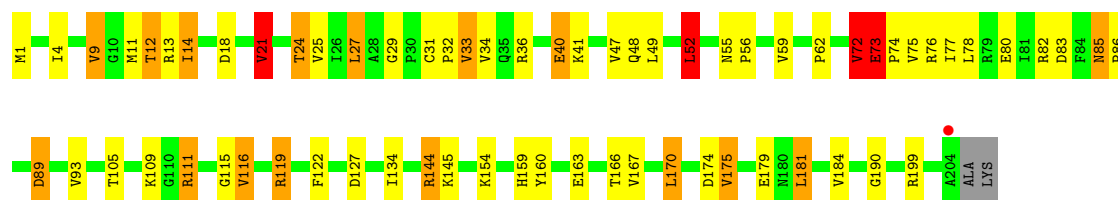
• Molecule 27: 50S Ribosomal Protein L2



• Molecule 28: 50S Ribosomal Protein L3

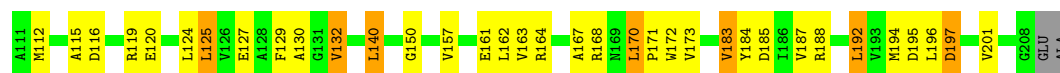


• Molecule 28: 50S Ribosomal Protein L3



• Molecule 29: 50S Ribosomal Protein L4

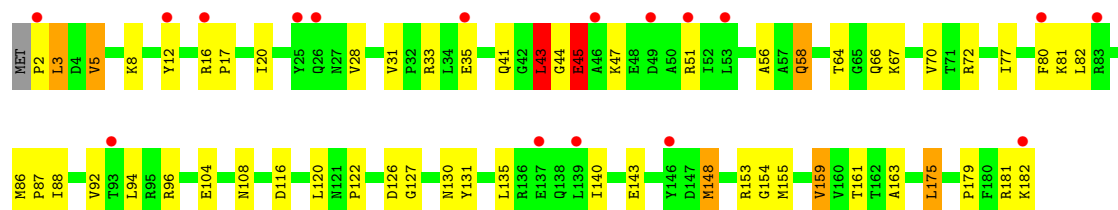




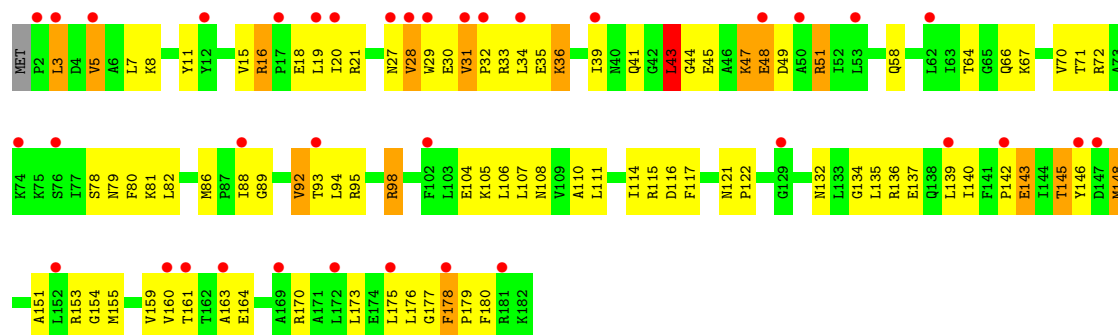
• Molecule 29: 50S Ribosomal Protein L4



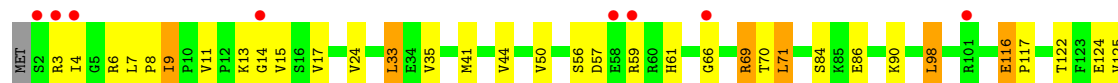
• Molecule 30: 50S Ribosomal Protein L5



• Molecule 30: 50S Ribosomal Protein L5

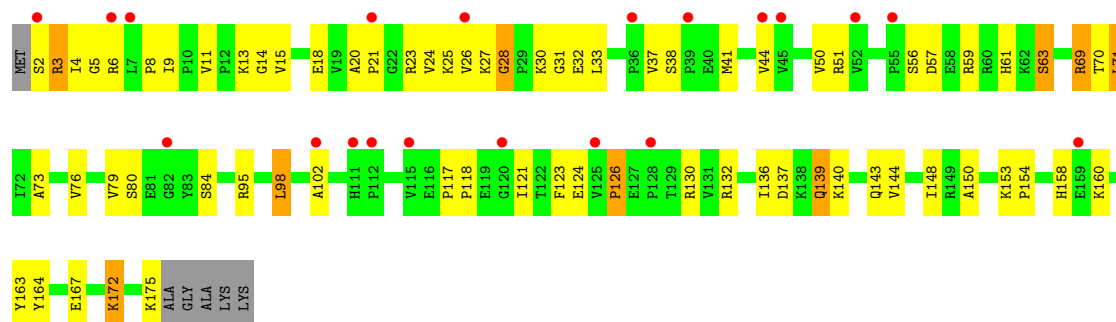


• Molecule 31: 50S Ribosomal Protein L6

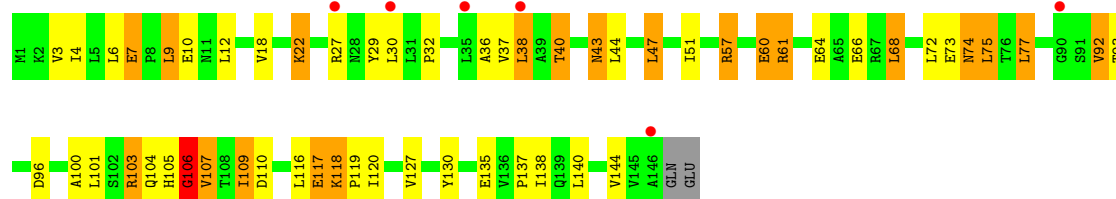




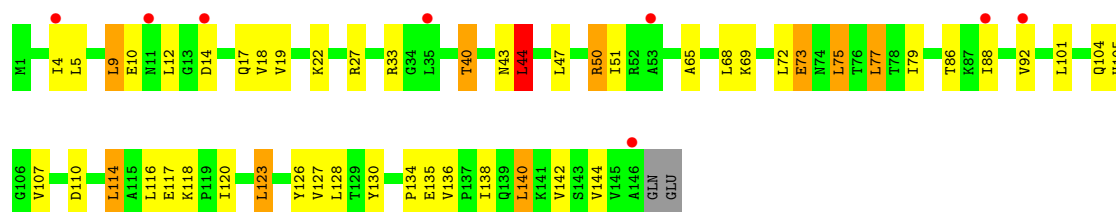
• Molecule 31: 50S Ribosomal Protein L6



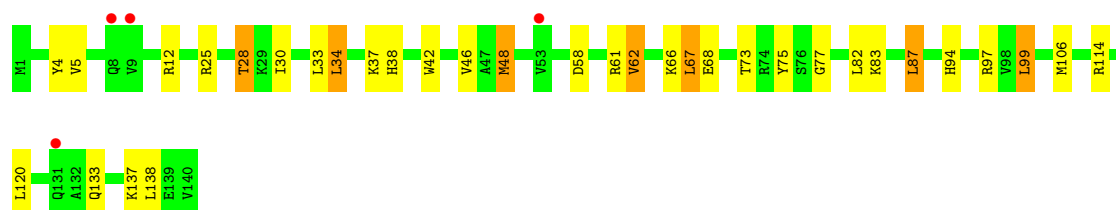
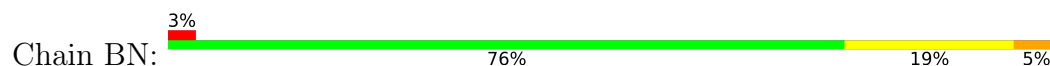
• Molecule 32: 50S Ribosomal Protein L9



• Molecule 32: 50S Ribosomal Protein L9



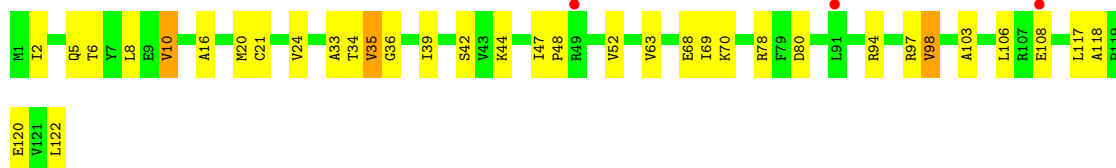
• Molecule 33: 50S Ribosomal Protein L13



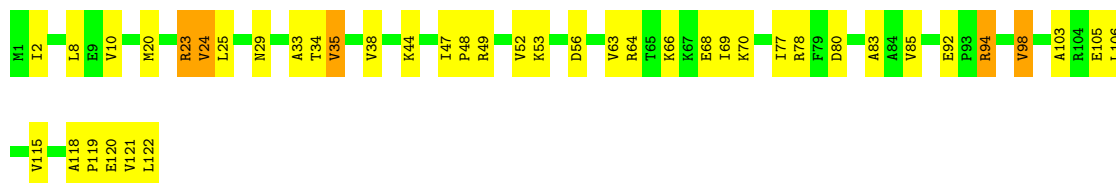
## • Molecule 33: 50S Ribosomal Protein L13

Chain DN:  76% 21% .

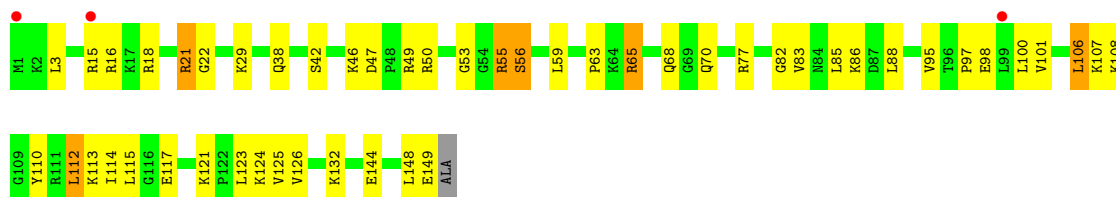
## • Molecule 34: 50S Ribosomal Protein L14

Chain BO:  2% 71% 26% .

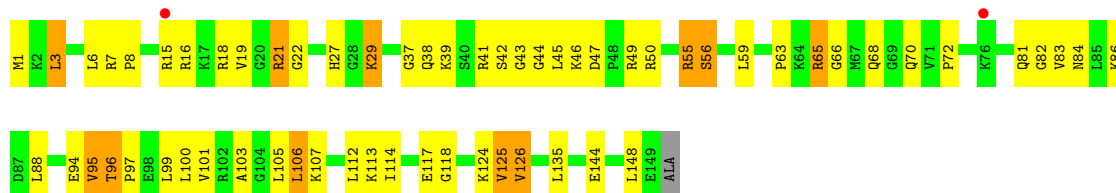
## • Molecule 34: 50S Ribosomal Protein L14

Chain DO:  66% 30% .

## • Molecule 35: 50S Ribosomal Protein L15

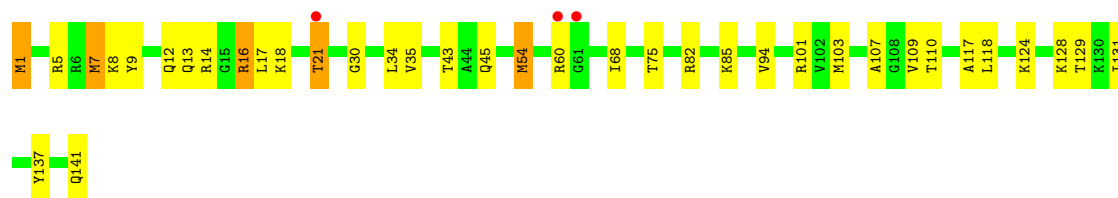
Chain BP:  2% 66% 29% . .

## • Molecule 35: 50S Ribosomal Protein L15

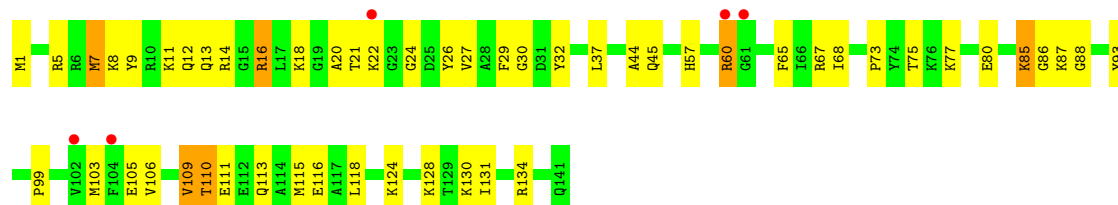
Chain DP:  % 58% 34% 7% .

## • Molecule 36: 50S Ribosomal Protein L16

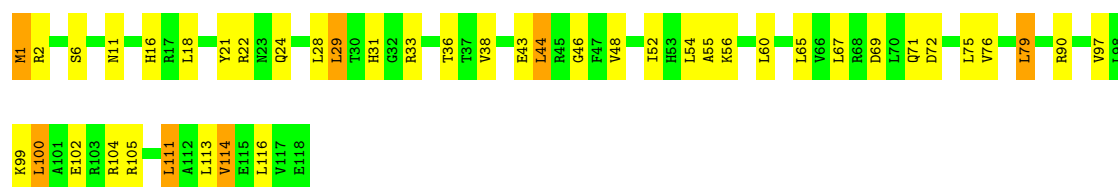
Chain BQ:  2% 74% 23% .



• Molecule 36: 50S Ribosomal Protein L16



• Molecule 37: 50S Ribosomal Protein L17



• Molecule 37: 50S Ribosomal Protein L17

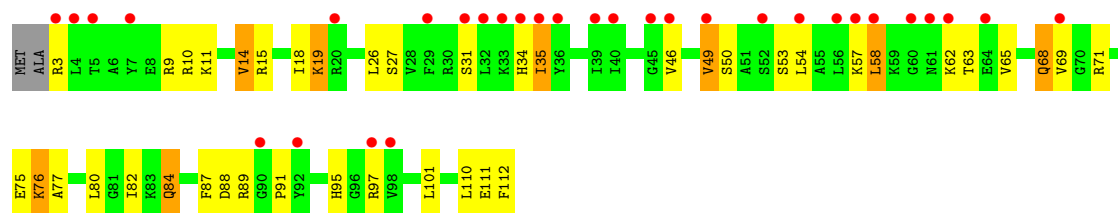


• Molecule 38: 50S Ribosomal Protein L18

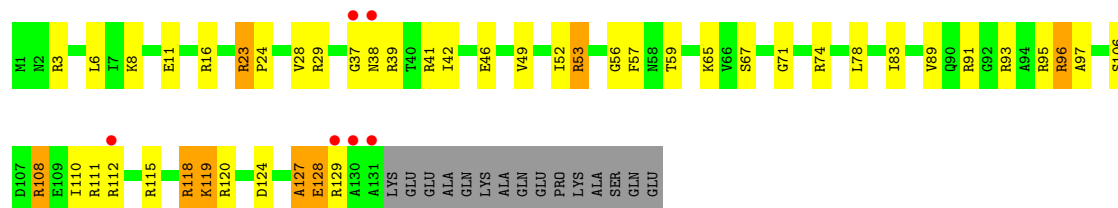


• Molecule 38: 50S Ribosomal Protein L18

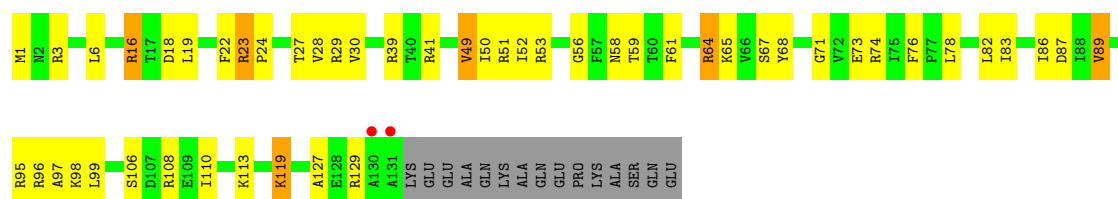




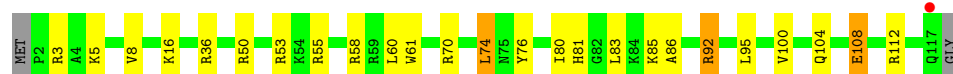
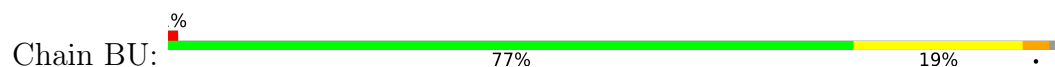
• Molecule 39: 50S Ribosomal Protein L19



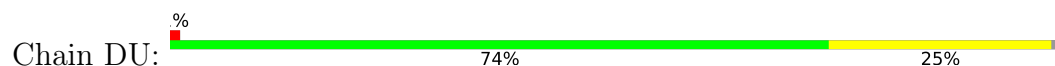
• Molecule 39: 50S Ribosomal Protein L19



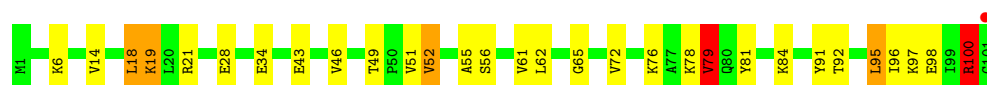
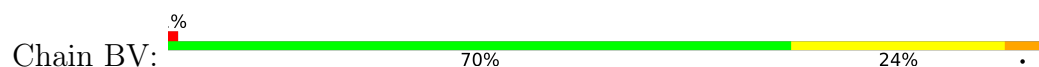
• Molecule 40: 50S Ribosomal Protein L20



• Molecule 40: 50S Ribosomal Protein L20



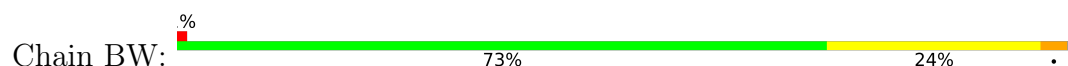
• Molecule 41: 50S Ribosomal Protein L21



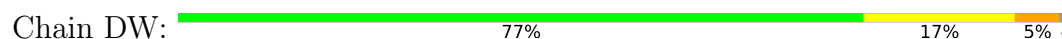
- Molecule 41: 50S Ribosomal Protein L21



- Molecule 42: 50S Ribosomal Protein L22



- Molecule 42: 50S Ribosomal Protein L22



- Molecule 43: 50S Ribosomal Protein L23



- Molecule 43: 50S Ribosomal Protein L23

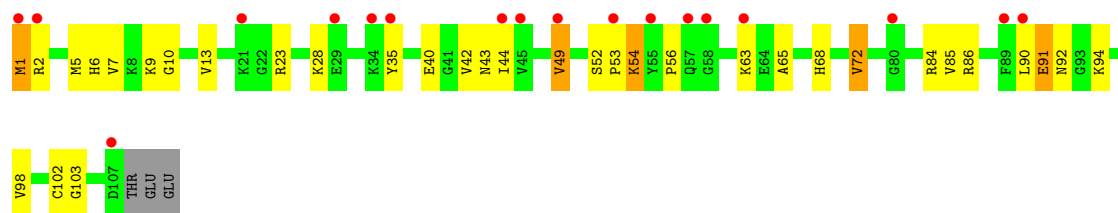


- Molecule 44: 50S Ribosomal Protein L24

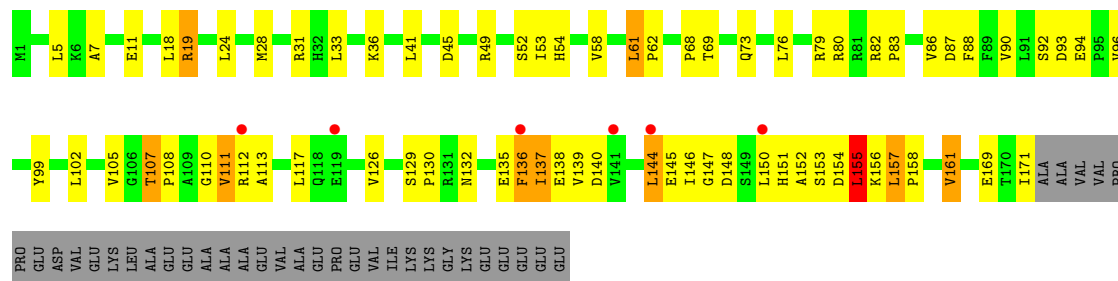


- Molecule 44: 50S Ribosomal Protein L24

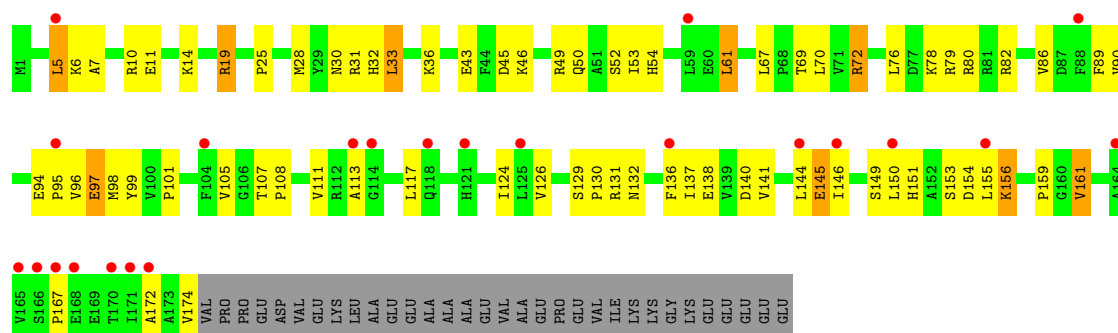




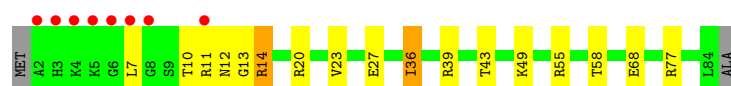
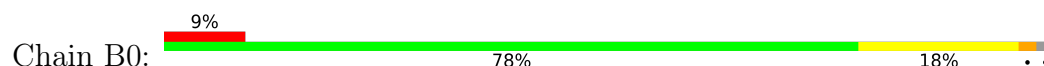
● Molecule 45: 50S Ribosomal Protein L25



● Molecule 45: 50S Ribosomal Protein L25



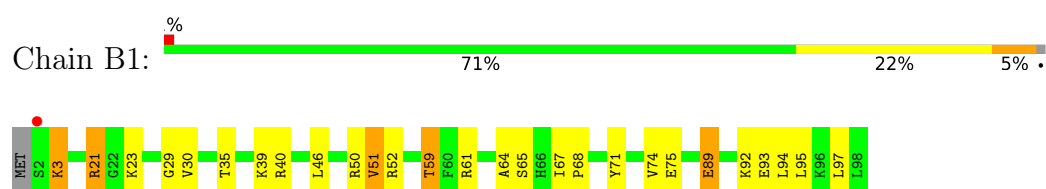
● Molecule 46: 50S Ribosomal Protein L27



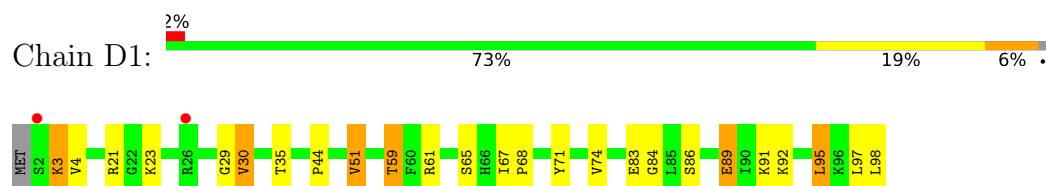
● Molecule 46: 50S Ribosomal Protein L27



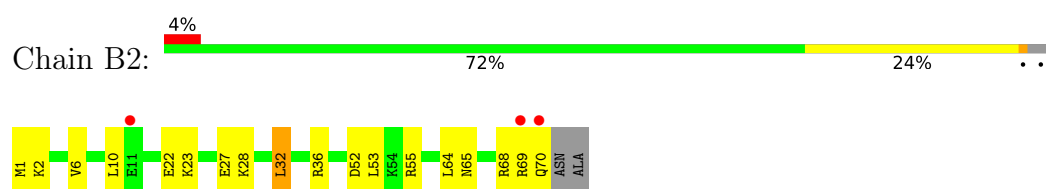
● Molecule 47: 50S Ribosomal Protein L28



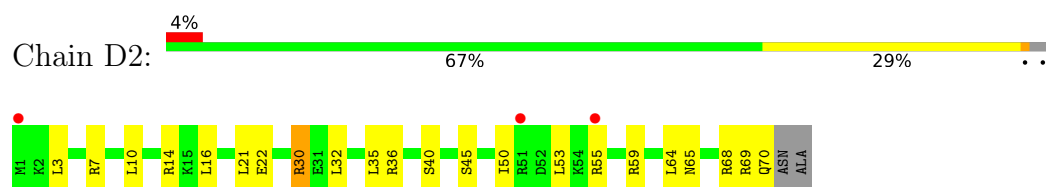
• Molecule 47: 50S Ribosomal Protein L28



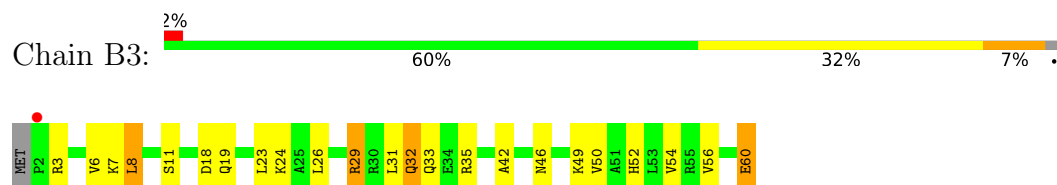
• Molecule 48: 50S Ribosomal Protein L29



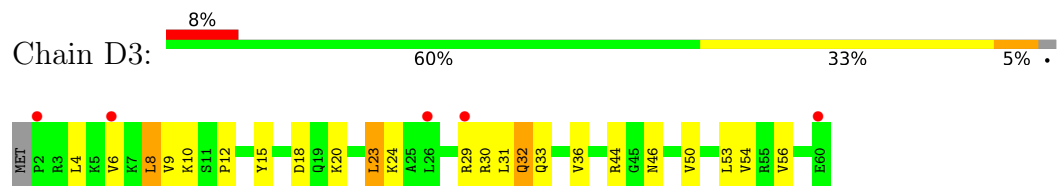
• Molecule 48: 50S Ribosomal Protein L29



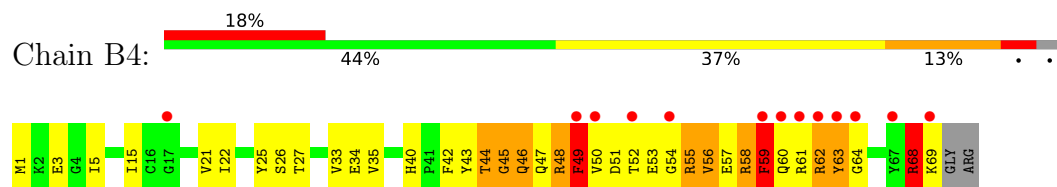
• Molecule 49: 50S Ribosomal Protein L30



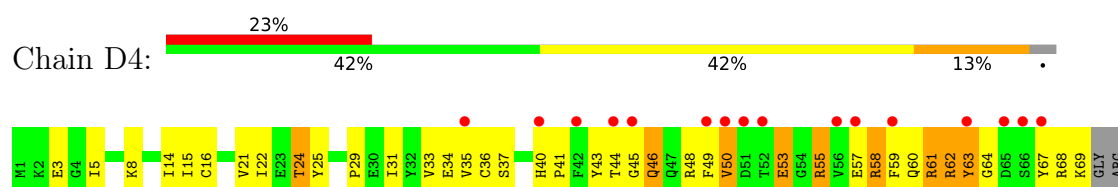
• Molecule 49: 50S Ribosomal Protein L30



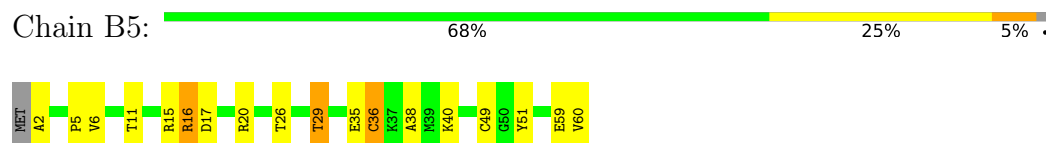
• Molecule 50: 50S Ribosomal Protein L31



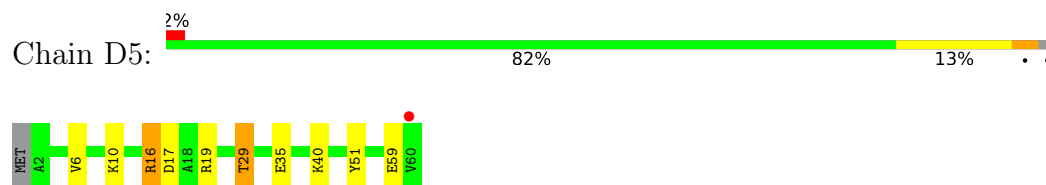
• Molecule 50: 50S Ribosomal Protein L31



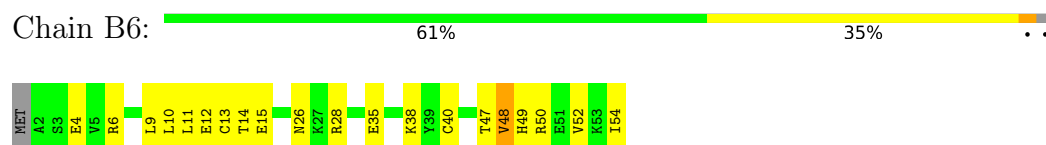
• Molecule 51: 50S Ribosomal Protein L32



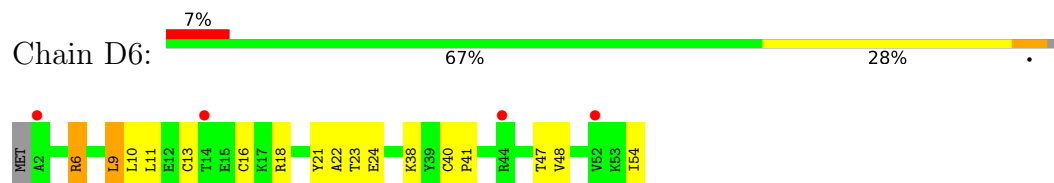
• Molecule 51: 50S Ribosomal Protein L32



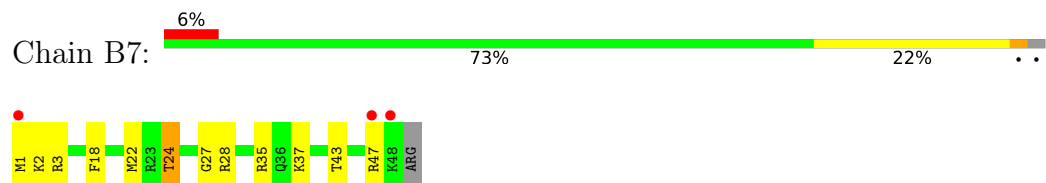
• Molecule 52: 50S Ribosomal Protein L33



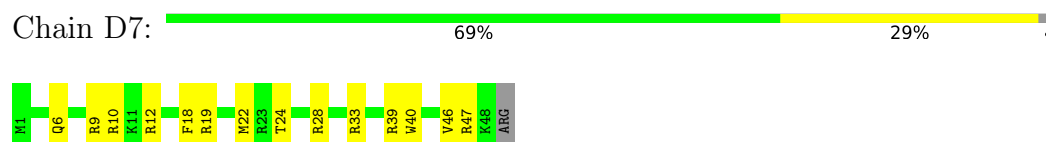
• Molecule 52: 50S Ribosomal Protein L33



• Molecule 53: 50S Ribosomal Protein L34

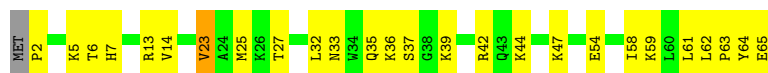


• Molecule 53: 50S Ribosomal Protein L34



• Molecule 54: 50S Ribosomal Protein L35

Chain B8:  58% 38% ..



