



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 29, 2026 – 01:02 AM UTC

PDB ID : 4V8D / pdb\_00004v8d  
Title : Structure analysis of ribosomal decoding (cognate tRNA-tyr complex).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : 2011-12-07  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

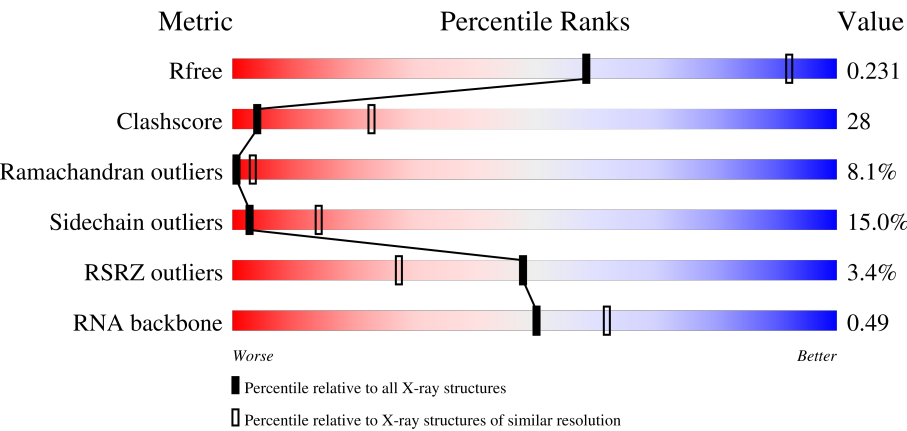
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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 <sub>free</sub>     | 180053                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |
| RNA backbone          | 3983                        | 1109 (3.20-2.80)                                      |

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    | 1506   | <div><div></div><div>38%46%16%</div></div>     |
| 1   | CA    | 1506   | <div><div>%</div><div>38%46%16%</div></div>    |
| 2   | AE    | 256    | <div><div>4%</div><div>27%49%15%7%</div></div> |
| 2   | CE    | 256    | <div><div>4%</div><div>30%46%16%7%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AF    | 239    |                  |
| 3   | CF    | 239    |                  |
| 4   | AG    | 208    |                  |
| 4   | CG    | 208    |                  |
| 5   | AH    | 162    |                  |
| 5   | CH    | 162    |                  |
| 6   | AI    | 101    |                  |
| 6   | CI    | 101    |                  |
| 7   | AJ    | 156    |                  |
| 7   | CJ    | 156    |                  |
| 8   | AK    | 138    |                  |
| 8   | CK    | 138    |                  |
| 9   | AL    | 128    |                  |
| 9   | CL    | 128    |                  |
| 10  | AM    | 105    |                  |
| 10  | CM    | 105    |                  |
| 11  | AN    | 129    |                  |
| 11  | CN    | 129    |                  |
| 12  | AO    | 132    |                  |
| 12  | CO    | 132    |                  |
| 13  | AP    | 126    |                  |
| 13  | CP    | 126    |                  |
| 14  | AQ    | 61     |                  |
| 14  | CQ    | 61     |                  |
| 15  | AR    | 89     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | CR    | 89     |                  |
| 16  | AS    | 88     |                  |
| 16  | CS    | 88     |                  |
| 17  | AT    | 105    |                  |
| 17  | CT    | 105    |                  |
| 18  | AU    | 88     |                  |
| 18  | CU    | 88     |                  |
| 19  | AV    | 93     |                  |
| 19  | CV    | 93     |                  |
| 20  | AW    | 106    |                  |
| 20  | CW    | 106    |                  |
| 21  | AX    | 27     |                  |
| 21  | CX    | 27     |                  |
| 22  | AB    | 85     |                  |
| 22  | AD    | 85     |                  |
| 22  | CB    | 85     |                  |
| 22  | CD    | 85     |                  |
| 23  | AC    | 77     |                  |
| 23  | CC    | 77     |                  |
| 24  | A1    | 16     |                  |
| 24  | C1    | 16     |                  |
| 25  | BA    | 2912   |                  |
| 25  | DA    | 2912   |                  |
| 26  | BB    | 122    |                  |
| 26  | DB    | 122    |                  |

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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  | BK    | 148    |                  |
| 32  | DK    | 148    |                  |
| 33  | BM    | 140    |                  |
| 33  | DM    | 140    |                  |
| 34  | BN    | 122    |                  |
| 34  | DN    | 122    |                  |
| 35  | BO    | 150    |                  |
| 35  | DO    | 150    |                  |
| 36  | BP    | 141    |                  |
| 36  | DP    | 141    |                  |
| 37  | B0    | 118    |                  |
| 37  | D0    | 118    |                  |
| 38  | BQ    | 112    |                  |
| 38  | DQ    | 112    |                  |
| 39  | BR    | 146    |                  |

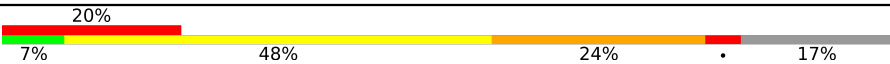
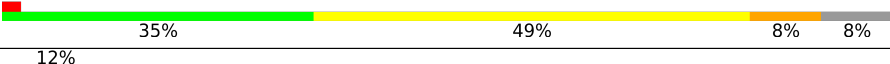
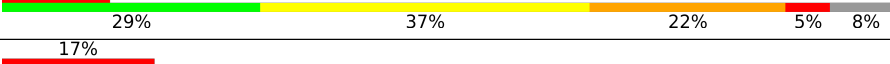
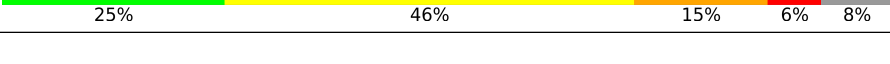
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | DR    | 146    |                  |
| 40  | B1    | 118    |                  |
| 40  | D1    | 118    |                  |
| 41  | B2    | 101    |                  |
| 41  | D2    | 101    |                  |
| 42  | BS    | 113    |                  |
| 42  | DS    | 113    |                  |
| 43  | BT    | 96     |                  |
| 43  | DT    | 96     |                  |
| 44  | BU    | 110    |                  |
| 44  | DU    | 110    |                  |
| 45  | BV    | 206    |                  |
| 45  | DV    | 206    |                  |
| 46  | B3    | 85     |                  |
| 46  | D3    | 85     |                  |
| 47  | BZ    | 98     |                  |
| 47  | DZ    | 98     |                  |
| 48  | BW    | 72     |                  |
| 48  | DW    | 72     |                  |
| 49  | BX    | 60     |                  |
| 49  | DX    | 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     |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | AA    | 1633 | -         | -        | -       | X                |
| 55  | MG   | AA    | 1643 | -         | -        | -       | X                |
| 55  | MG   | AA    | 1751 | -         | -        | -       | X                |
| 55  | MG   | AA    | 1757 | -         | -        | -       | X                |
| 55  | MG   | AA    | 1777 | -         | -        | -       | X                |
| 55  | MG   | AA    | 1804 | -         | -        | -       | X                |
| 55  | MG   | AA    | 1810 | -         | -        | -       | X                |
| 55  | MG   | BA    | 3126 | -         | -        | -       | X                |
| 55  | MG   | BA    | 3270 | -         | -        | -       | X                |
| 55  | MG   | BA    | 3382 | -         | -        | -       | X                |
| 55  | MG   | BA    | 3424 | -         | -        | -       | X                |
| 55  | MG   | BA    | 3472 | -         | -        | -       | X                |
| 55  | MG   | BA    | 3540 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1675 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1684 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1716 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1729 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1733 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1776 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1785 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1806 | -         | -        | -       | X                |
| 55  | MG   | CA    | 1808 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3114 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3125 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3225 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3239 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3243 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | DA    | 3270 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3279 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3310 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3320 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3358 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3366 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3370 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3371 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3403 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3406 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3439 | -         | -        | -       | X                |



## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299676 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    | 1502     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32284 | 14370 | 5982 | 10431 | 1501 |         |         |       |
| 1   | CA    | 1502     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32287 | 14370 | 5982 | 10433 | 1502 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | AL    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |  |         |         |       |
| 9   | CL    | 127      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |  |         |         |       |

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AP    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 928   | 574 | 191 | 161 | 2 |         |         |       |
| 13  | CP    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 577 | 192 | 162 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14  | AQ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 476   | 303 | 99 | 70 | 4 |         |         |       |
| 14  | CQ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 476   | 303 | 99 | 70 | 4 |         |         |       |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AU    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 591   | 376 | 117 | 98 |         |         |       |
| 18  | CU    | 72       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 591   | 376 | 117 | 98 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AV    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 398 | 115 | 109 | 2 |         |         |       |
| 19  | CV    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 398 | 115 | 109 | 2 |         |         |       |

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

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

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

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

- Molecule 22 is a RNA chain called TRNA-TYR.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 22  | AB    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |
| 22  | AD    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |
| 22  | CB    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |
| 22  | CD    | 85       | Total | C   | N   | O   | P  | S | 0       | 0       | 0     |
|     |       |          | 1814  | 813 | 323 | 592 | 85 | 1 |         |         |       |

- Molecule 23 is a RNA chain called TRNA-FMET.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23  | AC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1643  | 732 | 298 | 536 | 77 |         |         |       |
| 23  | CC    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1643  | 732 | 298 | 536 | 77 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| AC    | 18      | C        | U      | conflict | GB AP012306.1 |
| CC    | 18      | C        | U      | conflict | GB AP012306.1 |

- Molecule 24 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 24  | A1    | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 346   | 156 | 69 | 105 | 16 |         |         |       |
| 24  | C1    | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 346   | 156 | 69 | 105 | 16 |         |         |       |

- Molecule 25 is a RNA chain called RNA (2912-MER).

| Mol | Chain | Residues | Atoms          |            |            |            |           | ZeroOcc | AltConf | Trace |
|-----|-------|----------|----------------|------------|------------|------------|-----------|---------|---------|-------|
| 25  | BA    | 2912     | Total<br>62707 | C<br>27911 | N<br>11722 | O<br>20163 | P<br>2911 | 0       | 0       | 0     |
| 25  | DA    | 2907     | Total<br>62607 | C<br>27866 | N<br>11712 | O<br>20123 | P<br>2906 | 0       | 0       | 0     |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| BA    | 161     | U        | -      | insertion | GB AP008226.1 |
| BA    | 654A    | A        | G      | conflict  | GB AP008226.1 |
| BA    | 654E    | C        | G      | conflict  | GB AP008226.1 |
| BA    | 654P    | G        | C      | conflict  | GB AP008226.1 |
| BA    | 654T    | A        | C      | conflict  | GB AP008226.1 |
| BA    | 1058    | U        | G      | conflict  | GB AP008226.1 |
| BA    | 1080    | A        | C      | conflict  | GB AP008226.1 |
| DA    | 166     | U        | -      | insertion | GB AP008226.1 |
| DA    | 654A    | A        | G      | conflict  | GB AP008226.1 |
| DA    | 654E    | C        | G      | conflict  | GB AP008226.1 |
| DA    | 654P    | G        | C      | conflict  | GB AP008226.1 |
| DA    | 654T    | A        | C      | conflict  | GB AP008226.1 |
| DA    | 1058    | U        | G      | conflict  | GB AP008226.1 |
| DA    | 1080    | A        | C      | conflict  | GB AP008226.1 |

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

| Mol | Chain | Residues | Atoms         |           |          |          |          | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|---------|-------|
| 26  | BB    | 122      | Total<br>2617 | C<br>1166 | N<br>486 | O<br>844 | P<br>121 | 0       | 0       | 0     |
| 26  | DB    | 122      | Total<br>2617 | C<br>1166 | N<br>486 | O<br>844 | P<br>121 | 0       | 0       | 0     |

- Molecule 27 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 27  | BD    | 272      | Total<br>2115 | C<br>1335 | N<br>420 | O<br>357 | S<br>3 | 0       | 0       | 0     |
| 27  | DD    | 272      | Total<br>2115 | C<br>1335 | N<br>420 | O<br>357 | S<br>3 | 0       | 0       | 0     |

- Molecule 28 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 28  | DE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | BF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |
| 29  | DF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |

- 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     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 30  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |
| 31  | DH    | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 32  | DK    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | DM    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BN    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 34  | DN    | 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  | BO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 35  | DO    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BP    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 36  | DP    | 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  | B0    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 37  | D0    | 117      | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |   |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 38  | BQ    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |
| 38  | DQ    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |



- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BR    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 39  | DR    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | B1    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 40  | D1    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | B2    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 41  | D2    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |
| 42  | DS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43  | BT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |
| 43  | DT    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |
| 44  | DU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BV    | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1397  | 892 | 251 | 251 | 3 |         |         |       |
| 45  | DV    | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1428  | 911 | 255 | 259 | 3 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | B3    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 607   | 376 | 128 | 102 | 1 |         |         |       |
| 46  | D3    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 613   | 379 | 129 | 104 | 1 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 47  | DZ    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 48  | BW    | 66       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 558   | 346 | 113 | 98 | 1 |         |         |       |
| 48  | DW    | 66       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 558   | 346 | 113 | 98 | 1 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49  | BX    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49  | DX    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B4    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 533   | 335 | 96 | 97 | 5 |         |         |       |
| 50  | D4    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 515   | 326 | 93 | 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     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 51  | D5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B6    | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 389   | 241 | 79 | 65 | 4 |         |         |       |
| 52  | D6    | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 389   | 241 | 79 | 65 | 4 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | B7    | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 391   | 240 | 97 | 52 | 2 |         |         |       |
| 53  | D7    | 45       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 391   | 240 | 97 | 52 | 2 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54  | B8    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 480   | 306 | 98 | 74 | 2 |         |         |       |
| 54  | D8    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 480   | 306 | 98 | 74 | 2 |         |         |       |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 55  | AA    | 220      | Total<br>220 | Mg<br>220 | 1       | 0       |
| 55  | AG    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | AN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | AR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | AS    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | AB    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 55  | AC    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 55  | AD    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | A1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | BA    | 568      | Total<br>568 | Mg<br>568 | 2       | 0       |
| 55  | BB    | 18       | Total<br>18  | Mg<br>18  | 0       | 0       |
| 55  | BD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | BE    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | BF    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | BO    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | B0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | B1    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | B2    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | B3    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | BW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | B5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 55  | B6    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | B7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | CA    | 219      | Total<br>219 | Mg<br>219 | 0       | 0       |
| 55  | CG    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | CK    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | CR    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | CB    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 55  | CC    | 9        | Total<br>9   | Mg<br>9   | 0       | 0       |
| 55  | CD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | DA    | 488      | Total<br>488 | Mg<br>488 | 0       | 0       |
| 55  | DB    | 20       | Total<br>20  | Mg<br>20  | 0       | 0       |
| 55  | DD    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | DE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | DO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | D0    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | D1    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | D3    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | D5    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | D7    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | D8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

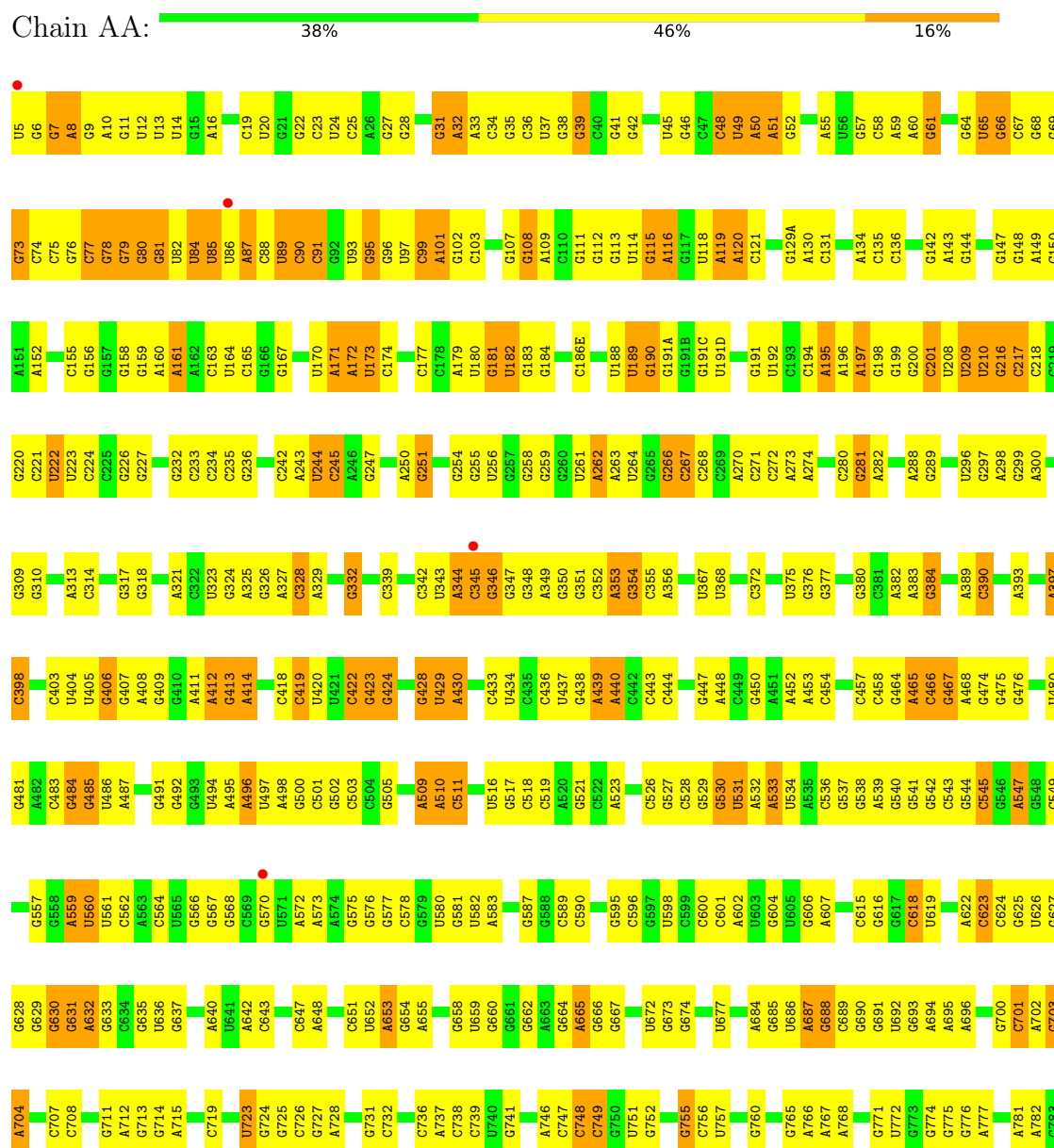
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

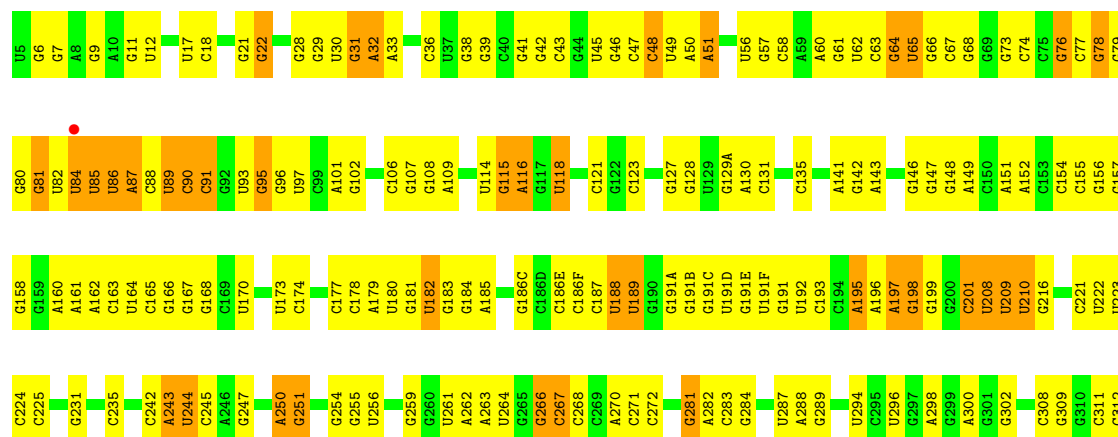
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 56  | AG    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 56  | AQ    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 56  | CG    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 56  | CQ    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