- Molecule 54: 50S Ribosomal Protein L35

Chain D8:  58% 38% ..



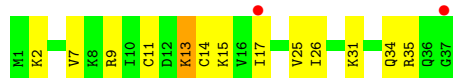
- Molecule 55: 50S Ribosomal Protein L36

Chain B9:  3% 70% 30%



- Molecule 55: 50S Ribosomal Protein L36

Chain D9:  5% 65% 32% .



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 208.93Å 446.95Å 619.78Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 144.86 – 2.70<br>144.86 – 2.70                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (144.86-2.70)<br>99.6 (144.86-2.70)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.18                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.32 (at 2.69Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.8.2_1309                                           | Depositor        |
| R, $R_{free}$                                                           | 0.215 , 0.262<br>0.216 , 0.263                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 78302 reflections (5.00%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.258                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 55.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 290807                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 59.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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    | 0.51         | 14/36024 (0.0%) | 0.47        | 7/56222 (0.0%) |
| 1   | CA    | 0.24         | 0/36170         | 0.46        | 1/56452 (0.0%) |
| 2   | AB    | 0.43         | 0/1881          | 1.03        | 10/2542 (0.4%) |
| 2   | CB    | 0.45         | 0/1860          | 1.05        | 8/2518 (0.3%)  |
| 3   | AC    | 0.40         | 0/1576          | 0.88        | 2/2130 (0.1%)  |
| 3   | CC    | 0.43         | 0/1566          | 0.99        | 4/2119 (0.2%)  |
| 4   | AD    | 0.42         | 0/1689          | 0.89        | 2/2267 (0.1%)  |
| 4   | CD    | 0.40         | 0/1704          | 0.87        | 2/2284 (0.1%)  |
| 5   | AE    | 0.42         | 0/1145          | 0.87        | 0/1543         |
| 5   | CE    | 0.42         | 0/1149          | 0.97        | 3/1548 (0.2%)  |
| 6   | AF    | 0.39         | 0/819           | 0.80        | 0/1111         |
| 6   | CF    | 0.42         | 0/829           | 0.84        | 0/1123         |
| 7   | AG    | 0.39         | 0/1250          | 0.86        | 0/1679         |
| 7   | CG    | 0.38         | 0/1254          | 0.93        | 2/1683 (0.1%)  |
| 8   | AH    | 0.40         | 0/1108          | 0.87        | 0/1494         |
| 8   | CH    | 0.38         | 0/1108          | 0.87        | 0/1494         |
| 9   | AI    | 0.37         | 0/1002          | 0.87        | 2/1346 (0.1%)  |
| 9   | CI    | 0.43         | 0/997           | 0.95        | 5/1343 (0.4%)  |
| 10  | AJ    | 0.42         | 0/722           | 0.93        | 0/982          |
| 10  | CJ    | 0.48         | 0/727           | 1.02        | 2/988 (0.2%)   |
| 11  | AK    | 0.43         | 0/844           | 0.88        | 0/1145         |
| 11  | CK    | 0.39         | 0/848           | 0.90        | 1/1149 (0.1%)  |
| 12  | AL    | 0.42         | 0/946           | 0.82        | 0/1274         |
| 12  | CL    | 0.41         | 0/946           | 0.94        | 4/1274 (0.3%)  |
| 13  | AM    | 0.38         | 0/947           | 0.92        | 1/1272 (0.1%)  |
| 13  | CM    | 0.41         | 0/930           | 0.87        | 0/1250         |
| 14  | AN    | 0.37         | 0/501           | 0.93        | 2/664 (0.3%)   |
| 14  | CN    | 0.38         | 0/501           | 0.84        | 0/664          |
| 15  | AO    | 0.41         | 0/739           | 0.86        | 0/985          |
| 15  | CO    | 0.37         | 0/739           | 0.82        | 0/985          |
| 16  | AP    | 0.41         | 0/697           | 0.83        | 0/939          |
| 16  | CP    | 0.42         | 0/693           | 0.83        | 0/935          |

| Mol | Chain | Bond lengths |              | Bond angles |                 |
|-----|-------|--------------|--------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5      | RMSZ        | # Z  >5         |
| 17  | AQ    | 0.39         | 0/836        | 0.81        | 0/1117          |
| 17  | CQ    | 0.35         | 0/836        | 0.79        | 2/1117 (0.2%)   |
| 18  | AR    | 0.39         | 0/560        | 0.83        | 0/746           |
| 18  | CR    | 0.36         | 0/560        | 0.78        | 0/746           |
| 19  | AS    | 0.39         | 0/667        | 0.86        | 0/900           |
| 19  | CS    | 0.46         | 0/661        | 1.03        | 3/893 (0.3%)    |
| 20  | AT    | 0.39         | 0/730        | 0.94        | 0/965           |
| 20  | CT    | 0.40         | 0/729        | 0.88        | 1/965 (0.1%)    |
| 21  | AU    | 0.36         | 0/203        | 0.83        | 0/266           |
| 21  | CU    | 0.42         | 0/203        | 0.88        | 1/266 (0.4%)    |
| 22  | AV    | 0.31         | 0/188        | 0.52        | 0/290           |
| 22  | CV    | 0.30         | 0/122        | 0.48        | 0/188           |
| 23  | AX    | 0.29         | 0/1725       | 0.45        | 0/2689          |
| 23  | CX    | 0.29         | 0/1725       | 0.47        | 0/2689          |
| 24  | AY    | 0.28         | 0/428        | 0.35        | 0/661           |
| 24  | CY    | 0.26         | 0/115        | 0.31        | 0/176           |
| 25  | BA    | 0.37         | 0/68083      | 0.51        | 2/106274 (0.0%) |
| 25  | DA    | 0.28         | 0/67542      | 0.48        | 1/105428 (0.0%) |
| 26  | BB    | 0.29         | 0/2878       | 0.45        | 0/4490          |
| 26  | DB    | 0.30         | 0/2878       | 0.48        | 0/4490          |
| 27  | BD    | 0.57         | 0/2186       | 0.92        | 3/2944 (0.1%)   |
| 27  | DD    | 0.49         | 0/2186       | 0.92        | 3/2944 (0.1%)   |
| 28  | BE    | 0.60         | 0/1592       | 0.93        | 2/2149 (0.1%)   |
| 28  | DE    | 0.49         | 0/1592       | 1.02        | 11/2149 (0.5%)  |
| 29  | BF    | 0.55         | 0/1619       | 0.88        | 0/2193          |
| 29  | DF    | 0.45         | 0/1615       | 0.95        | 5/2188 (0.2%)   |
| 30  | BG    | 0.43         | 0/1450       | 0.90        | 3/1959 (0.2%)   |
| 30  | DG    | 0.43         | 0/1449       | 0.98        | 4/1958 (0.2%)   |
| 31  | BH    | 0.48         | 0/1356       | 0.88        | 1/1834 (0.1%)   |
| 31  | DH    | 0.42         | 0/1356       | 0.93        | 3/1834 (0.2%)   |
| 32  | BI    | 0.44         | 0/1100       | 0.95        | 8/1501 (0.5%)   |
| 32  | DI    | 0.41         | 0/1076       | 0.88        | 1/1471 (0.1%)   |
| 33  | BN    | 0.53         | 0/1144       | 0.84        | 0/1543          |
| 33  | DN    | 0.43         | 0/1144       | 0.89        | 0/1543          |
| 34  | BO    | 0.59         | 0/943        | 0.88        | 2/1269 (0.2%)   |
| 34  | DO    | 0.46         | 0/943        | 0.88        | 2/1269 (0.2%)   |
| 35  | BP    | 0.55         | 0/1152       | 0.87        | 2/1533 (0.1%)   |
| 35  | DP    | 0.45         | 0/1152       | 1.00        | 8/1533 (0.5%)   |
| 36  | BQ    | 0.57         | 0/1143       | 0.84        | 0/1527          |
| 36  | DQ    | 0.46         | 0/1143       | 0.88        | 0/1527          |
| 37  | BR    | 0.62         | 1/982 (0.1%) | 0.90        | 0/1312          |
| 37  | DR    | 0.46         | 0/982        | 0.81        | 1/1312 (0.1%)   |
| 38  | BS    | 0.47         | 0/887        | 0.92        | 0/1180          |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | DS    | 0.44         | 0/880            | 0.91        | 0/1172            |
| 39  | BT    | 0.49         | 0/1105           | 0.87        | 0/1477            |
| 39  | DT    | 0.44         | 0/1097           | 0.84        | 0/1468            |
| 40  | BU    | 0.60         | 0/977            | 0.86        | 0/1301            |
| 40  | DU    | 0.41         | 0/977            | 0.80        | 0/1301            |
| 41  | BV    | 0.55         | 0/782            | 0.88        | 0/1049            |
| 41  | DV    | 0.41         | 0/782            | 0.84        | 0/1049            |
| 42  | BW    | 0.67         | 0/897            | 0.87        | 0/1205            |
| 42  | DW    | 0.47         | 0/897            | 0.83        | 2/1205 (0.2%)     |
| 43  | BX    | 0.55         | 0/764            | 0.87        | 1/1025 (0.1%)     |
| 43  | DX    | 0.42         | 0/764            | 0.82        | 0/1025            |
| 44  | BY    | 0.50         | 0/819            | 0.91        | 0/1095            |
| 44  | DY    | 0.39         | 0/819            | 0.91        | 1/1095 (0.1%)     |
| 45  | BZ    | 0.49         | 0/1379           | 1.01        | 5/1873 (0.3%)     |
| 45  | DZ    | 0.40         | 0/1390           | 0.94        | 4/1890 (0.2%)     |
| 46  | B0    | 0.54         | 0/662            | 0.91        | 1/881 (0.1%)      |
| 46  | D0    | 0.40         | 0/662            | 0.86        | 3/881 (0.3%)      |
| 47  | B1    | 0.50         | 0/762            | 0.82        | 0/1014            |
| 47  | D1    | 0.44         | 0/762            | 0.86        | 0/1014            |
| 48  | B2    | 0.49         | 0/590            | 0.88        | 0/781             |
| 48  | D2    | 0.35         | 0/590            | 0.80        | 0/781             |
| 49  | B3    | 0.54         | 0/474            | 0.96        | 2/635 (0.3%)      |
| 49  | D3    | 0.40         | 0/469            | 0.88        | 0/630             |
| 50  | B4    | 0.46         | 0/571            | 1.07        | 5/768 (0.7%)      |
| 50  | D4    | 0.42         | 0/545            | 0.99        | 3/737 (0.4%)      |
| 51  | B5    | 0.62         | 0/469            | 0.98        | 0/635             |
| 51  | D5    | 0.45         | 0/469            | 0.80        | 0/635             |
| 52  | B6    | 0.65         | 0/460            | 0.91        | 0/613             |
| 52  | D6    | 0.45         | 0/456            | 0.78        | 0/608             |
| 53  | B7    | 0.61         | 0/426            | 0.84        | 0/561             |
| 53  | D7    | 0.52         | 0/426            | 0.87        | 2/561 (0.4%)      |
| 54  | B8    | 0.59         | 0/519            | 0.87        | 0/684             |
| 54  | D8    | 0.47         | 0/525            | 0.81        | 0/691             |
| 55  | B9    | 0.58         | 0/310            | 0.91        | 1/407 (0.2%)      |
| 55  | D9    | 0.46         | 0/310            | 0.90        | 0/407             |
| All | All   | 0.39         | 15/310558 (0.0%) | 0.62        | 157/464586 (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 |
|-----|-------|---------------------|---------------------|
| 1   | AA    | 0                   | 1                   |
| 7   | CG    | 0                   | 2                   |
| 38  | BS    | 0                   | 1                   |
| 50  | B4    | 0                   | 1                   |
| 50  | D4    | 0                   | 1                   |
| All | All   | 0                   | 6                   |

The worst 5 of 15 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | AA    | 439 | A    | C5-C4 | 50.86 | 2.40        | 1.38     |
| 1   | AA    | 496 | A    | C6-N1 | 40.12 | 2.15        | 1.35     |
| 1   | AA    | 496 | A    | C2-N3 | 24.68 | 1.82        | 1.33     |
| 1   | AA    | 439 | A    | C5-C6 | 18.99 | 1.79        | 1.41     |
| 1   | AA    | 439 | A    | C6-N1 | 18.63 | 1.72        | 1.35     |

The worst 5 of 157 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | AA    | 496 | A    | C2-N3-C4 | 16.17  | 159.12      | 110.60   |
| 1   | AA    | 496 | A    | N1-C2-N3 | -15.00 | 84.31       | 129.30   |
| 2   | CB    | 231 | GLU  | CA-C-N   | -12.93 | 107.23      | 120.03   |
| 2   | CB    | 231 | GLU  | C-N-CA   | -12.93 | 107.23      | 120.03   |
| 1   | AA    | 496 | A    | C5-C6-N6 | -9.80  | 94.30       | 123.70   |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AA    | 439 | A    | Sidechain |
| 50  | B4    | 59  | PHE  | Peptide   |
| 38  | BS    | 58  | LEU  | Peptide   |
| 7   | CG    | 78  | ARG  | Peptide   |
| 7   | CG    | 79  | 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    | 32183 | 0        | 16244    | 644     | 0            |
| 1   | CA    | 32312 | 0        | 16308    | 680     | 0            |
| 2   | AB    | 1846  | 0        | 1867     | 91      | 0            |
| 2   | CB    | 1825  | 0        | 1828     | 92      | 0            |
| 3   | AC    | 1552  | 0        | 1546     | 53      | 0            |
| 3   | CC    | 1542  | 0        | 1517     | 53      | 0            |
| 4   | AD    | 1659  | 0        | 1676     | 75      | 0            |
| 4   | CD    | 1674  | 0        | 1714     | 54      | 0            |
| 5   | AE    | 1129  | 0        | 1185     | 32      | 0            |
| 5   | CE    | 1133  | 0        | 1191     | 37      | 0            |
| 6   | AF    | 806   | 0        | 793      | 19      | 0            |
| 6   | CF    | 816   | 0        | 808      | 17      | 0            |
| 7   | AG    | 1231  | 0        | 1238     | 25      | 0            |
| 7   | CG    | 1235  | 0        | 1249     | 39      | 0            |
| 8   | AH    | 1088  | 0        | 1126     | 28      | 0            |
| 8   | CH    | 1088  | 0        | 1126     | 26      | 0            |
| 9   | AI    | 983   | 0        | 986      | 31      | 0            |
| 9   | CI    | 978   | 0        | 966      | 47      | 0            |
| 10  | AJ    | 709   | 0        | 650      | 35      | 0            |
| 10  | CJ    | 714   | 0        | 672      | 34      | 0            |
| 11  | AK    | 829   | 0        | 825      | 21      | 0            |
| 11  | CK    | 833   | 0        | 836      | 18      | 0            |
| 12  | AL    | 930   | 0        | 980      | 25      | 0            |
| 12  | CL    | 930   | 0        | 980      | 28      | 0            |
| 13  | AM    | 937   | 0        | 977      | 28      | 0            |
| 13  | CM    | 920   | 0        | 950      | 37      | 0            |
| 14  | AN    | 492   | 0        | 529      | 22      | 0            |
| 14  | CN    | 492   | 0        | 529      | 24      | 0            |
| 15  | AO    | 728   | 0        | 760      | 23      | 0            |
| 15  | CO    | 728   | 0        | 760      | 23      | 0            |
| 16  | AP    | 681   | 0        | 697      | 23      | 0            |
| 16  | CP    | 677   | 0        | 686      | 17      | 0            |
| 17  | AQ    | 823   | 0        | 891      | 11      | 0            |
| 17  | CQ    | 823   | 0        | 891      | 11      | 0            |
| 18  | AR    | 555   | 0        | 618      | 13      | 0            |
| 18  | CR    | 555   | 0        | 618      | 14      | 0            |
| 19  | AS    | 652   | 0        | 662      | 25      | 0            |
| 19  | CS    | 646   | 0        | 644      | 41      | 0            |
| 20  | AT    | 728   | 0        | 798      | 21      | 0            |
| 20  | CT    | 727   | 0        | 796      | 17      | 0            |
| 21  | AU    | 199   | 0        | 208      | 5       | 0            |
| 21  | CU    | 199   | 0        | 208      | 9       | 0            |
| 22  | AV    | 169   | 0        | 86       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | CV    | 109   | 0        | 55       | 5       | 0            |
| 23  | AX    | 1625  | 0        | 828      | 20      | 0            |
| 23  | CX    | 1625  | 0        | 829      | 26      | 0            |
| 24  | AY    | 385   | 0        | 199      | 11      | 0            |
| 24  | CY    | 104   | 0        | 56       | 6       | 0            |
| 25  | BA    | 60792 | 0        | 30653    | 707     | 0            |
| 25  | DA    | 60311 | 0        | 30414    | 1002    | 0            |
| 26  | BB    | 2573  | 0        | 1306     | 23      | 0            |
| 26  | DB    | 2573  | 0        | 1306     | 73      | 0            |
| 27  | BD    | 2136  | 0        | 2218     | 61      | 0            |
| 27  | DD    | 2136  | 0        | 2218     | 67      | 0            |
| 28  | BE    | 1559  | 0        | 1618     | 26      | 0            |
| 28  | DE    | 1559  | 0        | 1618     | 46      | 0            |
| 29  | BF    | 1584  | 0        | 1625     | 48      | 0            |
| 29  | DF    | 1580  | 0        | 1619     | 52      | 0            |
| 30  | BG    | 1425  | 0        | 1443     | 45      | 0            |
| 30  | DG    | 1424  | 0        | 1434     | 69      | 0            |
| 31  | BH    | 1330  | 0        | 1407     | 24      | 0            |
| 31  | DH    | 1330  | 0        | 1407     | 50      | 0            |
| 32  | BI    | 1085  | 0        | 1114     | 39      | 0            |
| 32  | DI    | 1061  | 0        | 1080     | 30      | 0            |
| 33  | BN    | 1117  | 0        | 1183     | 20      | 0            |
| 33  | DN    | 1117  | 0        | 1184     | 17      | 0            |
| 34  | BO    | 933   | 0        | 996      | 24      | 0            |
| 34  | DO    | 933   | 0        | 996      | 28      | 0            |
| 35  | BP    | 1135  | 0        | 1212     | 34      | 0            |
| 35  | DP    | 1135  | 0        | 1212     | 54      | 0            |
| 36  | BQ    | 1122  | 0        | 1179     | 27      | 0            |
| 36  | DQ    | 1122  | 0        | 1179     | 39      | 0            |
| 37  | BR    | 968   | 0        | 1033     | 22      | 0            |
| 37  | DR    | 968   | 0        | 1033     | 28      | 0            |
| 38  | BS    | 877   | 0        | 938      | 26      | 0            |
| 38  | DS    | 870   | 0        | 923      | 29      | 0            |
| 39  | BT    | 1091  | 0        | 1151     | 38      | 0            |
| 39  | DT    | 1083  | 0        | 1136     | 38      | 0            |
| 40  | BU    | 959   | 0        | 1019     | 18      | 0            |
| 40  | DU    | 959   | 0        | 1019     | 19      | 0            |
| 41  | BV    | 771   | 0        | 830      | 14      | 0            |
| 41  | DV    | 771   | 0        | 830      | 19      | 0            |
| 42  | BW    | 886   | 0        | 940      | 19      | 0            |
| 42  | DW    | 886   | 0        | 940      | 16      | 0            |
| 43  | BX    | 750   | 0        | 814      | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | DX    | 750   | 0        | 814      | 19      | 0            |
| 44  | BY    | 806   | 0        | 881      | 22      | 0            |
| 44  | DY    | 806   | 0        | 881      | 22      | 0            |
| 45  | BZ    | 1349  | 0        | 1355     | 46      | 0            |
| 45  | DZ    | 1360  | 0        | 1363     | 47      | 0            |
| 46  | B0    | 653   | 0        | 674      | 15      | 0            |
| 46  | D0    | 653   | 0        | 674      | 23      | 0            |
| 47  | B1    | 755   | 0        | 826      | 23      | 0            |
| 47  | D1    | 755   | 0        | 826      | 19      | 0            |
| 48  | B2    | 588   | 0        | 643      | 10      | 0            |
| 48  | D2    | 588   | 0        | 643      | 12      | 0            |
| 49  | B3    | 469   | 0        | 518      | 11      | 0            |
| 49  | D3    | 464   | 0        | 514      | 12      | 0            |
| 50  | B4    | 558   | 0        | 544      | 37      | 0            |
| 50  | D4    | 532   | 0        | 503      | 26      | 0            |
| 51  | B5    | 455   | 0        | 465      | 10      | 0            |
| 51  | D5    | 455   | 0        | 465      | 8       | 0            |
| 52  | B6    | 453   | 0        | 473      | 9       | 0            |
| 52  | D6    | 449   | 0        | 469      | 10      | 0            |
| 53  | B7    | 418   | 0        | 467      | 9       | 0            |
| 53  | D7    | 418   | 0        | 467      | 9       | 0            |
| 54  | B8    | 511   | 0        | 571      | 22      | 0            |
| 54  | D8    | 517   | 0        | 582      | 17      | 0            |
| 55  | B9    | 307   | 0        | 335      | 9       | 0            |
| 55  | D9    | 307   | 0        | 335      | 7       | 0            |
| 56  | AA    | 190   | 0        | 0        | 0       | 0            |
| 56  | AD    | 1     | 0        | 0        | 0       | 0            |
| 56  | AE    | 3     | 0        | 0        | 0       | 0            |
| 56  | AF    | 1     | 0        | 0        | 0       | 0            |
| 56  | AM    | 1     | 0        | 0        | 0       | 0            |
| 56  | AN    | 1     | 0        | 0        | 0       | 0            |
| 56  | AQ    | 1     | 0        | 0        | 0       | 0            |
| 56  | AX    | 9     | 0        | 0        | 0       | 0            |
| 56  | B0    | 5     | 0        | 0        | 0       | 0            |
| 56  | B2    | 1     | 0        | 0        | 0       | 0            |
| 56  | B3    | 1     | 0        | 0        | 0       | 0            |
| 56  | B4    | 1     | 0        | 0        | 0       | 0            |
| 56  | B5    | 4     | 0        | 0        | 0       | 0            |
| 56  | B6    | 2     | 0        | 0        | 0       | 0            |
| 56  | B7    | 5     | 0        | 0        | 0       | 0            |
| 56  | B8    | 2     | 0        | 0        | 0       | 0            |
| 56  | B9    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | BA    | 814   | 0        | 0        | 0       | 0            |
| 56  | BB    | 22    | 0        | 0        | 0       | 0            |
| 56  | BD    | 9     | 0        | 0        | 0       | 0            |
| 56  | BE    | 7     | 0        | 0        | 0       | 0            |
| 56  | BF    | 9     | 0        | 0        | 0       | 0            |
| 56  | BG    | 2     | 0        | 0        | 0       | 0            |
| 56  | BN    | 7     | 0        | 0        | 0       | 0            |
| 56  | BO    | 1     | 0        | 0        | 0       | 0            |
| 56  | BP    | 4     | 0        | 0        | 0       | 0            |
| 56  | BQ    | 4     | 0        | 0        | 0       | 0            |
| 56  | BR    | 3     | 0        | 0        | 0       | 0            |
| 56  | BU    | 9     | 0        | 0        | 0       | 0            |
| 56  | BV    | 4     | 0        | 0        | 0       | 0            |
| 56  | BW    | 4     | 0        | 0        | 0       | 0            |
| 56  | BX    | 2     | 0        | 0        | 0       | 0            |
| 56  | BY    | 3     | 0        | 0        | 0       | 0            |
| 56  | BZ    | 2     | 0        | 0        | 0       | 0            |
| 56  | CA    | 175   | 0        | 0        | 0       | 0            |
| 56  | CE    | 2     | 0        | 0        | 0       | 0            |
| 56  | CF    | 1     | 0        | 0        | 0       | 0            |
| 56  | CJ    | 1     | 0        | 0        | 0       | 0            |
| 56  | CT    | 1     | 0        | 0        | 0       | 0            |
| 56  | CX    | 2     | 0        | 0        | 0       | 0            |
| 56  | D0    | 2     | 0        | 0        | 0       | 0            |
| 56  | D1    | 1     | 0        | 0        | 0       | 0            |
| 56  | D3    | 1     | 0        | 0        | 0       | 0            |
| 56  | D8    | 1     | 0        | 0        | 0       | 0            |
| 56  | DA    | 674   | 0        | 0        | 0       | 0            |
| 56  | DB    | 10    | 0        | 0        | 0       | 0            |
| 56  | DD    | 8     | 0        | 0        | 0       | 0            |
| 56  | DE    | 5     | 0        | 0        | 0       | 0            |
| 56  | DF    | 5     | 0        | 0        | 0       | 0            |
| 56  | DG    | 1     | 0        | 0        | 0       | 0            |
| 56  | DN    | 1     | 0        | 0        | 0       | 0            |
| 56  | DO    | 1     | 0        | 0        | 0       | 0            |
| 56  | DP    | 2     | 0        | 0        | 0       | 0            |
| 56  | DQ    | 3     | 0        | 0        | 0       | 0            |
| 56  | DR    | 1     | 0        | 0        | 0       | 0            |
| 56  | DU    | 4     | 0        | 0        | 0       | 0            |
| 56  | DV    | 3     | 0        | 0        | 0       | 0            |
| 56  | DW    | 2     | 0        | 0        | 0       | 0            |
| 56  | DY    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 57  | AA    | 40    | 0        | 38       | 6       | 0            |
| 57  | CA    | 40    | 0        | 38       | 4       | 0            |
| 58  | AD    | 8     | 0        | 0        | 1       | 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    | 175   | 0        | 0        | 13      | 0            |
| 61  | AJ    | 2     | 0        | 0        | 0       | 0            |
| 61  | AL    | 1     | 0        | 0        | 0       | 0            |
| 61  | AM    | 1     | 0        | 0        | 0       | 0            |
| 61  | AO    | 1     | 0        | 0        | 0       | 0            |
| 61  | AV    | 1     | 0        | 0        | 0       | 0            |
| 61  | AX    | 8     | 0        | 0        | 0       | 0            |
| 61  | B0    | 4     | 0        | 0        | 0       | 0            |
| 61  | B1    | 1     | 0        | 0        | 0       | 0            |
| 61  | B3    | 1     | 0        | 0        | 0       | 0            |
| 61  | B5    | 4     | 0        | 0        | 1       | 0            |
| 61  | B6    | 1     | 0        | 0        | 0       | 0            |
| 61  | B7    | 1     | 0        | 0        | 0       | 0            |
| 61  | B8    | 10    | 0        | 0        | 1       | 0            |
| 61  | BA    | 1294  | 0        | 0        | 49      | 0            |
| 61  | BB    | 34    | 0        | 0        | 1       | 0            |
| 61  | BD    | 16    | 0        | 0        | 1       | 0            |
| 61  | BE    | 12    | 0        | 0        | 1       | 0            |
| 61  | BF    | 7     | 0        | 0        | 1       | 0            |
| 61  | BG    | 3     | 0        | 0        | 0       | 0            |
| 61  | BI    | 1     | 0        | 0        | 0       | 0            |
| 61  | BN    | 1     | 0        | 0        | 0       | 0            |
| 61  | BO    | 4     | 0        | 0        | 0       | 0            |
| 61  | BP    | 15    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61  | BQ    | 5      | 0        | 0        | 0       | 0            |
| 61  | BR    | 1      | 0        | 0        | 0       | 0            |
| 61  | BU    | 2      | 0        | 0        | 0       | 0            |
| 61  | BV    | 2      | 0        | 0        | 0       | 0            |
| 61  | BW    | 3      | 0        | 0        | 0       | 0            |
| 61  | BX    | 5      | 0        | 0        | 0       | 0            |
| 61  | CA    | 137    | 0        | 0        | 12      | 0            |
| 61  | CD    | 1      | 0        | 0        | 0       | 0            |
| 61  | CJ    | 2      | 0        | 0        | 0       | 0            |
| 61  | CL    | 1      | 0        | 0        | 1       | 0            |
| 61  | CN    | 1      | 0        | 0        | 0       | 0            |
| 61  | CT    | 1      | 0        | 0        | 0       | 0            |
| 61  | CX    | 2      | 0        | 0        | 0       | 0            |
| 61  | D0    | 7      | 0        | 0        | 0       | 0            |
| 61  | D1    | 1      | 0        | 0        | 0       | 0            |
| 61  | D3    | 1      | 0        | 0        | 0       | 0            |
| 61  | D8    | 4      | 0        | 0        | 0       | 0            |
| 61  | DA    | 924    | 0        | 0        | 75      | 0            |
| 61  | DB    | 8      | 0        | 0        | 0       | 0            |
| 61  | DD    | 18     | 0        | 0        | 3       | 0            |
| 61  | DE    | 9      | 0        | 0        | 1       | 0            |
| 61  | DF    | 5      | 0        | 0        | 0       | 0            |
| 61  | DN    | 1      | 0        | 0        | 0       | 0            |
| 61  | DO    | 1      | 0        | 0        | 0       | 0            |
| 61  | DP    | 14     | 0        | 0        | 1       | 0            |
| 61  | DR    | 1      | 0        | 0        | 0       | 0            |
| 61  | DT    | 1      | 0        | 0        | 0       | 0            |
| 61  | DU    | 3      | 0        | 0        | 0       | 0            |
| 61  | DV    | 1      | 0        | 0        | 0       | 0            |
| 61  | DW    | 1      | 0        | 0        | 0       | 0            |
| 61  | DX    | 1      | 0        | 0        | 0       | 0            |
| 61  | DY    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 290807 | 0        | 193177   | 5227    | 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 5227 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 1:AA:439:A:N3 | 1:AA:439:A:C2 | 1.68                     | 1.62              |

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| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 1:AA:439:A:C5 | 1:AA:439:A:C6 | 1.79                     | 1.62              |
| 1:AA:439:A:N3 | 1:AA:439:A:C4 | 1.70                     | 1.56              |
| 1:AA:439:A:C6 | 1:AA:439:A:N1 | 1.72                     | 1.55              |
| 1:AA:439:A:C2 | 1:AA:439:A:N1 | 1.70                     | 1.54              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | AB    | 229/256 (90%) | 194 (85%) | 24 (10%) | 11 (5%)  | 2           | 3   |
| 2   | CB    | 229/256 (90%) | 195 (85%) | 24 (10%) | 10 (4%)  | 2           | 4   |
| 3   | AC    | 204/239 (85%) | 179 (88%) | 23 (11%) | 2 (1%)   | 12          | 32  |
| 3   | CC    | 204/239 (85%) | 178 (87%) | 23 (11%) | 3 (2%)   | 8           | 22  |
| 4   | AD    | 206/209 (99%) | 189 (92%) | 15 (7%)  | 2 (1%)   | 12          | 32  |
| 4   | CD    | 206/209 (99%) | 190 (92%) | 14 (7%)  | 2 (1%)   | 12          | 32  |
| 5   | AE    | 146/162 (90%) | 139 (95%) | 5 (3%)   | 2 (1%)   | 9           | 23  |
| 5   | CE    | 146/162 (90%) | 136 (93%) | 8 (6%)   | 2 (1%)   | 9           | 23  |
| 6   | AF    | 98/101 (97%)  | 88 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 6   | CF    | 98/101 (97%)  | 91 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 7   | AG    | 153/156 (98%) | 139 (91%) | 11 (7%)  | 3 (2%)   | 6           | 16  |
| 7   | CG    | 153/156 (98%) | 137 (90%) | 15 (10%) | 1 (1%)   | 18          | 41  |
| 8   | AH    | 135/138 (98%) | 130 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 8   | CH    | 135/138 (98%) | 129 (96%) | 5 (4%)   | 1 (1%)   | 18          | 41  |
| 9   | AI    | 125/128 (98%) | 107 (86%) | 14 (11%) | 4 (3%)   | 3           | 7   |
| 9   | CI    | 125/128 (98%) | 109 (87%) | 12 (10%) | 4 (3%)   | 3           | 7   |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 10  | AJ    | 95/105 (90%)  | 80 (84%)  | 9 (10%)  | 6 (6%)   | 1           | 2   |
| 10  | CJ    | 94/105 (90%)  | 83 (88%)  | 6 (6%)   | 5 (5%)   | 1           | 3   |
| 11  | AK    | 112/129 (87%) | 103 (92%) | 7 (6%)   | 2 (2%)   | 6           | 18  |
| 11  | CK    | 112/129 (87%) | 101 (90%) | 8 (7%)   | 3 (3%)   | 4           | 10  |
| 12  | AL    | 120/132 (91%) | 111 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 12  | CL    | 120/132 (91%) | 113 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 13  | AM    | 118/126 (94%) | 103 (87%) | 13 (11%) | 2 (2%)   | 7           | 19  |
| 13  | CM    | 116/126 (92%) | 101 (87%) | 11 (10%) | 4 (3%)   | 3           | 7   |
| 14  | AN    | 58/61 (95%)   | 55 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 14  | CN    | 58/61 (95%)   | 55 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 15  | AO    | 86/89 (97%)   | 80 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 15  | CO    | 86/89 (97%)   | 78 (91%)  | 7 (8%)   | 1 (1%)   | 10          | 27  |
| 16  | AP    | 80/88 (91%)   | 73 (91%)  | 7 (9%)   | 0        | 100         | 100 |
| 16  | CP    | 80/88 (91%)   | 74 (92%)  | 5 (6%)   | 1 (1%)   | 9           | 25  |
| 17  | AQ    | 97/105 (92%)  | 92 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 17  | CQ    | 97/105 (92%)  | 90 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 18  | AR    | 66/88 (75%)   | 63 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 18  | CR    | 66/88 (75%)   | 64 (97%)  | 1 (2%)   | 1 (2%)   | 8           | 22  |
| 19  | AS    | 81/93 (87%)   | 70 (86%)  | 11 (14%) | 0        | 100         | 100 |
| 19  | CS    | 81/93 (87%)   | 68 (84%)  | 11 (14%) | 2 (2%)   | 4           | 11  |
| 20  | AT    | 94/106 (89%)  | 82 (87%)  | 6 (6%)   | 6 (6%)   | 1           | 1   |
| 20  | CT    | 94/106 (89%)  | 84 (89%)  | 5 (5%)   | 5 (5%)   | 1           | 3   |
| 21  | AU    | 21/27 (78%)   | 17 (81%)  | 4 (19%)  | 0        | 100         | 100 |
| 21  | CU    | 21/27 (78%)   | 16 (76%)  | 4 (19%)  | 1 (5%)   | 2           | 3   |
| 27  | BD    | 273/276 (99%) | 258 (94%) | 14 (5%)  | 1 (0%)   | 30          | 54  |
| 27  | DD    | 273/276 (99%) | 257 (94%) | 14 (5%)  | 2 (1%)   | 18          | 41  |
| 28  | BE    | 202/206 (98%) | 194 (96%) | 7 (4%)   | 1 (0%)   | 24          | 48  |
| 28  | DE    | 202/206 (98%) | 193 (96%) | 7 (4%)   | 2 (1%)   | 12          | 32  |
| 29  | BF    | 201/210 (96%) | 196 (98%) | 4 (2%)   | 1 (0%)   | 24          | 48  |
| 29  | DF    | 201/210 (96%) | 195 (97%) | 4 (2%)   | 2 (1%)   | 12          | 32  |
| 30  | BG    | 179/182 (98%) | 165 (92%) | 11 (6%)  | 3 (2%)   | 7           | 19  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 30  | DG    | 179/182 (98%) | 161 (90%) | 14 (8%)  | 4 (2%)   | 5           | 14  |
| 31  | BH    | 172/180 (96%) | 161 (94%) | 10 (6%)  | 1 (1%)   | 21          | 44  |
| 31  | DH    | 172/180 (96%) | 160 (93%) | 11 (6%)  | 1 (1%)   | 21          | 44  |
| 32  | BI    | 144/148 (97%) | 129 (90%) | 12 (8%)  | 3 (2%)   | 5           | 15  |
| 32  | DI    | 144/148 (97%) | 130 (90%) | 12 (8%)  | 2 (1%)   | 9           | 23  |
| 33  | BN    | 138/140 (99%) | 135 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 33  | DN    | 138/140 (99%) | 133 (96%) | 4 (3%)   | 1 (1%)   | 18          | 41  |
| 34  | BO    | 120/122 (98%) | 114 (95%) | 5 (4%)   | 1 (1%)   | 16          | 37  |
| 34  | DO    | 120/122 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 35  | BP    | 147/150 (98%) | 140 (95%) | 6 (4%)   | 1 (1%)   | 18          | 41  |
| 35  | DP    | 147/150 (98%) | 137 (93%) | 9 (6%)   | 1 (1%)   | 18          | 41  |
| 36  | BQ    | 139/141 (99%) | 132 (95%) | 6 (4%)   | 1 (1%)   | 18          | 41  |
| 36  | DQ    | 139/141 (99%) | 132 (95%) | 5 (4%)   | 2 (1%)   | 9           | 23  |
| 37  | BR    | 116/118 (98%) | 109 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 37  | DR    | 116/118 (98%) | 110 (95%) | 5 (4%)   | 1 (1%)   | 14          | 35  |
| 38  | BS    | 108/112 (96%) | 98 (91%)  | 9 (8%)   | 1 (1%)   | 14          | 35  |
| 38  | DS    | 108/112 (96%) | 98 (91%)  | 9 (8%)   | 1 (1%)   | 14          | 35  |
| 39  | BT    | 129/146 (88%) | 122 (95%) | 5 (4%)   | 2 (2%)   | 7           | 20  |
| 39  | DT    | 129/146 (88%) | 125 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 40  | BU    | 114/118 (97%) | 113 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 40  | DU    | 114/118 (97%) | 112 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 41  | BV    | 99/101 (98%)  | 92 (93%)  | 5 (5%)   | 2 (2%)   | 6           | 16  |
| 41  | DV    | 99/101 (98%)  | 94 (95%)  | 4 (4%)   | 1 (1%)   | 12          | 32  |
| 42  | BW    | 110/113 (97%) | 109 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 42  | DW    | 110/113 (97%) | 109 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 43  | BX    | 93/96 (97%)   | 88 (95%)  | 4 (4%)   | 1 (1%)   | 11          | 29  |
| 43  | DX    | 93/96 (97%)   | 88 (95%)  | 3 (3%)   | 2 (2%)   | 5           | 14  |
| 44  | BY    | 105/110 (96%) | 97 (92%)  | 6 (6%)   | 2 (2%)   | 6           | 17  |
| 44  | DY    | 105/110 (96%) | 99 (94%)  | 5 (5%)   | 1 (1%)   | 12          | 32  |
| 45  | BZ    | 169/206 (82%) | 147 (87%) | 18 (11%) | 4 (2%)   | 4           | 12  |
| 45  | DZ    | 172/206 (84%) | 154 (90%) | 17 (10%) | 1 (1%)   | 21          | 44  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 46  | B0    | 81/85 (95%)       | 76 (94%)    | 4 (5%)   | 1 (1%)   | 10          | 27  |
| 46  | D0    | 81/85 (95%)       | 76 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 47  | B1    | 95/98 (97%)       | 92 (97%)    | 2 (2%)   | 1 (1%)   | 11          | 29  |
| 47  | D1    | 95/98 (97%)       | 92 (97%)    | 2 (2%)   | 1 (1%)   | 11          | 29  |
| 48  | B2    | 68/72 (94%)       | 68 (100%)   | 0        | 0        | 100         | 100 |
| 48  | D2    | 68/72 (94%)       | 68 (100%)   | 0        | 0        | 100         | 100 |
| 49  | B3    | 57/60 (95%)       | 55 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 49  | D3    | 57/60 (95%)       | 54 (95%)    | 3 (5%)   | 0        | 100         | 100 |
| 50  | B4    | 67/71 (94%)       | 50 (75%)    | 10 (15%) | 7 (10%)  | 0           | 0   |
| 50  | D4    | 67/71 (94%)       | 53 (79%)    | 7 (10%)  | 7 (10%)  | 0           | 0   |
| 51  | B5    | 57/60 (95%)       | 56 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 51  | D5    | 57/60 (95%)       | 56 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 52  | B6    | 51/54 (94%)       | 49 (96%)    | 1 (2%)   | 1 (2%)   | 6           | 16  |
| 52  | D6    | 51/54 (94%)       | 48 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| 53  | B7    | 46/49 (94%)       | 45 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 53  | D7    | 46/49 (94%)       | 45 (98%)    | 0        | 1 (2%)   | 5           | 14  |
| 54  | B8    | 62/65 (95%)       | 62 (100%)   | 0        | 0        | 100         | 100 |
| 54  | D8    | 62/65 (95%)       | 62 (100%)   | 0        | 0        | 100         | 100 |
| 55  | B9    | 35/37 (95%)       | 34 (97%)    | 1 (3%)   | 0        | 100         | 100 |
| 55  | D9    | 35/37 (95%)       | 33 (94%)    | 2 (6%)   | 0        | 100         | 100 |
| All | All   | 11402/12128 (94%) | 10561 (93%) | 687 (6%) | 154 (1%) | 9           | 23  |

5 of 154 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 9   | GLU  |
| 2   | AB    | 10  | LEU  |
| 2   | AB    | 125 | PRO  |
| 4   | AD    | 166 | LYS  |
| 7   | AG    | 80  | VAL  |

### 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%) | 152 (79%) | 40 (21%) | 1           | 3  |
| 2   | CB    | 187/220 (85%) | 154 (82%) | 33 (18%) | 2           | 5  |
| 3   | AC    | 143/188 (76%) | 128 (90%) | 15 (10%) | 6           | 17 |
| 3   | CC    | 140/188 (74%) | 121 (86%) | 19 (14%) | 3           | 9  |
| 4   | AD    | 170/181 (94%) | 150 (88%) | 20 (12%) | 5           | 13 |
| 4   | CD    | 173/181 (96%) | 156 (90%) | 17 (10%) | 7           | 19 |
| 5   | AE    | 113/123 (92%) | 103 (91%) | 10 (9%)  | 9           | 23 |
| 5   | CE    | 114/123 (93%) | 102 (90%) | 12 (10%) | 6           | 17 |
| 6   | AF    | 83/90 (92%)   | 78 (94%)  | 5 (6%)   | 17          | 41 |
| 6   | CF    | 85/90 (94%)   | 79 (93%)  | 6 (7%)   | 13          | 33 |
| 7   | AG    | 119/127 (94%) | 105 (88%) | 14 (12%) | 5           | 13 |
| 7   | CG    | 120/127 (94%) | 108 (90%) | 12 (10%) | 7           | 19 |
| 8   | AH    | 114/119 (96%) | 104 (91%) | 10 (9%)  | 9           | 23 |
| 8   | CH    | 114/119 (96%) | 104 (91%) | 10 (9%)  | 9           | 23 |
| 9   | AI    | 90/99 (91%)   | 78 (87%)  | 12 (13%) | 4           | 10 |
| 9   | CI    | 89/99 (90%)   | 79 (89%)  | 10 (11%) | 6           | 15 |
| 10  | AJ    | 66/92 (72%)   | 58 (88%)  | 8 (12%)  | 5           | 12 |
| 10  | CJ    | 69/92 (75%)   | 62 (90%)  | 7 (10%)  | 7           | 18 |
| 11  | AK    | 82/99 (83%)   | 75 (92%)  | 7 (8%)   | 10          | 25 |
| 11  | CK    | 83/99 (84%)   | 74 (89%)  | 9 (11%)  | 6           | 16 |
| 12  | AL    | 97/109 (89%)  | 89 (92%)  | 8 (8%)   | 10          | 27 |
| 12  | CL    | 97/109 (89%)  | 90 (93%)  | 7 (7%)   | 13          | 32 |
| 13  | AM    | 91/101 (90%)  | 78 (86%)  | 13 (14%) | 3           | 8  |
| 13  | CM    | 89/101 (88%)  | 76 (85%)  | 13 (15%) | 3           | 8  |
| 14  | AN    | 49/50 (98%)   | 42 (86%)  | 7 (14%)  | 3           | 8  |
| 14  | CN    | 49/50 (98%)   | 41 (84%)  | 8 (16%)  | 2           | 6  |
| 15  | AO    | 78/80 (98%)   | 69 (88%)  | 9 (12%)  | 5           | 14 |
| 15  | CO    | 78/80 (98%)   | 72 (92%)  | 6 (8%)   | 12          | 30 |
| 16  | AP    | 69/74 (93%)   | 58 (84%)  | 11 (16%) | 2           | 7  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 16  | CP    | 68/74 (92%)    | 58 (85%)  | 10 (15%) | 3           | 8   |
| 17  | AQ    | 94/97 (97%)    | 88 (94%)  | 6 (6%)   | 16          | 38  |
| 17  | CQ    | 94/97 (97%)    | 89 (95%)  | 5 (5%)   | 20          | 46  |
| 18  | AR    | 59/77 (77%)    | 53 (90%)  | 6 (10%)  | 7           | 18  |
| 18  | CR    | 59/77 (77%)    | 53 (90%)  | 6 (10%)  | 7           | 18  |
| 19  | AS    | 69/80 (86%)    | 64 (93%)  | 5 (7%)   | 13          | 32  |
| 19  | CS    | 67/80 (84%)    | 59 (88%)  | 8 (12%)  | 5           | 13  |
| 20  | AT    | 70/82 (85%)    | 63 (90%)  | 7 (10%)  | 7           | 19  |
| 20  | CT    | 70/82 (85%)    | 61 (87%)  | 9 (13%)  | 4           | 10  |
| 21  | AU    | 18/22 (82%)    | 16 (89%)  | 2 (11%)  | 6           | 15  |
| 21  | CU    | 18/22 (82%)    | 18 (100%) | 0        | 100         | 100 |
| 27  | BD    | 215/218 (99%)  | 195 (91%) | 20 (9%)  | 8           | 21  |
| 27  | DD    | 215/218 (99%)  | 197 (92%) | 18 (8%)  | 10          | 26  |
| 28  | BE    | 164/166 (99%)  | 140 (85%) | 24 (15%) | 3           | 8   |
| 28  | DE    | 164/166 (99%)  | 137 (84%) | 27 (16%) | 2           | 6   |
| 29  | BF    | 160/166 (96%)  | 139 (87%) | 21 (13%) | 4           | 10  |
| 29  | DF    | 159/166 (96%)  | 139 (87%) | 20 (13%) | 4           | 11  |
| 30  | BG    | 143/156 (92%)  | 126 (88%) | 17 (12%) | 5           | 13  |
| 30  | DG    | 142/156 (91%)  | 124 (87%) | 18 (13%) | 4           | 11  |
| 31  | BH    | 144/148 (97%)  | 130 (90%) | 14 (10%) | 8           | 20  |
| 31  | DH    | 144/148 (97%)  | 131 (91%) | 13 (9%)  | 9           | 23  |
| 32  | BI    | 110/124 (89%)  | 86 (78%)  | 24 (22%) | 1           | 3   |
| 32  | DI    | 104/124 (84%)  | 87 (84%)  | 17 (16%) | 2           | 6   |
| 33  | BN    | 118/119 (99%)  | 102 (86%) | 16 (14%) | 3           | 9   |
| 33  | DN    | 118/119 (99%)  | 105 (89%) | 13 (11%) | 6           | 15  |
| 34  | BO    | 100/100 (100%) | 93 (93%)  | 7 (7%)   | 14          | 34  |
| 34  | DO    | 100/100 (100%) | 91 (91%)  | 9 (9%)   | 9           | 23  |
| 35  | BP    | 115/116 (99%)  | 101 (88%) | 14 (12%) | 5           | 12  |
| 35  | DP    | 115/116 (99%)  | 102 (89%) | 13 (11%) | 5           | 14  |
| 36  | BQ    | 111/111 (100%) | 100 (90%) | 11 (10%) | 7           | 19  |
| 36  | DQ    | 111/111 (100%) | 101 (91%) | 10 (9%)  | 9           | 23  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 37  | BR    | 101/101 (100%) | 83 (82%)  | 18 (18%) | 2           | 5  |
| 37  | DR    | 101/101 (100%) | 84 (83%)  | 17 (17%) | 2           | 6  |
| 38  | BS    | 87/88 (99%)    | 79 (91%)  | 8 (9%)   | 8           | 22 |
| 38  | DS    | 85/88 (97%)    | 74 (87%)  | 11 (13%) | 4           | 10 |
| 39  | BT    | 115/127 (91%)  | 103 (90%) | 12 (10%) | 7           | 17 |
| 39  | DT    | 113/127 (89%)  | 102 (90%) | 11 (10%) | 8           | 20 |
| 40  | BU    | 93/94 (99%)    | 84 (90%)  | 9 (10%)  | 8           | 20 |
| 40  | DU    | 93/94 (99%)    | 87 (94%)  | 6 (6%)   | 15          | 37 |
| 41  | BV    | 80/82 (98%)    | 65 (81%)  | 15 (19%) | 1           | 4  |
| 41  | DV    | 80/82 (98%)    | 64 (80%)  | 16 (20%) | 1           | 4  |
| 42  | BW    | 90/92 (98%)    | 84 (93%)  | 6 (7%)   | 15          | 36 |
| 42  | DW    | 90/92 (98%)    | 83 (92%)  | 7 (8%)   | 11          | 29 |
| 43  | BX    | 77/78 (99%)    | 72 (94%)  | 5 (6%)   | 15          | 37 |
| 43  | DX    | 77/78 (99%)    | 72 (94%)  | 5 (6%)   | 15          | 37 |
| 44  | BY    | 85/91 (93%)    | 77 (91%)  | 8 (9%)   | 8           | 21 |
| 44  | DY    | 85/91 (93%)    | 79 (93%)  | 6 (7%)   | 13          | 33 |
| 45  | BZ    | 145/179 (81%)  | 129 (89%) | 16 (11%) | 6           | 15 |
| 45  | DZ    | 145/179 (81%)  | 129 (89%) | 16 (11%) | 6           | 15 |
| 46  | B0    | 65/67 (97%)    | 61 (94%)  | 4 (6%)   | 16          | 39 |
| 46  | D0    | 65/67 (97%)    | 60 (92%)  | 5 (8%)   | 12          | 30 |
| 47  | B1    | 80/83 (96%)    | 72 (90%)  | 8 (10%)  | 7           | 19 |
| 47  | D1    | 80/83 (96%)    | 73 (91%)  | 7 (9%)   | 9           | 23 |
| 48  | B2    | 65/67 (97%)    | 60 (92%)  | 5 (8%)   | 12          | 30 |
| 48  | D2    | 65/67 (97%)    | 58 (89%)  | 7 (11%)  | 6           | 16 |
| 49  | B3    | 51/52 (98%)    | 43 (84%)  | 8 (16%)  | 2           | 7  |
| 49  | D3    | 50/52 (96%)    | 43 (86%)  | 7 (14%)  | 3           | 9  |
| 50  | B4    | 60/63 (95%)    | 50 (83%)  | 10 (17%) | 2           | 6  |
| 50  | D4    | 53/63 (84%)    | 45 (85%)  | 8 (15%)  | 3           | 7  |
| 51  | B5    | 50/52 (96%)    | 41 (82%)  | 9 (18%)  | 2           | 5  |
| 51  | D5    | 50/52 (96%)    | 45 (90%)  | 5 (10%)  | 7           | 19 |
| 52  | B6    | 51/52 (98%)    | 45 (88%)  | 6 (12%)  | 5           | 13 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|------------------|------------|------------|-------------|-----|
| 52  | D6    | 50/52 (96%)      | 46 (92%)   | 4 (8%)     | 11          | 28  |
| 53  | B7    | 41/42 (98%)      | 39 (95%)   | 2 (5%)     | 22          | 49  |
| 53  | D7    | 41/42 (98%)      | 41 (100%)  | 0          | 100         | 100 |
| 54  | B8    | 53/55 (96%)      | 48 (91%)   | 5 (9%)     | 8           | 21  |
| 54  | D8    | 54/55 (98%)      | 48 (89%)   | 6 (11%)    | 6           | 15  |
| 55  | B9    | 34/34 (100%)     | 33 (97%)   | 1 (3%)     | 37          | 67  |
| 55  | D9    | 34/34 (100%)     | 30 (88%)   | 4 (12%)    | 5           | 13  |
| All | All   | 9315/10066 (92%) | 8264 (89%) | 1051 (11%) | 5           | 14  |

5 of 1051 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | DS    | 69  | VAL  |
| 41  | DV    | 28  | GLU  |
| 38  | DS    | 68  | GLN  |
| 52  | D6    | 48  | VAL  |
| 37  | BR    | 29  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CF    | 73  | ASN  |
| 27  | DD    | 87  | ASN  |
| 7   | CG    | 64  | GLN  |
| 12  | CL    | 78  | GLN  |
| 29  | DF    | 40  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1494/1521 (98%) | 367 (24%)         | 26 (1%)         |
| 1   | CA    | 1501/1521 (98%) | 374 (24%)         | 32 (2%)         |
| 22  | AV    | 7/24 (29%)      | 0                 | 0               |
| 22  | CV    | 4/24 (16%)      | 1 (25%)           | 0               |
| 23  | AX    | 75/77 (97%)     | 25 (33%)          | 0               |
| 23  | CX    | 75/77 (97%)     | 23 (30%)          | 0               |
| 24  | AY    | 16/76 (21%)     | 7 (43%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 24  | CY    | 4/76 (5%)       | 0                 | 0               |
| 25  | BA    | 2814/2915 (96%) | 477 (16%)         | 31 (1%)         |
| 25  | DA    | 2791/2915 (95%) | 524 (18%)         | 27 (0%)         |
| 26  | BB    | 119/121 (98%)   | 24 (20%)          | 0               |
| 26  | DB    | 119/121 (98%)   | 25 (21%)          | 0               |
| All | All   | 9019/9468 (95%) | 1847 (20%)        | 116 (1%)        |

5 of 1847 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    | 32  | A    |

5 of 116 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 60   | A    |
| 25  | DA    | 2126 | A    |
| 1   | CA    | 992  | U    |
| 25  | DA    | 2110 | G    |
| 25  | DA    | 856  | C    |

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

8 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 |
| 23  | PSU  | AX    | 55  | 23   | 18,21,22     | 1.36 | 2 (11%)  | 21,30,33    | 2.05 | 4 (19%)  |
| 23  | 5MU  | CX    | 54  | 23   | 19,22,23     | 1.42 | 4 (21%)  | 27,32,35    | 2.00 | 6 (22%)  |
| 23  | 4SU  | AX    | 8   | 23   | 18,21,22     | 2.29 | 5 (27%)  | 25,30,33    | 1.69 | 4 (16%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | 4SU  | CX    | 8   | 23   | 18,21,22     | 1.99 | 5 (27%)  | 25,30,33    | 1.36 | 4 (16%)  |
| 23  | 5MC  | AX    | 32  | 23   | 19,22,23     | 1.79 | 3 (15%)  | 26,32,35    | 1.38 | 4 (15%)  |
| 23  | 5MC  | CX    | 32  | 23   | 19,22,23     | 1.54 | 3 (15%)  | 26,32,35    | 1.22 | 4 (15%)  |
| 23  | PSU  | CX    | 55  | 23   | 18,21,22     | 1.39 | 2 (11%)  | 21,30,33    | 1.94 | 5 (23%)  |
| 23  | 5MU  | AX    | 54  | 23   | 19,22,23     | 1.51 | 4 (21%)  | 27,32,35    | 1.63 | 5 (18%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 23  | PSU  | AX    | 55  | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | 5MU  | CX    | 54  | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | 4SU  | AX    | 8   | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | 4SU  | CX    | 8   | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | 5MC  | AX    | 32  | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | 5MC  | CX    | 32  | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | PSU  | CX    | 55  | 23   | -       | 0/7/25/26 | 0/2/2/2 |
| 23  | 5MU  | AX    | 54  | 23   | -       | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 28 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23  | AX    | 32  | 5MC  | C5-C4 | 6.40  | 1.49        | 1.44     |
| 23  | AX    | 8   | 4SU  | C4-N3 | -5.59 | 1.31        | 1.37     |
| 23  | CX    | 32  | 5MC  | C5-C4 | 5.41  | 1.48        | 1.44     |
| 23  | AX    | 8   | 4SU  | C4-S4 | -4.96 | 1.59        | 1.68     |
| 23  | CX    | 8   | 4SU  | C4-N3 | -4.63 | 1.32        | 1.37     |

The worst 5 of 36 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 23  | AX    | 55  | PSU  | N1-C2-N3 | 6.18  | 121.68      | 115.17   |
| 23  | CX    | 55  | PSU  | N1-C2-N3 | 6.13  | 121.63      | 115.17   |
| 23  | CX    | 54  | 5MU  | N3-C2-N1 | 5.12  | 121.56      | 114.89   |
| 23  | AX    | 8   | 4SU  | C6-C5-C4 | -5.10 | 115.54      | 119.95   |
| 23  | CX    | 54  | 5MU  | C4-N3-C2 | -4.63 | 121.27      | 127.34   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | AX    | 8   | 4SU  | 1       | 0            |
| 23  | CX    | 8   | 4SU  | 1       | 0            |
| 23  | CX    | 55  | PSU  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2061 ligands modelled in this entry, 2057 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 57  | PCY  | AA    | 3191 | -    | 34,42,42     | 1.94 | 5 (14%)     | 41,65,65    | 1.51 | 8 (19%)     |
| 58  | SF4  | CD    | 501  | 4    | 0,12,12      | -    | -           | -           | -    | -           |
| 57  | PCY  | CA    | 3176 | -    | 34,42,42     | 1.77 | 5 (14%)     | 41,65,65    | 0.95 | 3 (7%)      |
| 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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 57  | PCY  | AA    | 3191 | -    | -       | 18/33/67/67 | 0/3/3/3 |
| 58  | SF4  | CD    | 501  | 4    | -       | -           | 0/6/5/5 |
| 57  | PCY  | CA    | 3176 | -    | -       | 6/33/67/67  | 0/3/3/3 |
| 58  | SF4  | AD    | 501  | 4    | -       | -           | 0/6/5/5 |

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

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 57  | AA    | 3191 | PCY  | C34-C30 | -6.06 | 1.39        | 1.51     |
| 57  | CA    | 3176 | PCY  | C34-C30 | -5.75 | 1.40        | 1.51     |
| 57  | AA    | 3191 | PCY  | C28-C32 | -5.38 | 1.39        | 1.49     |
| 57  | AA    | 3191 | PCY  | C17-N20 | 4.78  | 1.51        | 1.45     |
| 57  | CA    | 3176 | PCY  | C28-C32 | -4.73 | 1.40        | 1.49     |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57  | AA    | 3191 | PCY  | O21-C18-C15 | 4.06  | 115.29      | 107.79   |
| 57  | AA    | 3191 | PCY  | O21-C23-C27 | 4.04  | 121.35      | 112.35   |
| 57  | AA    | 3191 | PCY  | C18-O21-C23 | -2.84 | 110.93      | 116.55   |
| 57  | AA    | 3191 | PCY  | C30-C27-C23 | 2.45  | 127.43      | 120.47   |
| 57  | CA    | 3176 | PCY  | C18-O21-C23 | -2.35 | 111.90      | 116.55   |

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 57  | AA    | 3191 | PCY  | N2-C3-C6-C11 |
| 57  | AA    | 3191 | PCY  | N2-C3-C6-O12 |
| 57  | AA    | 3191 | PCY  | C7-C3-C6-C11 |
| 57  | AA    | 3191 | PCY  | C7-C3-C6-O12 |
| 57  | AA    | 3191 | PCY  | C8-C3-C6-C11 |

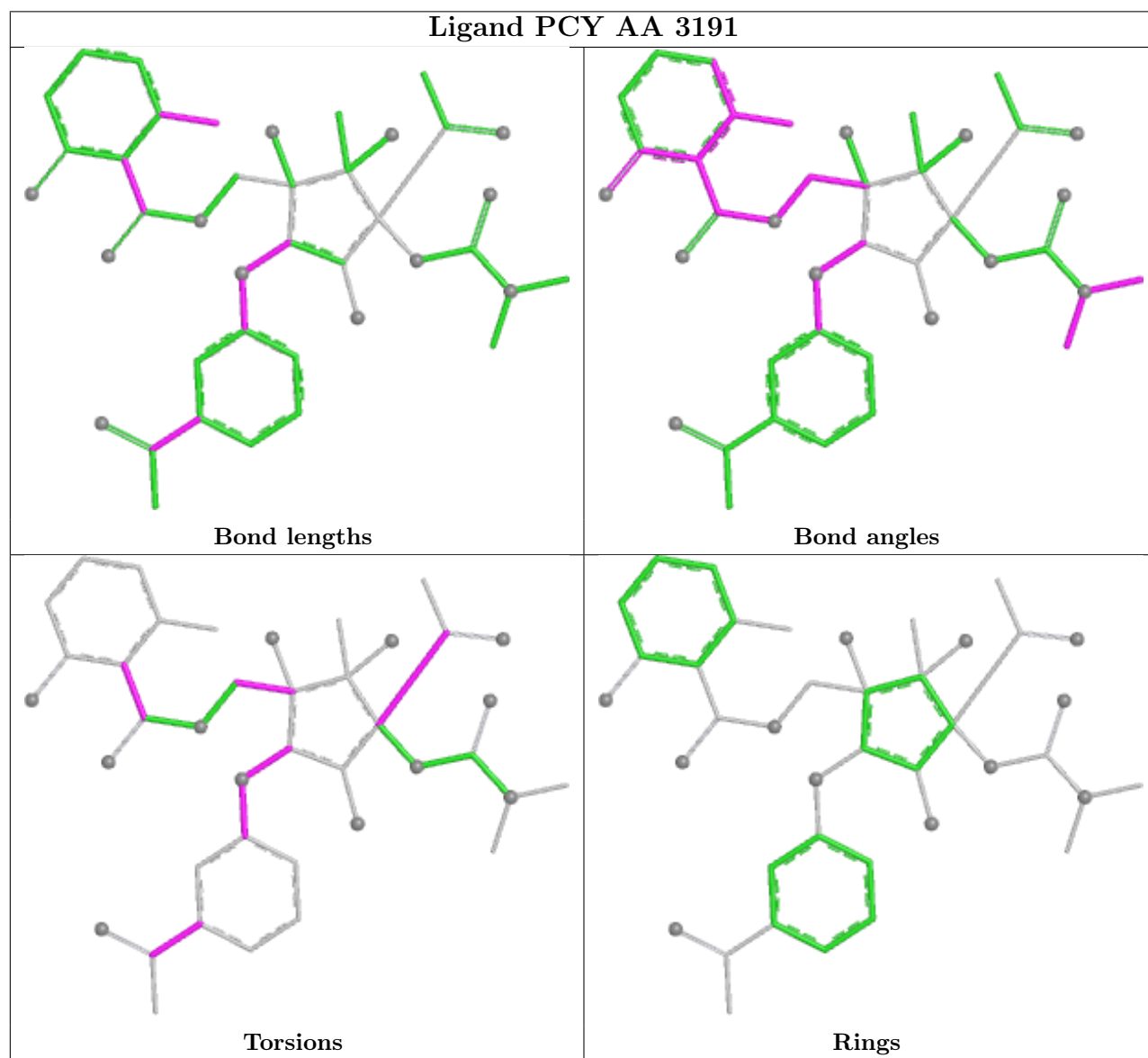
There are no ring outliers.