### 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

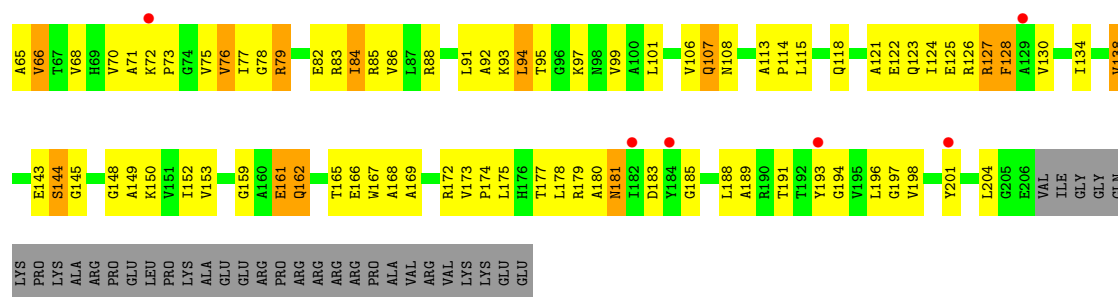




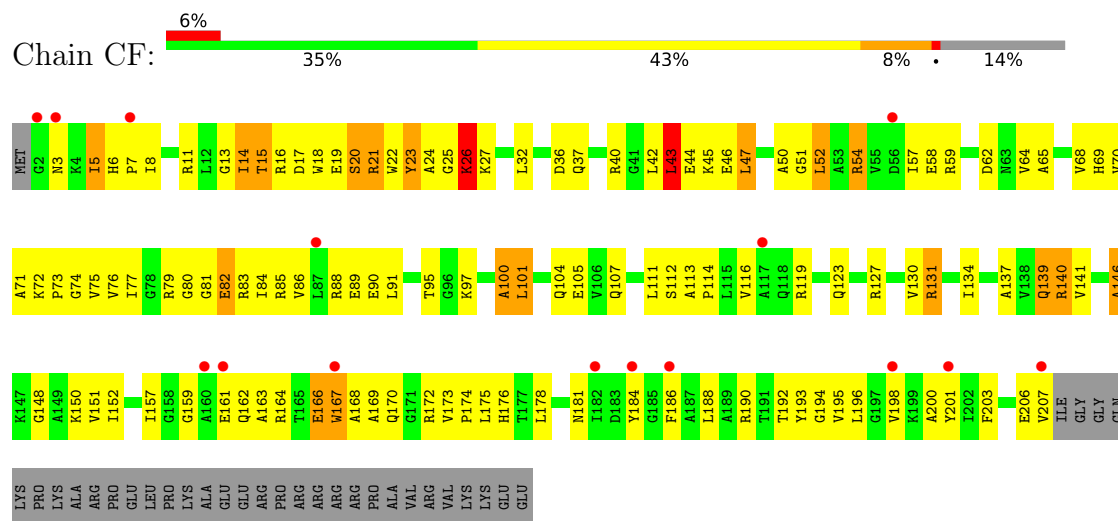


|       |       |       |       |        |      |      |      |      |      |      |
|-------|-------|-------|-------|--------|------|------|------|------|------|------|
| U1301 | A1229 | C1098 | G1034 | G973   | G903 | C817 | G724 | C634 | C554 | A313 |
| U1302 | C1230 | G1099 | A1035 | A974   | C904 | C818 | G725 | C635 | C555 | G316 |
| C1303 | G1233 | C1100 | G1036 | G975   | U905 | A819 | C726 | U636 | C556 |      |
| G1304 | A1170 | A1101 | C1037 | G976   | G906 | U820 | G727 | U637 | C557 | A321 |
| A1306 | A1238 | G1103 | C1038 | A977   | A909 | A821 | A728 | U638 | G558 | C322 |
| U1307 | A1239 | G1104 | U1040 | C978   | C910 | U827 | G730 | G639 | A559 | U823 |
| U1308 | U1240 | A1105 | A1041 | C979   | C910 | A828 | G731 | A640 | U560 | G324 |
| G1311 | G1176 | G1106 | G1042 | C980   | A913 | G829 |      | U646 | U561 | A325 |
| G1312 | G1177 | G1107 | C1043 | U981   | A914 | G830 | C735 |      | C562 | A478 |
|       | G1178 | G1108 | A1044 | U982   | A915 |      | C736 | G649 |      |      |
| A1245 | A1179 | C1039 | C1045 | A983   | G916 | U833 | A737 | G650 | U570 | C328 |
| A1248 | A1180 | C985  | A1046 | C984   | G917 | C834 | C738 | G651 | U571 | A329 |
| C1249 | G1161 | A986  | G1047 | C985   | A918 | U835 | G739 | U652 | A572 | C330 |
| C1250 | G1162 | G987  | U1048 | A986   | A919 | G836 | U740 | A653 | A573 | G331 |
| A1251 | G1184 |       | U1049 |        | U920 | G837 | G741 | G654 | A574 | G332 |
| A1252 | G1185 |       | G1050 | C990   | U921 | G838 | G742 | A655 | U575 | G333 |
|       | G1186 |       | C1051 | C991   | G922 | U841 |      |      | G576 |      |
| A1255 | G1187 |       | U1052 | U992   | G926 | C842 | C745 | G662 | G577 | C336 |
| A1256 | G1187 |       | G1053 | G993   | G927 | U843 |      | A663 | C578 | C337 |
| A1324 | G1190 |       | C1054 | A994   | U927 | C848 | C748 | U664 | C579 | A338 |
| C1325 | G1191 |       | A1055 | C995   |      | C849 | C749 | A665 | U580 | C339 |
| C1326 | G1192 |       | U1056 |        | C932 | U850 | G750 | G666 | C502 | U340 |
| C1327 | C1193 |       | G1057 | G998   | G933 | C851 | U751 | G667 | C504 | A415 |
| C1328 | U1194 |       | C1058 | C998A  | C934 | G852 | G752 | G668 | C505 | A344 |
| A1329 | C1195 |       | C1059 | U999   | A935 | C853 | A753 | U669 | G584 | C345 |
| U1330 | U1196 |       | G1060 | A1000  | C936 | C854 | C754 |      | G585 |      |
| C1331 | G1197 |       | U1061 | G1001  | C937 | G855 | G755 |      | C586 | G347 |
|       | G1198 |       | C1062 | A1002  | A938 | C856 |      | G674 | C600 |      |
| C1332 | G1199 |       | C1063 | G1003  | G939 | C857 | G765 | A675 | U591 | G350 |
| C1333 | U1200 |       | G1064 | A1004  | C940 | C858 | A766 | G676 | G592 | G351 |
| C1335 | G1201 |       | U1065 | A1005  | G941 | A859 |      | U677 | G593 | C352 |
| C1336 | C1202 |       | C1066 | C1006  | G942 | A860 | G769 |      | C600 | A353 |
| C1337 | G1203 |       | A1067 | C1007  | G945 | C861 | G774 | G684 | C518 | G354 |
| A1338 | G1272 |       | C1068 | C1008  | G946 | C862 |      | G685 | C519 |      |
| A1339 | G1273 |       | C1069 | G1009  | A947 | U863 | A777 | U686 | U429 | U359 |
|       | G1274 |       | U1070 | A1010  | G947 | A864 |      | A687 | A430 | A360 |
| C1342 | U1205 |       | C1071 | A1015  | C948 |      |      | G688 | G524 | G361 |
| G1343 | G1206 |       | G1072 | A1016  | A949 | C869 | A781 | C689 | C525 | G362 |
| A1346 | C1207 |       | U1073 | G1017  | U950 | U870 | A782 | C689 | C526 | A363 |
| G1347 | C1208 |       | G1074 | C1018  | G951 | U871 |      | G690 | G527 | A364 |
| U1348 | C1209 |       | C1075 | C1019  | U952 | A872 | G785 | C610 | C528 | U365 |
| A1349 | G1210 |       | C1076 | U1020  | G953 | A873 |      | A611 | G529 | C366 |
| A1350 | U1211 |       | G1077 | G1021  | G954 | C874 | G791 | C612 | G530 | U367 |
| U1351 | U1212 |       | U1078 | G1022  | U955 |      | A792 |      | U531 |      |
| C1352 | A1213 |       | G1079 | G1023  | U956 | C878 | U793 | C618 | A532 | C372 |
| C1353 | G1214 |       | A1080 | G1024  | U957 | C879 | A794 | U619 | A533 | A373 |
| A1285 | C1215 |       | U1081 | U1025  | A958 | C880 |      | C620 | U534 | A374 |
| A1286 | A1146 |       | G1081 | A959   |      |      | G797 | A704 | A535 | U375 |
| A1287 | C1217 |       |       | G1026  | U960 | C883 | C798 | U705 | C536 | G376 |
| A1288 | C1218 |       | G1084 | C1027  | U961 | U884 |      | C706 | G537 | G377 |
| A1289 | U1219 |       | U1085 | C1028  | U962 | C885 | U804 | C707 | G538 | G378 |
| G1290 | G1220 |       | U1086 | C1028A | G963 |      | C805 | C708 | A539 | C379 |
| G1291 | G1221 |       | A1151 | G1028B | A964 | G890 | C806 | G711 | G540 | G380 |
| U1292 | G1222 |       | U1091 | G1029  | G965 | U891 |      | A712 | G541 | C381 |
| G1293 | C1223 |       | A1092 | C1030  | A966 | A892 | C811 | G713 | G542 | A453 |
|       | A1157 |       | G1093 | G1031  | G967 |      | C812 |      | C454 | A382 |
| A1297 | A1225 |       | G1094 | A1032  | C967 | A900 | U813 | C719 | C455 | A383 |
| C1298 | C1226 |       | U1095 | G1032A | A968 | A901 |      | G546 | C456 | G394 |
| C1299 | A1227 |       | C1096 | U1032B | A969 | G902 | A816 |      | C457 | A389 |
| G1300 | C1228 |       | C1097 | G1033  |      |      |      |      | C458 |      |

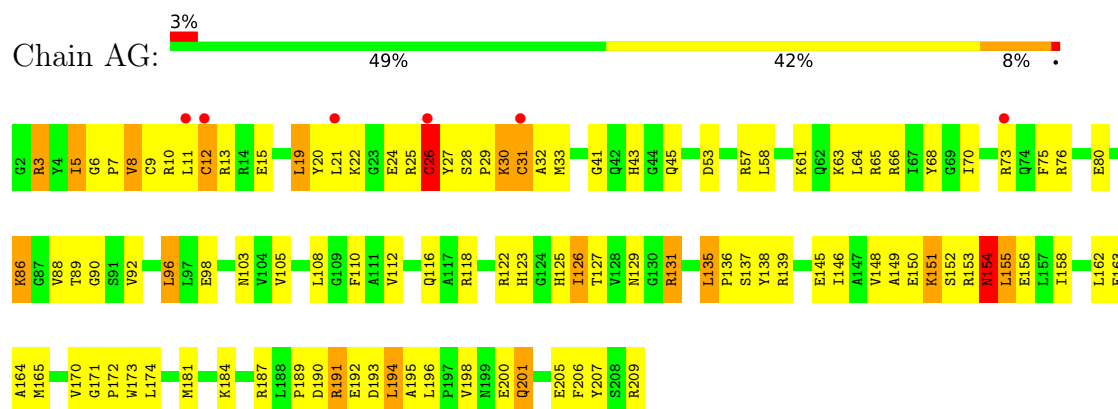




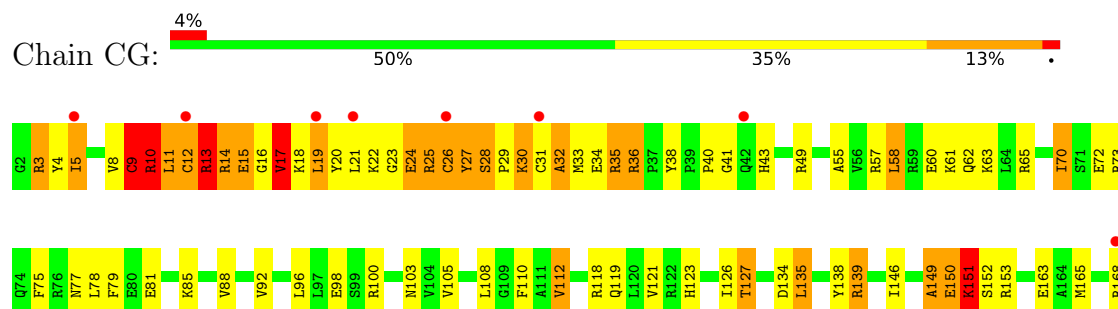
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

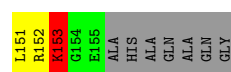
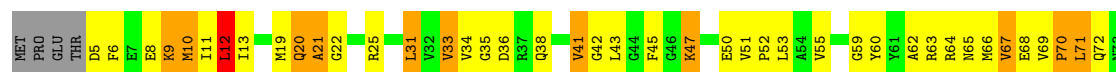


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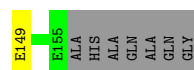
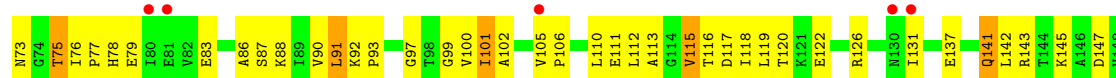
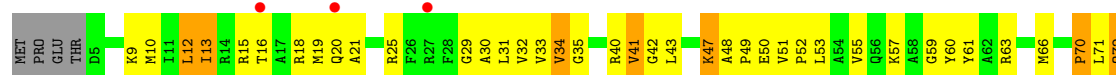




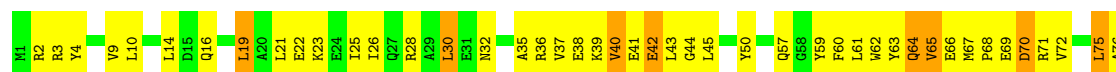
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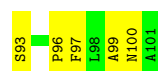
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



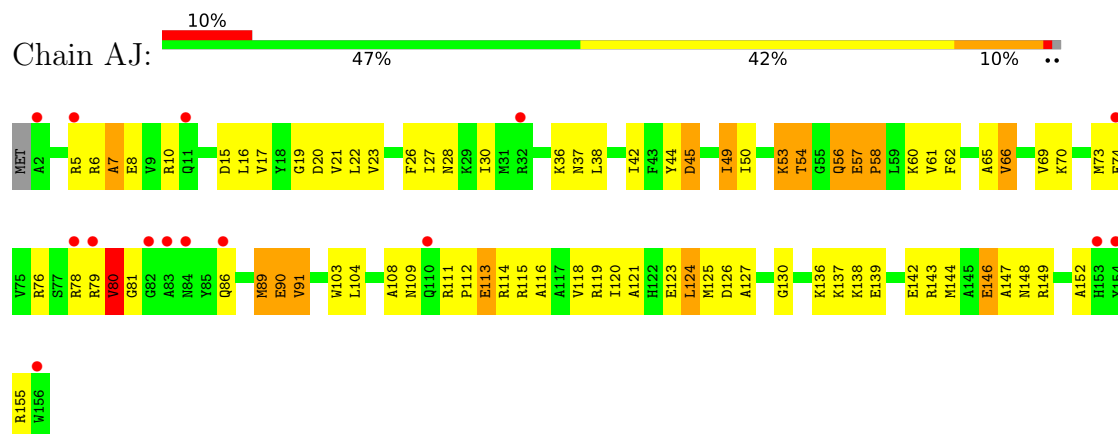
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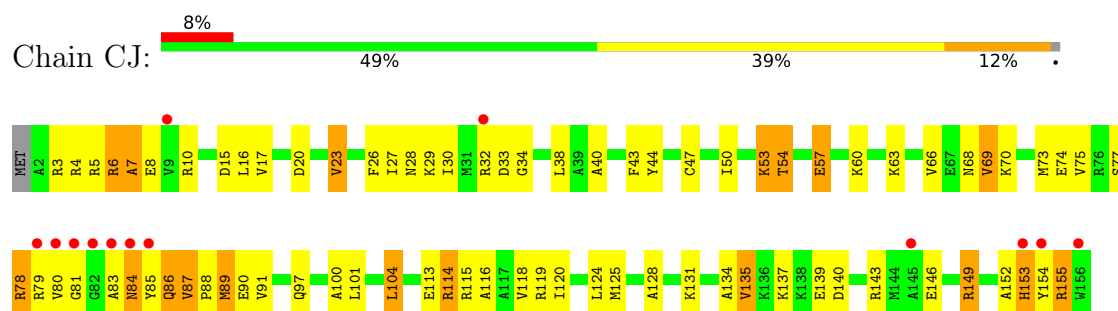
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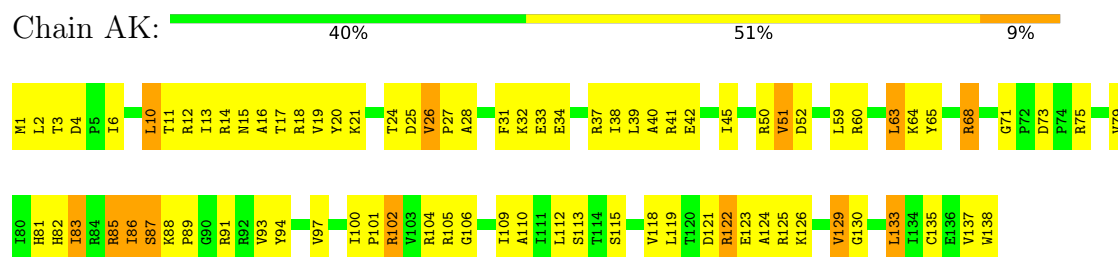
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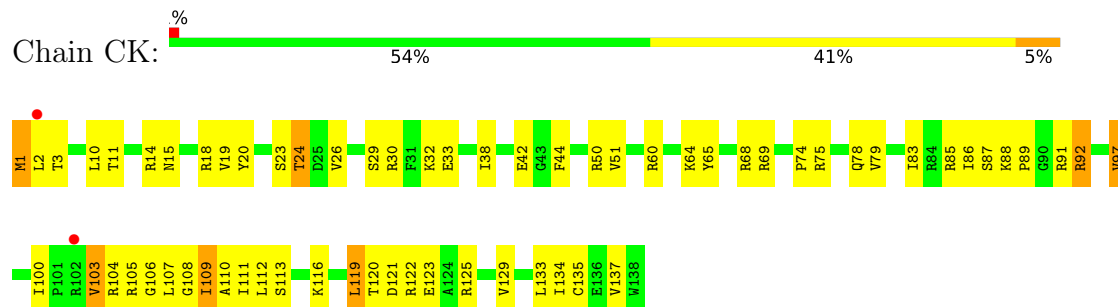
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

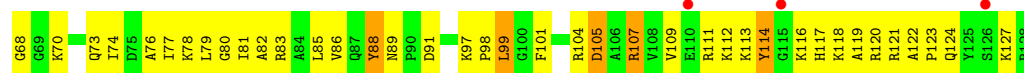
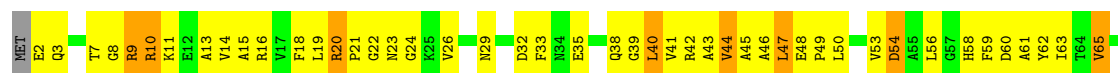


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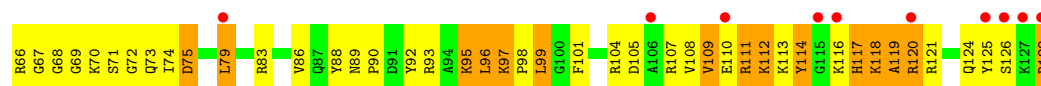


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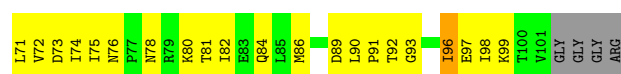




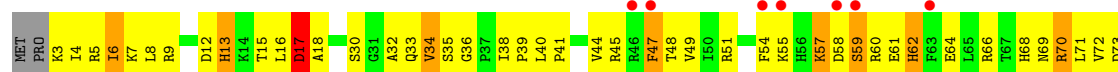
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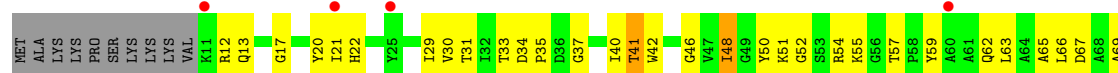
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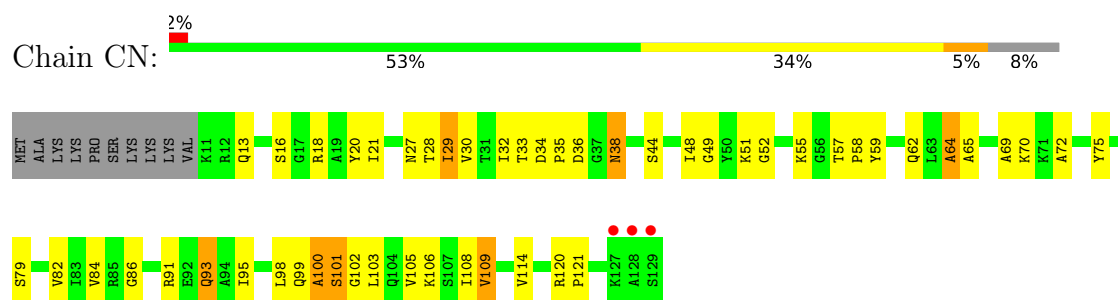
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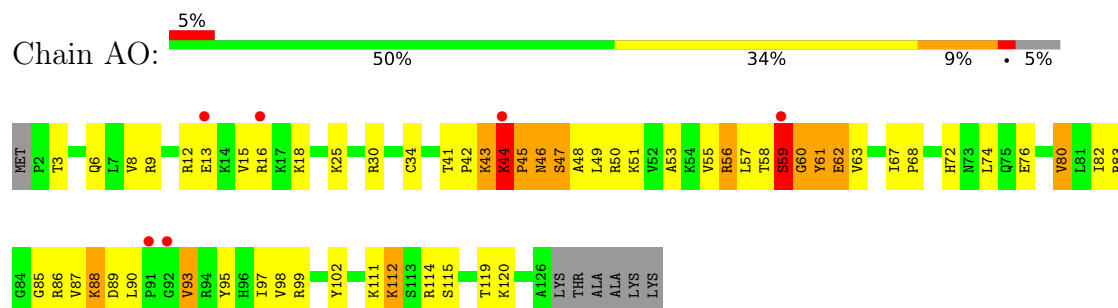
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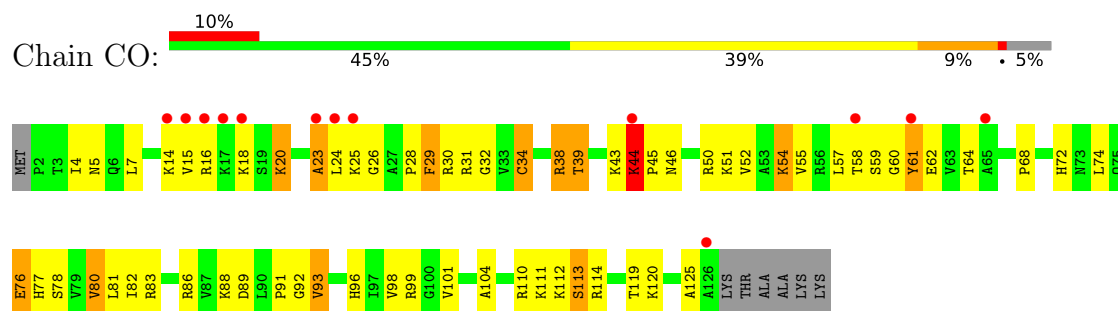
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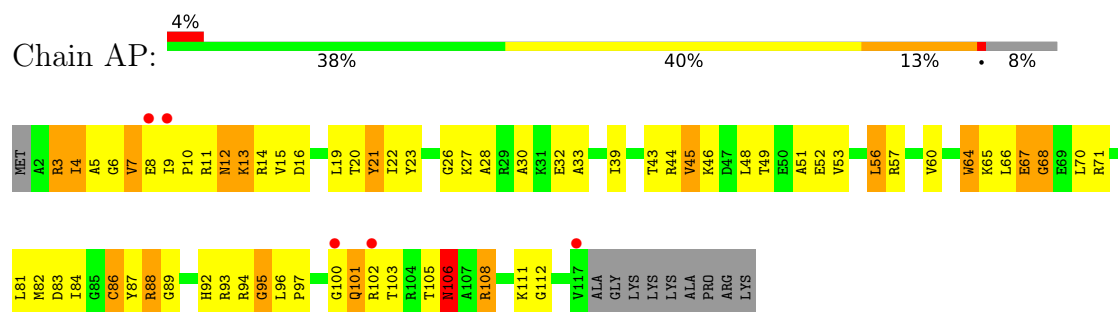
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



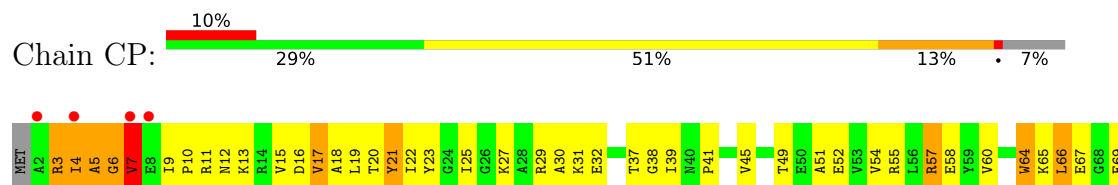
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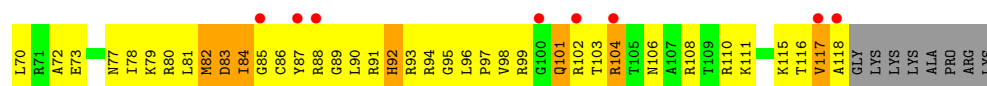


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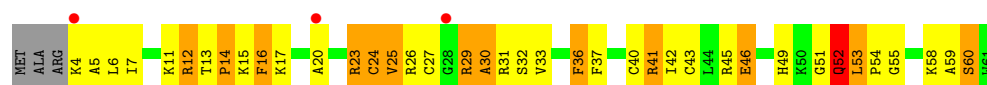


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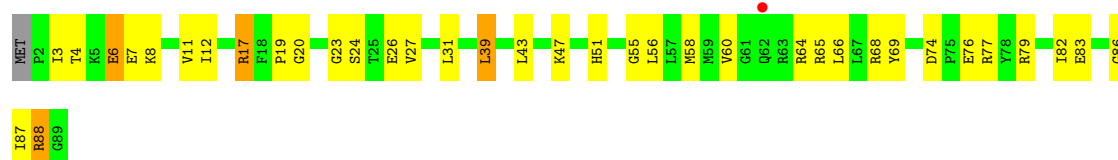
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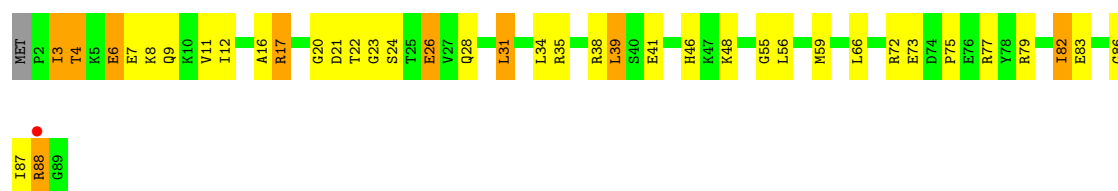
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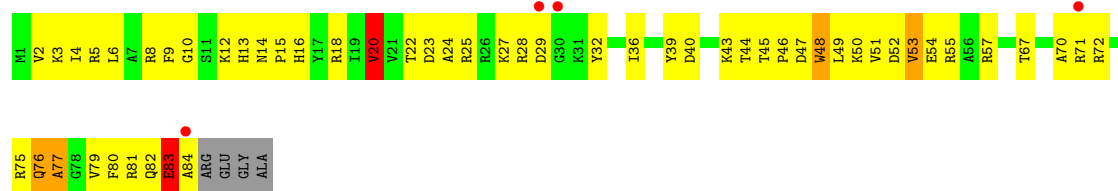
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

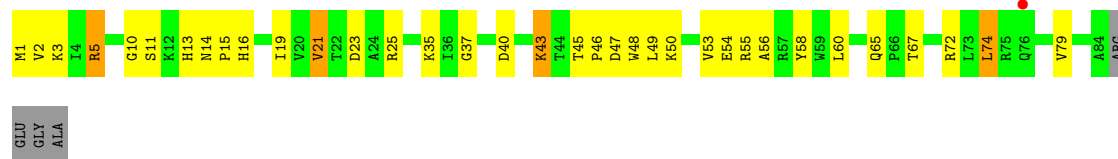


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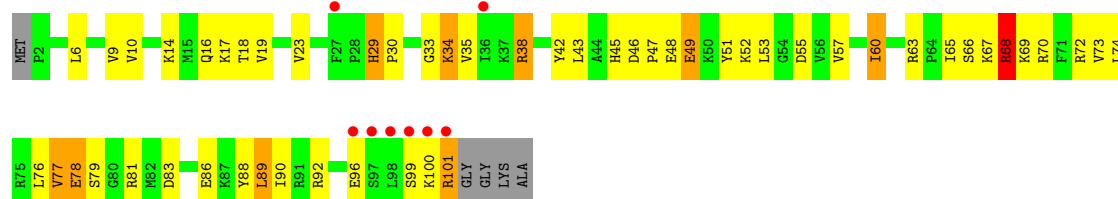


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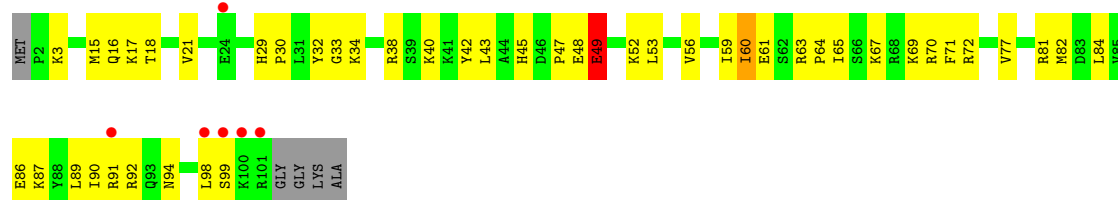




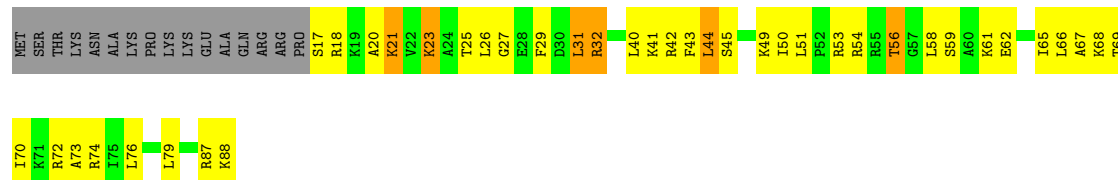
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



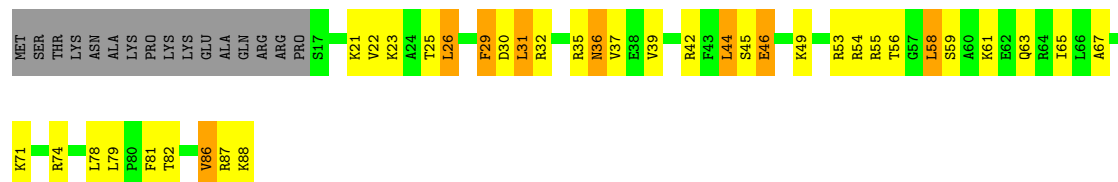
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



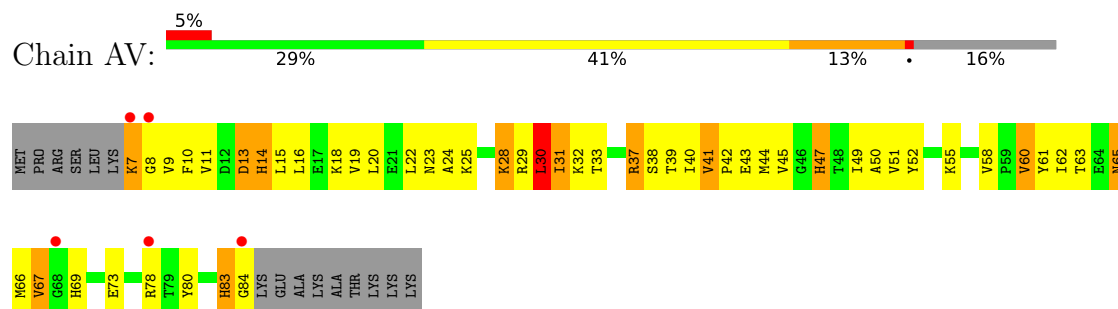
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



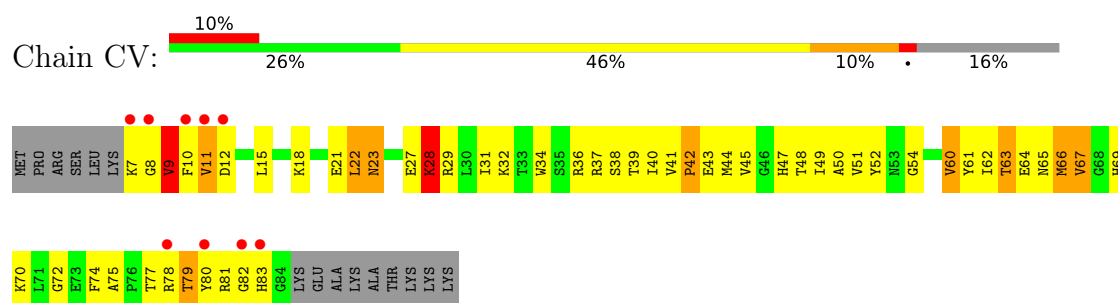
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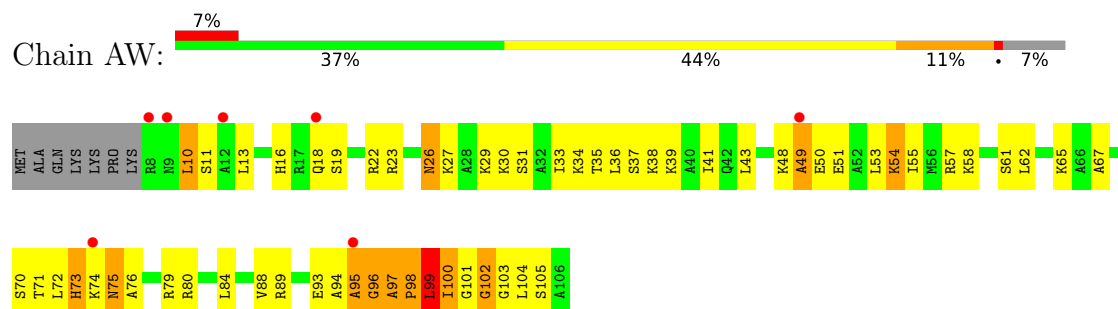
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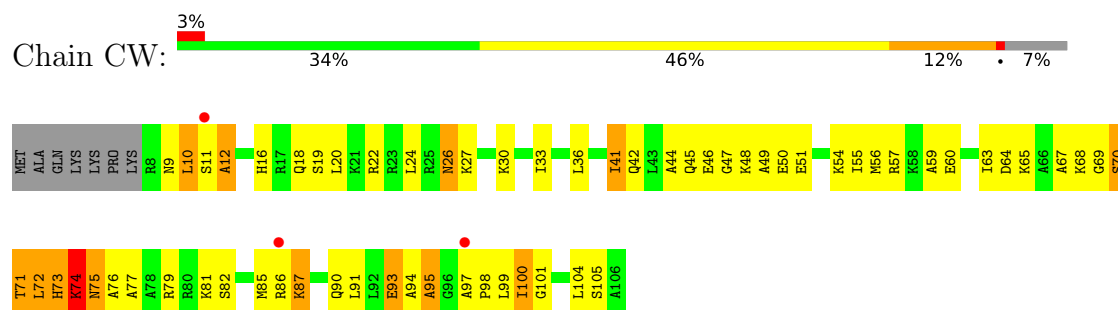
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• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



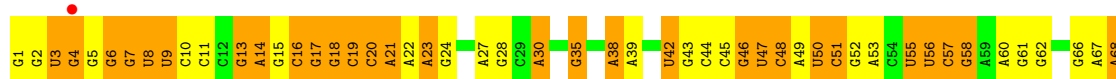
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CX: 



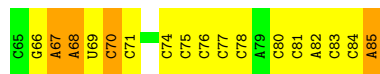
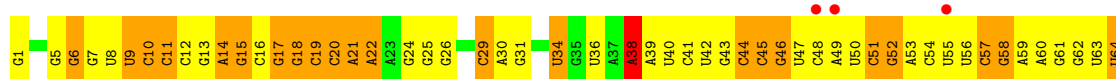
- Molecule 22: TRNA-TYR

Chain AB: 



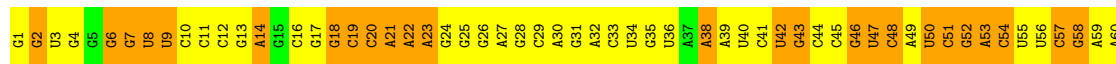
- Molecule 22: TRNA-TYR

Chain AD: 

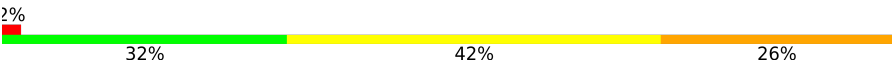


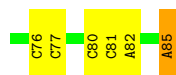
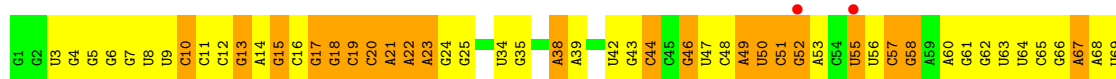
- Molecule 22: TRNA-TYR