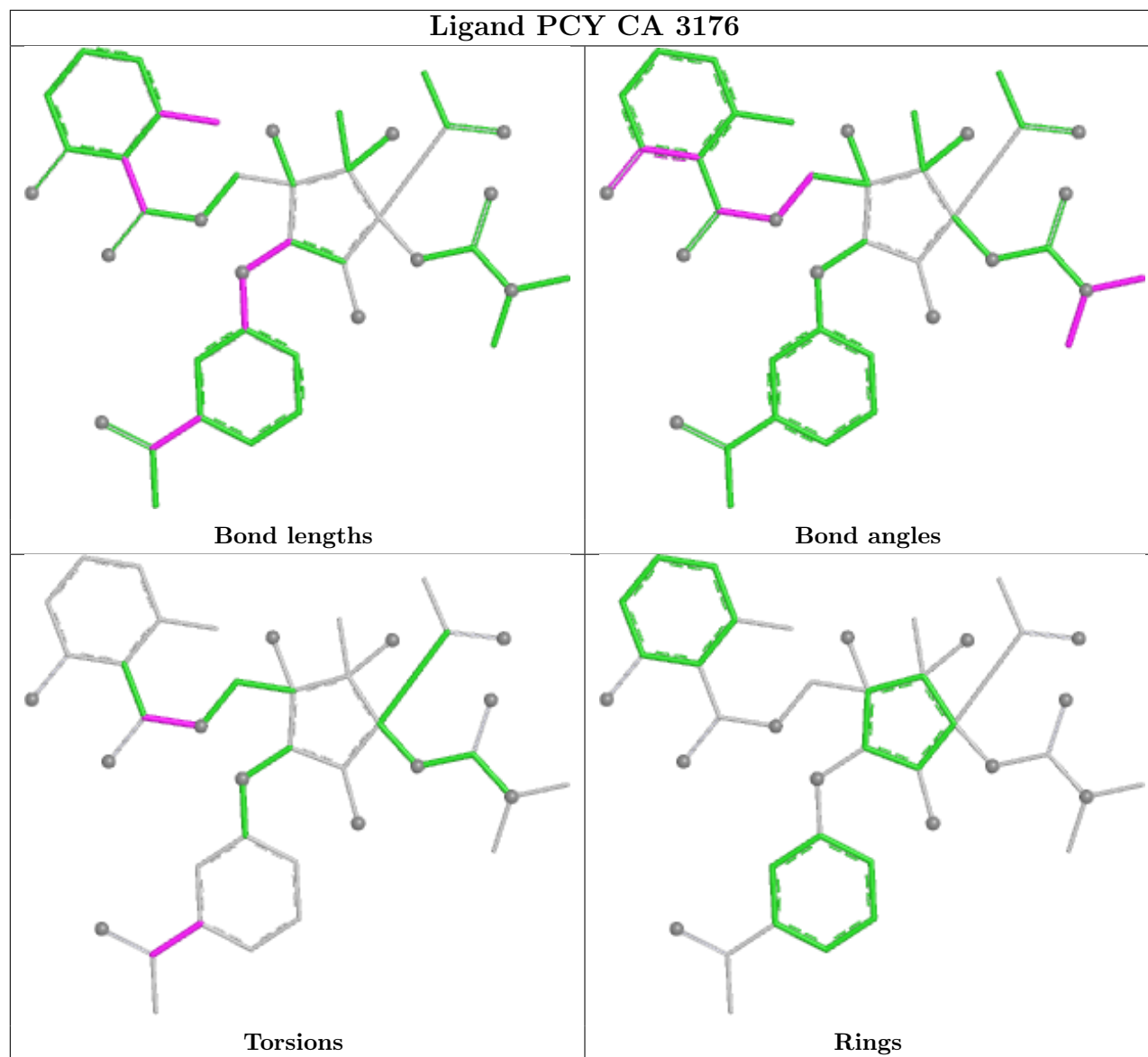
3 monomers are involved in 11 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57  | AA    | 3191 | PCY  | 6       | 0            |
| 57  | CA    | 3176 | PCY  | 4       | 0            |
| 58  | AD    | 501  | SF4  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |    |    | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|----|----|-----------------------|---------|
| 1   | AA    | 1497/1521 (98%) | 0.50   | 52 (3%)   | 47 | 43 | 40, 76, 97, 113       | 0       |
| 1   | CA    | 1503/1521 (98%) | 0.57   | 106 (7%)  | 22 | 19 | 42, 77, 97, 113       | 0       |
| 2   | AB    | 231/256 (90%)   | 1.24   | 39 (16%)  | 4  | 3  | 71, 85, 93, 98        | 0       |
| 2   | CB    | 231/256 (90%)   | 1.71   | 77 (33%)  | 1  | 1  | 71, 86, 94, 98        | 0       |
| 3   | AC    | 206/239 (86%)   | 1.06   | 23 (11%)  | 10 | 8  | 69, 83, 91, 95        | 0       |
| 3   | CC    | 206/239 (86%)   | 1.55   | 50 (24%)  | 2  | 1  | 69, 84, 92, 96        | 0       |
| 4   | AD    | 208/209 (99%)   | 1.30   | 37 (17%)  | 4  | 3  | 60, 76, 86, 91        | 0       |
| 4   | CD    | 208/209 (99%)   | 0.77   | 6 (2%)    | 53 | 50 | 60, 76, 84, 89        | 0       |
| 5   | AE    | 148/162 (91%)   | 0.86   | 12 (8%)   | 18 | 15 | 56, 72, 81, 88        | 0       |
| 5   | CE    | 148/162 (91%)   | 1.04   | 14 (9%)   | 14 | 11 | 58, 74, 83, 89        | 0       |
| 6   | AF    | 100/101 (99%)   | 0.71   | 1 (1%)    | 79 | 78 | 61, 74, 82, 85        | 0       |
| 6   | CF    | 100/101 (99%)   | 1.05   | 12 (12%)  | 9  | 7  | 62, 75, 83, 86        | 0       |
| 7   | AG    | 155/156 (99%)   | 1.00   | 21 (13%)  | 7  | 6  | 69, 79, 89, 98        | 0       |
| 7   | CG    | 155/156 (99%)   | 1.42   | 31 (20%)  | 3  | 2  | 70, 80, 90, 99        | 0       |
| 8   | AH    | 137/138 (99%)   | 0.81   | 7 (5%)    | 33 | 29 | 61, 74, 81, 85        | 0       |
| 8   | CH    | 137/138 (99%)   | 1.19   | 19 (13%)  | 6  | 5  | 63, 75, 83, 88        | 0       |
| 9   | AI    | 127/128 (99%)   | 1.21   | 17 (13%)  | 7  | 6  | 63, 85, 91, 94        | 0       |
| 9   | CI    | 127/128 (99%)   | 2.05   | 63 (49%)  | 0  | 0  | 70, 86, 92, 96        | 0       |
| 10  | AJ    | 97/105 (92%)    | 1.57   | 28 (28%)  | 1  | 1  | 73, 87, 94, 97        | 0       |
| 10  | CJ    | 96/105 (91%)    | 2.02   | 43 (44%)  | 0  | 0  | 76, 89, 95, 96        | 0       |
| 11  | AK    | 114/129 (88%)   | 0.79   | 6 (5%)    | 32 | 28 | 52, 72, 84, 87        | 0       |
| 11  | CK    | 114/129 (88%)   | 0.85   | 9 (7%)    | 18 | 16 | 54, 74, 84, 87        | 0       |
| 12  | AL    | 122/132 (92%)   | 0.78   | 5 (4%)    | 41 | 37 | 52, 67, 77, 81        | 0       |
| 12  | CL    | 122/132 (92%)   | 0.92   | 12 (9%)   | 13 | 11 | 53, 67, 76, 81        | 0       |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | AM    | 120/126 (95%)   | 1.03   | 8 (6%) 24 21  | 53, 75, 85, 93        | 0     |
| 13  | CM    | 118/126 (93%)   | 1.74   | 42 (35%) 1 1  | 71, 88, 94, 98        | 0     |
| 14  | AN    | 60/61 (98%)     | 1.26   | 10 (16%) 4 3  | 74, 80, 88, 90        | 0     |
| 14  | CN    | 60/61 (98%)     | 2.63   | 44 (73%) 0 0  | 75, 83, 88, 92        | 0     |
| 15  | AO    | 88/89 (98%)     | 0.99   | 8 (9%) 15 12  | 55, 69, 81, 85        | 0     |
| 15  | CO    | 88/89 (98%)     | 0.82   | 6 (6%) 23 20  | 58, 71, 82, 86        | 0     |
| 16  | AP    | 82/88 (93%)     | 1.54   | 19 (23%) 2 2  | 64, 75, 84, 91        | 0     |
| 16  | CP    | 82/88 (93%)     | 1.39   | 17 (20%) 2 2  | 63, 73, 83, 89        | 0     |
| 17  | AQ    | 99/105 (94%)    | 0.86   | 7 (7%) 22 19  | 55, 70, 79, 81        | 0     |
| 17  | CQ    | 99/105 (94%)    | 1.07   | 6 (6%) 27 24  | 58, 71, 80, 84        | 0     |
| 18  | AR    | 68/88 (77%)     | 0.74   | 2 (2%) 53 50  | 62, 74, 84, 89        | 0     |
| 18  | CR    | 68/88 (77%)     | 0.83   | 3 (4%) 39 35  | 64, 74, 84, 91        | 0     |
| 19  | AS    | 83/93 (89%)     | 1.65   | 22 (26%) 1 1  | 75, 85, 93, 94        | 0     |
| 19  | CS    | 83/93 (89%)     | 1.95   | 33 (39%) 1 0  | 78, 87, 93, 96        | 0     |
| 20  | AT    | 96/106 (90%)    | 1.01   | 12 (12%) 8 7  | 63, 72, 82, 87        | 0     |
| 20  | CT    | 96/106 (90%)    | 1.06   | 7 (7%) 21 18  | 61, 73, 82, 87        | 0     |
| 21  | AU    | 23/27 (85%)     | 1.79   | 10 (43%) 0 0  | 71, 77, 79, 81        | 0     |
| 21  | CU    | 23/27 (85%)     | 1.88   | 8 (34%) 1 1   | 72, 79, 81, 83        | 0     |
| 22  | AV    | 8/24 (33%)      | 1.70   | 4 (50%) 0 0   | 62, 89, 94, 97        | 0     |
| 22  | CV    | 5/24 (20%)      | 1.40   | 1 (20%) 3 2   | 65, 73, 91, 96        | 0     |
| 23  | AX    | 72/77 (93%)     | 0.54   | 3 (4%) 40 37  | 40, 71, 88, 98        | 0     |
| 23  | CX    | 72/77 (93%)     | 0.39   | 1 (1%) 73 72  | 43, 74, 90, 97        | 0     |
| 24  | AY    | 18/76 (23%)     | 1.35   | 3 (16%) 4 3   | 62, 104, 109, 109     | 0     |
| 24  | CY    | 5/76 (6%)       | 2.61   | 4 (80%) 0 0   | 74, 101, 102, 106     | 0     |
| 25  | BA    | 2822/2915 (96%) | -0.29  | 97 (3%) 48 44 | 18, 41, 91, 109       | 0     |
| 25  | DA    | 2800/2915 (96%) | -0.29  | 79 (2%) 55 51 | 22, 45, 91, 112       | 0     |
| 26  | BB    | 120/121 (99%)   | 0.17   | 0 100 100     | 31, 63, 75, 88        | 0     |
| 26  | DB    | 120/121 (99%)   | 1.07   | 19 (15%) 5 4  | 38, 69, 81, 91        | 0     |
| 27  | BD    | 275/276 (99%)   | 0.02   | 2 (0%) 84 83  | 20, 39, 58, 77        | 0     |
| 27  | DD    | 275/276 (99%)   | -0.07  | 2 (0%) 84 83  | 22, 42, 60, 78        | 0     |
| 28  | BE    | 204/206 (99%)   | 0.11   | 1 (0%) 87 86  | 19, 44, 64, 86        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | DE    | 204/206 (99%)  | 0.13   | 1 (0%) 87 86  | 22, 48, 66, 86        | 0     |
| 29  | BF    | 203/210 (96%)  | 0.19   | 1 (0%) 87 86  | 21, 50, 74, 91        | 0     |
| 29  | DF    | 203/210 (96%)  | 0.16   | 3 (1%) 72 70  | 24, 55, 77, 90        | 0     |
| 30  | BG    | 181/182 (99%)  | 0.94   | 17 (9%) 14 12 | 55, 71, 83, 96        | 0     |
| 30  | DG    | 181/182 (99%)  | 1.32   | 37 (20%) 3 2  | 60, 75, 84, 95        | 0     |
| 31  | BH    | 174/180 (96%)  | 0.82   | 10 (5%) 29 26 | 45, 64, 75, 84        | 0     |
| 31  | DH    | 174/180 (96%)  | 1.14   | 20 (11%) 9 8  | 53, 68, 79, 86        | 0     |
| 32  | BI    | 146/148 (98%)  | 0.65   | 6 (4%) 41 37  | 48, 75, 84, 88        | 0     |
| 32  | DI    | 146/148 (98%)  | 0.87   | 8 (5%) 30 27  | 51, 75, 84, 88        | 0     |
| 33  | BN    | 140/140 (100%) | 0.44   | 4 (2%) 53 50  | 28, 45, 69, 79        | 0     |
| 33  | DN    | 140/140 (100%) | 0.37   | 0 100 100     | 33, 49, 71, 81        | 0     |
| 34  | BO    | 122/122 (100%) | 0.06   | 3 (2%) 58 55  | 31, 45, 63, 70        | 0     |
| 34  | DO    | 122/122 (100%) | 0.00   | 0 100 100     | 34, 48, 64, 70        | 0     |
| 35  | BP    | 149/150 (99%)  | 0.36   | 3 (2%) 65 62  | 18, 53, 74, 82        | 0     |
| 35  | DP    | 149/150 (99%)  | 0.32   | 2 (1%) 75 73  | 20, 56, 76, 84        | 0     |
| 36  | BQ    | 141/141 (100%) | 0.26   | 3 (2%) 63 61  | 29, 48, 65, 77        | 0     |
| 36  | DQ    | 141/141 (100%) | 0.41   | 5 (3%) 47 43  | 32, 52, 69, 78        | 0     |
| 37  | BR    | 118/118 (100%) | -0.34  | 0 100 100     | 19, 32, 49, 62        | 0     |
| 37  | DR    | 118/118 (100%) | 0.20   | 1 (0%) 82 81  | 35, 53, 66, 78        | 0     |
| 38  | BS    | 110/112 (98%)  | 0.01   | 0 100 100     | 30, 47, 65, 70        | 0     |
| 38  | DS    | 110/112 (98%)  | 1.50   | 31 (28%) 1 1  | 63, 77, 88, 93        | 0     |
| 39  | BT    | 131/146 (89%)  | 0.03   | 6 (4%) 37 34  | 30, 43, 71, 85        | 0     |
| 39  | DT    | 131/146 (89%)  | 0.44   | 2 (1%) 72 70  | 43, 59, 78, 88        | 0     |
| 40  | BU    | 116/118 (98%)  | -0.45  | 1 (0%) 81 80  | 15, 27, 48, 62        | 0     |
| 40  | DU    | 116/118 (98%)  | 0.38   | 1 (0%) 81 80  | 38, 59, 76, 87        | 0     |
| 41  | BV    | 101/101 (100%) | -0.46  | 1 (0%) 79 78  | 14, 35, 57, 76        | 0     |
| 41  | DV    | 101/101 (100%) | 0.48   | 1 (0%) 79 78  | 43, 71, 84, 90        | 0     |
| 42  | BW    | 112/113 (99%)  | -0.49  | 1 (0%) 81 80  | 17, 28, 50, 75        | 0     |
| 42  | DW    | 112/113 (99%)  | 0.04   | 0 100 100     | 34, 50, 68, 92        | 0     |
| 43  | BX    | 95/96 (98%)    | -0.20  | 1 (1%) 78 76  | 17, 35, 65, 78        | 0     |
| 43  | DX    | 95/96 (98%)    | 0.88   | 9 (9%) 14 11  | 44, 62, 77, 90        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | BY    | 107/110 (97%)     | 0.18   | 1 (0%) 81 80    | 28, 47, 67, 85        | 0     |
| 44  | DY    | 107/110 (97%)     | 1.16   | 18 (16%) 4 3    | 51, 72, 83, 88        | 0     |
| 45  | BZ    | 171/206 (83%)     | 0.50   | 6 (3%) 47 43    | 36, 62, 81, 90        | 0     |
| 45  | DZ    | 174/206 (84%)     | 1.28   | 23 (13%) 7 6    | 66, 83, 93, 96        | 0     |
| 46  | B0    | 83/85 (97%)       | 0.02   | 8 (9%) 13 11    | 12, 33, 66, 84        | 0     |
| 46  | D0    | 83/85 (97%)       | 0.87   | 9 (10%) 11 9    | 34, 64, 78, 91        | 0     |
| 47  | B1    | 97/98 (98%)       | 0.01   | 1 (1%) 79 78    | 19, 43, 69, 72        | 0     |
| 47  | D1    | 97/98 (98%)       | 0.45   | 2 (2%) 63 61    | 37, 57, 78, 82        | 0     |
| 48  | B2    | 70/72 (97%)       | 0.08   | 3 (4%) 40 36    | 30, 46, 63, 77        | 0     |
| 48  | D2    | 70/72 (97%)       | 0.83   | 3 (4%) 40 36    | 56, 71, 80, 85        | 0     |
| 49  | B3    | 59/60 (98%)       | -0.31  | 1 (1%) 69 67    | 20, 31, 56, 83        | 0     |
| 49  | D3    | 59/60 (98%)       | 0.58   | 5 (8%) 16 14    | 47, 62, 77, 91        | 0     |
| 50  | B4    | 69/71 (97%)       | 1.02   | 13 (18%) 3 3    | 55, 77, 92, 99        | 0     |
| 50  | D4    | 69/71 (97%)       | 1.41   | 16 (23%) 2 2    | 77, 91, 99, 105       | 0     |
| 51  | B5    | 59/60 (98%)       | -0.47  | 0 100 100       | 11, 28, 53, 67        | 0     |
| 51  | D5    | 59/60 (98%)       | -0.02  | 1 (1%) 69 67    | 27, 52, 68, 81        | 0     |
| 52  | B6    | 53/54 (98%)       | -0.17  | 0 100 100       | 27, 39, 56, 66        | 0     |
| 52  | D6    | 53/54 (98%)       | 0.66   | 4 (7%) 20 17    | 45, 62, 73, 79        | 0     |
| 53  | B7    | 48/49 (97%)       | -0.09  | 3 (6%) 26 23    | 16, 23, 52, 68        | 0     |
| 53  | D7    | 48/49 (97%)       | -0.13  | 0 100 100       | 29, 40, 64, 77        | 0     |
| 54  | B8    | 64/65 (98%)       | -0.27  | 0 100 100       | 24, 31, 43, 61        | 0     |
| 54  | D8    | 64/65 (98%)       | 0.41   | 0 100 100       | 44, 53, 63, 72        | 0     |
| 55  | B9    | 37/37 (100%)      | 0.27   | 1 (2%) 56 53    | 28, 45, 67, 72        | 0     |
| 55  | D9    | 37/37 (100%)      | 0.72   | 2 (5%) 31 27    | 44, 55, 68, 75        | 0     |
| All | All   | 20640/21596 (95%) | 0.41   | 1468 (7%) 22 19 | 11, 64, 91, 113       | 0     |

The worst 5 of 1468 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | CT    | 9    | ASN  | 7.6  |
| 25  | BA    | 2143 | G    | 7.5  |
| 14  | CN    | 2    | ALA  | 6.6  |
| 2   | CB    | 165  | VAL  | 6.3  |
| 25  | BA    | 2135 | U    | 6.1  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 23  | 4SU  | CX    | 8   | 20/21 | 0.81 | 0.11 | 73,81,98,100               | 0     |
| 23  | PSU  | CX    | 55  | 20/21 | 0.82 | 0.13 | 56,73,80,86                | 0     |
| 23  | 5MU  | CX    | 54  | 21/22 | 0.84 | 0.13 | 69,80,93,106               | 0     |
| 23  | PSU  | AX    | 55  | 20/21 | 0.91 | 0.11 | 56,70,78,80                | 0     |
| 23  | 5MC  | CX    | 32  | 21/22 | 0.91 | 0.12 | 66,75,83,86                | 0     |
| 23  | 5MU  | AX    | 54  | 21/22 | 0.92 | 0.11 | 60,72,80,91                | 0     |
| 23  | 4SU  | AX    | 8   | 20/21 | 0.94 | 0.10 | 47,67,77,84                | 0     |
| 23  | 5MC  | AX    | 32  | 21/22 | 0.95 | 0.13 | 38,59,69,83                | 0     |