Chain CB: 

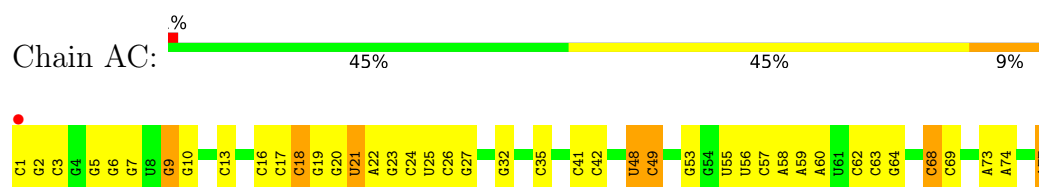


- Molecule 22: TRNA-TYR

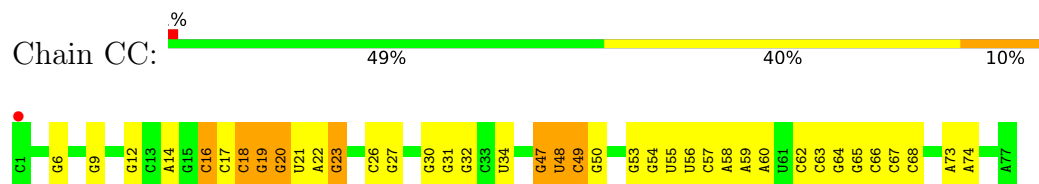
Chain CD: 



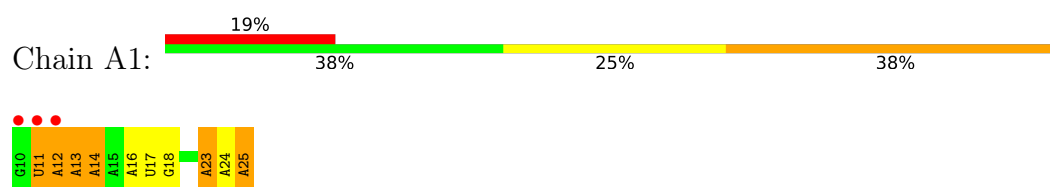
- Molecule 23: TRNA-FMET



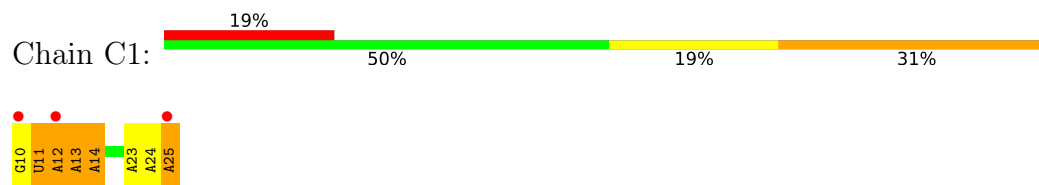
- Molecule 23: TRNA-FMET



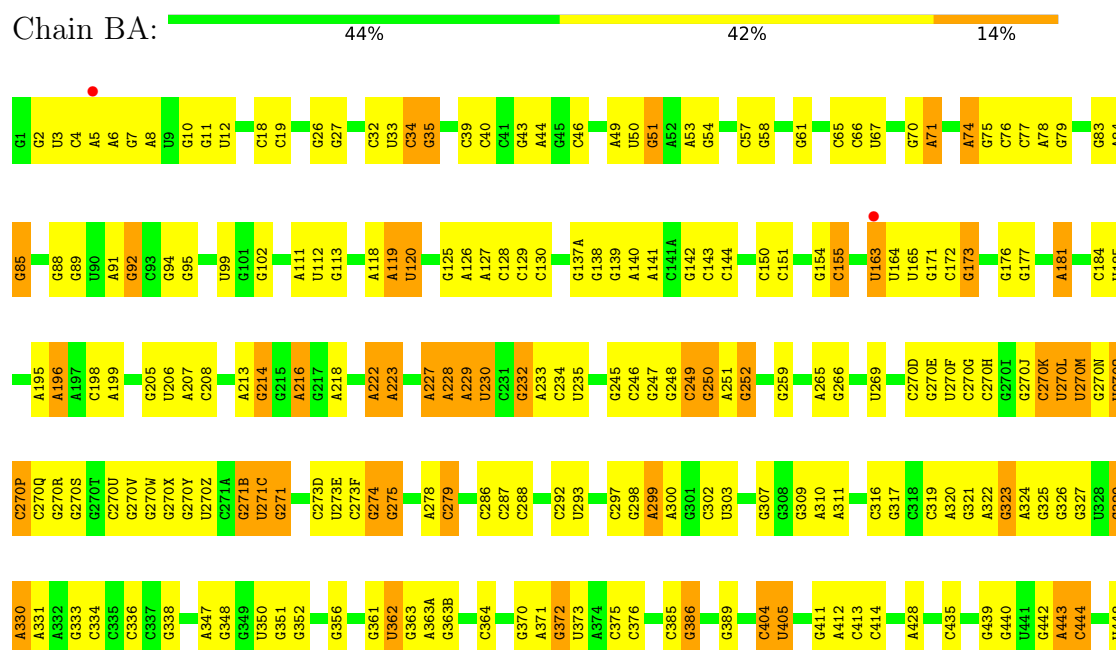
- Molecule 24: MRNA



- Molecule 24: MRNA

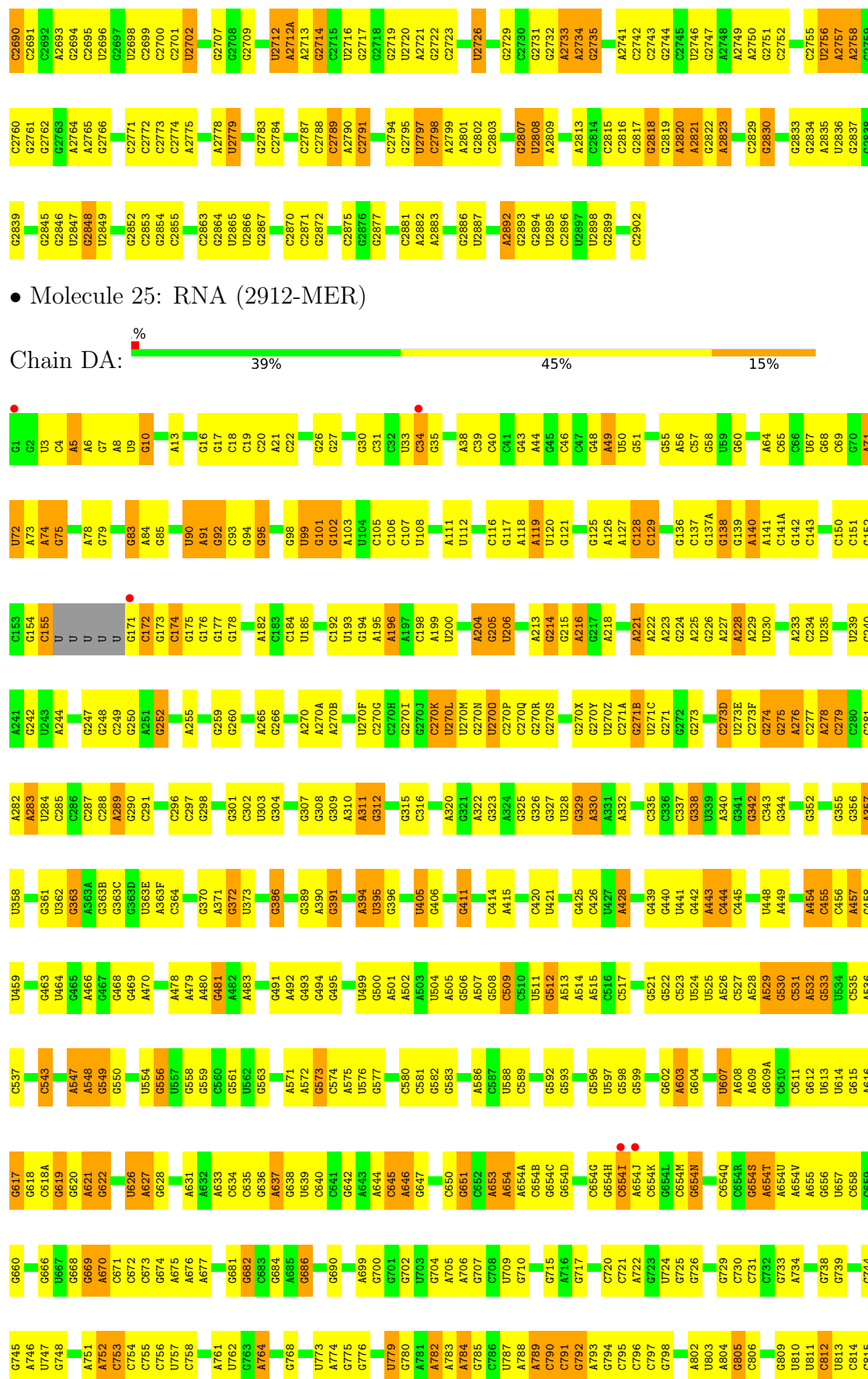


- Molecule 25: RNA (2912-MER)



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |        |       |       |       |       |       |       |       |        |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1421 | A1427 | C1428 | C1430 | U1431 | A1434 | G1442 | G1443 | A1444 | C1445 | G1446 | G1447 | G1448 | A1449 | G1449A | C1450 | C1451 | G1458 | G1459 | A1460 | G1461 | C1464 | G1465  | A1466 | G1467 | C1468 | A1469 | G1470 | A1471 | A1472 | C1473 | C1474 | G1475 | C1476 | A1477 | G1478 | C1479 | G1483 | A1486 | G1487 | C1493 | A1494 | A1495 | A1496 | U1497 | C1498 | G1499 | G1500 | C1505 |       |       |       |       |       |       |       |       |       |       |       |
| G1264 | U1265 | G1266 | A1269 | C1270 | G1271 | A1272 | U1273 | A1278 | G1279 | A1284 | G1285 | A1286 | A1287 | U1288  | G1289 | C1290 | G1291 | U1292 | C1293 | G1296 | C1297 | G1298  | C1299 | A1300 | A1301 | G1302 | C1303 | G1309 | G1310 | G1311 | U1312 | U1313 | C1314 | C1315 | U1316 | A1317 | G1318 | C1319 | C1320 | U1323 | U1324 | C1327 | G1328 | U1329 | C1330 | A1331 | G1332 | U1341 | G1348 | A1349 |       |       |       |       |       |       |       |       |       |
| U1352 | A1353 | A1354 | G1355 | G1356 | U1357 | G1358 | A1359 | A1360 | G1363 | G1364 | A1365 | G1368 | G1369 | C1370  | G1371 | U1372 | A1373 | G1374 | A1379 | G1380 | G1381 | G1382  | C1383 | A1384 | G1385 | G1386 | C1387 | G1388 | G1389 | U1394 | A1395 | U1396 | U1397 | G1400 | G1401 | G1402 | C1403 | C1404 | U1405 | U1406 | C1407 | C1408 | G1409 | G1410 | C1411 | A1412 | G1413 | G1416 | C1417 | G1418 | A1419 | U1420 |       |       |       |       |       |       |       |
| G1107 | U1108 | C1109 | G1110 | A1111 | G1112 | U1113 | C1121 | G1122 | G1125 | A1126 | A1127 | A1128 | U1129 | G1130  | G1131 | C1135 | G1136 | G1137 | G1138 | G1139 | U1142 | A1142A | A1143 | G1144 | C1145 | C1146 | C1147 | A1148 | G1151 | C1152 | C1153 | A1156 | G1157 | C1158 | C1161 | G1162 | G1163 | U1164 | U1165 | C1166 | G1171 | G1173 | A1174 | U1175 | G1176 | A1177 | C1178 | C1179 | C1180 | C1185 |       |       |       |       |       |       |       |       |       |
| A1046 | G1047 | A1048 | C1049 | A1050 | G1051 | C1052 | C1053 | A1054 | G1055 | U1056 | A1057 | U1058 | G1059 | U1060  | U1061 | G1062 | G1063 | C1064 | U1065 | U1066 | A1067 | G1068  | A1069 | A1070 | G1071 | C1072 | A1073 | G1074 | C1075 | C1076 | U1077 | U1078 | A1079 | G1080 | U1081 | U1082 | U1083 | A1084 | A1085 | U1086 | G1087 | A1088 | G1089 | U1090 | G1091 | C1092 | G1093 | U1094 | A1095 | A1096 | U1097 | C1100 | U1101 | G1103 | C1102 | A1103 | C1104 | U1105 | A1106 |
| C967  | G968  | U969  | C970  | G971  | G972  | A973  | G974  | C974A | G975  | G978  | A983  | C986  | G987  | G988   | G989  | A990  | C991  | G992  | G993  | C994  | G995  | A996   | G1003 | C1004 | G1005 | C1006 | A1009 | G1010 | G1011 | U1012 | C1013 | U1014 | G1015 | G1016 | U1019 | A1020 | A1021 | G1022 | U1023 | G1024 | G1025 | U1026 | A1027 | A1028 | U1029 | U1033 | G1034 | G1042 | G1043 | C1044 | A1045 |       |       |       |       |       |       |       |       |
| A887  | C888  | A889  | G890  | C891  | G892  | C893  | C894  | U895  | C897  | C898  | A899  | U899  | A900  | A901   | C902  | C903  | G904  | U905  | G906  | U907  | C908  | A909   | A910  | C911  | C912  | U913  | C914  | G915  | G916  | A917  | C918  | G919  | C925  | G932  | A933  | G938  | A941  | G942  | U943  | G944  | A945  | G946  | G950  | C951  | G952  | A953  | G956  | U957  | U958  | A959  | A960  | C961  | G966  |       |       |       |       |       |       |
| C812  | U813  | C814  | C817  | G818  | A819  | A820  | A821  | U826  | U827  | U828  | A829  | G830  | C831  | G832   | U833  | C834  | U839  | C844  | C845  | C846  | U847  | G848   | A849  | C850  | U851  | C852  | C853  | C856  | C857  | U858  | C859  | U860  | A861  | A862  | A863  | C864  | C865  | A866  | C867  | U868  | C869  | A870  | C873  | A878  | C879  | C880  | C881  | C882  | C883  | C884  | C885  | C886  |       |       |       |       |       |       |       |
| G733  | G738  | G739  | U740  | G743  | G744  | G745  | G746  | U747  | U748  | A751  | A752  | C753  | C754  | C755   | C756  | A764  | G765  | C766  | A767  | G768  | C769  | A771   | A772  | A773  | G775  | G776  | A777  | U778  | G779  | C780  | A781  | A782  | A783  | A784  | C785  | C786  | U787  | A788  | A789  | C790  | C791  | G792  | A793  | G794  | C795  | C796  | C797  | A802  | G805  | C806  | U811  |       |       |       |       |       |       |       |       |
| C654I | A654J | C654K | C654L | C654M | C654N | C654O | C654P | C654Q | C654R | C654S | A654T | A655  | C656  | U657   | C658  | C659  | G660  | C664  | C668  | C669  | A670  | C671   | C672  | C673  | C674  | A675  | A676  | C686  | C690  | C691  | C692  | C693  | U694  | C695  | C696  | C697  | C698  | A699  | G700  | U714  | G715  | A716  | G717  | C720  | C721  | A722  | G723  | U724  | G725  | G726  | C730  |       |       |       |       |       |       |       |       |
| G592  | G593  | C598  | G602  | A603  | G604  | C605  | A606  | G607  | G612  | U613  | U614  | G615  | A616  | G617   | C618  | C618A | G619  | A620  | C621  | G622  | G625  | U626   | G627  | G628  | G629  | C630  | A631  | A632  | A633  | C634  | C635  | C636  | A637  | G638  | U639  | C640  | C641  | G642  | A643  | A644  | C645  | A646  | G647  | C650  | C651  | G652  | C653  | A654  | A654A | C654B | C654C | G654D | C654G | C654H | C591  |       |       |       |       |
| C523  | U524  | U525  | A526  | C527  | G528  | A529  | C530  | C531  | A532  | G533  | U534  | C535  | A536  | C537   | G539  | G540  | C542  | C543  | C544  | G545  | C546  | A547   | A548  | G549  | G550  | G551  | U552  | U553  | U554  | C555  | C556  | U557  | G558  | G559  | C560  | G561  | U562  | C563  | C564  | C565  | U566  | A571  | A572  | C573  | C574  | A575  | C580  | C581  | G582  | C583  | A513  | A514  | C515  | C516  | C517  | G521  | G522  |       |       |