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56  | MG   | AA    | 3147 | 1/1   | 0.56 | 0.18 | 72,72,72,72                | 0     |
| 56  | MG   | CJ    | 5001 | 1/1   | 0.58 | 0.14 | 94,94,94,94                | 0     |
| 56  | MG   | DB    | 3001 | 1/1   | 0.58 | 0.13 | 77,77,77,77                | 0     |
| 56  | MG   | AA    | 3177 | 1/1   | 0.62 | 0.23 | 80,80,80,80                | 0     |
| 56  | MG   | DA    | 3640 | 1/1   | 0.64 | 0.19 | 64,64,64,64                | 0     |
| 56  | MG   | DA    | 3533 | 1/1   | 0.64 | 0.14 | 52,52,52,52                | 0     |
| 56  | MG   | DA    | 3655 | 1/1   | 0.67 | 0.54 | 74,74,74,74                | 0     |
| 56  | MG   | DA    | 3612 | 1/1   | 0.67 | 0.21 | 58,58,58,58                | 0     |
| 56  | MG   | BA    | 3447 | 1/1   | 0.68 | 0.21 | 59,59,59,59                | 0     |
| 56  | MG   | CA    | 3124 | 1/1   | 0.68 | 0.20 | 75,75,75,75                | 0     |
| 56  | MG   | DA    | 3607 | 1/1   | 0.69 | 0.22 | 63,63,63,63                | 0     |
| 56  | MG   | BE    | 306  | 1/1   | 0.69 | 0.28 | 93,93,93,93                | 0     |
| 56  | MG   | DA    | 3634 | 1/1   | 0.69 | 0.19 | 61,61,61,61                | 0     |
| 56  | MG   | DA    | 3657 | 1/1   | 0.70 | 0.20 | 56,56,56,56                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3174 | 1/1   | 0.70 | 0.15 | 80,80,80,80                 | 0     |
| 56  | MG   | CA    | 3054 | 1/1   | 0.72 | 0.39 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3657 | 1/1   | 0.72 | 0.27 | 52,52,52,52                 | 0     |
| 56  | MG   | AA    | 3171 | 1/1   | 0.72 | 0.18 | 67,67,67,67                 | 0     |
| 56  | MG   | CA    | 3131 | 1/1   | 0.73 | 0.35 | 81,81,81,81                 | 0     |
| 56  | MG   | CX    | 3002 | 1/1   | 0.73 | 0.43 | 81,81,81,81                 | 0     |
| 56  | MG   | CA    | 3084 | 1/1   | 0.74 | 0.28 | 71,71,71,71                 | 0     |
| 56  | MG   | AA    | 3067 | 1/1   | 0.74 | 0.40 | 72,72,72,72                 | 0     |
| 57  | PCY  | CA    | 3176 | 40/40 | 0.74 | 0.22 | 72,89,98,102                | 0     |
| 56  | MG   | BA    | 3703 | 1/1   | 0.75 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3562 | 1/1   | 0.75 | 0.19 | 72,72,72,72                 | 0     |
| 56  | MG   | BA    | 3598 | 1/1   | 0.75 | 0.24 | 53,53,53,53                 | 0     |
| 56  | MG   | AA    | 3059 | 1/1   | 0.75 | 0.27 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3466 | 1/1   | 0.75 | 0.24 | 66,66,66,66                 | 0     |
| 56  | MG   | AA    | 3040 | 1/1   | 0.76 | 0.16 | 72,72,72,72                 | 0     |
| 56  | MG   | BA    | 3659 | 1/1   | 0.76 | 0.32 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3671 | 1/1   | 0.76 | 0.23 | 59,59,59,59                 | 0     |
| 56  | MG   | AA    | 3163 | 1/1   | 0.76 | 0.24 | 58,58,58,58                 | 0     |
| 56  | MG   | CE    | 201  | 1/1   | 0.76 | 0.30 | 73,73,73,73                 | 0     |
| 56  | MG   | BA    | 3555 | 1/1   | 0.76 | 0.11 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3043 | 1/1   | 0.76 | 0.32 | 76,76,76,76                 | 0     |
| 56  | MG   | DA    | 3211 | 1/1   | 0.76 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3082 | 1/1   | 0.76 | 0.32 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3484 | 1/1   | 0.76 | 0.16 | 32,32,32,32                 | 0     |
| 56  | MG   | AA    | 3153 | 1/1   | 0.77 | 0.19 | 81,81,81,81                 | 0     |
| 56  | MG   | BA    | 3692 | 1/1   | 0.77 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3521 | 1/1   | 0.77 | 0.19 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3768 | 1/1   | 0.77 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3179 | 1/1   | 0.77 | 0.26 | 61,61,61,61                 | 0     |
| 57  | PCY  | AA    | 3191 | 40/40 | 0.77 | 0.21 | 59,86,97,99                 | 0     |
| 56  | MG   | DA    | 3319 | 1/1   | 0.77 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3737 | 1/1   | 0.78 | 0.16 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3498 | 1/1   | 0.78 | 0.21 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3505 | 1/1   | 0.78 | 0.18 | 33,33,33,33                 | 0     |
| 56  | MG   | AA    | 3125 | 1/1   | 0.78 | 0.14 | 72,72,72,72                 | 0     |
| 56  | MG   | CA    | 3063 | 1/1   | 0.78 | 0.32 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3384 | 1/1   | 0.78 | 0.22 | 63,63,63,63                 | 0     |
| 56  | MG   | AA    | 3100 | 1/1   | 0.78 | 0.26 | 66,66,66,66                 | 0     |
| 56  | MG   | DA    | 3110 | 1/1   | 0.79 | 0.33 | 64,64,64,64                 | 0     |
| 56  | MG   | CA    | 3144 | 1/1   | 0.79 | 0.26 | 68,68,68,68                 | 0     |
| 56  | MG   | CA    | 3171 | 1/1   | 0.79 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | CA    | 3100 | 1/1   | 0.79 | 0.17 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | AA    | 3184 | 1/1   | 0.79 | 0.13 | 66,66,66,66                 | 0     |
| 56  | MG   | DA    | 3527 | 1/1   | 0.79 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3034 | 1/1   | 0.79 | 0.21 | 70,70,70,70                 | 0     |
| 56  | MG   | DA    | 3537 | 1/1   | 0.79 | 0.25 | 58,58,58,58                 | 0     |
| 56  | MG   | CA    | 3142 | 1/1   | 0.79 | 0.17 | 81,81,81,81                 | 0     |
| 56  | MG   | DA    | 3567 | 1/1   | 0.80 | 0.19 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3514 | 1/1   | 0.80 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3341 | 1/1   | 0.80 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3435 | 1/1   | 0.80 | 0.30 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3512 | 1/1   | 0.80 | 0.23 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3626 | 1/1   | 0.80 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3650 | 1/1   | 0.80 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3103 | 1/1   | 0.80 | 0.15 | 71,71,71,71                 | 0     |
| 56  | MG   | CA    | 3149 | 1/1   | 0.80 | 0.31 | 74,74,74,74                 | 0     |
| 56  | MG   | B4    | 502  | 1/1   | 0.80 | 0.21 | 77,77,77,77                 | 0     |
| 56  | MG   | BA    | 3592 | 1/1   | 0.81 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | AA    | 3169 | 1/1   | 0.81 | 0.18 | 73,73,73,73                 | 0     |
| 56  | MG   | AA    | 3170 | 1/1   | 0.81 | 0.25 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3559 | 1/1   | 0.81 | 0.21 | 61,61,61,61                 | 0     |
| 56  | MG   | CA    | 3091 | 1/1   | 0.81 | 0.24 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3760 | 1/1   | 0.81 | 0.14 | 43,43,43,43                 | 0     |
| 56  | MG   | CA    | 3107 | 1/1   | 0.81 | 0.12 | 77,77,77,77                 | 0     |
| 56  | MG   | DA    | 3175 | 1/1   | 0.81 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | AX    | 3002 | 1/1   | 0.81 | 0.18 | 69,69,69,69                 | 0     |
| 56  | MG   | BB    | 205  | 1/1   | 0.81 | 0.29 | 76,76,76,76                 | 0     |
| 56  | MG   | AA    | 3127 | 1/1   | 0.81 | 0.17 | 79,79,79,79                 | 0     |
| 56  | MG   | BA    | 3437 | 1/1   | 0.81 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3438 | 1/1   | 0.81 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3043 | 1/1   | 0.81 | 0.31 | 67,67,67,67                 | 0     |
| 56  | MG   | AA    | 3094 | 1/1   | 0.81 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | CA    | 3019 | 1/1   | 0.82 | 0.29 | 62,62,62,62                 | 0     |
| 56  | MG   | CT    | 3001 | 1/1   | 0.82 | 0.31 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3725 | 1/1   | 0.82 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 3049 | 1/1   | 0.82 | 0.15 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3109 | 1/1   | 0.82 | 0.30 | 68,68,68,68                 | 0     |
| 56  | MG   | AA    | 3105 | 1/1   | 0.82 | 0.23 | 71,71,71,71                 | 0     |
| 56  | MG   | BA    | 3663 | 1/1   | 0.82 | 0.26 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3202 | 1/1   | 0.82 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3108 | 1/1   | 0.82 | 0.27 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3222 | 1/1   | 0.82 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3159 | 1/1   | 0.82 | 0.25 | 71,71,71,71                 | 0     |
| 56  | MG   | DA    | 3324 | 1/1   | 0.82 | 0.15 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3288 | 1/1   | 0.82 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3402 | 1/1   | 0.82 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3426 | 1/1   | 0.82 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | DB    | 3008 | 1/1   | 0.82 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | DD    | 308  | 1/1   | 0.82 | 0.33 | 72,72,72,72                 | 0     |
| 56  | MG   | DV    | 3003 | 1/1   | 0.82 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3096 | 1/1   | 0.82 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3525 | 1/1   | 0.82 | 0.13 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3579 | 1/1   | 0.83 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3469 | 1/1   | 0.83 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3083 | 1/1   | 0.83 | 0.29 | 72,72,72,72                 | 0     |
| 56  | MG   | DA    | 3488 | 1/1   | 0.83 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3499 | 1/1   | 0.83 | 0.23 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3583 | 1/1   | 0.83 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3518 | 1/1   | 0.83 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | AA    | 3185 | 1/1   | 0.83 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | BP    | 203  | 1/1   | 0.83 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3150 | 1/1   | 0.83 | 0.22 | 52,52,52,52                 | 0     |
| 56  | MG   | B0    | 101  | 1/1   | 0.83 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3606 | 1/1   | 0.83 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3185 | 1/1   | 0.83 | 0.16 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3122 | 1/1   | 0.83 | 0.26 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3626 | 1/1   | 0.83 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3607 | 1/1   | 0.83 | 0.22 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3693 | 1/1   | 0.83 | 0.16 | 74,74,74,74                 | 0     |
| 56  | MG   | CA    | 3025 | 1/1   | 0.83 | 0.31 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3617 | 1/1   | 0.83 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | CA    | 3053 | 1/1   | 0.83 | 0.27 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3400 | 1/1   | 0.83 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3265 | 1/1   | 0.83 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3389 | 1/1   | 0.83 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3067 | 1/1   | 0.83 | 0.24 | 72,72,72,72                 | 0     |
| 56  | MG   | CA    | 3078 | 1/1   | 0.83 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | AX    | 3007 | 1/1   | 0.84 | 0.20 | 69,69,69,69                 | 0     |
| 56  | MG   | DA    | 3221 | 1/1   | 0.84 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3677 | 1/1   | 0.84 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3257 | 1/1   | 0.84 | 0.37 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3296 | 1/1   | 0.84 | 0.17 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3599 | 1/1   | 0.84 | 0.15 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3066 | 1/1   | 0.84 | 0.23 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3090 | 1/1   | 0.84 | 0.27 | 67,67,67,67                 | 0     |
| 56  | MG   | CA    | 3011 | 1/1   | 0.84 | 0.27 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3097 | 1/1   | 0.84 | 0.26 | 52,52,52,52                 | 0     |
| 56  | MG   | AA    | 3157 | 1/1   | 0.84 | 0.19 | 84,84,84,84                 | 0     |
| 56  | MG   | BA    | 3112 | 1/1   | 0.84 | 0.11 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3437 | 1/1   | 0.84 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3558 | 1/1   | 0.84 | 0.28 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3221 | 1/1   | 0.84 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | AA    | 3020 | 1/1   | 0.84 | 0.44 | 71,71,71,71                 | 0     |
| 56  | MG   | CA    | 3134 | 1/1   | 0.84 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | CA    | 3138 | 1/1   | 0.84 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | CA    | 3139 | 1/1   | 0.84 | 0.28 | 69,69,69,69                 | 0     |
| 56  | MG   | BB    | 211  | 1/1   | 0.84 | 0.13 | 81,81,81,81                 | 0     |
| 56  | MG   | DA    | 3229 | 1/1   | 0.85 | 0.28 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3249 | 1/1   | 0.85 | 0.29 | 65,65,65,65                 | 0     |
| 56  | MG   | CA    | 3030 | 1/1   | 0.85 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3268 | 1/1   | 0.85 | 0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3420 | 1/1   | 0.85 | 0.22 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3605 | 1/1   | 0.85 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3059 | 1/1   | 0.85 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3583 | 1/1   | 0.85 | 0.09 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3364 | 1/1   | 0.85 | 0.16 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3389 | 1/1   | 0.85 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3506 | 1/1   | 0.85 | 0.10 | 31,31,31,31                 | 0     |
| 56  | MG   | B5    | 105  | 1/1   | 0.85 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | DA    | 3412 | 1/1   | 0.85 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3629 | 1/1   | 0.85 | 0.13 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3631 | 1/1   | 0.85 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3417 | 1/1   | 0.85 | 0.19 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3418 | 1/1   | 0.85 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | CA    | 3007 | 1/1   | 0.85 | 0.21 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3158 | 1/1   | 0.85 | 0.15 | 75,75,75,75                 | 0     |
| 56  | MG   | CA    | 3116 | 1/1   | 0.85 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | CA    | 3164 | 1/1   | 0.85 | 0.19 | 73,73,73,73                 | 0     |
| 56  | MG   | CA    | 3169 | 1/1   | 0.85 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3392 | 1/1   | 0.85 | 0.15 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3721 | 1/1   | 0.85 | 0.08 | 9,9,9,9                     | 0     |
| 56  | MG   | BA    | 3503 | 1/1   | 0.85 | 0.22 | 64,64,64,64                 | 0     |
| 56  | MG   | AA    | 3141 | 1/1   | 0.86 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3080 | 1/1   | 0.86 | 0.42 | 71,71,71,71                 | 0     |
| 56  | MG   | BA    | 3455 | 1/1   | 0.86 | 0.10 | 32,32,32,32                 | 0     |
| 56  | MG   | B7    | 104  | 1/1   | 0.86 | 0.19 | 64,64,64,64                 | 0     |
| 56  | MG   | CA    | 3151 | 1/1   | 0.86 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3423 | 1/1   | 0.86 | 0.11 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3152 | 1/1   | 0.86 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3433 | 1/1   | 0.86 | 0.13 | 34,34,34,34                 | 0     |
| 56  | MG   | CA    | 3155 | 1/1   | 0.86 | 0.22 | 76,76,76,76                 | 0     |
| 56  | MG   | BA    | 3458 | 1/1   | 0.86 | 0.38 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3109 | 1/1   | 0.86 | 0.35 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3150 | 1/1   | 0.86 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3165 | 1/1   | 0.86 | 0.24 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3479 | 1/1   | 0.86 | 0.18 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3175 | 1/1   | 0.86 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3199 | 1/1   | 0.86 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | CA    | 3052 | 1/1   | 0.86 | 0.16 | 69,69,69,69                 | 0     |
| 56  | MG   | DA    | 3502 | 1/1   | 0.86 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3216 | 1/1   | 0.86 | 0.13 | 62,62,62,62                 | 0     |
| 56  | MG   | AA    | 3122 | 1/1   | 0.86 | 0.14 | 80,80,80,80                 | 0     |
| 56  | MG   | CA    | 3061 | 1/1   | 0.86 | 0.16 | 64,64,64,64                 | 0     |
| 56  | MG   | BA    | 3698 | 1/1   | 0.86 | 0.16 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3699 | 1/1   | 0.86 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | AA    | 3183 | 1/1   | 0.86 | 0.22 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3569 | 1/1   | 0.86 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3274 | 1/1   | 0.86 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | AA    | 3138 | 1/1   | 0.86 | 0.10 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3603 | 1/1   | 0.86 | 0.23 | 55,55,55,55                 | 0     |
| 56  | MG   | AA    | 3139 | 1/1   | 0.86 | 0.13 | 72,72,72,72                 | 0     |
| 56  | MG   | BA    | 3744 | 1/1   | 0.86 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3381 | 1/1   | 0.86 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3621 | 1/1   | 0.86 | 0.33 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3767 | 1/1   | 0.86 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | CA    | 3099 | 1/1   | 0.86 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | AA    | 3166 | 1/1   | 0.86 | 0.16 | 74,74,74,74                 | 0     |
| 56  | MG   | CA    | 3103 | 1/1   | 0.86 | 0.11 | 79,79,79,79                 | 0     |
| 56  | MG   | BA    | 3770 | 1/1   | 0.86 | 0.20 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3648 | 1/1   | 0.86 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3650 | 1/1   | 0.86 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3813 | 1/1   | 0.86 | 0.13 | 58,58,58,58                 | 0     |
| 56  | MG   | AA    | 3167 | 1/1   | 0.86 | 0.19 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3670 | 1/1   | 0.86 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | BB    | 209  | 1/1   | 0.86 | 0.29 | 69,69,69,69                 | 0     |
| 56  | MG   | CA    | 3129 | 1/1   | 0.86 | 0.19 | 69,69,69,69                 | 0     |
| 56  | MG   | DD    | 302  | 1/1   | 0.86 | 0.17 | 73,73,73,73                 | 0     |
| 56  | MG   | BA    | 3595 | 1/1   | 0.86 | 0.46 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3140 | 1/1   | 0.86 | 0.22 | 36,36,36,36                 | 0     |
| 56  | MG   | DY    | 502  | 1/1   | 0.86 | 0.16 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3377 | 1/1   | 0.86 | 0.19 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3083 | 1/1   | 0.86 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3711 | 1/1   | 0.87 | 0.22 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3044 | 1/1   | 0.87 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3173 | 1/1   | 0.87 | 0.25 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3728 | 1/1   | 0.87 | 0.12 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3082 | 1/1   | 0.87 | 0.30 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3455 | 1/1   | 0.87 | 0.23 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3458 | 1/1   | 0.87 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | AA    | 3098 | 1/1   | 0.87 | 0.24 | 71,71,71,71                 | 0     |
| 56  | MG   | BA    | 3745 | 1/1   | 0.87 | 0.17 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3755 | 1/1   | 0.87 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3759 | 1/1   | 0.87 | 0.10 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3044 | 1/1   | 0.87 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 3016 | 1/1   | 0.87 | 0.30 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3294 | 1/1   | 0.87 | 0.24 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3525 | 1/1   | 0.87 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3612 | 1/1   | 0.87 | 0.19 | 58,58,58,58                 | 0     |
| 56  | MG   | AA    | 3102 | 1/1   | 0.87 | 0.17 | 64,64,64,64                 | 0     |
| 56  | MG   | CA    | 3093 | 1/1   | 0.87 | 0.28 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3547 | 1/1   | 0.87 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3793 | 1/1   | 0.87 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3359 | 1/1   | 0.87 | 0.21 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3648 | 1/1   | 0.87 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3371 | 1/1   | 0.87 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3575 | 1/1   | 0.87 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | AA    | 3073 | 1/1   | 0.87 | 0.20 | 71,71,71,71                 | 0     |
| 56  | MG   | BB    | 220  | 1/1   | 0.87 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | CA    | 3117 | 1/1   | 0.87 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | BB    | 221  | 1/1   | 0.87 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3038 | 1/1   | 0.87 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3266 | 1/1   | 0.87 | 0.31 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3084 | 1/1   | 0.87 | 0.31 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3276 | 1/1   | 0.87 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3290 | 1/1   | 0.87 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | AA    | 3012 | 1/1   | 0.87 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3632 | 1/1   | 0.87 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3673 | 1/1   | 0.87 | 0.11 | 28,28,28,28                 | 0     |
| 56  | MG   | DA    | 3330 | 1/1   | 0.87 | 0.20 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3339 | 1/1   | 0.87 | 0.16 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3027 | 1/1   | 0.87 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3347 | 1/1   | 0.87 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3690 | 1/1   | 0.87 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3427 | 1/1   | 0.87 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3009 | 1/1   | 0.87 | 0.31 | 66,66,66,66                 | 0     |
| 56  | MG   | CA    | 3148 | 1/1   | 0.87 | 0.12 | 88,88,88,88                 | 0     |
| 56  | MG   | BA    | 3561 | 1/1   | 0.87 | 0.18 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3013 | 1/1   | 0.87 | 0.16 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3571 | 1/1   | 0.87 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3575 | 1/1   | 0.87 | 0.13 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3419 | 1/1   | 0.87 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3434 | 1/1   | 0.87 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3624 | 1/1   | 0.88 | 0.14 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3420 | 1/1   | 0.88 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | AA    | 3078 | 1/1   | 0.88 | 0.13 | 72,72,72,72                 | 0     |
| 56  | MG   | BA    | 3644 | 1/1   | 0.88 | 0.15 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3431 | 1/1   | 0.88 | 0.12 | 64,64,64,64                 | 0     |
| 56  | MG   | CA    | 3062 | 1/1   | 0.88 | 0.26 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3766 | 1/1   | 0.88 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3378 | 1/1   | 0.88 | 0.11 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3075 | 1/1   | 0.88 | 0.29 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3446 | 1/1   | 0.88 | 0.15 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 3180 | 1/1   | 0.88 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3081 | 1/1   | 0.88 | 0.25 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3465 | 1/1   | 0.88 | 0.21 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3034 | 1/1   | 0.88 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3185 | 1/1   | 0.88 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3478 | 1/1   | 0.88 | 0.20 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3772 | 1/1   | 0.88 | 0.17 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3062 | 1/1   | 0.88 | 0.25 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3083 | 1/1   | 0.88 | 0.23 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3098 | 1/1   | 0.88 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3194 | 1/1   | 0.88 | 0.22 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3524 | 1/1   | 0.88 | 0.22 | 59,59,59,59                 | 0     |
| 56  | MG   | CA    | 3086 | 1/1   | 0.88 | 0.33 | 76,76,76,76                 | 0     |
| 56  | MG   | CA    | 3087 | 1/1   | 0.88 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3124 | 1/1   | 0.88 | 0.16 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3534 | 1/1   | 0.88 | 0.11 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3131 | 1/1   | 0.88 | 0.18 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3541 | 1/1   | 0.88 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | CA    | 3088 | 1/1   | 0.88 | 0.23 | 66,66,66,66                 | 0     |
| 56  | MG   | AA    | 3124 | 1/1   | 0.88 | 0.21 | 71,71,71,71                 | 0     |
| 56  | MG   | BB    | 201  | 1/1   | 0.88 | 0.21 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3563 | 1/1   | 0.88 | 0.23 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3092 | 1/1   | 0.88 | 0.30 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3047 | 1/1   | 0.88 | 0.24 | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 3096 | 1/1   | 0.88 | 0.25 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3582 | 1/1   | 0.88 | 0.13 | 64,64,64,64                 | 0     |
| 56  | MG   | BA    | 3566 | 1/1   | 0.88 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3589 | 1/1   | 0.88 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3590 | 1/1   | 0.88 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3241 | 1/1   | 0.88 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3259 | 1/1   | 0.88 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3255 | 1/1   | 0.88 | 0.26 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3440 | 1/1   | 0.88 | 0.12 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3609 | 1/1   | 0.88 | 0.24 | 61,61,61,61                 | 0     |
| 56  | MG   | BO    | 5001 | 1/1   | 0.88 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3580 | 1/1   | 0.88 | 0.15 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3623 | 1/1   | 0.88 | 0.22 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3262 | 1/1   | 0.88 | 0.34 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3286 | 1/1   | 0.88 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | AA    | 3048 | 1/1   | 0.88 | 0.27 | 59,59,59,59                 | 0     |
| 56  | MG   | CA    | 3128 | 1/1   | 0.88 | 0.24 | 68,68,68,68                 | 0     |
| 56  | MG   | DA    | 3321 | 1/1   | 0.88 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | AA    | 3136 | 1/1   | 0.88 | 0.18 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3716 | 1/1   | 0.88 | 0.20 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3649 | 1/1   | 0.88 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3005 | 1/1   | 0.88 | 0.36 | 73,73,73,73                 | 0     |
| 56  | MG   | BA    | 3477 | 1/1   | 0.88 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3656 | 1/1   | 0.88 | 0.09 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3604 | 1/1   | 0.88 | 0.16 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3666 | 1/1   | 0.88 | 0.20 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3074 | 1/1   | 0.88 | 0.25 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3111 | 1/1   | 0.88 | 0.17 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3738 | 1/1   | 0.88 | 0.16 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3392 | 1/1   | 0.88 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3109 | 1/1   | 0.88 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3135 | 1/1   | 0.88 | 0.08 | 61,61,61,61                 | 0     |
| 56  | MG   | CA    | 3042 | 1/1   | 0.88 | 0.30 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3747 | 1/1   | 0.88 | 0.14 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3748 | 1/1   | 0.88 | 0.15 | 69,69,69,69                 | 0     |
| 56  | MG   | BA    | 3028 | 1/1   | 0.89 | 0.26 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3006 | 1/1   | 0.89 | 0.11 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3697 | 1/1   | 0.89 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3161 | 1/1   | 0.89 | 0.21 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3029 | 1/1   | 0.89 | 0.13 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3040 | 1/1   | 0.89 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3014 | 1/1   | 0.89 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3704 | 1/1   | 0.89 | 0.24 | 36,36,36,36                 | 0     |
| 56  | MG   | CA    | 3021 | 1/1   | 0.89 | 0.24 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3567 | 1/1   | 0.89 | 0.11 | 45,45,45,45                 | 0     |
| 56  | MG   | CA    | 3168 | 1/1   | 0.89 | 0.27 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3387 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | CA    | 3036 | 1/1   | 0.89 | 0.34 | 72,72,72,72                 | 0     |
| 56  | MG   | DA    | 3445 | 1/1   | 0.89 | 0.15 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3717 | 1/1   | 0.89 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3454 | 1/1   | 0.89 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3004 | 1/1   | 0.89 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | CA    | 3045 | 1/1   | 0.89 | 0.31 | 68,68,68,68                 | 0     |
| 56  | MG   | DA    | 3459 | 1/1   | 0.89 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | CA    | 3047 | 1/1   | 0.89 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | CA    | 3049 | 1/1   | 0.89 | 0.12 | 71,71,71,71                 | 0     |
| 56  | MG   | DA    | 3017 | 1/1   | 0.89 | 0.15 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3472 | 1/1   | 0.89 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3576 | 1/1   | 0.89 | 0.13 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3055 | 1/1   | 0.89 | 0.31 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3057 | 1/1   | 0.89 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3396 | 1/1   | 0.89 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3494 | 1/1   | 0.89 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | CA    | 3058 | 1/1   | 0.89 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3059 | 1/1   | 0.89 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3510 | 1/1   | 0.89 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3512 | 1/1   | 0.89 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3740 | 1/1   | 0.89 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3741 | 1/1   | 0.89 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3584 | 1/1   | 0.89 | 0.14 | 34,34,34,34                 | 0     |
| 56  | MG   | AA    | 3162 | 1/1   | 0.89 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3115 | 1/1   | 0.89 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3118 | 1/1   | 0.89 | 0.20 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3104 | 1/1   | 0.89 | 0.33 | 70,70,70,70                 | 0     |
| 56  | MG   | DA    | 3542 | 1/1   | 0.89 | 0.23 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3225 | 1/1   | 0.89 | 0.13 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3132 | 1/1   | 0.89 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3146 | 1/1   | 0.89 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 3097 | 1/1   | 0.89 | 0.41 | 71,71,71,71                 | 0     |
| 56  | MG   | BA    | 3242 | 1/1   | 0.89 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3606 | 1/1   | 0.89 | 0.19 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3452 | 1/1   | 0.89 | 0.18 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3255 | 1/1   | 0.89 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3218 | 1/1   | 0.89 | 0.14 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3457 | 1/1   | 0.89 | 0.17 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3092 | 1/1   | 0.89 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3225 | 1/1   | 0.89 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3464 | 1/1   | 0.89 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3240 | 1/1   | 0.89 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3634 | 1/1   | 0.89 | 0.21 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3639 | 1/1   | 0.89 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | AA    | 3142 | 1/1   | 0.89 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3264 | 1/1   | 0.89 | 0.24 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3130 | 1/1   | 0.89 | 0.15 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3055 | 1/1   | 0.89 | 0.40 | 69,69,69,69                 | 0     |
| 56  | MG   | AX    | 3003 | 1/1   | 0.89 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | DA    | 3630 | 1/1   | 0.89 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3292 | 1/1   | 0.89 | 0.17 | 40,40,40,40                 | 0     |
| 56  | MG   | AA    | 3001 | 1/1   | 0.89 | 0.16 | 77,77,77,77                 | 0     |
| 56  | MG   | DA    | 3309 | 1/1   | 0.89 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3637 | 1/1   | 0.89 | 0.06 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3666 | 1/1   | 0.89 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3118 | 1/1   | 0.89 | 0.19 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3322 | 1/1   | 0.89 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | BF    | 304  | 1/1   | 0.89 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3654 | 1/1   | 0.89 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3295 | 1/1   | 0.89 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3127 | 1/1   | 0.89 | 0.32 | 65,65,65,65                 | 0     |
| 56  | MG   | AA    | 3156 | 1/1   | 0.89 | 0.13 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3665 | 1/1   | 0.89 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3315 | 1/1   | 0.89 | 0.21 | 59,59,59,59                 | 0     |
| 56  | MG   | B0    | 105  | 1/1   | 0.89 | 0.13 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3673 | 1/1   | 0.89 | 0.18 | 68,68,68,68                 | 0     |
| 56  | MG   | DA    | 3365 | 1/1   | 0.89 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3376 | 1/1   | 0.89 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | CA    | 3132 | 1/1   | 0.89 | 0.24 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3388 | 1/1   | 0.89 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | DG    | 3001 | 1/1   | 0.89 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | DP    | 202  | 1/1   | 0.89 | 0.23 | 55,55,55,55                 | 0     |
| 56  | MG   | DV    | 3002 | 1/1   | 0.89 | 0.20 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3682 | 1/1   | 0.89 | 0.19 | 39,39,39,39                 | 0     |
| 56  | MG   | DW    | 201  | 1/1   | 0.89 | 0.12 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3125 | 1/1   | 0.89 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3399 | 1/1   | 0.89 | 0.12 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3547 | 1/1   | 0.89 | 0.09 | 64,64,64,64                 | 0     |
| 60  | K    | CX    | 3001 | 1/1   | 0.89 | 0.14 | 77,77,77,77                 | 0     |
| 56  | MG   | BA    | 3290 | 1/1   | 0.90 | 0.23 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3025 | 1/1   | 0.90 | 0.30 | 69,69,69,69                 | 0     |
| 56  | MG   | CA    | 3163 | 1/1   | 0.90 | 0.10 | 78,78,78,78                 | 0     |
| 56  | MG   | BA    | 3121 | 1/1   | 0.90 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | AA    | 3026 | 1/1   | 0.90 | 0.18 | 71,71,71,71                 | 0     |
| 56  | MG   | AA    | 3008 | 1/1   | 0.90 | 0.07 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3529 | 1/1   | 0.90 | 0.15 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3310 | 1/1   | 0.90 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3032 | 1/1   | 0.90 | 0.11 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3312 | 1/1   | 0.90 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3706 | 1/1   | 0.90 | 0.08 | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 3039 | 1/1   | 0.90 | 0.22 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3319 | 1/1   | 0.90 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3442 | 1/1   | 0.90 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3443 | 1/1   | 0.90 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3032 | 1/1   | 0.90 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3033 | 1/1   | 0.90 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3453 | 1/1   | 0.90 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3356 | 1/1   | 0.90 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3162 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3363 | 1/1   | 0.90 | 0.10 | 66,66,66,66                 | 0     |
| 56  | MG   | AA    | 3149 | 1/1   | 0.90 | 0.12 | 68,68,68,68                 | 0     |
| 56  | MG   | BA    | 3733 | 1/1   | 0.90 | 0.08 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3076 | 1/1   | 0.90 | 0.11 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3377 | 1/1   | 0.90 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3089 | 1/1   | 0.90 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3059 | 1/1   | 0.90 | 0.15 | 75,75,75,75                 | 0     |
| 56  | MG   | DA    | 3100 | 1/1   | 0.90 | 0.29 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3578 | 1/1   | 0.90 | 0.13 | 20,20,20,20                 | 0     |
| 56  | MG   | AA    | 3174 | 1/1   | 0.90 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3489 | 1/1   | 0.90 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3493 | 1/1   | 0.90 | 0.25 | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 3048 | 1/1   | 0.90 | 0.21 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3193 | 1/1   | 0.90 | 0.27 | 62,62,62,62                 | 0     |
| 56  | MG   | CA    | 3072 | 1/1   | 0.90 | 0.34 | 62,62,62,62                 | 0     |
| 56  | MG   | AA    | 3091 | 1/1   | 0.90 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3587 | 1/1   | 0.90 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3590 | 1/1   | 0.90 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3135 | 1/1   | 0.90 | 0.24 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3195 | 1/1   | 0.90 | 0.26 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3531 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3056 | 1/1   | 0.90 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3204 | 1/1   | 0.90 | 0.13 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3184 | 1/1   | 0.90 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3085 | 1/1   | 0.90 | 0.23 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3194 | 1/1   | 0.90 | 0.18 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3201 | 1/1   | 0.90 | 0.31 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3548 | 1/1   | 0.90 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3549 | 1/1   | 0.90 | 0.12 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3399 | 1/1   | 0.90 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3211 | 1/1   | 0.90 | 0.18 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3212 | 1/1   | 0.90 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3214 | 1/1   | 0.90 | 0.27 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3422 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3570 | 1/1   | 0.90 | 0.11 | 59,59,59,59                 | 0     |
| 56  | MG   | AA    | 3057 | 1/1   | 0.90 | 0.43 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3219 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3789 | 1/1   | 0.90 | 0.16 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3226 | 1/1   | 0.90 | 0.17 | 57,57,57,57                 | 0     |
| 56  | MG   | AA    | 3096 | 1/1   | 0.90 | 0.39 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3233 | 1/1   | 0.90 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3234 | 1/1   | 0.90 | 0.22 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3239 | 1/1   | 0.90 | 0.20 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3806 | 1/1   | 0.90 | 0.32 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3618 | 1/1   | 0.90 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3010 | 1/1   | 0.90 | 0.13 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3616 | 1/1   | 0.90 | 0.10 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3237 | 1/1   | 0.90 | 0.37 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3260 | 1/1   | 0.90 | 0.30 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3624 | 1/1   | 0.90 | 0.23 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3631 | 1/1   | 0.90 | 0.21 | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 3158 | 1/1   | 0.90 | 0.12 | 71,71,71,71                 | 0     |
| 56  | MG   | BA    | 3636 | 1/1   | 0.90 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3453 | 1/1   | 0.90 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3278 | 1/1   | 0.90 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3282 | 1/1   | 0.90 | 0.19 | 42,42,42,42                 | 0     |
| 56  | MG   | AA    | 3066 | 1/1   | 0.90 | 0.23 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3639 | 1/1   | 0.90 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3123 | 1/1   | 0.90 | 0.16 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3643 | 1/1   | 0.90 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3305 | 1/1   | 0.90 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3250 | 1/1   | 0.90 | 0.22 | 42,42,42,42                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3125 | 1/1   | 0.90 | 0.08 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3652 | 1/1   | 0.90 | 0.18 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3320 | 1/1   | 0.90 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | AD    | 502  | 1/1   | 0.90 | 0.28 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3654 | 1/1   | 0.90 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | BU    | 201  | 1/1   | 0.90 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | BU    | 206  | 1/1   | 0.90 | 0.42 | 61,61,61,61                 | 0     |
| 56  | MG   | BZ    | 301  | 1/1   | 0.90 | 0.13 | 58,58,58,58                 | 0     |
| 56  | MG   | AA    | 3017 | 1/1   | 0.90 | 0.34 | 69,69,69,69                 | 0     |
| 56  | MG   | DA    | 3343 | 1/1   | 0.90 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3344 | 1/1   | 0.90 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | DB    | 3002 | 1/1   | 0.90 | 0.20 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3345 | 1/1   | 0.90 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3103 | 1/1   | 0.90 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3479 | 1/1   | 0.90 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | DE    | 302  | 1/1   | 0.90 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3495 | 1/1   | 0.90 | 0.11 | 58,58,58,58                 | 0     |
| 56  | MG   | DP    | 201  | 1/1   | 0.90 | 0.24 | 58,58,58,58                 | 0     |
| 56  | MG   | CA    | 3143 | 1/1   | 0.90 | 0.24 | 77,77,77,77                 | 0     |
| 56  | MG   | AA    | 3019 | 1/1   | 0.90 | 0.14 | 66,66,66,66                 | 0     |
| 56  | MG   | AX    | 3006 | 1/1   | 0.90 | 0.17 | 71,71,71,71                 | 0     |
| 56  | MG   | BA    | 3277 | 1/1   | 0.90 | 0.20 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3678 | 1/1   | 0.90 | 0.28 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3398 | 1/1   | 0.90 | 0.29 | 52,52,52,52                 | 0     |
| 56  | MG   | AA    | 3011 | 1/1   | 0.90 | 0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3010 | 1/1   | 0.90 | 0.24 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3019 | 1/1   | 0.91 | 0.11 | 39,39,39,39                 | 0     |
| 56  | MG   | CA    | 3160 | 1/1   | 0.91 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | CA    | 3162 | 1/1   | 0.91 | 0.08 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3318 | 1/1   | 0.91 | 0.08 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3391 | 1/1   | 0.91 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3020 | 1/1   | 0.91 | 0.13 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3685 | 1/1   | 0.91 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3687 | 1/1   | 0.91 | 0.18 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3321 | 1/1   | 0.91 | 0.11 | 21,21,21,21                 | 0     |
| 56  | MG   | BA    | 3534 | 1/1   | 0.91 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3405 | 1/1   | 0.91 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3355 | 1/1   | 0.91 | 0.14 | 28,28,28,28                 | 0     |
| 56  | MG   | AA    | 3095 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3180 | 1/1   | 0.91 | 0.24 | 46,46,46,46                 | 0     |
| 56  | MG   | AA    | 3168 | 1/1   | 0.91 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | CX    | 3003 | 1/1   | 0.91 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3014 | 1/1   | 0.91 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3424 | 1/1   | 0.91 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3015 | 1/1   | 0.91 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3700 | 1/1   | 0.91 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3019 | 1/1   | 0.91 | 0.11 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3368 | 1/1   | 0.91 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3186 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3033 | 1/1   | 0.91 | 0.30 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3037 | 1/1   | 0.91 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | AA    | 3021 | 1/1   | 0.91 | 0.19 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3046 | 1/1   | 0.91 | 0.21 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3041 | 1/1   | 0.91 | 0.34 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3715 | 1/1   | 0.91 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | AA    | 3070 | 1/1   | 0.91 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3066 | 1/1   | 0.91 | 0.21 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3068 | 1/1   | 0.91 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3022 | 1/1   | 0.91 | 0.07 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3719 | 1/1   | 0.91 | 0.11 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3087 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3720 | 1/1   | 0.91 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3091 | 1/1   | 0.91 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | AA    | 3054 | 1/1   | 0.91 | 0.15 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3724 | 1/1   | 0.91 | 0.09 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3482 | 1/1   | 0.91 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3050 | 1/1   | 0.91 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3057 | 1/1   | 0.91 | 0.16 | 52,52,52,52                 | 0     |
| 56  | MG   | AA    | 3076 | 1/1   | 0.91 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3731 | 1/1   | 0.91 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3116 | 1/1   | 0.91 | 0.13 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3395 | 1/1   | 0.91 | 0.14 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3735 | 1/1   | 0.91 | 0.08 | 20,20,20,20                 | 0     |
| 56  | MG   | DA    | 3128 | 1/1   | 0.91 | 0.23 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3511 | 1/1   | 0.91 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3129 | 1/1   | 0.91 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3517 | 1/1   | 0.91 | 0.09 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3736 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3585 | 1/1   | 0.91 | 0.08 | 58,58,58,58                 | 0     |
| 56  | MG   | CA    | 3068 | 1/1   | 0.91 | 0.30 | 64,64,64,64                 | 0     |
| 56  | MG   | AA    | 3077 | 1/1   | 0.91 | 0.25 | 54,54,54,54                 | 0     |
| 56  | MG   | CA    | 3073 | 1/1   | 0.91 | 0.16 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3168 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3536 | 1/1   | 0.91 | 0.08 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | AA    | 3039 | 1/1   | 0.91 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3181 | 1/1   | 0.91 | 0.27 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3182 | 1/1   | 0.91 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | CA    | 3077 | 1/1   | 0.91 | 0.31 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3411 | 1/1   | 0.91 | 0.17 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3186 | 1/1   | 0.91 | 0.27 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3556 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3187 | 1/1   | 0.91 | 0.27 | 51,51,51,51                 | 0     |
| 56  | MG   | AA    | 3181 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3200 | 1/1   | 0.91 | 0.21 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3565 | 1/1   | 0.91 | 0.18 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3596 | 1/1   | 0.91 | 0.20 | 68,68,68,68                 | 0     |
| 56  | MG   | BA    | 3597 | 1/1   | 0.91 | 0.13 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3210 | 1/1   | 0.91 | 0.14 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3574 | 1/1   | 0.91 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3229 | 1/1   | 0.91 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3754 | 1/1   | 0.91 | 0.17 | 60,60,60,60                 | 0     |
| 56  | MG   | AA    | 3182 | 1/1   | 0.91 | 0.25 | 64,64,64,64                 | 0     |
| 56  | MG   | BA    | 3431 | 1/1   | 0.91 | 0.10 | 63,63,63,63                 | 0     |
| 56  | MG   | AA    | 3155 | 1/1   | 0.91 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 3056 | 1/1   | 0.91 | 0.29 | 54,54,54,54                 | 0     |
| 56  | MG   | AA    | 3002 | 1/1   | 0.91 | 0.15 | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 3615 | 1/1   | 0.91 | 0.13 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3254 | 1/1   | 0.91 | 0.22 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3608 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3094 | 1/1   | 0.91 | 0.40 | 68,68,68,68                 | 0     |
| 56  | MG   | BA    | 3771 | 1/1   | 0.91 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | AA    | 3187 | 1/1   | 0.91 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3778 | 1/1   | 0.91 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3242 | 1/1   | 0.91 | 0.28 | 68,68,68,68                 | 0     |
| 56  | MG   | BA    | 3781 | 1/1   | 0.91 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3622 | 1/1   | 0.91 | 0.10 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3627 | 1/1   | 0.91 | 0.11 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3256 | 1/1   | 0.91 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3112 | 1/1   | 0.91 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3085 | 1/1   | 0.91 | 0.26 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3800 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | AE    | 202  | 1/1   | 0.91 | 0.09 | 74,74,74,74                 | 0     |
| 56  | MG   | DA    | 3635 | 1/1   | 0.91 | 0.19 | 47,47,47,47                 | 0     |
| 56  | MG   | AF    | 3001 | 1/1   | 0.91 | 0.16 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3087 | 1/1   | 0.91 | 0.34 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3461 | 1/1   | 0.91 | 0.08 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3279 | 1/1   | 0.91 | 0.27 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3646 | 1/1   | 0.91 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3280 | 1/1   | 0.91 | 0.28 | 62,62,62,62                 | 0     |
| 56  | MG   | BB    | 206  | 1/1   | 0.91 | 0.18 | 58,58,58,58                 | 0     |
| 56  | MG   | AA    | 3018 | 1/1   | 0.91 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3280 | 1/1   | 0.91 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | DA    | 3293 | 1/1   | 0.91 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3294 | 1/1   | 0.91 | 0.08 | 36,36,36,36                 | 0     |
| 56  | MG   | BB    | 216  | 1/1   | 0.91 | 0.21 | 63,63,63,63                 | 0     |
| 56  | MG   | BB    | 219  | 1/1   | 0.91 | 0.11 | 74,74,74,74                 | 0     |
| 56  | MG   | DA    | 3664 | 1/1   | 0.91 | 0.25 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3310 | 1/1   | 0.91 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3316 | 1/1   | 0.91 | 0.08 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3646 | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3120 | 1/1   | 0.91 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3649 | 1/1   | 0.91 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | BE    | 307  | 1/1   | 0.91 | 0.08 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3492 | 1/1   | 0.91 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | DB    | 3009 | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |
| 56  | MG   | DB    | 3010 | 1/1   | 0.91 | 0.23 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3326 | 1/1   | 0.91 | 0.15 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3165 | 1/1   | 0.91 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3338 | 1/1   | 0.91 | 0.13 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3061 | 1/1   | 0.91 | 0.19 | 54,54,54,54                 | 0     |
| 56  | MG   | CA    | 3147 | 1/1   | 0.91 | 0.24 | 70,70,70,70                 | 0     |
| 56  | MG   | BA    | 3133 | 1/1   | 0.91 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | AX    | 3009 | 1/1   | 0.91 | 0.18 | 74,74,74,74                 | 0     |
| 56  | MG   | BA    | 3137 | 1/1   | 0.91 | 0.21 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3147 | 1/1   | 0.91 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | AX    | 3010 | 1/1   | 0.91 | 0.11 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3674 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3369 | 1/1   | 0.91 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3370 | 1/1   | 0.91 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3415 | 1/1   | 0.92 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3632 | 1/1   | 0.92 | 0.21 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3079 | 1/1   | 0.92 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3633 | 1/1   | 0.92 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | AA    | 3029 | 1/1   | 0.92 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3144 | 1/1   | 0.92 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | AA    | 3189 | 1/1   | 0.92 | 0.32 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3643 | 1/1   | 0.92 | 0.13 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3430 | 1/1   | 0.92 | 0.10 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3360 | 1/1   | 0.92 | 0.09 | 21,21,21,21                 | 0     |
| 56  | MG   | BA    | 3645 | 1/1   | 0.92 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3106 | 1/1   | 0.92 | 0.07 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3107 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3222 | 1/1   | 0.92 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3779 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | CA    | 3079 | 1/1   | 0.92 | 0.48 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3122 | 1/1   | 0.92 | 0.23 | 46,46,46,46                 | 0     |
| 56  | MG   | AA    | 3146 | 1/1   | 0.92 | 0.23 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3450 | 1/1   | 0.92 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3792 | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3231 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3795 | 1/1   | 0.92 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3796 | 1/1   | 0.92 | 0.15 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3041 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | BA    | 3656 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 56  | MG   | CA    | 3089 | 1/1   | 0.92 | 0.28 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3147 | 1/1   | 0.92 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3807 | 1/1   | 0.92 | 0.18 | 66,66,66,66                 | 0     |
| 56  | MG   | DA    | 3152 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3054 | 1/1   | 0.92 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3170 | 1/1   | 0.92 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3537 | 1/1   | 0.92 | 0.12 | 21,21,21,21                 | 0     |
| 56  | MG   | BA    | 3538 | 1/1   | 0.92 | 0.10 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3545 | 1/1   | 0.92 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | AA    | 3030 | 1/1   | 0.92 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 3551 | 1/1   | 0.92 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3246 | 1/1   | 0.92 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3501 | 1/1   | 0.92 | 0.08 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3247 | 1/1   | 0.92 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3504 | 1/1   | 0.92 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3192 | 1/1   | 0.92 | 0.08 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3559 | 1/1   | 0.92 | 0.08 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3144 | 1/1   | 0.92 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3513 | 1/1   | 0.92 | 0.08 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3251 | 1/1   | 0.92 | 0.32 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3252 | 1/1   | 0.92 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 3064 | 1/1   | 0.92 | 0.07 | 54,54,54,54                 | 0     |
| 56  | MG   | CA    | 3120 | 1/1   | 0.92 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | BF    | 306  | 1/1   | 0.92 | 0.20 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3213 | 1/1   | 0.92 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | BG    | 3002 | 1/1   | 0.92 | 0.08 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3215 | 1/1   | 0.92 | 0.31 | 49,49,49,49                 | 0     |
| 56  | MG   | BN    | 3002 | 1/1   | 0.92 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3572 | 1/1   | 0.92 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3401 | 1/1   | 0.92 | 0.15 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3545 | 1/1   | 0.92 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3151 | 1/1   | 0.92 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3417 | 1/1   | 0.92 | 0.13 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3419 | 1/1   | 0.92 | 0.09 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3554 | 1/1   | 0.92 | 0.13 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3230 | 1/1   | 0.92 | 0.21 | 52,52,52,52                 | 0     |
| 56  | MG   | BZ    | 302  | 1/1   | 0.92 | 0.23 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3256 | 1/1   | 0.92 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3236 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3564 | 1/1   | 0.92 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3157 | 1/1   | 0.92 | 0.39 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3566 | 1/1   | 0.92 | 0.11 | 62,62,62,62                 | 0     |
| 56  | MG   | AA    | 3129 | 1/1   | 0.92 | 0.14 | 70,70,70,70                 | 0     |
| 56  | MG   | DA    | 3568 | 1/1   | 0.92 | 0.08 | 66,66,66,66                 | 0     |
| 56  | MG   | B5    | 101  | 1/1   | 0.92 | 0.25 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3243 | 1/1   | 0.92 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3244 | 1/1   | 0.92 | 0.30 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3062 | 1/1   | 0.92 | 0.09 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3577 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 3154 | 1/1   | 0.92 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | CA    | 3002 | 1/1   | 0.92 | 0.14 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3584 | 1/1   | 0.92 | 0.12 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3168 | 1/1   | 0.92 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3258 | 1/1   | 0.92 | 0.32 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3594 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3597 | 1/1   | 0.92 | 0.07 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3259 | 1/1   | 0.92 | 0.30 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3439 | 1/1   | 0.92 | 0.10 | 71,71,71,71                 | 0     |
| 56  | MG   | DA    | 3605 | 1/1   | 0.92 | 0.10 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3172 | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3008 | 1/1   | 0.92 | 0.40 | 60,60,60,60                 | 0     |
| 56  | MG   | CA    | 3153 | 1/1   | 0.92 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | AA    | 3176 | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | CA    | 3157 | 1/1   | 0.92 | 0.19 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3046 | 1/1   | 0.92 | 0.27 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3134 | 1/1   | 0.92 | 0.10 | 65,65,65,65                 | 0     |
| 56  | MG   | AA    | 3103 | 1/1   | 0.92 | 0.20 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3192 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3625 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3016 | 1/1   | 0.92 | 0.21 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3291 | 1/1   | 0.92 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3726 | 1/1   | 0.92 | 0.17 | 65,65,65,65                 | 0     |
| 56  | MG   | AA    | 3092 | 1/1   | 0.92 | 0.36 | 54,54,54,54                 | 0     |
| 56  | MG   | CA    | 3024 | 1/1   | 0.92 | 0.23 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3100 | 1/1   | 0.92 | 0.27 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3026 | 1/1   | 0.92 | 0.18 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3029 | 1/1   | 0.92 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3611 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3638 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3026 | 1/1   | 0.92 | 0.17 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3613 | 1/1   | 0.92 | 0.19 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3039 | 1/1   | 0.92 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3645 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3002 | 1/1   | 0.92 | 0.19 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3325 | 1/1   | 0.92 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3006 | 1/1   | 0.92 | 0.40 | 58,58,58,58                 | 0     |
| 56  | MG   | CA    | 3040 | 1/1   | 0.92 | 0.15 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3614 | 1/1   | 0.92 | 0.30 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3197 | 1/1   | 0.92 | 0.25 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3739 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3026 | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3616 | 1/1   | 0.92 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3478 | 1/1   | 0.92 | 0.13 | 59,59,59,59                 | 0     |
| 56  | MG   | AA    | 3015 | 1/1   | 0.92 | 0.07 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3360 | 1/1   | 0.92 | 0.14 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3036 | 1/1   | 0.92 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3051 | 1/1   | 0.92 | 0.32 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3367 | 1/1   | 0.92 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3043 | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | DB    | 3003 | 1/1   | 0.92 | 0.10 | 56,56,56,56                 | 0     |
| 56  | MG   | DB    | 3004 | 1/1   | 0.92 | 0.20 | 53,53,53,53                 | 0     |
| 56  | MG   | DB    | 3006 | 1/1   | 0.92 | 0.26 | 60,60,60,60                 | 0     |
| 56  | MG   | AA    | 3106 | 1/1   | 0.92 | 0.09 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3372 | 1/1   | 0.92 | 0.09 | 24,24,24,24                 | 0     |
| 56  | MG   | AA    | 3079 | 1/1   | 0.92 | 0.33 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3052 | 1/1   | 0.92 | 0.05 | 26,26,26,26                 | 0     |
| 56  | MG   | DD    | 306  | 1/1   | 0.92 | 0.46 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3385 | 1/1   | 0.92 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | DA    | 3054 | 1/1   | 0.92 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3496 | 1/1   | 0.92 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DO    | 5001 | 1/1   | 0.92 | 0.18 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3055 | 1/1   | 0.92 | 0.23 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3061 | 1/1   | 0.92 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | DR    | 5001 | 1/1   | 0.92 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | DU    | 3001 | 1/1   | 0.92 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | DU    | 3004 | 1/1   | 0.92 | 0.18 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3393 | 1/1   | 0.92 | 0.07 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3750 | 1/1   | 0.92 | 0.16 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3629 | 1/1   | 0.92 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | DW    | 202  | 1/1   | 0.92 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3344 | 1/1   | 0.92 | 0.23 | 55,55,55,55                 | 0     |
| 56  | MG   | D1    | 101  | 1/1   | 0.92 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | D8    | 5001 | 1/1   | 0.92 | 0.18 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3070 | 1/1   | 0.92 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3073 | 1/1   | 0.92 | 0.25 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3074 | 1/1   | 0.92 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3485 | 1/1   | 0.93 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3148 | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3444 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3121 | 1/1   | 0.93 | 0.09 | 81,81,81,81                 | 0     |
| 56  | MG   | BA    | 3366 | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3163 | 1/1   | 0.93 | 0.21 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3166 | 1/1   | 0.93 | 0.17 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3190 | 1/1   | 0.93 | 0.19 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3191 | 1/1   | 0.93 | 0.18 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3457 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3172 | 1/1   | 0.93 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | CA    | 3001 | 1/1   | 0.93 | 0.08 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3180 | 1/1   | 0.93 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3375 | 1/1   | 0.93 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3467 | 1/1   | 0.93 | 0.25 | 48,48,48,48                 | 0     |
| 56  | MG   | AA    | 3006 | 1/1   | 0.93 | 0.10 | 71,71,71,71                 | 0     |
| 56  | MG   | DA    | 3470 | 1/1   | 0.93 | 0.15 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3257 | 1/1   | 0.93 | 0.24 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3002 | 1/1   | 0.93 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3018 | 1/1   | 0.93 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | AA    | 3101 | 1/1   | 0.93 | 0.18 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3191 | 1/1   | 0.93 | 0.18 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3485 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3486 | 1/1   | 0.93 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | CA    | 3135 | 1/1   | 0.93 | 0.16 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3193 | 1/1   | 0.93 | 0.20 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3491 | 1/1   | 0.93 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3136 | 1/1   | 0.93 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3195 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3497 | 1/1   | 0.93 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3198 | 1/1   | 0.93 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3065 | 1/1   | 0.93 | 0.19 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3519 | 1/1   | 0.93 | 0.20 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3276 | 1/1   | 0.93 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3508 | 1/1   | 0.93 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3509 | 1/1   | 0.93 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3203 | 1/1   | 0.93 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3523 | 1/1   | 0.93 | 0.17 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3014 | 1/1   | 0.93 | 0.25 | 62,62,62,62                 | 0     |
| 56  | MG   | CA    | 3146 | 1/1   | 0.93 | 0.18 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3025 | 1/1   | 0.93 | 0.19 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3518 | 1/1   | 0.93 | 0.15 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3398 | 1/1   | 0.93 | 0.11 | 51,51,51,51                 | 0     |
| 56  | MG   | CA    | 3022 | 1/1   | 0.93 | 0.30 | 60,60,60,60                 | 0     |
| 56  | MG   | CA    | 3023 | 1/1   | 0.93 | 0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3220 | 1/1   | 0.93 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3536 | 1/1   | 0.93 | 0.11 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3637 | 1/1   | 0.93 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | CA    | 3154 | 1/1   | 0.93 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3638 | 1/1   | 0.93 | 0.18 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3028 | 1/1   | 0.93 | 0.27 | 55,55,55,55                 | 0     |
| 56  | MG   | AA    | 3044 | 1/1   | 0.93 | 0.34 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3544 | 1/1   | 0.93 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3231 | 1/1   | 0.93 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3640 | 1/1   | 0.93 | 0.11 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3031 | 1/1   | 0.93 | 0.14 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3150 | 1/1   | 0.93 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3034 | 1/1   | 0.93 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3539 | 1/1   | 0.93 | 0.12 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3241 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3561 | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 56  | MG   | CA    | 3165 | 1/1   | 0.93 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | CA    | 3038 | 1/1   | 0.93 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | BA    | 3764 | 1/1   | 0.93 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3248 | 1/1   | 0.93 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3541 | 1/1   | 0.93 | 0.15 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3250 | 1/1   | 0.93 | 0.21 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3544 | 1/1   | 0.93 | 0.16 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3175 | 1/1   | 0.93 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3410 | 1/1   | 0.93 | 0.16 | 31,31,31,31                 | 0     |
| 56  | MG   | AA    | 3081 | 1/1   | 0.93 | 0.22 | 51,51,51,51                 | 0     |
| 56  | MG   | AE    | 203  | 1/1   | 0.93 | 0.24 | 73,73,73,73                 | 0     |
| 56  | MG   | DA    | 3576 | 1/1   | 0.93 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3651 | 1/1   | 0.93 | 0.07 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3580 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3262 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3048 | 1/1   | 0.93 | 0.13 | 77,77,77,77                 | 0     |
| 56  | MG   | AA    | 3062 | 1/1   | 0.93 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3586 | 1/1   | 0.93 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | CA    | 3050 | 1/1   | 0.93 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3011 | 1/1   | 0.93 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3593 | 1/1   | 0.93 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | AQ    | 3001 | 1/1   | 0.93 | 0.20 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3780 | 1/1   | 0.93 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3297 | 1/1   | 0.93 | 0.22 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3786 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3285 | 1/1   | 0.93 | 0.25 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3024 | 1/1   | 0.93 | 0.37 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3787 | 1/1   | 0.93 | 0.20 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3307 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3292 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3660 | 1/1   | 0.93 | 0.18 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3615 | 1/1   | 0.93 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3662 | 1/1   | 0.93 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3430 | 1/1   | 0.93 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | AA    | 3032 | 1/1   | 0.93 | 0.26 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3039 | 1/1   | 0.93 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3668 | 1/1   | 0.93 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3318 | 1/1   | 0.93 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3166 | 1/1   | 0.93 | 0.16 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3233 | 1/1   | 0.93 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3135 | 1/1   | 0.93 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3053 | 1/1   | 0.93 | 0.19 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3238 | 1/1   | 0.93 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3056 | 1/1   | 0.93 | 0.21 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3445 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3446 | 1/1   | 0.93 | 0.10 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3060 | 1/1   | 0.93 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3169 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3340 | 1/1   | 0.93 | 0.06 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3342 | 1/1   | 0.93 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3644 | 1/1   | 0.93 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3067 | 1/1   | 0.93 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3046 | 1/1   | 0.93 | 0.15 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3069 | 1/1   | 0.93 | 0.16 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3586 | 1/1   | 0.93 | 0.11 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3362 | 1/1   | 0.93 | 0.20 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3071 | 1/1   | 0.93 | 0.09 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3653 | 1/1   | 0.93 | 0.18 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3696 | 1/1   | 0.93 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3351 | 1/1   | 0.93 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3588 | 1/1   | 0.93 | 0.06 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3077 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3659 | 1/1   | 0.93 | 0.18 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3662 | 1/1   | 0.93 | 0.11 | 38,38,38,38                 | 0     |
| 56  | MG   | BF    | 302  | 1/1   | 0.93 | 0.27 | 56,56,56,56                 | 0     |
| 56  | MG   | BF    | 303  | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3353 | 1/1   | 0.93 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3379 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3672 | 1/1   | 0.93 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3459 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3387 | 1/1   | 0.93 | 0.13 | 39,39,39,39                 | 0     |
| 56  | MG   | BF    | 309  | 1/1   | 0.93 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3094 | 1/1   | 0.93 | 0.22 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3097 | 1/1   | 0.93 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | DB    | 3005 | 1/1   | 0.93 | 0.22 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3460 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | AA    | 3107 | 1/1   | 0.93 | 0.19 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3102 | 1/1   | 0.93 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | BN    | 3007 | 1/1   | 0.93 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3178 | 1/1   | 0.93 | 0.33 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3097 | 1/1   | 0.93 | 0.12 | 64,64,64,64                 | 0     |
| 56  | MG   | BA    | 3473 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3411 | 1/1   | 0.93 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | BR    | 201  | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3113 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3712 | 1/1   | 0.93 | 0.21 | 29,29,29,29                 | 0     |
| 56  | MG   | CA    | 3104 | 1/1   | 0.93 | 0.08 | 60,60,60,60                 | 0     |
| 56  | MG   | CA    | 3105 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3122 | 1/1   | 0.93 | 0.22 | 53,53,53,53                 | 0     |
| 56  | MG   | DU    | 3003 | 1/1   | 0.93 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3714 | 1/1   | 0.93 | 0.12 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3126 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3603 | 1/1   | 0.93 | 0.19 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3113 | 1/1   | 0.93 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3115 | 1/1   | 0.93 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | AA    | 3027 | 1/1   | 0.93 | 0.16 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3119 | 1/1   | 0.93 | 0.13 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3436 | 1/1   | 0.93 | 0.10 | 70,70,70,70                 | 0     |
| 56  | MG   | DA    | 3142 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3113 | 1/1   | 0.93 | 0.18 | 67,67,67,67                 | 0     |
| 59  | ZN   | B5    | 104  | 1/1   | 0.93 | 0.10 | 82,82,82,82                 | 0     |
| 56  | MG   | DA    | 3440 | 1/1   | 0.93 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3023 | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | CA    | 3069 | 1/1   | 0.94 | 0.17 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3025 | 1/1   | 0.94 | 0.26 | 52,52,52,52                 | 0     |
| 56  | MG   | CA    | 3071 | 1/1   | 0.94 | 0.15 | 57,57,57,57                 | 0     |
| 56  | MG   | AA    | 3005 | 1/1   | 0.94 | 0.37 | 77,77,77,77                 | 0     |
| 56  | MG   | AN    | 502  | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | CA    | 3074 | 1/1   | 0.94 | 0.22 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3035 | 1/1   | 0.94 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3308 | 1/1   | 0.94 | 0.15 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3099 | 1/1   | 0.94 | 0.21 | 67,67,67,67                 | 0     |
| 56  | MG   | BA    | 3412 | 1/1   | 0.94 | 0.18 | 19,19,19,19                 | 0     |
| 56  | MG   | DA    | 3041 | 1/1   | 0.94 | 0.21 | 56,56,56,56                 | 0     |
| 56  | MG   | BF    | 305  | 1/1   | 0.94 | 0.06 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3506 | 1/1   | 0.94 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3620 | 1/1   | 0.94 | 0.17 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3621 | 1/1   | 0.94 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3252 | 1/1   | 0.94 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3051 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3034 | 1/1   | 0.94 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3101 | 1/1   | 0.94 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3514 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | AA    | 3178 | 1/1   | 0.94 | 0.12 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3055 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3106 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3630 | 1/1   | 0.94 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3263 | 1/1   | 0.94 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 3112 | 1/1   | 0.94 | 0.13 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3327 | 1/1   | 0.94 | 0.11 | 37,37,37,37                 | 0     |
| 56  | MG   | BU    | 204  | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3269 | 1/1   | 0.94 | 0.21 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3271 | 1/1   | 0.94 | 0.21 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3540 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3274 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3331 | 1/1   | 0.94 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | BV    | 204  | 1/1   | 0.94 | 0.18 | 47,47,47,47                 | 0     |
| 56  | MG   | BW    | 201  | 1/1   | 0.94 | 0.19 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3336 | 1/1   | 0.94 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3281 | 1/1   | 0.94 | 0.11 | 49,49,49,49                 | 0     |