|       |       |       |       |        |        |       |        |        |       |       |      |      |
|-------|-------|-------|-------|--------|--------|-------|--------|--------|-------|-------|------|------|
| A1812 | G1725 | G1622 | C1533 | G1455  | G1389  | A1308 | C1221  | G1149  | G1015 | C951  | G883 | C816 |
| G1813 | G1728 | G1625 | G1534 | C1458  | A1392  | G1309 | C1222  | C1150  | G1016 | C952  | C884 | C817 |
| G1814 | G1729 | G1635 | G1535 | C1459  | A1393  | G1310 | C1223  | C1151  | G1086 | G952  | C885 | C818 |
| A1815 | U1730 | G1635 | A1536 | G1459  | A1394  | C1314 | C1225  | C1152  | G1087 | G953  | C886 | A819 |
| G1816 | G1731 | G1635 | G1537 | A1460  | U1395  | C1315 | C1226  | C1153  | A1088 | A1020 | A887 | G820 |
| U1818 | A1732 | G1638 | G1538 | G1461  | U1396  | C1316 | A1227  | C1154  | G1089 | A1021 | C888 | A821 |
| A1819 | U1639 | U1639 | G1539 | C1464  | A1397  | U1317 | G1228  | A1155  | G956  | G1022 | C889 | G824 |
| U1820 | C1640 | G1640 | G1542 | C1467  | C1398  | A1317 | G1229  | A1156  | A957  | U1023 | A890 | A825 |
| A1821 | C1741 | G1645 | A1543 | C1468  | G1401  | G1318 | G1229A | U1159  | U958  | G1024 | A892 | C826 |
| G1826 | G1748 | G1647 | A1544 | A1469  | C1402  | G1319 | C1230  | C1160  | G1093 | U1025 | A893 | U827 |
| A1829 | A1749 | G1648 | A1545 | G1470  | C1403  | U1323 | G1231  | C1161  | U959  | U1026 | C894 | U828 |
| C1830 | G1753 | G1651 | C1548 | A1471  | C1404  | G1325 | G1232  | G1162  | A1095 | A1027 | U895 | A829 |
| G1831 | G1754 | A1651 | C1549 | A1472  | U1405  | U1326 | A1241  | G1163  | A1096 | A1028 | A896 | G830 |
| C1832 | A1755 | A1652 | C1550 | G1473  | U1406  | G1327 | G1248  | U1165  | A1098 | G1036 | C897 | G831 |
| U1833 | G1756 | G1653 | G1551 | C1474  | C1407  | G1328 | U1249  | C1166  | G1099 | G972  | A899 | G832 |
| G1839 | U1757 | A1654 | G1552 | G1475  | C1408  | U1329 | G1250  | U1167  | U960  | G973  | A900 | U833 |
| C1843 | G1758 | C1657 | C1556 | C1476  | C1409  | C1330 | C1251  | G1168  | G974  | A973  | C902 | C834 |
| A1847 | A1760 | G1657 | C1557 | A1477  | A1412  | A1331 | G1252  | G1169  | C974A | C974  | C903 | A835 |
| A1848 | C1761 | C1658 | A1558 | G1478  | G1413  | G1332 | A1253  | U1170  | G1039 | C975  | C904 | C838 |
| G1851 | A1762 | A1664 | G1560 | G1480  | G1416  | A1336 | G1254  | G1171  | C1040 | C976  | U905 | U839 |
| U1852 | G1763 | G1666 | G1568 | U1482  | C1417  | G1337 | U1255  | C1173  | C1041 | C977  | G906 | C844 |
| C1852 | G1769 | A1667 | A1569 | G1483  | G1418  | G1338 | G1256  | A1174  | G1110 | G977  | U907 | C845 |
| A1853 | U1770 | A1668 | A1570 | G1486  | A1419  | U1340 | G1259  | C1175  | C1042 | G978  | C908 | C846 |
| U1854 | C1771 | A1669 | A1571 | A1488  | U1420  | U1341 | C1261  | C1176  | A1045 | A980  | A910 | U847 |
| G1858 | G1772 | C1670 | C1577 | A1490  | G1421  | A1342 | A1262  | C1177  | G1047 | C982  | A911 | G848 |
| A1859 | A1773 | U1671 | U1578 | C1493  | G1422  | G1343 | G1263  | C1180  | C1048 | G983  | C912 | A849 |
| C1860 | C1773 | C1672 | U1578 | A1494  | G1426  | G1344 | G1264  | C1181  | C1049 | A984  | C914 | U851 |
| U1864 | A1778 | G1673 | C1582 | A1496  | A1427  | G1345 | A1265  | G1182  | A1050 | C985  | C915 | G854 |
| G1872 | G1781 | C1674 | C1583 | A1498  | A1428  | G1346 | G1266  | C1187  | G1055 | G986  | G916 | G855 |
| C1882 | A1783 | G1675 | A1584 | U1496  | G1429  | G1347 | U1267  | U1188  | A1056 | G987  | A917 | C856 |
| A1884 | C1782 | G1678 | U1585 | C1503  | G1430  | G1348 | A1268  | A1189  | G1056 | G989  | G919 | C857 |
| G1888 | A1791 | G1681 | C1586 | U1504  | U1431  | A1349 | G1269  | G1190  | G1057 | A990  | G920 | U858 |
| A1889 | G1792 | G1682 | C1587 | C1505  | C1432  | U1352 | C1270  | G1191  | C991  | C991  | G921 | G859 |
| G1899 | U1793 | C1686 | U1588 | A1508  | U1433  | G1356 | G1271  | G1192  | C992  | C992  | U860 | U860 |
| A1900 | C1794 | G1687 | U1590 | C1509  | G1434  | U1357 | A1272  | A1194  | G1059 | G993  | C924 | A861 |
| U1901 | U1796 | A1693 | C1591 | A1510  | G1435  | G1358 | U1273  | C1195  | C994  | C994  | C925 | G862 |
| C1902 | C1797 | G1699 | U1602 | A1511  | C1437  | A1359 | A1278  | C1196  | U1060 | C995  | A926 | A863 |
| G1903 | A1800 | A1701 | G1606 | G1512  | U1438  | A1360 | G1279  | U1198  | G1062 | A996  | G928 | G864 |
| U1906 | G1802 | G1710 | G1520 | C1513  | A1444  | G1369 | U1292  | U1199  | G1063 | G997  | G929 | C865 |
| C1914 | U1805 | C1712 | G1521 | U1514  | C1445  | A1365 | G1285  | C1200  | C1064 | C998  | A866 | A866 |
| U1915 | U1716 | G1717 | G1522 | C1515  | G1446  | A1366 | U1288  | C1201  | U999  | U999  | G931 | C867 |
| A1916 | A1810 | G1718 | U1523 | U1516  | G1447  | A1367 | U1299  | A1142  | U1065 | A1000 | G932 | U868 |
| G1917 | G1811 | G1718 | G1524 | A1449A | G1448  | G1380 | A1301  | A1142A | A1067 | A1001 | A932 | U869 |
| C1918 | U1812 | G1719 | G1525 | G1450  | A1449  | A1384 | U1300  | G1143  | G1068 | G1002 | A933 | A870 |
| U1919 | U1813 | G1720 | G1526 | C1451  | G1450  | G1385 | A1301  | C1145  | G1074 | G1003 | G934 | U871 |
| A1920 | U1814 | G1721 | U1527 | A1453  | C1451  | G1386 | A1302  | C1146  | C1075 | C1004 | G936 | G874 |
| G1921 | U1815 | G1722 | A1528 | U1454  | A1454  | C1387 | G1303  | C1147  | G1076 | G1011 | A945 | G875 |
| U1922 | U1816 | G1723 | G1529 | G1455  | G1455  | C1388 | U1454  | A1148  | U1012 | G1012 | G946 | G876 |
| C1923 | U1817 | G1724 | G1530 | G1456  | G1456  | G1389 | U1455  | A1149  | U1013 | G1013 | G947 | U877 |
| U1924 | U1818 | G1725 | G1531 | G1457  | G1457  | G1390 | U1456  | A1150  | U1014 | U1014 | G948 | A878 |
| A1925 | U1819 | G1726 | G1532 | G1458  | G1458  | G1391 | U1457  | A1151  | U1015 | U1015 | G949 | G879 |
| G1926 | U1820 | G1727 | G1533 | G1459  | G1459  | G1392 | U1458  | A1152  | U1016 | U1016 | G950 | G880 |
| U1927 | U1821 | G1728 | G1534 | G1460  | G1460  | G1393 | U1459  | A1153  | U1017 | U1017 | G951 | G881 |
| C1928 | U1822 | G1729 | G1535 | G1461  | G1461  | G1394 | U1460  | A1154  | U1018 | U1018 | G952 | G882 |
| U1929 | U1823 | G1730 | G1536 | G1462  | G1462  | G1395 | U1461  | A1155  | U1019 | U1019 | G953 | G883 |
| A1930 | U1824 | G1731 | G1537 | G1463  | G1463  | G1396 | U1462  | A1156  | U1020 | U1020 | G954 | A819 |
| G1931 | U1825 | G1732 | G1538 | G1464  | G1464  | G1397 | U1463  | A1157  | U1021 | U1021 | G955 | G820 |
| C1932 | U1826 | G1733 | G1539 | G1465  | G1465  | G1398 | U1464  | A1158  | U1022 | U1022 | G956 | A821 |
| U1933 | U1827 | G1734 | G1540 | G1466  | G1466  | G1399 | U1465  | A1159  | U1023 | U1023 | G957 | G824 |
| G1934 | U1828 | G1735 | G1541 | G1467  | G1467  | G1400 | U1466  | U1160  | U1024 | U1024 | A890 | A825 |
| U1915 | U1829 | C1736 | G1542 | C1468  | C1468  | U1401 | G1229  | C1161  | G1093 | U1025 | A892 | C826 |
| A1916 | C1830 | C1741 | A1543 | A1469  | A1469  | C1402 | C1230  | C1162  | U959  | U1026 | C894 | U827 |
| G1917 | G1831 | A1749 | A1544 | G1470  | G1470  | C1403 | G1231  | G1163  | A1095 | A1027 | U895 | A829 |
| C1918 | A1832 | G1753 | A1545 | A1471  | C1404  | G1325 | G1232  | U1165  | A1096 | A1028 | A896 | G830 |
| U1919 | U1833 | G1754 | C1548 | A1472  | U1405  | U1326 | A1241  | G1166  | A1098 | G1036 | C897 | G831 |
| G1920 | G1839 | G1755 | C1549 | G1473  | U1406  | G1327 | G1248  | U1167  | G1099 | G972  | A899 | G832 |
| C1921 | A1847 | A1756 | C1550 | C1474  | C1407  | G1328 | U1249  | C1168  | U960  | G973  | A900 | U833 |
| U1922 | A1848 | G1757 | G1551 | G1475  | C1408  | U1329 | G1250  | U1169  | G974  | A973  | C902 | C834 |
| C1923 | G1851 | U1758 | G1552 | C1476  | C1409  | C1330 | C1251  | G1170  | C974A | C974  | C903 | A835 |
| U1924 | U1852 | G1759 | C1556 | A1477  | A1412  | A1331 | G1252  | G1171  | G1039 | C975  | C904 | C838 |
| A1925 | C1852 | C1761 | A1558 | G1478  | G1413  | G1332 | A1253  | G1172  | C1040 | C976  | U905 | U839 |
| G1926 | A1853 | A1762 | G1560 | G1480  | G1416  | A1336 | G1254  | C1173  | C1041 | C977  | G906 | C844 |
| C1927 | U1854 | G1763 | G1568 | U1482  | C1417  | G1337 | U1255  | A1174  | G1110 | G977  | U907 | C845 |
| U1928 | U1855 | G1769 | A1569 | G1483  | G1418  | G1338 | G1256  | C1175  | C1042 | G978  | C908 | C846 |
| C1929 | C1856 | A1770 | A1570 | G1486  | A1419  | U1340 | G1259  | C1176  | A1045 | A980  | A910 | U847 |
| U1930 | A1857 | U1771 | A1571 | A1488  | U1420  | U1341 | C1261  | C1177  | G1047 | C982  | A911 | G848 |
| G1931 | G1858 | G1772 | C1577 | A1490  | G1421  | A1342 | A1262  | C1180  | C1048 | G983  | C912 | A849 |
| C1932 | A1859 | C1773 | U1578 | C1493  | G1422  | G1343 | G1263  | C1181  | C1049 | A984  | C914 | U851 |
| U1933 | C1860 | U1778 | U1578 | A1494  | G1426  | G1344 | G1264  | G1182  | A1050 | C985  | C915 | G854 |
| A1934 | U1860 | C1779 | C1582 | A1496  | A1427  | G1345 | A1265  | C1187  | G1055 | G986  | G916 | G855 |
| G1935 | G1861 | G1781 | C1583 | A1498  | A1428  | G1346 | G1266  | U1188  | A1056 | G987  | A917 | C856 |
| C1936 | A1862 | A1783 | A1584 | U1496  | G1429  | G1347 | U1267  | A1189  | G1056 | G989  | G919 | C857 |
| U1937 | C1863 | C1782 | U1585 | C1503  | G1430  | A1349 | G1269  | G1190  | G1057 | A990  | G920 | U858 |
| G1938 | U1864 | G1678 | U1586 | U1504  | U1431  | U1352 | C1270  | G1191  | C991  | C991  | G921 | G859 |
| A1939 | U1865 | G1681 | C1587 | C1505  | C1432  | G1356 | G1271  | G1192  | C992  | C992  | U860 | U860 |
| C1940 | A1866 | G1682 | C1588 | A1508  | U1433  | U1357 | A1272  | A1194  | G1059 | G993  | C924 | A861 |
| U1941 | C1867 | C1783 | U1589 | C1509  | G1434  | G1358 | U1273  | C1195  | C994  | C994  | C925 | G862 |
| C1942 | U1868 | A1785 | C1591 | A1510  | G1435  | G1358 | U1278  | C1196  | U1060 | C995  | A926 | A863 |
| G1943 | A1869 | A1786 | C1592 | A1511  | C1437  | A1359 | A1279  | U1198  | G1062 | A996  | G928 | G864 |
| U1944 | C1870 | G1787 | U1593 | G1512  | U1438  | A1360 | G1279  | U1199  | G1063 | G997  | G929 | C865 |
| C1945 | U1871 | G1683 | G1594 | C1513  | A1439  | G1365 | U1285  | C1200  | C1064 | C998  | A866 | A866 |
| A1946 | U1872 | G1684 | U1595 | U1514  | C1445  | A1366 | G1288  | C1201  | U999  | U999  | G931 | C867 |
| G1947 | C1873 | G1685 | C1596 | C1515  | G1446  | A1367 | U1299  | A1142  | U1065 | A1000 | G932 | U868 |
| U1948 | A1874 | U1789 | C1598 | U1516  | G1447  | G1368 | A1301  | A1142A | A1067 | A1001 | A932 | U869 |
| C1949 | U1875 | C1790 | U1602 | A1444A | A1444  | G1369 | U1292  | G1143  | G1068 | G1002 | A933 | A870 |
| U1950 | C1876 | U1791 | G1606 | G1520  | C1445  | A1370 | U1292  | C1145  | A1070 | G1003 | G934 | U871 |
| G1951 | A1877 | A1792 | G1521 | G1521  | G1446  | A1379 | A1287  | C1146  | C1004 | C1004 | G936 | G874 |
| C1952 | U1878 | G1792 | G1522 | U1522  | G1447  | A1380 | C1297  | U1142  | G1072 | C1005 | A941 | G875 |
| U1953 | C1879 | C1793 | U1523 | G1448  | G1448  | G1380 | C1298  | A1142A | A1073 | C1006 | A942 | G876 |
| C1954 | A1880 | U1794 | G1524 | A1449  | G1449  | A1384 | A1299  | G1143  | G1074 | C1007 | U943 | U877 |
| U1955 | U1881 | G1795 | G1525 | G1449A | A1449A | A1385 | U1300  | C1144  | C1075 | A1010 | A944 | A878 |
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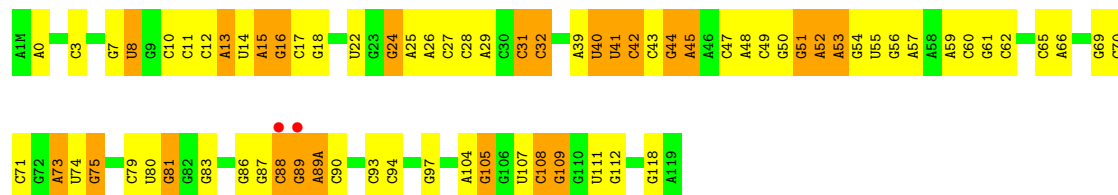




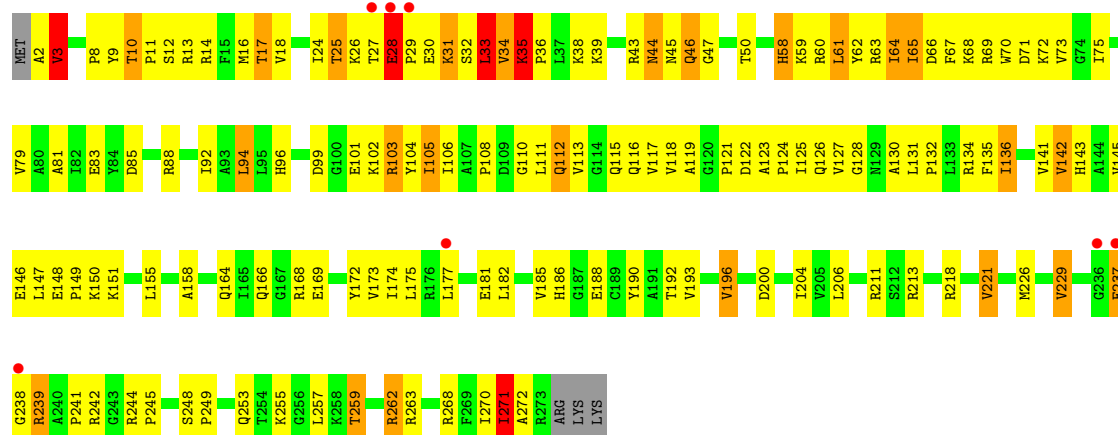
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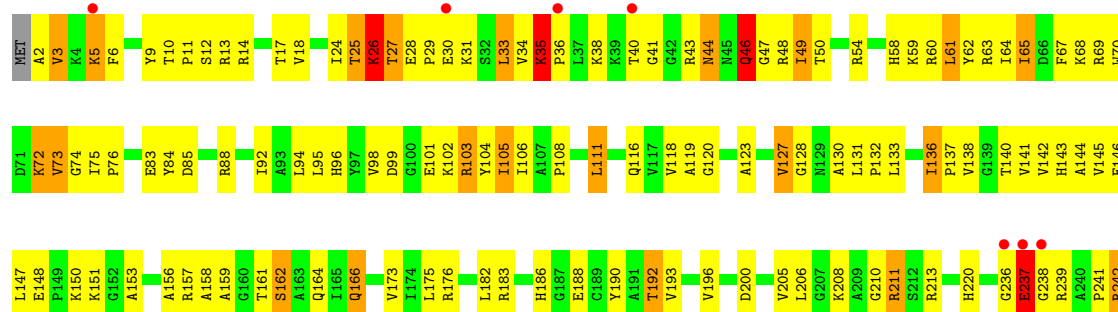
• Molecule 26: 5S RIBOSOMAL RNA



• Molecule 27: 50S ribosomal protein L2

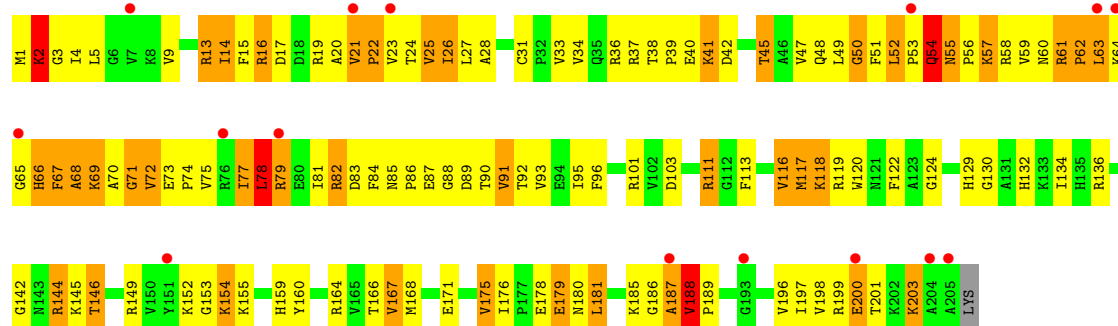


• Molecule 27: 50S ribosomal protein L2

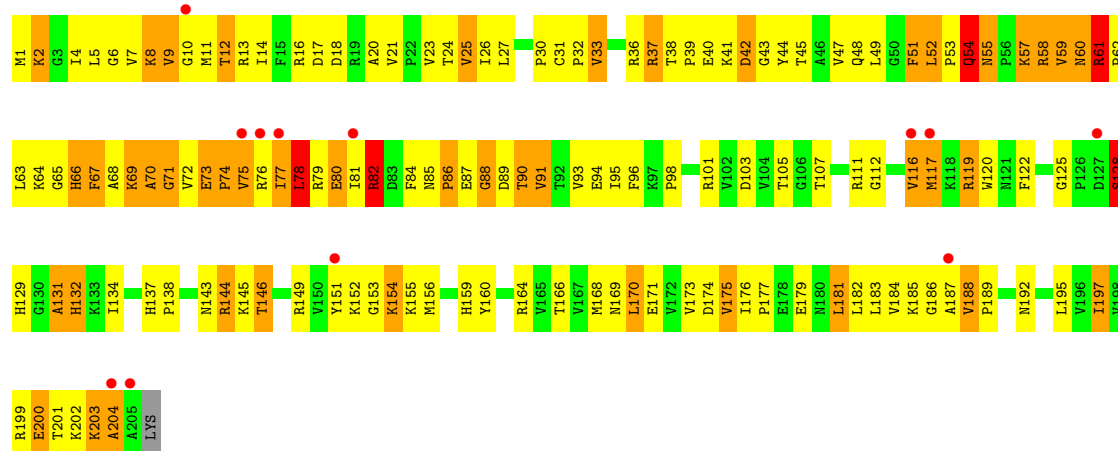




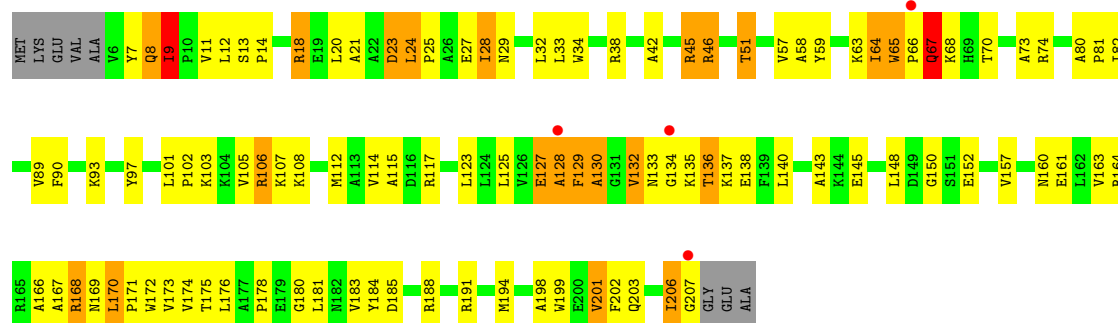
• Molecule 28: 50S ribosomal protein L3



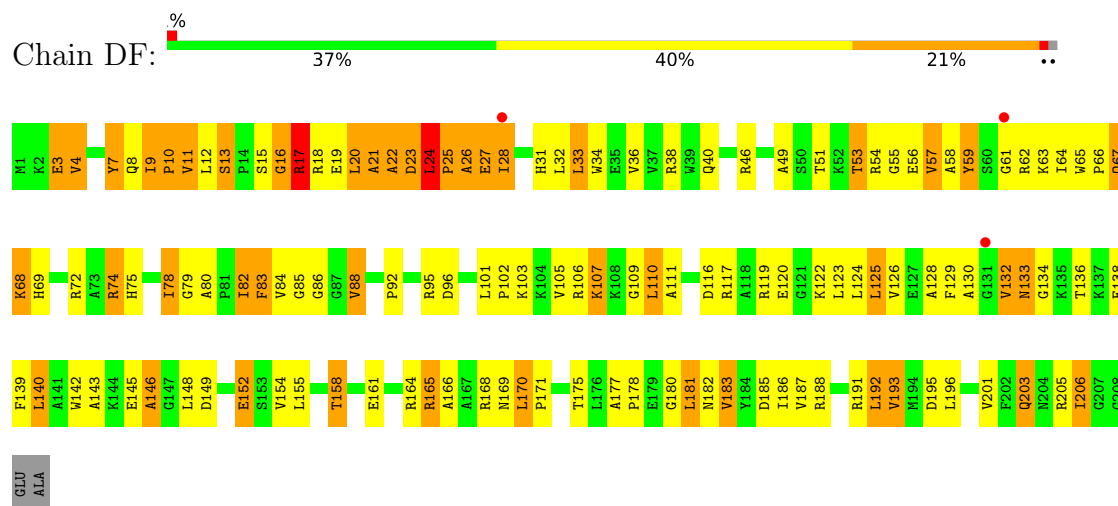
• Molecule 28: 50S ribosomal protein L3



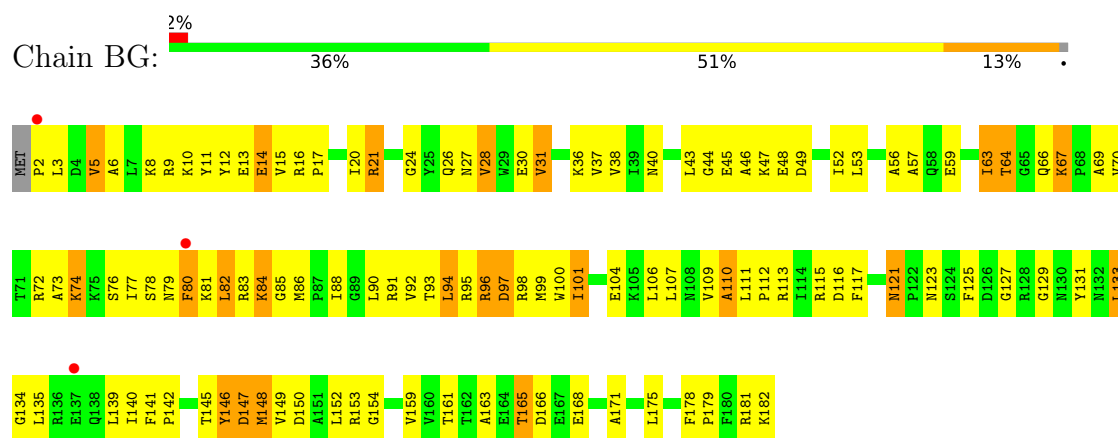
• Molecule 29: 50S ribosomal protein L4



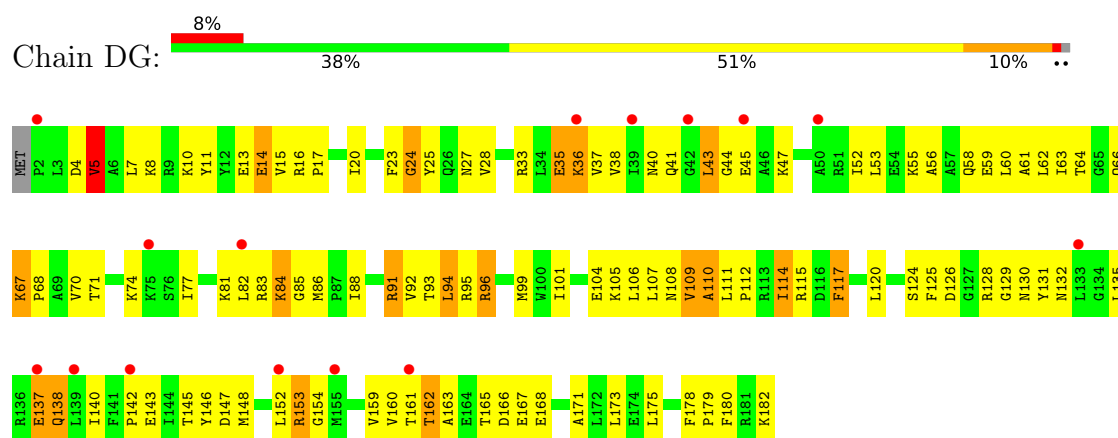
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5

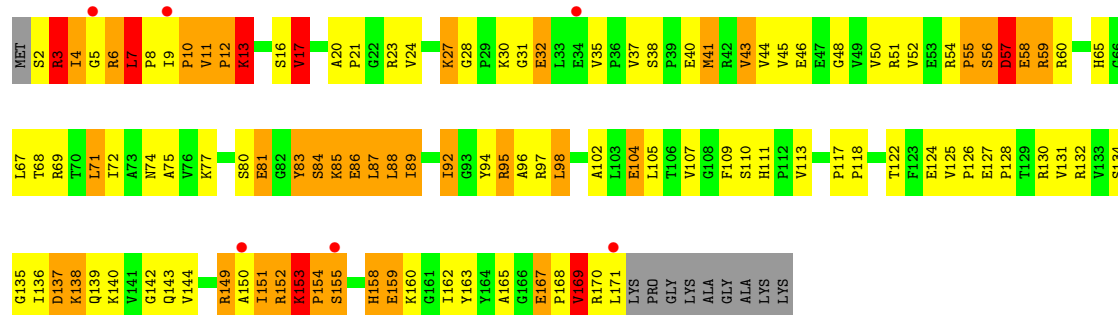


- Molecule 30: 50S ribosomal protein L5

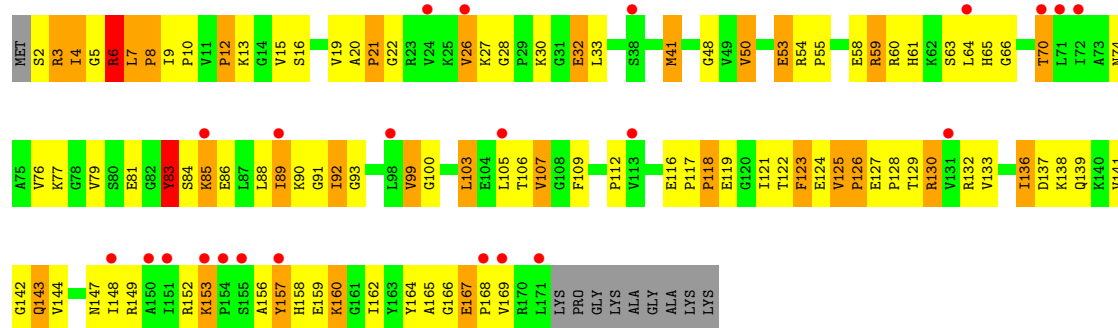


- Molecule 31: 50S ribosomal protein L6

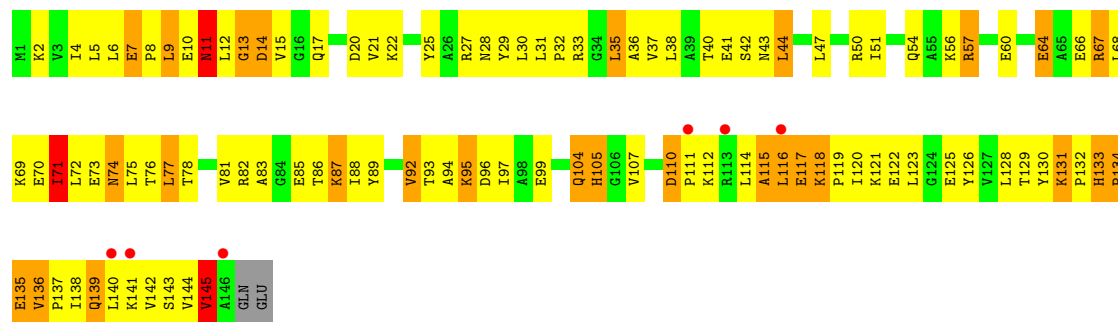




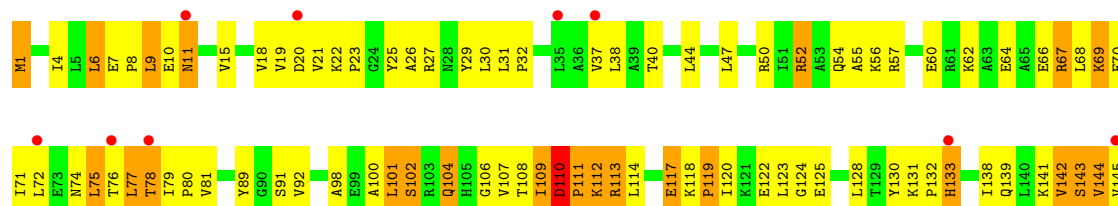
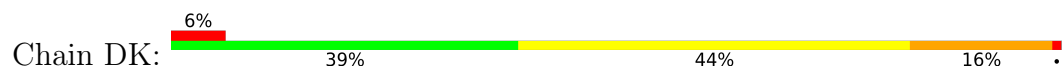
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

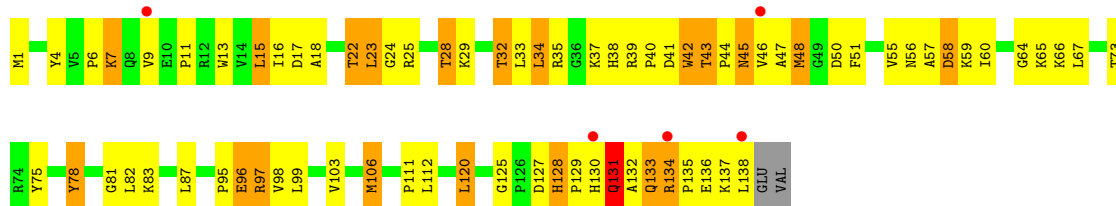


• Molecule 32: 50S ribosomal protein L9

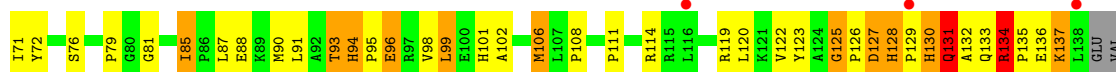
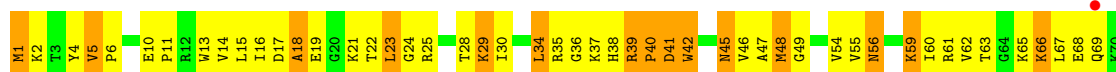




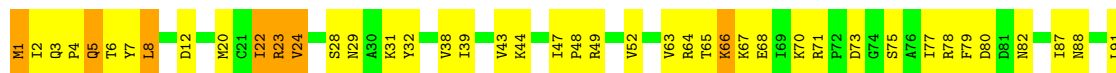
• Molecule 33: 50S ribosomal protein L13



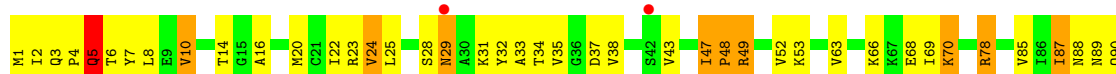
• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

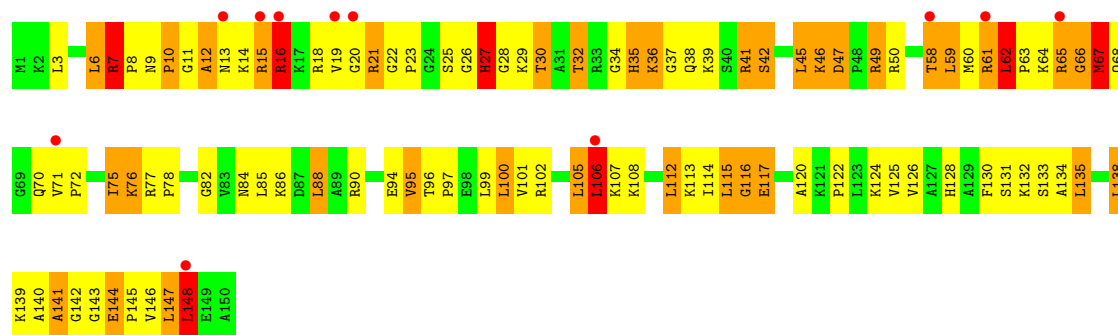


• Molecule 34: 50S ribosomal protein L14

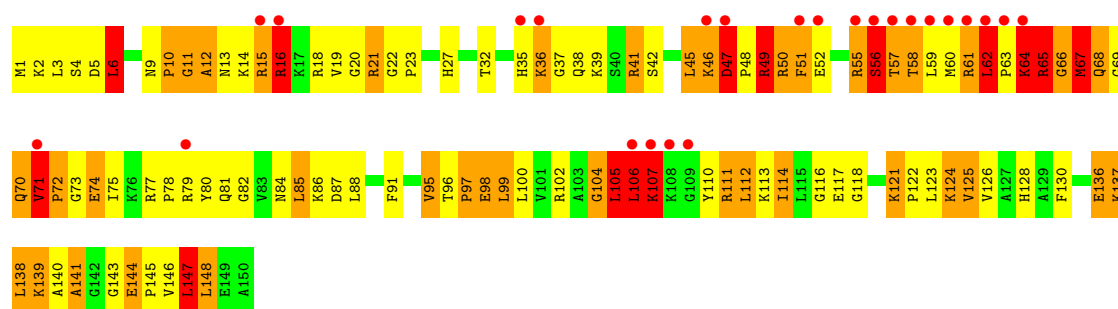
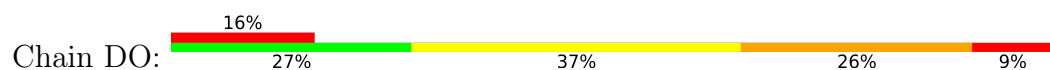


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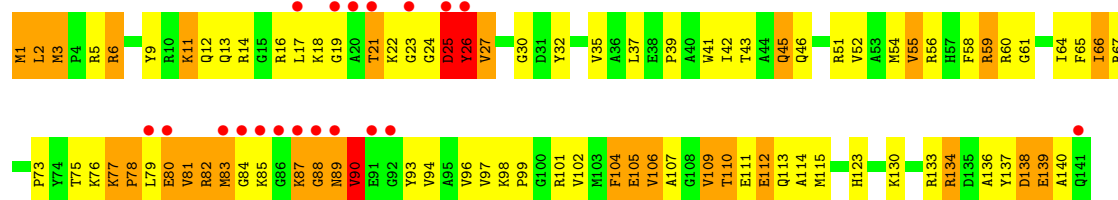




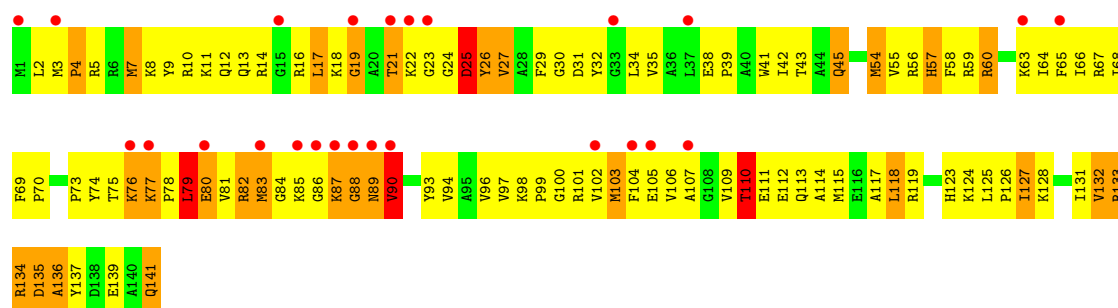
• Molecule 35: 50S ribosomal protein L15



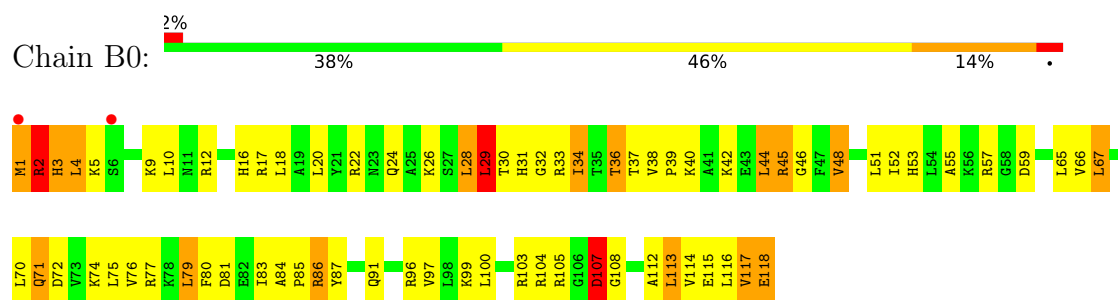
• Molecule 36: 50S ribosomal protein L16