| 56  | MG   | AA    | 3133 | 1/1   | 0.94 | 0.08 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3548 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | B0    | 103  | 1/1   | 0.94 | 0.11 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3557 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3558 | 1/1   | 0.94 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3072 | 1/1   | 0.94 | 0.23 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3560 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3068 | 1/1   | 0.94 | 0.34 | 62,62,62,62                 | 0     |
| 56  | MG   | B2    | 3001 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3047 | 1/1   | 0.94 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3187 | 1/1   | 0.94 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3296 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3300 | 1/1   | 0.94 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3642 | 1/1   | 0.94 | 0.08 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3308 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3080 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3108 | 1/1   | 0.94 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3113 | 1/1   | 0.94 | 0.14 | 39,39,39,39                 | 0     |
| 56  | MG   | B8    | 101  | 1/1   | 0.94 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3090 | 1/1   | 0.94 | 0.20 | 48,48,48,48                 | 0     |
| 56  | MG   | AA    | 3115 | 1/1   | 0.94 | 0.22 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3578 | 1/1   | 0.94 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3562 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 3119 | 1/1   | 0.94 | 0.06 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3647 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | CA    | 3119 | 1/1   | 0.94 | 0.14 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3585 | 1/1   | 0.94 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3751 | 1/1   | 0.94 | 0.08 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3358 | 1/1   | 0.94 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3333 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3337 | 1/1   | 0.94 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3104 | 1/1   | 0.94 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3454 | 1/1   | 0.94 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3340 | 1/1   | 0.94 | 0.07 | 30,30,30,30                 | 0     |
| 56  | MG   | AA    | 3009 | 1/1   | 0.94 | 0.08 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3258 | 1/1   | 0.94 | 0.28 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3761 | 1/1   | 0.94 | 0.21 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3111 | 1/1   | 0.94 | 0.07 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3126 | 1/1   | 0.94 | 0.08 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3357 | 1/1   | 0.94 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3610 | 1/1   | 0.94 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3611 | 1/1   | 0.94 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3358 | 1/1   | 0.94 | 0.08 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3763 | 1/1   | 0.94 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | CA    | 3015 | 1/1   | 0.94 | 0.17 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3617 | 1/1   | 0.94 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3619 | 1/1   | 0.94 | 0.12 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3361 | 1/1   | 0.94 | 0.11 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3622 | 1/1   | 0.94 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | CA    | 3017 | 1/1   | 0.94 | 0.12 | 76,76,76,76                 | 0     |
| 56  | MG   | BA    | 3765 | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3133 | 1/1   | 0.94 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3577 | 1/1   | 0.94 | 0.17 | 18,18,18,18                 | 0     |
| 56  | MG   | AA    | 3082 | 1/1   | 0.94 | 0.33 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3628 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3006 | 1/1   | 0.94 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3264 | 1/1   | 0.94 | 0.22 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3582 | 1/1   | 0.94 | 0.12 | 19,19,19,19                 | 0     |
| 56  | MG   | DA    | 3381 | 1/1   | 0.94 | 0.07 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3141 | 1/1   | 0.94 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3016 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3372 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3476 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3373 | 1/1   | 0.94 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | AA    | 3093 | 1/1   | 0.94 | 0.23 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3785 | 1/1   | 0.94 | 0.13 | 81,81,81,81                 | 0     |
| 56  | MG   | DA    | 3156 | 1/1   | 0.94 | 0.25 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3158 | 1/1   | 0.94 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | CA    | 3033 | 1/1   | 0.94 | 0.16 | 60,60,60,60                 | 0     |
| 56  | MG   | DA    | 3647 | 1/1   | 0.94 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3164 | 1/1   | 0.94 | 0.24 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3376 | 1/1   | 0.94 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3408 | 1/1   | 0.94 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3651 | 1/1   | 0.94 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3409 | 1/1   | 0.94 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3480 | 1/1   | 0.94 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | CA    | 3037 | 1/1   | 0.94 | 0.18 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | AA    | 3172 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3173 | 1/1   | 0.94 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3593 | 1/1   | 0.94 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3177 | 1/1   | 0.94 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3179 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 56  | MG   | CA    | 3156 | 1/1   | 0.94 | 0.13 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3683 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3425 | 1/1   | 0.94 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3668 | 1/1   | 0.94 | 0.55 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3489 | 1/1   | 0.94 | 0.25 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3183 | 1/1   | 0.94 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3206 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3674 | 1/1   | 0.94 | 0.23 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3798 | 1/1   | 0.94 | 0.07 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3799 | 1/1   | 0.94 | 0.27 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3050 | 1/1   | 0.94 | 0.09 | 77,77,77,77                 | 0     |
| 56  | MG   | DA    | 3189 | 1/1   | 0.94 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3801 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3439 | 1/1   | 0.94 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3382 | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3599 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3281 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3071 | 1/1   | 0.94 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3197 | 1/1   | 0.94 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | DD    | 307  | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3217 | 1/1   | 0.94 | 0.13 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3080 | 1/1   | 0.94 | 0.26 | 51,51,51,51                 | 0     |
| 56  | MG   | DE    | 304  | 1/1   | 0.94 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3509 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 56  | MG   | CE    | 202  | 1/1   | 0.94 | 0.08 | 74,74,74,74                 | 0     |
| 56  | MG   | CA    | 3056 | 1/1   | 0.94 | 0.15 | 60,60,60,60                 | 0     |
| 56  | MG   | BB    | 210  | 1/1   | 0.94 | 0.23 | 55,55,55,55                 | 0     |
| 56  | MG   | DQ    | 3003 | 1/1   | 0.94 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3702 | 1/1   | 0.94 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | AE    | 201  | 1/1   | 0.94 | 0.34 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3461 | 1/1   | 0.94 | 0.16 | 57,57,57,57                 | 0     |
| 56  | MG   | DA    | 3463 | 1/1   | 0.94 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | BB    | 217  | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3003 | 1/1   | 0.94 | 0.18 | 48,48,48,48                 | 0     |
| 56  | MG   | AA    | 3128 | 1/1   | 0.94 | 0.10 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3468 | 1/1   | 0.94 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | AA    | 3160 | 1/1   | 0.94 | 0.18 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | CA    | 3064 | 1/1   | 0.94 | 0.18 | 59,59,59,59                 | 0     |
| 56  | MG   | CA    | 3066 | 1/1   | 0.94 | 0.15 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3707 | 1/1   | 0.94 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3018 | 1/1   | 0.94 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3481 | 1/1   | 0.94 | 0.07 | 24,24,24,24                 | 0     |
| 59  | ZN   | D4    | 501  | 1/1   | 0.94 | 0.07 | 151,151,151,151             | 0     |
| 56  | MG   | BD    | 3306 | 1/1   | 0.94 | 0.19 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3367 | 1/1   | 0.95 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | BB    | 218  | 1/1   | 0.95 | 0.07 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3434 | 1/1   | 0.95 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3143 | 1/1   | 0.95 | 0.27 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3077 | 1/1   | 0.95 | 0.21 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3369 | 1/1   | 0.95 | 0.11 | 40,40,40,40                 | 0     |
| 56  | MG   | CA    | 3106 | 1/1   | 0.95 | 0.07 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3526 | 1/1   | 0.95 | 0.11 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3151 | 1/1   | 0.95 | 0.09 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3441 | 1/1   | 0.95 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | BD    | 3304 | 1/1   | 0.95 | 0.07 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3153 | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3154 | 1/1   | 0.95 | 0.20 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3153 | 1/1   | 0.95 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3157 | 1/1   | 0.95 | 0.13 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3447 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 56  | MG   | BD    | 3307 | 1/1   | 0.95 | 0.27 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3160 | 1/1   | 0.95 | 0.20 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3530 | 1/1   | 0.95 | 0.12 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3532 | 1/1   | 0.95 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3165 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | BF    | 301  | 1/1   | 0.95 | 0.18 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3533 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3169 | 1/1   | 0.95 | 0.21 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3670 | 1/1   | 0.95 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3110 | 1/1   | 0.95 | 0.17 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3024 | 1/1   | 0.95 | 0.17 | 45,45,45,45                 | 0     |
| 56  | MG   | AA    | 3190 | 1/1   | 0.95 | 0.11 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3176 | 1/1   | 0.95 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | BF    | 308  | 1/1   | 0.95 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3178 | 1/1   | 0.95 | 0.07 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3471 | 1/1   | 0.95 | 0.18 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3675 | 1/1   | 0.95 | 0.15 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3474 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3477 | 1/1   | 0.95 | 0.06 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BG    | 3001 | 1/1   | 0.95 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3676 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3088 | 1/1   | 0.95 | 0.14 | 49,49,49,49                 | 0     |
| 56  | MG   | BN    | 3004 | 1/1   | 0.95 | 0.20 | 61,61,61,61                 | 0     |
| 56  | MG   | BN    | 3006 | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3148 | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3679 | 1/1   | 0.95 | 0.29 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3093 | 1/1   | 0.95 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3188 | 1/1   | 0.95 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | BP    | 204  | 1/1   | 0.95 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3380 | 1/1   | 0.95 | 0.05 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3094 | 1/1   | 0.95 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | BU    | 202  | 1/1   | 0.95 | 0.06 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3171 | 1/1   | 0.95 | 0.17 | 54,54,54,54                 | 0     |
| 56  | MG   | BU    | 205  | 1/1   | 0.95 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3088 | 1/1   | 0.95 | 0.18 | 42,42,42,42                 | 0     |
| 56  | MG   | BV    | 203  | 1/1   | 0.95 | 0.20 | 31,31,31,31                 | 0     |
| 56  | MG   | CA    | 3145 | 1/1   | 0.95 | 0.10 | 68,68,68,68                 | 0     |
| 56  | MG   | DA    | 3507 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3549 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3385 | 1/1   | 0.95 | 0.20 | 41,41,41,41                 | 0     |
| 56  | MG   | BY    | 202  | 1/1   | 0.95 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3209 | 1/1   | 0.95 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | BY    | 204  | 1/1   | 0.95 | 0.26 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3695 | 1/1   | 0.95 | 0.11 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3554 | 1/1   | 0.95 | 0.09 | 24,24,24,24                 | 0     |
| 56  | MG   | DA    | 3516 | 1/1   | 0.95 | 0.07 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3386 | 1/1   | 0.95 | 0.16 | 47,47,47,47                 | 0     |
| 56  | MG   | B0    | 102  | 1/1   | 0.95 | 0.15 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3519 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 56  | MG   | DA    | 3520 | 1/1   | 0.95 | 0.05 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3521 | 1/1   | 0.95 | 0.14 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3557 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3260 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3219 | 1/1   | 0.95 | 0.10 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3530 | 1/1   | 0.95 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3089 | 1/1   | 0.95 | 0.28 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3176 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3394 | 1/1   | 0.95 | 0.05 | 20,20,20,20                 | 0     |
| 56  | MG   | DA    | 3535 | 1/1   | 0.95 | 0.09 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3224 | 1/1   | 0.95 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | B5    | 102  | 1/1   | 0.95 | 0.15 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | B5    | 103  | 1/1   | 0.95 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3563 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3098 | 1/1   | 0.95 | 0.15 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3269 | 1/1   | 0.95 | 0.22 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3166 | 1/1   | 0.95 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3546 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3167 | 1/1   | 0.95 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3709 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 56  | MG   | DA    | 3237 | 1/1   | 0.95 | 0.05 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3569 | 1/1   | 0.95 | 0.20 | 56,56,56,56                 | 0     |
| 56  | MG   | AA    | 3152 | 1/1   | 0.95 | 0.07 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3032 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3573 | 1/1   | 0.95 | 0.08 | 24,24,24,24                 | 0     |
| 56  | MG   | AA    | 3090 | 1/1   | 0.95 | 0.19 | 41,41,41,41                 | 0     |
| 56  | MG   | AA    | 3065 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3245 | 1/1   | 0.95 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3105 | 1/1   | 0.95 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3282 | 1/1   | 0.95 | 0.23 | 41,41,41,41                 | 0     |
| 56  | MG   | CA    | 3012 | 1/1   | 0.95 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3283 | 1/1   | 0.95 | 0.07 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3254 | 1/1   | 0.95 | 0.18 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3001 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3722 | 1/1   | 0.95 | 0.07 | 17,17,17,17                 | 0     |
| 56  | MG   | BA    | 3286 | 1/1   | 0.95 | 0.26 | 41,41,41,41                 | 0     |
| 56  | MG   | AA    | 3013 | 1/1   | 0.95 | 0.12 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3041 | 1/1   | 0.95 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3424 | 1/1   | 0.95 | 0.11 | 55,55,55,55                 | 0     |
| 56  | MG   | CA    | 3020 | 1/1   | 0.95 | 0.18 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3016 | 1/1   | 0.95 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | AA    | 3123 | 1/1   | 0.95 | 0.12 | 51,51,51,51                 | 0     |
| 56  | MG   | AA    | 3003 | 1/1   | 0.95 | 0.12 | 63,63,63,63                 | 0     |
| 56  | MG   | DA    | 3267 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | AX    | 3005 | 1/1   | 0.95 | 0.24 | 64,64,64,64                 | 0     |
| 56  | MG   | AA    | 3023 | 1/1   | 0.95 | 0.27 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3270 | 1/1   | 0.95 | 0.39 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3114 | 1/1   | 0.95 | 0.13 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3273 | 1/1   | 0.95 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3300 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 56  | MG   | DA    | 3592 | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3200 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3277 | 1/1   | 0.95 | 0.25 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3030 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3031 | 1/1   | 0.95 | 0.24 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3600 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3602 | 1/1   | 0.95 | 0.08 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3117 | 1/1   | 0.95 | 0.22 | 35,35,35,35                 | 0     |
| 56  | MG   | AA    | 3159 | 1/1   | 0.95 | 0.10 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3742 | 1/1   | 0.95 | 0.15 | 21,21,21,21                 | 0     |
| 56  | MG   | DA    | 3283 | 1/1   | 0.95 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3207 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3449 | 1/1   | 0.95 | 0.11 | 32,32,32,32                 | 0     |
| 56  | MG   | DA    | 3287 | 1/1   | 0.95 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | AA    | 3028 | 1/1   | 0.95 | 0.20 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3214 | 1/1   | 0.95 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3614 | 1/1   | 0.95 | 0.16 | 61,61,61,61                 | 0     |
| 56  | MG   | AA    | 3161 | 1/1   | 0.95 | 0.19 | 59,59,59,59                 | 0     |
| 56  | MG   | AA    | 3143 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3323 | 1/1   | 0.95 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3618 | 1/1   | 0.95 | 0.06 | 64,64,64,64                 | 0     |
| 56  | MG   | BA    | 3324 | 1/1   | 0.95 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3620 | 1/1   | 0.95 | 0.15 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3297 | 1/1   | 0.95 | 0.11 | 24,24,24,24                 | 0     |
| 56  | MG   | DA    | 3047 | 1/1   | 0.95 | 0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3304 | 1/1   | 0.95 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3048 | 1/1   | 0.95 | 0.21 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3049 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3756 | 1/1   | 0.95 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3758 | 1/1   | 0.95 | 0.11 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3313 | 1/1   | 0.95 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3610 | 1/1   | 0.95 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | AA    | 3086 | 1/1   | 0.95 | 0.19 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3330 | 1/1   | 0.95 | 0.10 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3127 | 1/1   | 0.95 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3633 | 1/1   | 0.95 | 0.07 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3128 | 1/1   | 0.95 | 0.07 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3467 | 1/1   | 0.95 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3636 | 1/1   | 0.95 | 0.19 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3472 | 1/1   | 0.95 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3337 | 1/1   | 0.95 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3338 | 1/1   | 0.95 | 0.21 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3327 | 1/1   | 0.95 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3642 | 1/1   | 0.95 | 0.06 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3328 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3769 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3332 | 1/1   | 0.95 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3224 | 1/1   | 0.95 | 0.22 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3130 | 1/1   | 0.95 | 0.22 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3227 | 1/1   | 0.95 | 0.08 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3777 | 1/1   | 0.95 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3346 | 1/1   | 0.95 | 0.08 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3483 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3348 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |
| 56  | MG   | BA    | 3014 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3783 | 1/1   | 0.95 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | CA    | 3065 | 1/1   | 0.95 | 0.21 | 64,64,64,64                 | 0     |
| 56  | MG   | DA    | 3353 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3355 | 1/1   | 0.95 | 0.12 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3078 | 1/1   | 0.95 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3490 | 1/1   | 0.95 | 0.10 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3491 | 1/1   | 0.95 | 0.12 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3081 | 1/1   | 0.95 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3352 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3494 | 1/1   | 0.95 | 0.05 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3070 | 1/1   | 0.95 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3671 | 1/1   | 0.95 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3790 | 1/1   | 0.95 | 0.17 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3635 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3134 | 1/1   | 0.95 | 0.16 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3096 | 1/1   | 0.95 | 0.17 | 48,48,48,48                 | 0     |
| 56  | MG   | AA    | 3164 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3234 | 1/1   | 0.95 | 0.19 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3499 | 1/1   | 0.95 | 0.10 | 19,19,19,19                 | 0     |
| 56  | MG   | DA    | 3382 | 1/1   | 0.95 | 0.06 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3501 | 1/1   | 0.95 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3502 | 1/1   | 0.95 | 0.05 | 20,20,20,20                 | 0     |
| 56  | MG   | BA    | 3357 | 1/1   | 0.95 | 0.09 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3105 | 1/1   | 0.95 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | AA    | 3145 | 1/1   | 0.95 | 0.12 | 65,65,65,65                 | 0     |
| 56  | MG   | DD    | 303  | 1/1   | 0.95 | 0.17 | 51,51,51,51                 | 0     |
| 56  | MG   | AA    | 3072 | 1/1   | 0.95 | 0.21 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3808 | 1/1   | 0.95 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3507 | 1/1   | 0.95 | 0.18 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3814 | 1/1   | 0.95 | 0.16 | 42,42,42,42                 | 0     |
| 56  | MG   | DE    | 303  | 1/1   | 0.95 | 0.13 | 62,62,62,62                 | 0     |
| 56  | MG   | BA    | 3240 | 1/1   | 0.95 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | DE    | 305  | 1/1   | 0.95 | 0.14 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DF    | 301  | 1/1   | 0.95 | 0.26 | 47,47,47,47                 | 0     |
| 56  | MG   | DF    | 303  | 1/1   | 0.95 | 0.05 | 52,52,52,52                 | 0     |
| 56  | MG   | DF    | 305  | 1/1   | 0.95 | 0.17 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3114 | 1/1   | 0.95 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | DN    | 5001 | 1/1   | 0.95 | 0.06 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3403 | 1/1   | 0.95 | 0.08 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3404 | 1/1   | 0.95 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | BB    | 202  | 1/1   | 0.95 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | BB    | 203  | 1/1   | 0.95 | 0.16 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3072 | 1/1   | 0.95 | 0.08 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3410 | 1/1   | 0.95 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3362 | 1/1   | 0.95 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | BB    | 207  | 1/1   | 0.95 | 0.17 | 39,39,39,39                 | 0     |
| 56  | MG   | DV    | 3001 | 1/1   | 0.95 | 0.10 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3073 | 1/1   | 0.95 | 0.23 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3416 | 1/1   | 0.95 | 0.06 | 22,22,22,22                 | 0     |
| 56  | MG   | BA    | 3245 | 1/1   | 0.95 | 0.14 | 61,61,61,61                 | 0     |
| 56  | MG   | CA    | 3095 | 1/1   | 0.95 | 0.11 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3130 | 1/1   | 0.95 | 0.21 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3520 | 1/1   | 0.95 | 0.09 | 50,50,50,50                 | 0     |
| 56  | MG   | D3    | 3001 | 1/1   | 0.95 | 0.13 | 60,60,60,60                 | 0     |
| 56  | MG   | BB    | 212  | 1/1   | 0.95 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3133 | 1/1   | 0.95 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3134 | 1/1   | 0.95 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3655 | 1/1   | 0.95 | 0.12 | 54,54,54,54                 | 0     |
| 59  | ZN   | B6    | 103  | 1/1   | 0.95 | 0.06 | 62,62,62,62                 | 0     |
| 59  | ZN   | CN    | 501  | 1/1   | 0.95 | 0.07 | 103,103,103,103             | 0     |
| 56  | MG   | DA    | 3429 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3140 | 1/1   | 0.95 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | BQ    | 201  | 1/1   | 0.96 | 0.15 | 35,35,35,35                 | 0     |
| 56  | MG   | CA    | 3141 | 1/1   | 0.96 | 0.14 | 53,53,53,53                 | 0     |
| 56  | MG   | BQ    | 203  | 1/1   | 0.96 | 0.11 | 36,36,36,36                 | 0     |
| 56  | MG   | BQ    | 204  | 1/1   | 0.96 | 0.15 | 43,43,43,43                 | 0     |
| 56  | MG   | AA    | 3058 | 1/1   | 0.96 | 0.12 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3451 | 1/1   | 0.96 | 0.10 | 20,20,20,20                 | 0     |
| 56  | MG   | BA    | 3035 | 1/1   | 0.96 | 0.11 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3390 | 1/1   | 0.96 | 0.08 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3701 | 1/1   | 0.96 | 0.10 | 20,20,20,20                 | 0     |
| 56  | MG   | DA    | 3456 | 1/1   | 0.96 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3391 | 1/1   | 0.96 | 0.06 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3267 | 1/1   | 0.96 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | CA    | 3150 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BU    | 208  | 1/1   | 0.96 | 0.15 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3268 | 1/1   | 0.96 | 0.29 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3705 | 1/1   | 0.96 | 0.18 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3170 | 1/1   | 0.96 | 0.35 | 52,52,52,52                 | 0     |
| 56  | MG   | BW    | 202  | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 56  | MG   | BY    | 201  | 1/1   | 0.96 | 0.07 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3271 | 1/1   | 0.96 | 0.17 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3196 | 1/1   | 0.96 | 0.20 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3565 | 1/1   | 0.96 | 0.04 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3038 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3199 | 1/1   | 0.96 | 0.21 | 55,55,55,55                 | 0     |
| 56  | MG   | AA    | 3069 | 1/1   | 0.96 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3713 | 1/1   | 0.96 | 0.13 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3568 | 1/1   | 0.96 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3480 | 1/1   | 0.96 | 0.05 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3174 | 1/1   | 0.96 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3204 | 1/1   | 0.96 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3483 | 1/1   | 0.96 | 0.11 | 32,32,32,32                 | 0     |
| 56  | MG   | DA    | 3205 | 1/1   | 0.96 | 0.18 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3207 | 1/1   | 0.96 | 0.23 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3208 | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3403 | 1/1   | 0.96 | 0.04 | 22,22,22,22                 | 0     |
| 56  | MG   | AX    | 3008 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | AA    | 3045 | 1/1   | 0.96 | 0.31 | 54,54,54,54                 | 0     |
| 56  | MG   | AA    | 3083 | 1/1   | 0.96 | 0.19 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3416 | 1/1   | 0.96 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3496 | 1/1   | 0.96 | 0.15 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3179 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | CA    | 3173 | 1/1   | 0.96 | 0.12 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3500 | 1/1   | 0.96 | 0.16 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3217 | 1/1   | 0.96 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3418 | 1/1   | 0.96 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3503 | 1/1   | 0.96 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | B6    | 102  | 1/1   | 0.96 | 0.20 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3284 | 1/1   | 0.96 | 0.20 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3285 | 1/1   | 0.96 | 0.20 | 54,54,54,54                 | 0     |
| 56  | MG   | CF    | 3001 | 1/1   | 0.96 | 0.12 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3223 | 1/1   | 0.96 | 0.20 | 41,41,41,41                 | 0     |
| 56  | MG   | B9    | 502  | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3102 | 1/1   | 0.96 | 0.30 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3045 | 1/1   | 0.96 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3227 | 1/1   | 0.96 | 0.07 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3001 | 1/1   | 0.96 | 0.11 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3515 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3291 | 1/1   | 0.96 | 0.10 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3071 | 1/1   | 0.96 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3232 | 1/1   | 0.96 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3004 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3435 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3235 | 1/1   | 0.96 | 0.15 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3522 | 1/1   | 0.96 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3007 | 1/1   | 0.96 | 0.11 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3010 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3049 | 1/1   | 0.96 | 0.15 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3438 | 1/1   | 0.96 | 0.06 | 21,21,21,21                 | 0     |
| 56  | MG   | AA    | 3060 | 1/1   | 0.96 | 0.11 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3051 | 1/1   | 0.96 | 0.14 | 18,18,18,18                 | 0     |
| 56  | MG   | BA    | 3443 | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3444 | 1/1   | 0.96 | 0.17 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3746 | 1/1   | 0.96 | 0.09 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3247 | 1/1   | 0.96 | 0.07 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3010 | 1/1   | 0.96 | 0.12 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3305 | 1/1   | 0.96 | 0.07 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3749 | 1/1   | 0.96 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3543 | 1/1   | 0.96 | 0.15 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3600 | 1/1   | 0.96 | 0.11 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3253 | 1/1   | 0.96 | 0.14 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3602 | 1/1   | 0.96 | 0.12 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3753 | 1/1   | 0.96 | 0.08 | 27,27,27,27                 | 0     |
| 56  | MG   | AA    | 3117 | 1/1   | 0.96 | 0.16 | 34,34,34,34                 | 0     |
| 56  | MG   | AA    | 3118 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3450 | 1/1   | 0.96 | 0.07 | 10,10,10,10                 | 0     |
| 56  | MG   | CA    | 3027 | 1/1   | 0.96 | 0.29 | 61,61,61,61                 | 0     |
| 56  | MG   | BA    | 3757 | 1/1   | 0.96 | 0.06 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3198 | 1/1   | 0.96 | 0.13 | 28,28,28,28                 | 0     |
| 56  | MG   | DA    | 3038 | 1/1   | 0.96 | 0.12 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3057 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3040 | 1/1   | 0.96 | 0.14 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3314 | 1/1   | 0.96 | 0.14 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3042 | 1/1   | 0.96 | 0.21 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3017 | 1/1   | 0.96 | 0.14 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3762 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3317 | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3272 | 1/1   | 0.96 | 0.16 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3201 | 1/1   | 0.96 | 0.18 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3202 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3275 | 1/1   | 0.96 | 0.22 | 58,58,58,58                 | 0     |
| 56  | MG   | DA    | 3571 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3573 | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3320 | 1/1   | 0.96 | 0.07 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3203 | 1/1   | 0.96 | 0.18 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3322 | 1/1   | 0.96 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3061 | 1/1   | 0.96 | 0.24 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3468 | 1/1   | 0.96 | 0.08 | 45,45,45,45                 | 0     |
| 56  | MG   | AA    | 3051 | 1/1   | 0.96 | 0.18 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3325 | 1/1   | 0.96 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | CA    | 3046 | 1/1   | 0.96 | 0.17 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3284 | 1/1   | 0.96 | 0.19 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3774 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3776 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3623 | 1/1   | 0.96 | 0.04 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3289 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3475 | 1/1   | 0.96 | 0.10 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3063 | 1/1   | 0.96 | 0.21 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3064 | 1/1   | 0.96 | 0.14 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3065 | 1/1   | 0.96 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3326 | 1/1   | 0.96 | 0.07 | 22,22,22,22                 | 0     |
| 56  | MG   | BA    | 3627 | 1/1   | 0.96 | 0.19 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3628 | 1/1   | 0.96 | 0.06 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3299 | 1/1   | 0.96 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3604 | 1/1   | 0.96 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3124 | 1/1   | 0.96 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3303 | 1/1   | 0.96 | 0.08 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3328 | 1/1   | 0.96 | 0.09 | 11,11,11,11                 | 0     |
| 56  | MG   | BA    | 3064 | 1/1   | 0.96 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3213 | 1/1   | 0.96 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3335 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3126 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3312 | 1/1   | 0.96 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3075 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3314 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3315 | 1/1   | 0.96 | 0.06 | 44,44,44,44                 | 0     |
| 56  | MG   | AA    | 3121 | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3317 | 1/1   | 0.96 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | AA    | 3175 | 1/1   | 0.96 | 0.09 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3067 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3131 | 1/1   | 0.96 | 0.17 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3797 | 1/1   | 0.96 | 0.09 | 19,19,19,19                 | 0     |
| 56  | MG   | BA    | 3132 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3082 | 1/1   | 0.96 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3223 | 1/1   | 0.96 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3641 | 1/1   | 0.96 | 0.06 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3347 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3804 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3805 | 1/1   | 0.96 | 0.16 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3331 | 1/1   | 0.96 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3093 | 1/1   | 0.96 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3068 | 1/1   | 0.96 | 0.25 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3335 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3095 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3349 | 1/1   | 0.96 | 0.16 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3350 | 1/1   | 0.96 | 0.10 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3810 | 1/1   | 0.96 | 0.08 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3099 | 1/1   | 0.96 | 0.13 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3342 | 1/1   | 0.96 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3811 | 1/1   | 0.96 | 0.24 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3641 | 1/1   | 0.96 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3101 | 1/1   | 0.96 | 0.13 | 55,55,55,55                 | 0     |
| 56  | MG   | AA    | 3052 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 56  | MG   | AM    | 201  | 1/1   | 0.96 | 0.04 | 59,59,59,59                 | 0     |
| 56  | MG   | DA    | 3349 | 1/1   | 0.96 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3350 | 1/1   | 0.96 | 0.06 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3080 | 1/1   | 0.96 | 0.13 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3354 | 1/1   | 0.96 | 0.07 | 48,48,48,48                 | 0     |
| 56  | MG   | AA    | 3075 | 1/1   | 0.96 | 0.32 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3139 | 1/1   | 0.96 | 0.08 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3232 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3359 | 1/1   | 0.96 | 0.11 | 39,39,39,39                 | 0     |