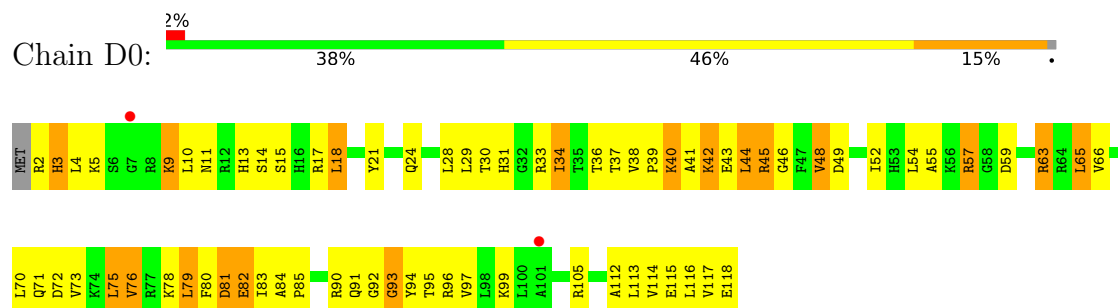
• Molecule 36: 50S ribosomal protein L16



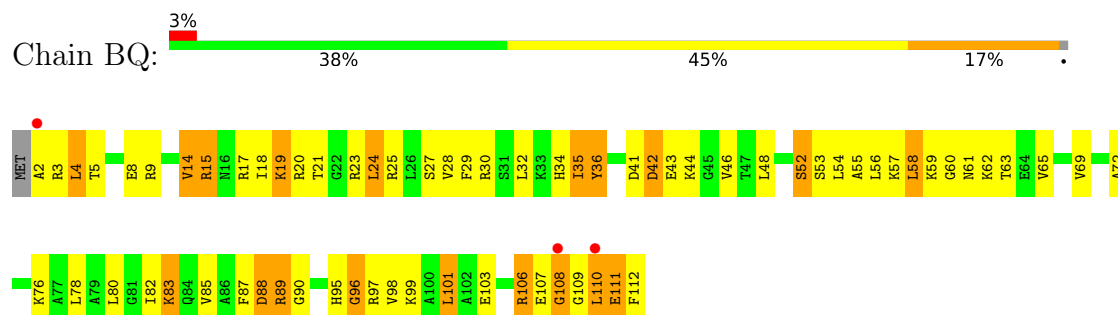
• Molecule 37: 50S ribosomal protein L17



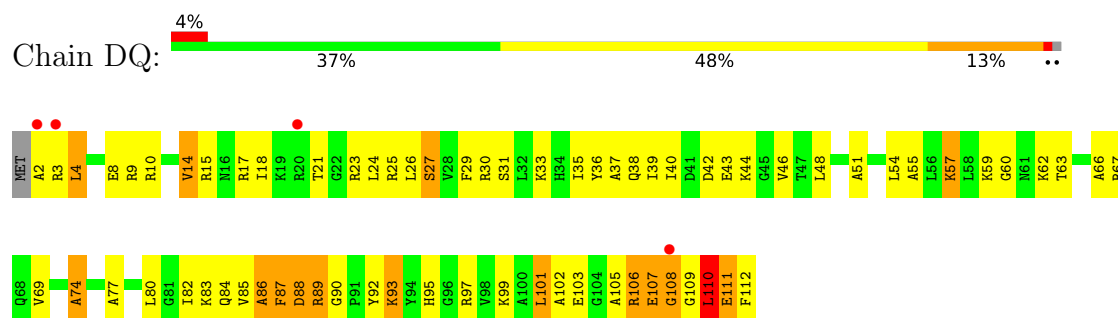
• Molecule 37: 50S ribosomal protein L17



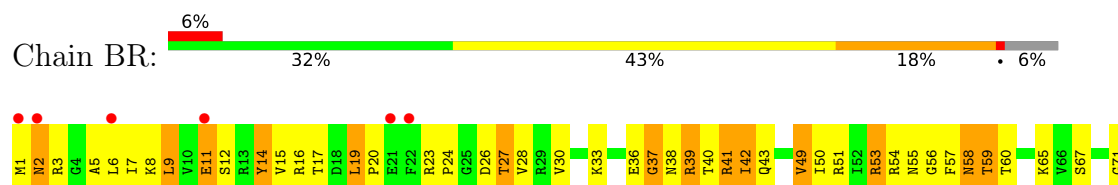
• Molecule 38: 50S ribosomal protein L18



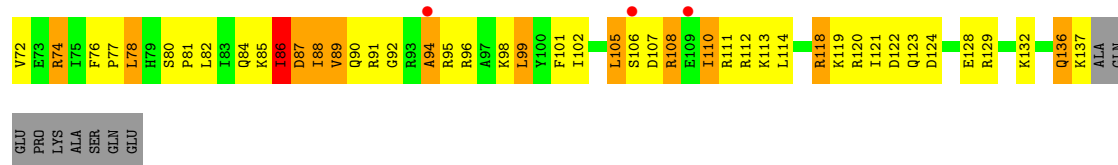
• Molecule 38: 50S ribosomal protein L18



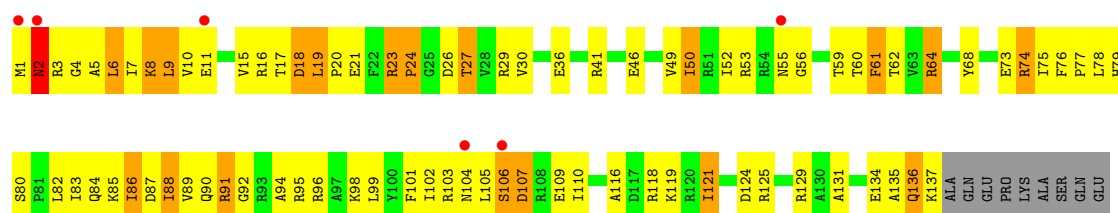
• Molecule 39: 50S ribosomal protein L19



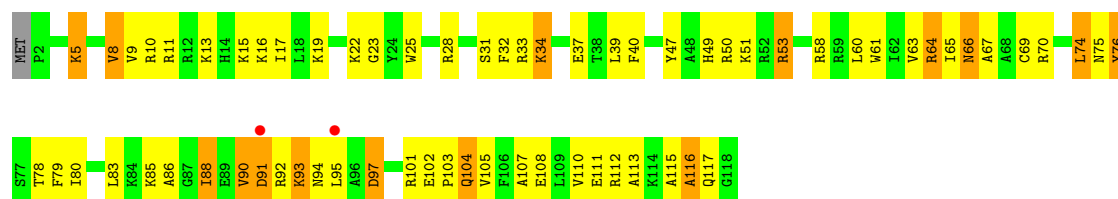
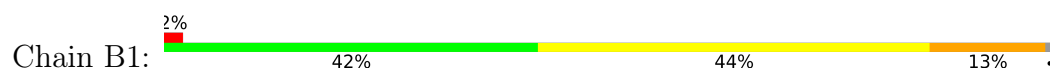




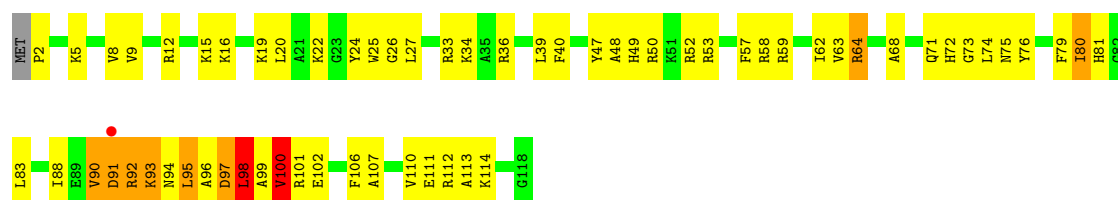
• Molecule 39: 50S ribosomal protein L19



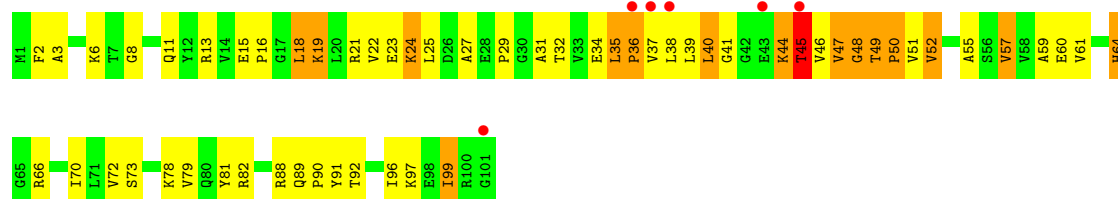
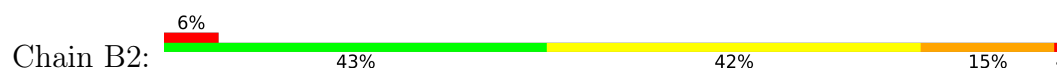
• Molecule 40: 50S ribosomal protein L20



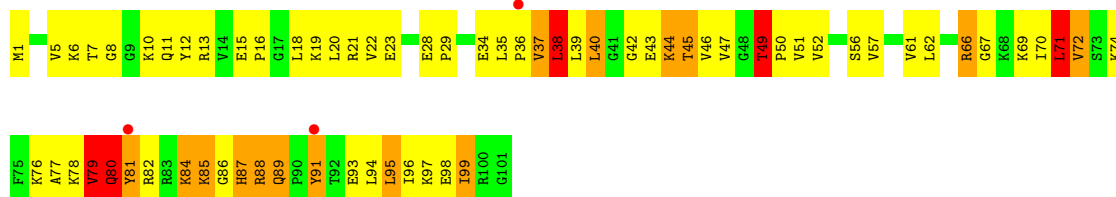
• Molecule 40: 50S ribosomal protein L20



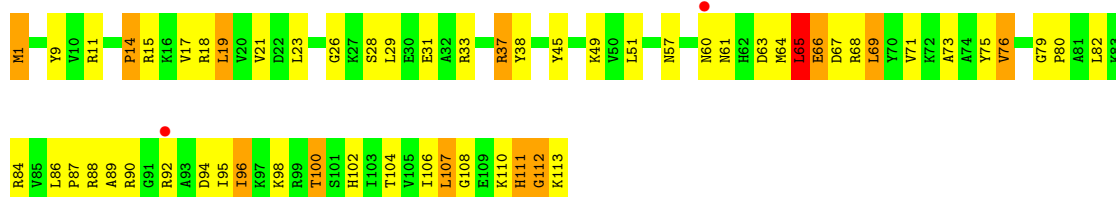
• Molecule 41: 50S ribosomal protein L21



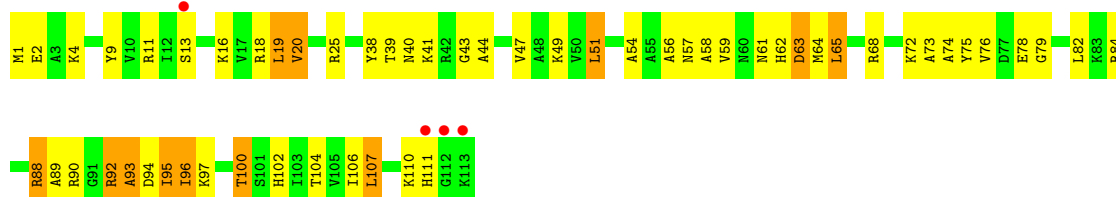
• Molecule 41: 50S ribosomal protein L21



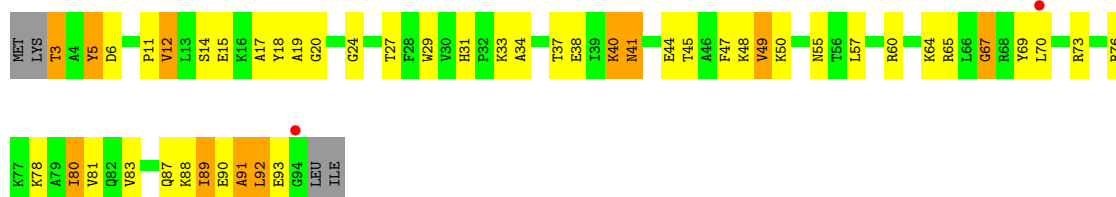
- Molecule 42: 50S ribosomal protein L22



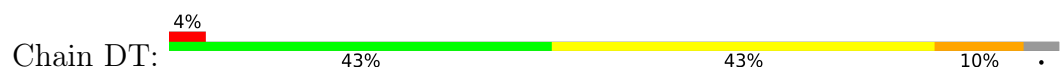
- Molecule 42: 50S ribosomal protein L22

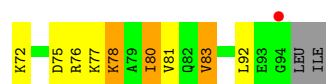


- Molecule 43: 50S ribosomal protein L23

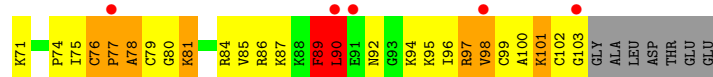
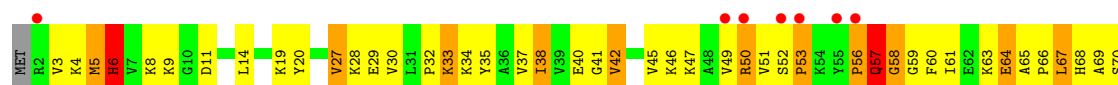


- Molecule 43: 50S ribosomal protein L23

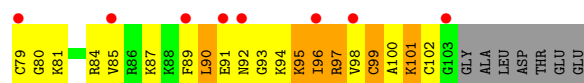
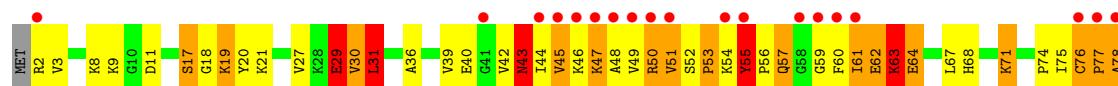




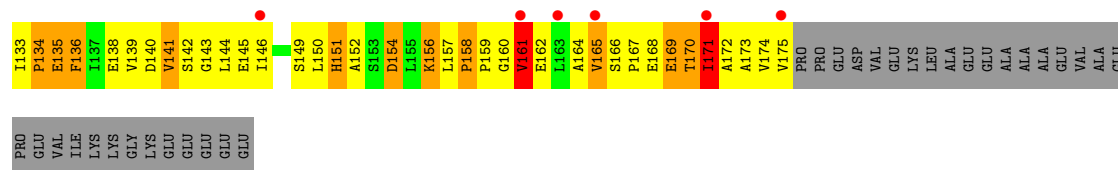
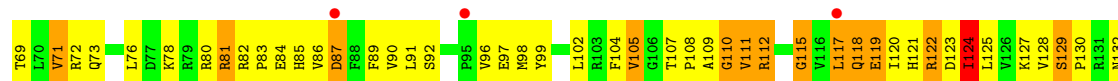
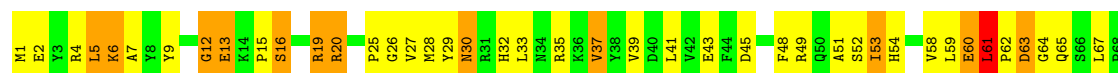
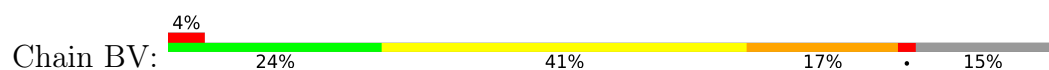
• Molecule 44: 50S ribosomal protein L24



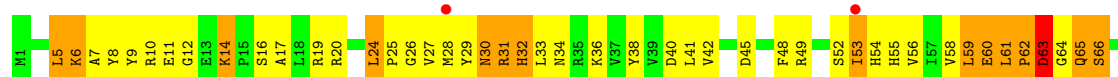
• Molecule 44: 50S ribosomal protein L24

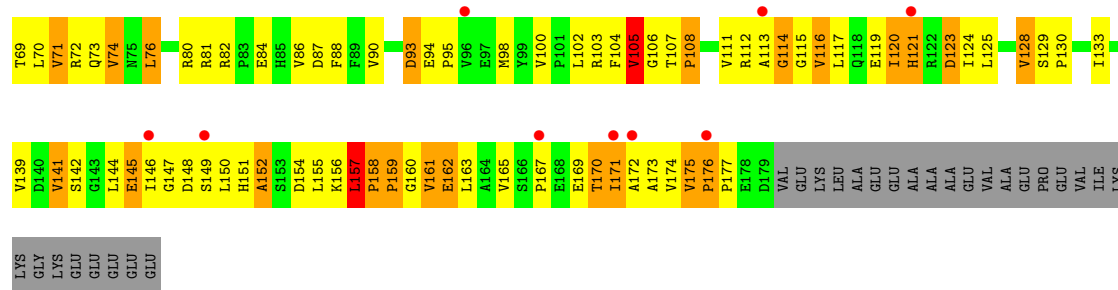


• Molecule 45: 50S ribosomal protein L25

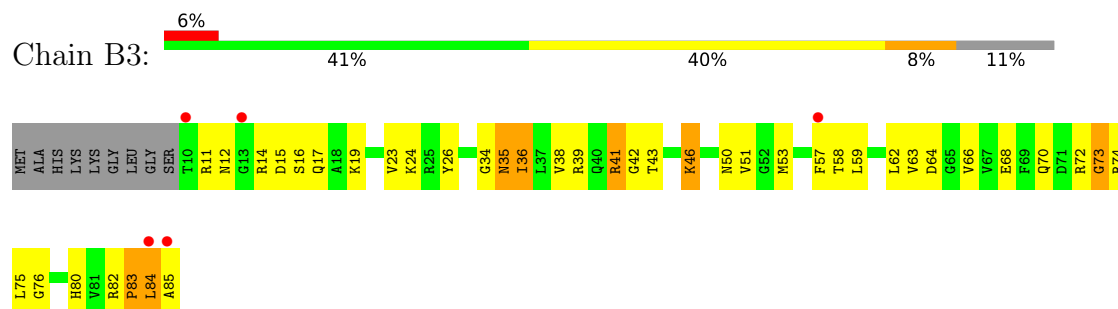


• Molecule 45: 50S ribosomal protein L25

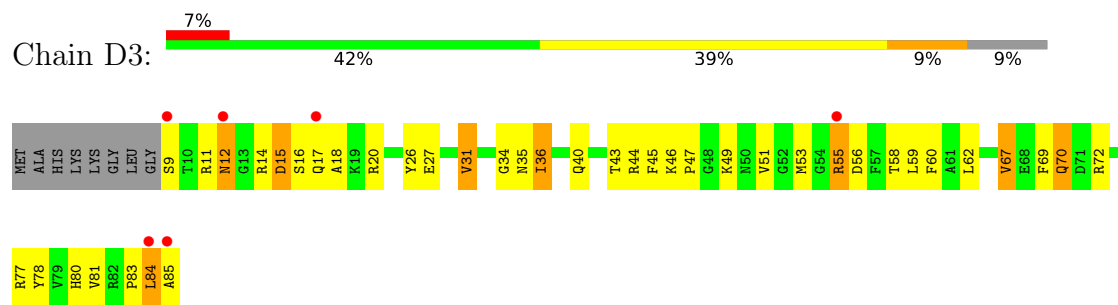




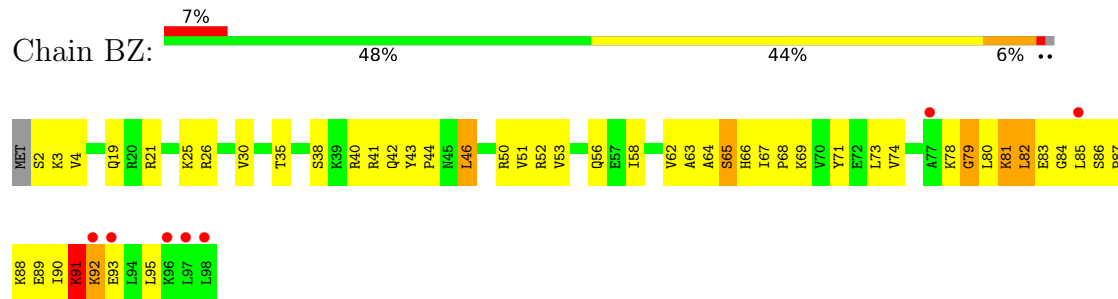
• Molecule 46: 50S ribosomal protein L27