| 56  | MG   | BB    | 204  | 1/1   | 0.96 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3508 | 1/1   | 0.96 | 0.05 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3363 | 1/1   | 0.96 | 0.13 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3652 | 1/1   | 0.96 | 0.09 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3112 | 1/1   | 0.96 | 0.18 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3658 | 1/1   | 0.96 | 0.08 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3366 | 1/1   | 0.96 | 0.05 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3661 | 1/1   | 0.96 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3653 | 1/1   | 0.96 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3140 | 1/1   | 0.96 | 0.16 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3141 | 1/1   | 0.96 | 0.16 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3236 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3117 | 1/1   | 0.96 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3142 | 1/1   | 0.96 | 0.15 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3121 | 1/1   | 0.96 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | BB    | 214  | 1/1   | 0.96 | 0.17 | 53,53,53,53                 | 0     |
| 56  | MG   | AA    | 3024 | 1/1   | 0.96 | 0.26 | 55,55,55,55                 | 0     |
| 56  | MG   | DA    | 3383 | 1/1   | 0.96 | 0.08 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3125 | 1/1   | 0.96 | 0.08 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3386 | 1/1   | 0.96 | 0.06 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3239 | 1/1   | 0.96 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3079 | 1/1   | 0.96 | 0.25 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3522 | 1/1   | 0.96 | 0.10 | 16,16,16,16                 | 0     |
| 56  | MG   | DA    | 3390 | 1/1   | 0.96 | 0.06 | 19,19,19,19                 | 0     |
| 56  | MG   | BA    | 3365 | 1/1   | 0.96 | 0.13 | 37,37,37,37                 | 0     |
| 56  | MG   | AA    | 3042 | 1/1   | 0.96 | 0.20 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3669 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3396 | 1/1   | 0.96 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | BD    | 3305 | 1/1   | 0.96 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | DD    | 305  | 1/1   | 0.96 | 0.36 | 39,39,39,39                 | 0     |
| 56  | MG   | AA    | 3007 | 1/1   | 0.96 | 0.13 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3527 | 1/1   | 0.96 | 0.06 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3138 | 1/1   | 0.96 | 0.07 | 63,63,63,63                 | 0     |
| 56  | MG   | BD    | 3308 | 1/1   | 0.96 | 0.20 | 60,60,60,60                 | 0     |
| 56  | MG   | BD    | 3309 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | BE    | 301  | 1/1   | 0.96 | 0.10 | 27,27,27,27                 | 0     |
| 56  | MG   | BE    | 302  | 1/1   | 0.96 | 0.20 | 40,40,40,40                 | 0     |
| 56  | MG   | BE    | 303  | 1/1   | 0.96 | 0.33 | 32,32,32,32                 | 0     |
| 56  | MG   | DF    | 302  | 1/1   | 0.96 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | BE    | 304  | 1/1   | 0.96 | 0.12 | 43,43,43,43                 | 0     |
| 56  | MG   | DF    | 304  | 1/1   | 0.96 | 0.16 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3672 | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 56  | MG   | DA    | 3149 | 1/1   | 0.96 | 0.26 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3152 | 1/1   | 0.96 | 0.16 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3030 | 1/1   | 0.96 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3531 | 1/1   | 0.96 | 0.09 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3154 | 1/1   | 0.96 | 0.17 | 37,37,37,37                 | 0     |
| 56  | MG   | DQ    | 3001 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3248 | 1/1   | 0.96 | 0.30 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3155 | 1/1   | 0.96 | 0.26 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3422 | 1/1   | 0.96 | 0.07 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3087 | 1/1   | 0.96 | 0.32 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BF    | 307  | 1/1   | 0.96 | 0.18 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3159 | 1/1   | 0.96 | 0.06 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3158 | 1/1   | 0.96 | 0.10 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3161 | 1/1   | 0.96 | 0.13 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3162 | 1/1   | 0.96 | 0.06 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3159 | 1/1   | 0.96 | 0.11 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3160 | 1/1   | 0.96 | 0.17 | 40,40,40,40                 | 0     |
| 56  | MG   | D0    | 102  | 1/1   | 0.96 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3379 | 1/1   | 0.96 | 0.11 | 39,39,39,39                 | 0     |
| 56  | MG   | BN    | 3001 | 1/1   | 0.96 | 0.34 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3688 | 1/1   | 0.96 | 0.06 | 16,16,16,16                 | 0     |
| 56  | MG   | BA    | 3031 | 1/1   | 0.96 | 0.13 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3090 | 1/1   | 0.96 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3171 | 1/1   | 0.96 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3163 | 1/1   | 0.96 | 0.11 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3164 | 1/1   | 0.96 | 0.25 | 35,35,35,35                 | 0     |
| 56  | MG   | AA    | 3036 | 1/1   | 0.96 | 0.40 | 69,69,69,69                 | 0     |
| 60  | K    | AX    | 3001 | 1/1   | 0.96 | 0.12 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3033 | 1/1   | 0.96 | 0.28 | 42,42,42,42                 | 0     |
| 56  | MG   | AA    | 3099 | 1/1   | 0.97 | 0.25 | 47,47,47,47                 | 0     |
| 56  | MG   | CA    | 3140 | 1/1   | 0.97 | 0.11 | 75,75,75,75                 | 0     |
| 56  | MG   | DA    | 3295 | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3123 | 1/1   | 0.97 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | B7    | 105  | 1/1   | 0.97 | 0.12 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3095 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3661 | 1/1   | 0.97 | 0.09 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3301 | 1/1   | 0.97 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3279 | 1/1   | 0.97 | 0.27 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3167 | 1/1   | 0.97 | 0.14 | 43,43,43,43                 | 0     |
| 56  | MG   | CA    | 3004 | 1/1   | 0.97 | 0.05 | 67,67,67,67                 | 0     |
| 56  | MG   | DA    | 3307 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3782 | 1/1   | 0.97 | 0.29 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3015 | 1/1   | 0.97 | 0.19 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3523 | 1/1   | 0.97 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3784 | 1/1   | 0.97 | 0.08 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3667 | 1/1   | 0.97 | 0.13 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3129 | 1/1   | 0.97 | 0.30 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3136 | 1/1   | 0.97 | 0.26 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3564 | 1/1   | 0.97 | 0.13 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3532 | 1/1   | 0.97 | 0.08 | 61,61,61,61                 | 0     |
| 56  | MG   | DA    | 3139 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3456 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | AA    | 3114 | 1/1   | 0.97 | 0.09 | 45,45,45,45                 | 0     |
| 56  | MG   | AA    | 3053 | 1/1   | 0.97 | 0.13 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3070 | 1/1   | 0.97 | 0.16 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3538 | 1/1   | 0.97 | 0.06 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3144 | 1/1   | 0.97 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3145 | 1/1   | 0.97 | 0.13 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3323 | 1/1   | 0.97 | 0.09 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3173 | 1/1   | 0.97 | 0.25 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3570 | 1/1   | 0.97 | 0.11 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3287 | 1/1   | 0.97 | 0.16 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3462 | 1/1   | 0.97 | 0.10 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3226 | 1/1   | 0.97 | 0.16 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3329 | 1/1   | 0.97 | 0.13 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3466 | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3552 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3681 | 1/1   | 0.97 | 0.12 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3555 | 1/1   | 0.97 | 0.05 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3803 | 1/1   | 0.97 | 0.13 | 33,33,33,33                 | 0     |
| 56  | MG   | AA    | 3116 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3228 | 1/1   | 0.97 | 0.30 | 56,56,56,56                 | 0     |
| 56  | MG   | DA    | 3336 | 1/1   | 0.97 | 0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3684 | 1/1   | 0.97 | 0.13 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3469 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3686 | 1/1   | 0.97 | 0.07 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3809 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3471 | 1/1   | 0.97 | 0.07 | 27,27,27,27                 | 0     |
| 56  | MG   | AA    | 3037 | 1/1   | 0.97 | 0.20 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3812 | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3689 | 1/1   | 0.97 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3581 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3346 | 1/1   | 0.97 | 0.10 | 48,48,48,48                 | 0     |
| 56  | MG   | CA    | 3035 | 1/1   | 0.97 | 0.13 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3167 | 1/1   | 0.97 | 0.14 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3572 | 1/1   | 0.97 | 0.06 | 68,68,68,68                 | 0     |
| 56  | MG   | BA    | 3691 | 1/1   | 0.97 | 0.08 | 68,68,68,68                 | 0     |
| 56  | MG   | DA    | 3352 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3293 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3053 | 1/1   | 0.97 | 0.09 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3694 | 1/1   | 0.97 | 0.15 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3356 | 1/1   | 0.97 | 0.14 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3579 | 1/1   | 0.97 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3075 | 1/1   | 0.97 | 0.10 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3104 | 1/1   | 0.97 | 0.13 | 23,23,23,23                 | 0     |
| 56  | MG   | DA    | 3005 | 1/1   | 0.97 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3076 | 1/1   | 0.97 | 0.12 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3361 | 1/1   | 0.97 | 0.05 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3298 | 1/1   | 0.97 | 0.24 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3588 | 1/1   | 0.97 | 0.05 | 65,65,65,65                 | 0     |
| 56  | MG   | DA    | 3008 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | CA    | 3044 | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3591 | 1/1   | 0.97 | 0.05 | 59,59,59,59                 | 0     |
| 56  | MG   | BA    | 3299 | 1/1   | 0.97 | 0.05 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3012 | 1/1   | 0.97 | 0.04 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3481 | 1/1   | 0.97 | 0.13 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3595 | 1/1   | 0.97 | 0.08 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3181 | 1/1   | 0.97 | 0.11 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3598 | 1/1   | 0.97 | 0.08 | 30,30,30,30                 | 0     |
| 56  | MG   | BB    | 213  | 1/1   | 0.97 | 0.09 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3371 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 56  | MG   | BA    | 3484 | 1/1   | 0.97 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3374 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3375 | 1/1   | 0.97 | 0.06 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3301 | 1/1   | 0.97 | 0.06 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3302 | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 56  | MG   | DA    | 3020 | 1/1   | 0.97 | 0.05 | 32,32,32,32                 | 0     |
| 56  | MG   | DA    | 3021 | 1/1   | 0.97 | 0.18 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3190 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3304 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3182 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 56  | MG   | AA    | 3186 | 1/1   | 0.97 | 0.11 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3613 | 1/1   | 0.97 | 0.04 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3708 | 1/1   | 0.97 | 0.20 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3028 | 1/1   | 0.97 | 0.14 | 45,45,45,45                 | 0     |
| 56  | MG   | BB    | 222  | 1/1   | 0.97 | 0.14 | 50,50,50,50                 | 0     |
| 56  | MG   | BD    | 3301 | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 56  | MG   | BD    | 3302 | 1/1   | 0.97 | 0.05 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3021 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 56  | MG   | CA    | 3060 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | AA    | 3126 | 1/1   | 0.97 | 0.14 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3388 | 1/1   | 0.97 | 0.05 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3311 | 1/1   | 0.97 | 0.08 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3188 | 1/1   | 0.97 | 0.15 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3401 | 1/1   | 0.97 | 0.04 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3189 | 1/1   | 0.97 | 0.17 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3206 | 1/1   | 0.97 | 0.16 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3243 | 1/1   | 0.97 | 0.12 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3609 | 1/1   | 0.97 | 0.07 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3718 | 1/1   | 0.97 | 0.13 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3244 | 1/1   | 0.97 | 0.25 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3146 | 1/1   | 0.97 | 0.06 | 19,19,19,19                 | 0     |
| 56  | MG   | DA    | 3045 | 1/1   | 0.97 | 0.32 | 60,60,60,60                 | 0     |
| 56  | MG   | BA    | 3110 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3413 | 1/1   | 0.97 | 0.04 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3414 | 1/1   | 0.97 | 0.06 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3148 | 1/1   | 0.97 | 0.06 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3081 | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3249 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3050 | 1/1   | 0.97 | 0.08 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3510 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | CA    | 3076 | 1/1   | 0.97 | 0.17 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3511 | 1/1   | 0.97 | 0.16 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3729 | 1/1   | 0.97 | 0.04 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3402 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3732 | 1/1   | 0.97 | 0.06 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3619 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3427 | 1/1   | 0.97 | 0.04 | 45,45,45,45                 | 0     |
| 56  | MG   | DA    | 3428 | 1/1   | 0.97 | 0.05 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3058 | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | AA    | 3188 | 1/1   | 0.97 | 0.19 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3228 | 1/1   | 0.97 | 0.14 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3517 | 1/1   | 0.97 | 0.08 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3406 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3408 | 1/1   | 0.97 | 0.05 | 21,21,21,21                 | 0     |
| 56  | MG   | BA    | 3058 | 1/1   | 0.97 | 0.09 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3196 | 1/1   | 0.97 | 0.07 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3086 | 1/1   | 0.97 | 0.17 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3115 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3660 | 1/1   | 0.97 | 0.04 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3116 | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3156 | 1/1   | 0.97 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | AA    | 3111 | 1/1   | 0.97 | 0.15 | 61,61,61,61                 | 0     |
| 56  | MG   | BQ    | 202  | 1/1   | 0.97 | 0.14 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3528 | 1/1   | 0.97 | 0.10 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3667 | 1/1   | 0.97 | 0.10 | 66,66,66,66                 | 0     |
| 56  | MG   | BA    | 3332 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3669 | 1/1   | 0.97 | 0.12 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3421 | 1/1   | 0.97 | 0.14 | 48,48,48,48                 | 0     |
| 56  | MG   | BR    | 202  | 1/1   | 0.97 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3449 | 1/1   | 0.97 | 0.05 | 33,33,33,33                 | 0     |
| 56  | MG   | CA    | 3098 | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 56  | MG   | BR    | 203  | 1/1   | 0.97 | 0.16 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3452 | 1/1   | 0.97 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3060 | 1/1   | 0.97 | 0.18 | 26,26,26,26                 | 0     |
| 56  | MG   | CA    | 3102 | 1/1   | 0.97 | 0.12 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3089 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3752 | 1/1   | 0.97 | 0.07 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3042 | 1/1   | 0.97 | 0.09 | 41,41,41,41                 | 0     |
| 56  | MG   | DB    | 3007 | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3263 | 1/1   | 0.97 | 0.28 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3205 | 1/1   | 0.97 | 0.14 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3460 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3084 | 1/1   | 0.97 | 0.07 | 47,47,47,47                 | 0     |
| 56  | MG   | DA    | 3462 | 1/1   | 0.97 | 0.05 | 31,31,31,31                 | 0     |
| 56  | MG   | DD    | 304  | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3086 | 1/1   | 0.97 | 0.17 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3464 | 1/1   | 0.97 | 0.04 | 24,24,24,24                 | 0     |
| 56  | MG   | BA    | 3091 | 1/1   | 0.97 | 0.22 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3088 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 56  | MG   | CA    | 3109 | 1/1   | 0.97 | 0.17 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3261 | 1/1   | 0.97 | 0.14 | 36,36,36,36                 | 0     |
| 56  | MG   | CA    | 3110 | 1/1   | 0.97 | 0.21 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3343 | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 56  | MG   | DA    | 3092 | 1/1   | 0.97 | 0.11 | 48,48,48,48                 | 0     |
| 56  | MG   | DA    | 3265 | 1/1   | 0.97 | 0.13 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3473 | 1/1   | 0.97 | 0.07 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3266 | 1/1   | 0.97 | 0.12 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3475 | 1/1   | 0.97 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3476 | 1/1   | 0.97 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | CA    | 3114 | 1/1   | 0.97 | 0.09 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3540 | 1/1   | 0.97 | 0.07 | 57,57,57,57                 | 0     |
| 56  | MG   | BX    | 101  | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3345 | 1/1   | 0.97 | 0.05 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3542 | 1/1   | 0.97 | 0.09 | 20,20,20,20                 | 0     |
| 56  | MG   | BA    | 3543 | 1/1   | 0.97 | 0.15 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3123 | 1/1   | 0.97 | 0.14 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3210 | 1/1   | 0.97 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | DU    | 3002 | 1/1   | 0.97 | 0.28 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3442 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | AA    | 3031 | 1/1   | 0.97 | 0.21 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3487 | 1/1   | 0.97 | 0.09 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3270 | 1/1   | 0.97 | 0.24 | 40,40,40,40                 | 0     |
| 56  | MG   | B0    | 104  | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3490 | 1/1   | 0.97 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3550 | 1/1   | 0.97 | 0.06 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3212 | 1/1   | 0.97 | 0.10 | 26,26,26,26                 | 0     |
| 56  | MG   | D0    | 101  | 1/1   | 0.97 | 0.07 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3108 | 1/1   | 0.97 | 0.07 | 46,46,46,46                 | 0     |
| 56  | MG   | B3    | 3001 | 1/1   | 0.97 | 0.09 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3552 | 1/1   | 0.97 | 0.06 | 46,46,46,46                 | 0     |
| 56  | MG   | CA    | 3130 | 1/1   | 0.97 | 0.15 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3553 | 1/1   | 0.97 | 0.09 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3273 | 1/1   | 0.97 | 0.24 | 41,41,41,41                 | 0     |
| 59  | ZN   | B4    | 501  | 1/1   | 0.97 | 0.04 | 99,99,99,99                 | 0     |
| 56  | MG   | AX    | 3004 | 1/1   | 0.97 | 0.12 | 53,53,53,53                 | 0     |
| 56  | MG   | DA    | 3288 | 1/1   | 0.97 | 0.08 | 48,48,48,48                 | 0     |
| 59  | ZN   | B9    | 501  | 1/1   | 0.97 | 0.04 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3775 | 1/1   | 0.97 | 0.05 | 34,34,34,34                 | 0     |
| 56  | MG   | B6    | 101  | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3658 | 1/1   | 0.97 | 0.08 | 51,51,51,51                 | 0     |
| 56  | MG   | B7    | 103  | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3119 | 1/1   | 0.98 | 0.12 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3215 | 1/1   | 0.98 | 0.09 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3601 | 1/1   | 0.98 | 0.09 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3451 | 1/1   | 0.98 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3383 | 1/1   | 0.98 | 0.08 | 20,20,20,20                 | 0     |
| 56  | MG   | CA    | 3101 | 1/1   | 0.98 | 0.14 | 54,54,54,54                 | 0     |
| 56  | MG   | DA    | 3022 | 1/1   | 0.98 | 0.04 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3127 | 1/1   | 0.98 | 0.13 | 36,36,36,36                 | 0     |
| 56  | MG   | BD    | 3303 | 1/1   | 0.98 | 0.04 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3348 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3333 | 1/1   | 0.98 | 0.04 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3334 | 1/1   | 0.98 | 0.07 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3351 | 1/1   | 0.98 | 0.11 | 32,32,32,32                 | 0     |
| 56  | MG   | AA    | 3137 | 1/1   | 0.98 | 0.06 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3238 | 1/1   | 0.98 | 0.09 | 54,54,54,54                 | 0     |
| 56  | MG   | AA    | 3035 | 1/1   | 0.98 | 0.09 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3029 | 1/1   | 0.98 | 0.06 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3608 | 1/1   | 0.98 | 0.11 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3218 | 1/1   | 0.98 | 0.10 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3253 | 1/1   | 0.98 | 0.21 | 47,47,47,47                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3137 | 1/1   | 0.98 | 0.22 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3535 | 1/1   | 0.98 | 0.15 | 31,31,31,31                 | 0     |
| 56  | MG   | DA    | 3246 | 1/1   | 0.98 | 0.08 | 31,31,31,31                 | 0     |
| 56  | MG   | CA    | 3111 | 1/1   | 0.98 | 0.10 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3074 | 1/1   | 0.98 | 0.09 | 31,31,31,31                 | 0     |
| 56  | MG   | CA    | 3018 | 1/1   | 0.98 | 0.06 | 52,52,52,52                 | 0     |
| 56  | MG   | DA    | 3492 | 1/1   | 0.98 | 0.05 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3220 | 1/1   | 0.98 | 0.15 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3251 | 1/1   | 0.98 | 0.11 | 46,46,46,46                 | 0     |
| 56  | MG   | BE    | 305  | 1/1   | 0.98 | 0.07 | 19,19,19,19                 | 0     |
| 56  | MG   | AA    | 3120 | 1/1   | 0.98 | 0.07 | 49,49,49,49                 | 0     |
| 56  | MG   | DA    | 3498 | 1/1   | 0.98 | 0.05 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3136 | 1/1   | 0.98 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | BA    | 3043 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3465 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3138 | 1/1   | 0.98 | 0.20 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3397 | 1/1   | 0.98 | 0.06 | 25,25,25,25                 | 0     |
| 56  | MG   | AA    | 3063 | 1/1   | 0.98 | 0.09 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3505 | 1/1   | 0.98 | 0.07 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3261 | 1/1   | 0.98 | 0.04 | 46,46,46,46                 | 0     |
| 56  | MG   | DA    | 3378 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3470 | 1/1   | 0.98 | 0.11 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3380 | 1/1   | 0.98 | 0.05 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3400 | 1/1   | 0.98 | 0.05 | 34,34,34,34                 | 0     |
| 56  | MG   | BA    | 3118 | 1/1   | 0.98 | 0.27 | 37,37,37,37                 | 0     |
| 56  | MG   | DA    | 3155 | 1/1   | 0.98 | 0.25 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3384 | 1/1   | 0.98 | 0.09 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3625 | 1/1   | 0.98 | 0.04 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3078 | 1/1   | 0.98 | 0.06 | 15,15,15,15                 | 0     |
| 56  | MG   | BA    | 3474 | 1/1   | 0.98 | 0.04 | 20,20,20,20                 | 0     |
| 56  | MG   | BA    | 3303 | 1/1   | 0.98 | 0.17 | 37,37,37,37                 | 0     |
| 56  | MG   | BN    | 3003 | 1/1   | 0.98 | 0.09 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3404 | 1/1   | 0.98 | 0.10 | 23,23,23,23                 | 0     |
| 56  | MG   | BN    | 3005 | 1/1   | 0.98 | 0.10 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3005 | 1/1   | 0.98 | 0.06 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3143 | 1/1   | 0.98 | 0.05 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3395 | 1/1   | 0.98 | 0.04 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3354 | 1/1   | 0.98 | 0.04 | 20,20,20,20                 | 0     |
| 56  | MG   | DA    | 3397 | 1/1   | 0.98 | 0.03 | 30,30,30,30                 | 0     |
| 56  | MG   | BP    | 202  | 1/1   | 0.98 | 0.06 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3528 | 1/1   | 0.98 | 0.04 | 39,39,39,39                 | 0     |
| 56  | MG   | DA    | 3663 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3529 | 1/1   | 0.98 | 0.06 | 57,57,57,57                 | 0     |
| 56  | MG   | BA    | 3230 | 1/1   | 0.98 | 0.21 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3788 | 1/1   | 0.98 | 0.07 | 10,10,10,10                 | 0     |
| 56  | MG   | AA    | 3151 | 1/1   | 0.98 | 0.05 | 56,56,56,56                 | 0     |
| 56  | MG   | BA    | 3414 | 1/1   | 0.98 | 0.11 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3791 | 1/1   | 0.98 | 0.05 | 18,18,18,18                 | 0     |
| 56  | MG   | BA    | 3710 | 1/1   | 0.98 | 0.16 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3415 | 1/1   | 0.98 | 0.09 | 34,34,34,34                 | 0     |
| 56  | MG   | DA    | 3174 | 1/1   | 0.98 | 0.23 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3309 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 56  | MG   | DA    | 3539 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3145 | 1/1   | 0.98 | 0.08 | 41,41,41,41                 | 0     |
| 56  | MG   | BA    | 3008 | 1/1   | 0.98 | 0.08 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3063 | 1/1   | 0.98 | 0.32 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3313 | 1/1   | 0.98 | 0.08 | 34,34,34,34                 | 0     |
| 56  | MG   | AA    | 3132 | 1/1   | 0.98 | 0.10 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3272 | 1/1   | 0.98 | 0.09 | 22,22,22,22                 | 0     |
| 56  | MG   | BA    | 3802 | 1/1   | 0.98 | 0.19 | 23,23,23,23                 | 0     |
| 56  | MG   | BU    | 209  | 1/1   | 0.98 | 0.21 | 27,27,27,27                 | 0     |
| 56  | MG   | BV    | 202  | 1/1   | 0.98 | 0.20 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3423 | 1/1   | 0.98 | 0.06 | 31,31,31,31                 | 0     |
| 56  | MG   | DD    | 301  | 1/1   | 0.98 | 0.06 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3550 | 1/1   | 0.98 | 0.09 | 22,22,22,22                 | 0     |
| 56  | MG   | DA    | 3551 | 1/1   | 0.98 | 0.04 | 47,47,47,47                 | 0     |
| 56  | MG   | BA    | 3497 | 1/1   | 0.98 | 0.03 | 44,44,44,44                 | 0     |
| 56  | MG   | DA    | 3553 | 1/1   | 0.98 | 0.04 | 46,46,46,46                 | 0     |
| 56  | MG   | BA    | 3364 | 1/1   | 0.98 | 0.15 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3425 | 1/1   | 0.98 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | BW    | 204  | 1/1   | 0.98 | 0.19 | 31,31,31,31                 | 0     |
| 56  | MG   | DE    | 301  | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | CA    | 3161 | 1/1   | 0.98 | 0.10 | 51,51,51,51                 | 0     |
| 56  | MG   | BA    | 3316 | 1/1   | 0.98 | 0.11 | 25,25,25,25                 | 0     |
| 56  | MG   | DA    | 3302 | 1/1   | 0.98 | 0.07 | 32,32,32,32                 | 0     |
| 56  | MG   | BX    | 102  | 1/1   | 0.98 | 0.08 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3149 | 1/1   | 0.98 | 0.21 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3085 | 1/1   | 0.98 | 0.12 | 23,23,23,23                 | 0     |
| 56  | MG   | DA    | 3306 | 1/1   | 0.98 | 0.19 | 35,35,35,35                 | 0     |
| 56  | MG   | DA    | 3432 | 1/1   | 0.98 | 0.05 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3504 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3432 | 1/1   | 0.98 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3433 | 1/1   | 0.98 | 0.08 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3275 | 1/1   | 0.98 | 0.17 | 34,34,34,34                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | DA    | 3311 | 1/1   | 0.98 | 0.06 | 19,19,19,19                 | 0     |
| 56  | MG   | CA    | 3170 | 1/1   | 0.98 | 0.11 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3022 | 1/1   | 0.98 | 0.03 | 25,25,25,25                 | 0     |
| 56  | MG   | DQ    | 3002 | 1/1   | 0.98 | 0.10 | 41,41,41,41                 | 0     |
| 56  | MG   | CA    | 3172 | 1/1   | 0.98 | 0.08 | 50,50,50,50                 | 0     |
| 56  | MG   | BA    | 3436 | 1/1   | 0.98 | 0.09 | 17,17,17,17                 | 0     |
| 56  | MG   | BA    | 3177 | 1/1   | 0.98 | 0.06 | 44,44,44,44                 | 0     |
| 56  | MG   | BA    | 3278 | 1/1   | 0.98 | 0.21 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3023 | 1/1   | 0.98 | 0.09 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3374 | 1/1   | 0.98 | 0.04 | 21,21,21,21                 | 0     |
| 56  | MG   | BA    | 3036 | 1/1   | 0.98 | 0.12 | 19,19,19,19                 | 0     |
| 56  | MG   | BA    | 3589 | 1/1   | 0.98 | 0.07 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3448 | 1/1   | 0.98 | 0.06 | 45,45,45,45                 | 0     |
| 56  | MG   | BB    | 208  | 1/1   | 0.98 | 0.08 | 36,36,36,36                 | 0     |
| 56  | MG   | BA    | 3208 | 1/1   | 0.98 | 0.13 | 19,19,19,19                 | 0     |
| 56  | MG   | BA    | 3743 | 1/1   | 0.98 | 0.07 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3664 | 1/1   | 0.98 | 0.10 | 17,17,17,17                 | 0     |
| 56  | MG   | BA    | 3665 | 1/1   | 0.98 | 0.06 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3587 | 1/1   | 0.98 | 0.12 | 52,52,52,52                 | 0     |
| 56  | MG   | B7    | 101  | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 56  | MG   | B7    | 102  | 1/1   | 0.98 | 0.10 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3052 | 1/1   | 0.98 | 0.12 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3011 | 1/1   | 0.98 | 0.04 | 33,33,33,33                 | 0     |
| 58  | SF4  | AD    | 501  | 8/8   | 0.98 | 0.05 | 62,74,91,95                 | 0     |
| 58  | SF4  | CD    | 501  | 8/8   | 0.98 | 0.04 | 64,77,89,111                | 0     |
| 59  | ZN   | AN    | 501  | 1/1   | 0.98 | 0.05 | 86,86,86,86                 | 0     |
| 56  | MG   | BA    | 3012 | 1/1   | 0.98 | 0.18 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3183 | 1/1   | 0.98 | 0.08 | 35,35,35,35                 | 0     |
| 56  | MG   | B8    | 102  | 1/1   | 0.98 | 0.07 | 41,41,41,41                 | 0     |
| 56  | MG   | DA    | 3334 | 1/1   | 0.98 | 0.05 | 45,45,45,45                 | 0     |
| 56  | MG   | BA    | 3448 | 1/1   | 0.98 | 0.08 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3524 | 1/1   | 0.98 | 0.10 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3184 | 1/1   | 0.98 | 0.17 | 37,37,37,37                 | 0     |
| 56  | MG   | CA    | 3003 | 1/1   | 0.98 | 0.09 | 51,51,51,51                 | 0     |
| 56  | MG   | DA    | 3407 | 1/1   | 0.99 | 0.02 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3429 | 1/1   | 0.99 | 0.03 | 23,23,23,23                 | 0     |
| 56  | MG   | DA    | 3009 | 1/1   | 0.99 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | BA    | 3546 | 1/1   | 0.99 | 0.05 | 38,38,38,38                 | 0     |
| 56  | MG   | DA    | 3120 | 1/1   | 0.99 | 0.07 | 34,34,34,34                 | 0     |
| 56  | MG   | BP    | 201  | 1/1   | 0.99 | 0.24 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3513 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 56  | MG   | DA    | 3013 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BB    | 215  | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3341 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 56  | MG   | BA    | 3515 | 1/1   | 0.99 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3482 | 1/1   | 0.99 | 0.08 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3298 | 1/1   | 0.99 | 0.04 | 55,55,55,55                 | 0     |
| 56  | MG   | BA    | 3407 | 1/1   | 0.99 | 0.09 | 40,40,40,40                 | 0     |
| 56  | MG   | DA    | 3421 | 1/1   | 0.99 | 0.02 | 31,31,31,31                 | 0     |
| 56  | MG   | BA    | 3007 | 1/1   | 0.99 | 0.06 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3409 | 1/1   | 0.99 | 0.07 | 21,21,21,21                 | 0     |
| 56  | MG   | BA    | 3486 | 1/1   | 0.99 | 0.05 | 22,22,22,22                 | 0     |
| 56  | MG   | BA    | 3591 | 1/1   | 0.99 | 0.08 | 48,48,48,48                 | 0     |
| 56  | MG   | BA    | 3289 | 1/1   | 0.99 | 0.30 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3556 | 1/1   | 0.99 | 0.06 | 48,48,48,48                 | 0     |
| 56  | MG   | BU    | 203  | 1/1   | 0.99 | 0.13 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3594 | 1/1   | 0.99 | 0.11 | 33,33,33,33                 | 0     |
| 56  | MG   | DA    | 3027 | 1/1   | 0.99 | 0.15 | 42,42,42,42                 | 0     |
| 56  | MG   | DA    | 3495 | 1/1   | 0.99 | 0.12 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3037 | 1/1   | 0.99 | 0.31 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3368 | 1/1   | 0.99 | 0.06 | 24,24,24,24                 | 0     |
| 56  | MG   | BA    | 3235 | 1/1   | 0.99 | 0.12 | 26,26,26,26                 | 0     |
| 56  | MG   | BU    | 207  | 1/1   | 0.99 | 0.24 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3085 | 1/1   | 0.99 | 0.12 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3413 | 1/1   | 0.99 | 0.08 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3373 | 1/1   | 0.99 | 0.06 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3560 | 1/1   | 0.99 | 0.10 | 38,38,38,38                 | 0     |
| 56  | MG   | BV    | 201  | 1/1   | 0.99 | 0.19 | 27,27,27,27                 | 0     |
| 56  | MG   | BA    | 3493 | 1/1   | 0.99 | 0.06 | 49,49,49,49                 | 0     |
| 56  | MG   | BA    | 3463 | 1/1   | 0.99 | 0.03 | 10,10,10,10                 | 0     |
| 56  | MG   | BA    | 3393 | 1/1   | 0.99 | 0.05 | 22,22,22,22                 | 0     |
| 56  | MG   | BA    | 3003 | 1/1   | 0.99 | 0.05 | 30,30,30,30                 | 0     |
| 56  | MG   | BA    | 3107 | 1/1   | 0.99 | 0.18 | 50,50,50,50                 | 0     |
| 56  | MG   | BW    | 203  | 1/1   | 0.99 | 0.10 | 37,37,37,37                 | 0     |
| 56  | MG   | BA    | 3680 | 1/1   | 0.99 | 0.05 | 53,53,53,53                 | 0     |
| 56  | MG   | BA    | 3441 | 1/1   | 0.99 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3306 | 1/1   | 0.99 | 0.14 | 18,18,18,18                 | 0     |
| 56  | MG   | BA    | 3500 | 1/1   | 0.99 | 0.08 | 32,32,32,32                 | 0     |
| 56  | MG   | BA    | 3723 | 1/1   | 0.99 | 0.04 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3069 | 1/1   | 0.99 | 0.14 | 39,39,39,39                 | 0     |
| 56  | MG   | BA    | 3084 | 1/1   | 0.99 | 0.11 | 33,33,33,33                 | 0     |
| 56  | MG   | BA    | 3209 | 1/1   | 0.99 | 0.07 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3013 | 1/1   | 0.99 | 0.10 | 26,26,26,26                 | 0     |
| 56  | MG   | DA    | 3216 | 1/1   | 0.99 | 0.13 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56  | MG   | BA    | 3009 | 1/1   | 0.99 | 0.04 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3730 | 1/1   | 0.99 | 0.08 | 13,13,13,13                 | 0     |
| 56  | MG   | DA    | 3394 | 1/1   | 0.99 | 0.04 | 40,40,40,40                 | 0     |
| 56  | MG   | BA    | 3773 | 1/1   | 0.99 | 0.04 | 38,38,38,38                 | 0     |
| 56  | MG   | BA    | 3574 | 1/1   | 0.99 | 0.04 | 28,28,28,28                 | 0     |
| 56  | MG   | DA    | 3526 | 1/1   | 0.99 | 0.17 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3339 | 1/1   | 0.99 | 0.07 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3370 | 1/1   | 0.99 | 0.04 | 27,27,27,27                 | 0     |
| 56  | MG   | DA    | 3596 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 59  | ZN   | BY    | 203  | 1/1   | 0.99 | 0.02 | 54,54,54,54                 | 0     |
| 56  | MG   | BA    | 3734 | 1/1   | 0.99 | 0.07 | 18,18,18,18                 | 0     |
| 56  | MG   | AA    | 3108 | 1/1   | 0.99 | 0.08 | 58,58,58,58                 | 0     |
| 56  | MG   | BA    | 3426 | 1/1   | 0.99 | 0.10 | 20,20,20,20                 | 0     |
| 56  | MG   | DA    | 3004 | 1/1   | 0.99 | 0.12 | 25,25,25,25                 | 0     |
| 56  | MG   | BA    | 3405 | 1/1   | 0.99 | 0.09 | 22,22,22,22                 | 0     |
| 59  | ZN   | DY    | 501  | 1/1   | 0.99 | 0.05 | 97,97,97,97                 | 0     |
| 56  | MG   | CA    | 3137 | 1/1   | 0.99 | 0.09 | 50,50,50,50                 | 0     |
| 59  | ZN   | D6    | 501  | 1/1   | 0.99 | 0.05 | 66,66,66,66                 | 0     |
| 59  | ZN   | D9    | 501  | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 56  | MG   | BA    | 3428 | 1/1   | 0.99 | 0.12 | 36,36,36,36                 | 0     |
| 56  | MG   | DA    | 3406 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 56  | MG   | AA    | 3131 | 1/1   | 1.00 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3601 | 1/1   | 1.00 | 0.02 | 26,26,26,26                 | 0     |
| 56  | MG   | BA    | 3487 | 1/1   | 1.00 | 0.07 | 23,23,23,23                 | 0     |
| 56  | MG   | BA    | 3516 | 1/1   | 1.00 | 0.09 | 28,28,28,28                 | 0     |
| 56  | MG   | BA    | 3727 | 1/1   | 1.00 | 0.02 | 34,34,34,34                 | 0     |
| 59  | ZN   | D5    | 501  | 1/1   | 1.00 | 0.03 | 52,52,52,52                 | 0     |
| 56  | MG   | BA    | 3794 | 1/1   | 1.00 | 0.07 | 29,29,29,29                 | 0     |
| 56  | MG   | DA    | 3581 | 1/1   | 1.00 | 0.03 | 35,35,35,35                 | 0     |
| 56  | MG   | BA    | 3488 | 1/1   | 1.00 | 0.06 | 16,16,16,16                 | 0     |
| 56  | MG   | BA    | 3329 | 1/1   | 1.00 | 0.06 | 24,24,24,24                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.