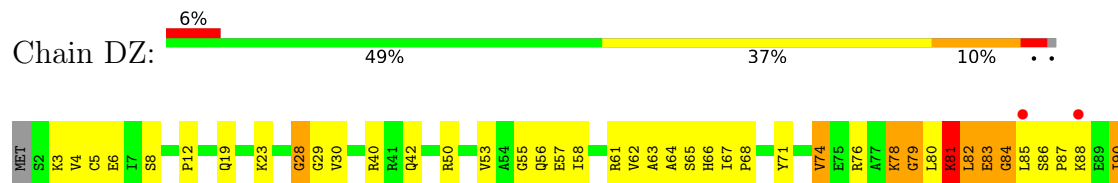
• Molecule 46: 50S ribosomal protein L27

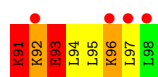


• Molecule 47: 50S ribosomal protein L28

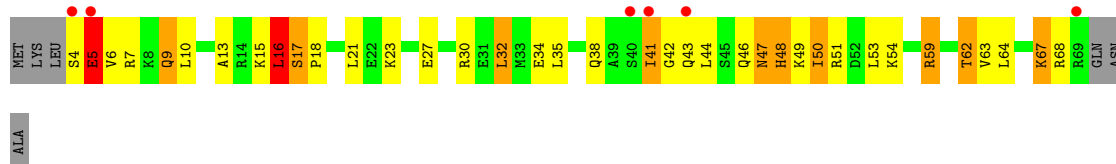
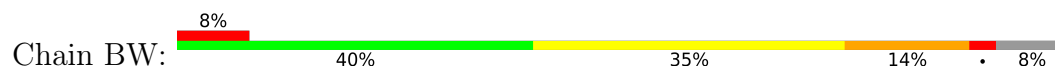


• Molecule 47: 50S ribosomal protein L28

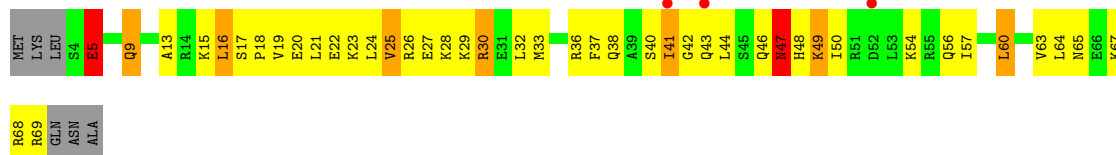




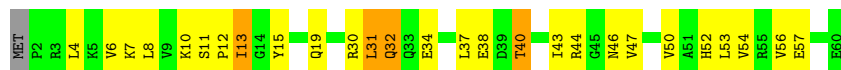
- Molecule 48: 50S ribosomal protein L29



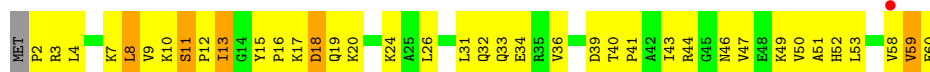
- Molecule 48: 50S ribosomal protein L29



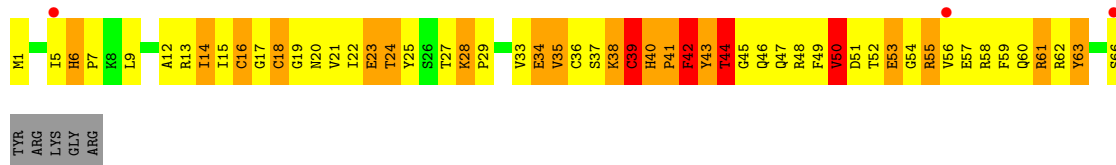
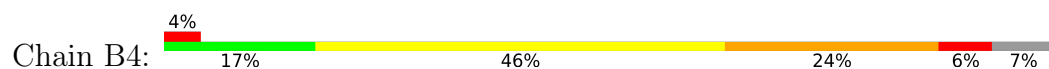
- Molecule 49: 50S ribosomal protein L30



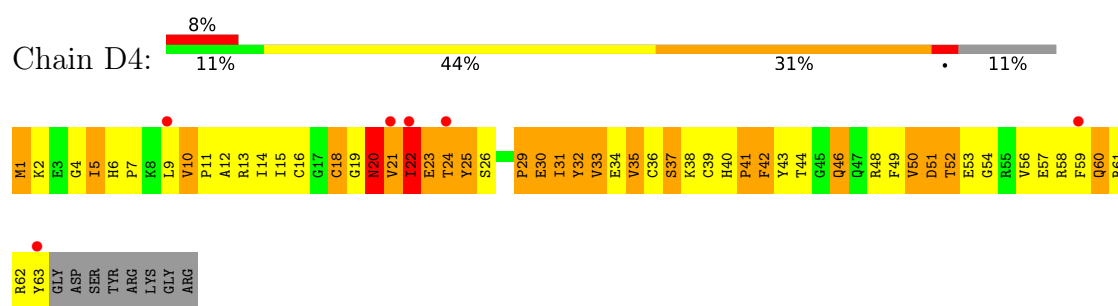
- Molecule 49: 50S ribosomal protein L30



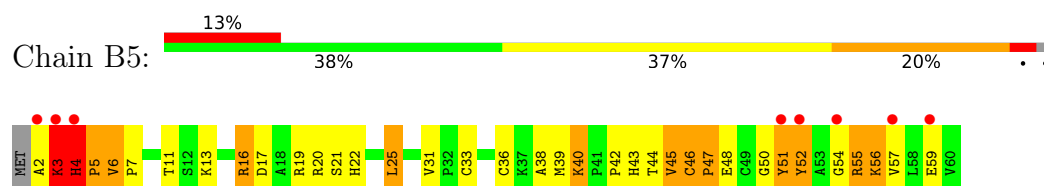
- Molecule 50: 50S ribosomal protein L31



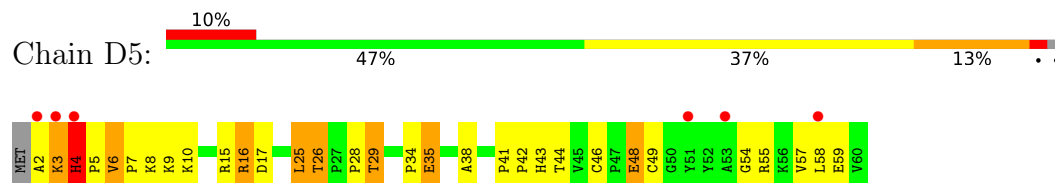
- Molecule 50: 50S ribosomal protein L31



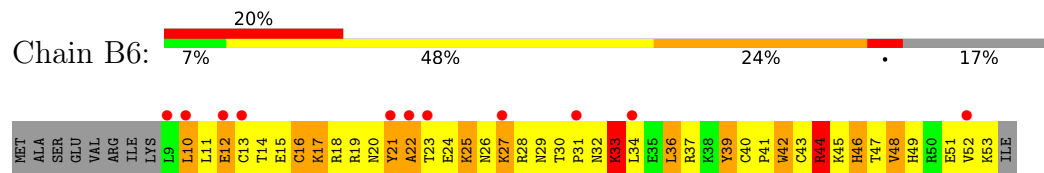
- Molecule 51: 50S ribosomal protein L32



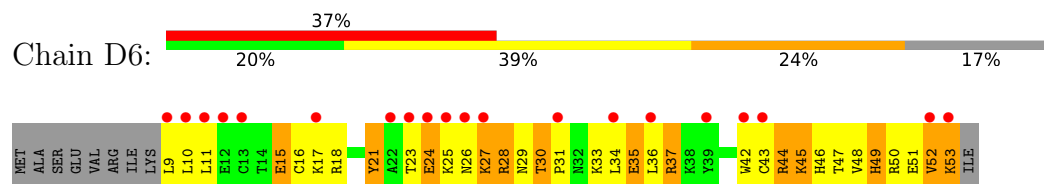
- Molecule 51: 50S ribosomal protein L32



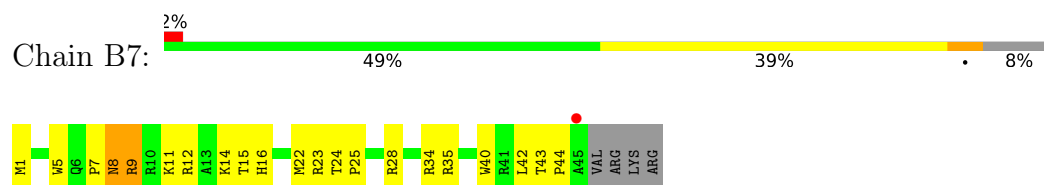
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34

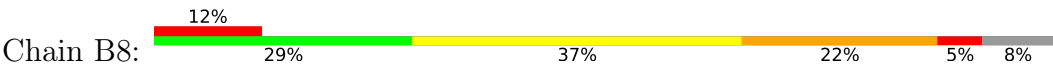


- Molecule 53: 50S ribosomal protein L34

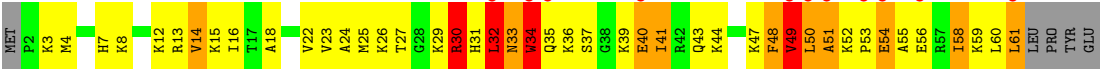




• Molecule 54: 50S ribosomal protein L35



• Molecule 54: 50S ribosomal protein L35



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.67Å 451.75Å 625.08Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 154.06 – 3.00<br>154.06 – 3.00                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (154.06-3.00)<br>93.5 (154.06-3.00)                   | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.22                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.20 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX dev_810                                              | Depositor        |
| R, $R_{free}$                                                           | 0.203 , 0.235<br>0.203 , 0.231                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (0.17%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 78.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.228                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 76.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 299676                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 100.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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 [i](#)

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

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | AA    | 0.16         | 0/36139 | 0.33        | 1/56406 (0.0%) |
| 1   | CA    | 0.16         | 0/36142 | 0.32        | 0/56410        |
| 2   | AE    | 0.27         | 0/1959  | 0.71        | 0/2642         |
| 2   | CE    | 0.27         | 0/1959  | 0.73        | 0/2642         |
| 3   | AF    | 0.29         | 0/1629  | 0.72        | 1/2195 (0.0%)  |
| 3   | CF    | 0.28         | 0/1636  | 0.73        | 0/2205         |
| 4   | AG    | 0.33         | 0/1733  | 0.77        | 1/2318 (0.0%)  |
| 4   | CG    | 0.31         | 0/1733  | 0.83        | 3/2318 (0.1%)  |
| 5   | AH    | 0.29         | 0/1171  | 0.76        | 1/1576 (0.1%)  |
| 5   | CH    | 0.30         | 0/1171  | 0.77        | 0/1576         |
| 6   | AI    | 0.30         | 0/856   | 0.70        | 0/1154         |
| 6   | CI    | 0.29         | 0/856   | 0.74        | 2/1154 (0.2%)  |
| 7   | AJ    | 0.28         | 0/1276  | 0.75        | 2/1709 (0.1%)  |
| 7   | CJ    | 0.29         | 0/1276  | 0.71        | 0/1709         |
| 8   | AK    | 0.29         | 0/1136  | 0.81        | 0/1527         |
| 8   | CK    | 0.28         | 0/1136  | 0.76        | 0/1527         |
| 9   | AL    | 0.27         | 0/1029  | 0.70        | 0/1379         |
| 9   | CL    | 0.28         | 0/1029  | 0.78        | 2/1379 (0.1%)  |
| 10  | AM    | 0.28         | 0/814   | 0.76        | 0/1095         |
| 10  | CM    | 0.27         | 0/814   | 0.80        | 0/1095         |
| 11  | AN    | 0.30         | 0/900   | 0.80        | 0/1213         |
| 11  | CN    | 0.31         | 0/900   | 0.80        | 2/1213 (0.2%)  |
| 12  | AO    | 0.33         | 0/991   | 0.81        | 2/1327 (0.2%)  |
| 12  | CO    | 0.32         | 0/991   | 0.77        | 1/1327 (0.1%)  |
| 13  | AP    | 0.28         | 0/938   | 0.76        | 0/1258         |
| 13  | CP    | 0.28         | 0/943   | 0.72        | 0/1265         |
| 14  | AQ    | 0.33         | 0/485   | 0.74        | 0/643          |
| 14  | CQ    | 0.28         | 0/485   | 0.69        | 0/643          |
| 15  | AR    | 0.31         | 0/745   | 0.69        | 0/992          |
| 15  | CR    | 0.30         | 0/745   | 0.68        | 0/992          |
| 16  | AS    | 0.29         | 0/721   | 0.76        | 2/970 (0.2%)   |
| 16  | CS    | 0.30         | 0/721   | 0.70        | 0/970          |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 17  | AT    | 0.27         | 0/847   | 0.75        | 2/1131 (0.2%) |
| 17  | CT    | 0.27         | 0/847   | 0.72        | 0/1131        |
| 18  | AU    | 0.29         | 0/596   | 0.78        | 1/790 (0.1%)  |
| 18  | CU    | 0.29         | 0/596   | 0.72        | 0/790         |
| 19  | AV    | 0.30         | 0/638   | 0.86        | 0/860         |
| 19  | CV    | 0.29         | 0/638   | 0.77        | 0/860         |
| 20  | AW    | 0.28         | 0/765   | 0.76        | 0/1007        |
| 20  | CW    | 0.30         | 0/765   | 0.83        | 1/1007 (0.1%) |
| 21  | AX    | 0.26         | 0/221   | 0.73        | 0/288         |
| 21  | CX    | 0.26         | 0/221   | 0.72        | 0/288         |
| 22  | AB    | 0.17         | 0/1992  | 0.29        | 0/3099        |
| 22  | AD    | 0.12         | 0/1992  | 0.27        | 0/3099        |
| 22  | CB    | 0.16         | 0/1992  | 0.29        | 0/3099        |
| 22  | CD    | 0.12         | 0/1992  | 0.27        | 0/3099        |
| 23  | AC    | 0.15         | 0/1835  | 0.29        | 0/2859        |
| 23  | CC    | 0.14         | 0/1835  | 0.30        | 0/2859        |
| 24  | A1    | 0.22         | 0/389   | 0.33        | 0/604         |
| 24  | C1    | 0.25         | 0/389   | 0.36        | 0/604         |
| 25  | BA    | 0.20         | 0/70233 | 0.36        | 0/109643      |
| 25  | DA    | 0.18         | 0/70122 | 0.34        | 0/109469      |
| 26  | BB    | 0.18         | 0/2928  | 0.35        | 0/4568        |
| 26  | DB    | 0.16         | 0/2928  | 0.35        | 0/4568        |
| 27  | BD    | 0.39         | 0/2165  | 0.91        | 5/2919 (0.2%) |
| 27  | DD    | 0.36         | 0/2165  | 0.84        | 4/2919 (0.1%) |
| 28  | BE    | 0.36         | 0/1601  | 0.93        | 9/2160 (0.4%) |
| 28  | DE    | 0.35         | 0/1601  | 0.91        | 9/2160 (0.4%) |
| 29  | BF    | 0.37         | 0/1620  | 0.85        | 5/2194 (0.2%) |
| 29  | DF    | 0.33         | 0/1662  | 0.87        | 4/2249 (0.2%) |
| 30  | BG    | 0.29         | 0/1499  | 0.75        | 2/2016 (0.1%) |
| 30  | DG    | 0.28         | 0/1499  | 0.71        | 0/2016        |
| 31  | BH    | 0.35         | 0/1332  | 0.83        | 3/1802 (0.2%) |
| 31  | DH    | 0.29         | 0/1332  | 0.77        | 0/1802        |
| 32  | BK    | 0.32         | 0/1151  | 0.79        | 1/1558 (0.1%) |
| 32  | DK    | 0.30         | 0/1151  | 0.85        | 6/1558 (0.4%) |
| 33  | BM    | 0.34         | 0/1131  | 0.80        | 1/1525 (0.1%) |
| 33  | DM    | 0.28         | 0/1131  | 0.82        | 4/1525 (0.3%) |
| 34  | BN    | 0.34         | 0/943   | 0.79        | 0/1269        |
| 34  | DN    | 0.32         | 0/943   | 0.79        | 2/1269 (0.2%) |
| 35  | BO    | 0.36         | 0/1162  | 0.92        | 2/1544 (0.1%) |
| 35  | DO    | 0.29         | 0/1162  | 0.71        | 0/1544        |
| 36  | BP    | 0.35         | 0/1143  | 0.78        | 0/1527        |
| 36  | DP    | 0.29         | 0/1143  | 0.72        | 1/1527 (0.1%) |
| 37  | B0    | 0.33         | 0/982   | 0.76        | 0/1312        |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 37  | D0    | 0.32         | 0/974    | 0.71        | 0/1302            |
| 38  | BQ    | 0.32         | 0/892    | 0.79        | 0/1187            |
| 38  | DQ    | 0.28         | 0/892    | 0.71        | 0/1187            |
| 39  | BR    | 0.35         | 0/1155   | 0.84        | 4/1542 (0.3%)     |
| 39  | DR    | 0.31         | 0/1155   | 0.78        | 2/1542 (0.1%)     |
| 40  | B1    | 0.34         | 0/982    | 0.84        | 4/1306 (0.3%)     |
| 40  | D1    | 0.31         | 0/982    | 0.81        | 2/1306 (0.2%)     |
| 41  | B2    | 0.32         | 0/790    | 0.74        | 0/1057            |
| 41  | D2    | 0.37         | 0/790    | 0.84        | 3/1057 (0.3%)     |
| 42  | BS    | 0.35         | 0/911    | 0.73        | 0/1220            |
| 42  | DS    | 0.35         | 0/911    | 0.71        | 0/1220            |
| 43  | BT    | 0.35         | 0/739    | 0.78        | 1/993 (0.1%)      |
| 43  | DT    | 0.32         | 0/739    | 0.79        | 2/993 (0.2%)      |
| 44  | BU    | 0.37         | 0/798    | 0.85        | 3/1064 (0.3%)     |
| 44  | DU    | 0.34         | 0/798    | 0.78        | 0/1064            |
| 45  | BV    | 0.28         | 0/1427   | 0.78        | 2/1935 (0.1%)     |
| 45  | DV    | 0.29         | 0/1460   | 0.80        | 2/1982 (0.1%)     |
| 46  | B3    | 0.31         | 0/615    | 0.81        | 2/819 (0.2%)      |
| 46  | D3    | 0.29         | 0/621    | 0.76        | 0/827             |
| 47  | BZ    | 0.34         | 0/770    | 0.77        | 0/1022            |
| 47  | DZ    | 0.33         | 0/770    | 0.81        | 0/1022            |
| 48  | BW    | 0.33         | 0/560    | 0.81        | 1/741 (0.1%)      |
| 48  | DW    | 0.30         | 0/560    | 0.77        | 1/741 (0.1%)      |
| 49  | BX    | 0.31         | 0/474    | 0.75        | 0/635             |
| 49  | DX    | 0.27         | 0/474    | 0.89        | 4/635 (0.6%)      |
| 50  | B4    | 0.28         | 0/545    | 0.72        | 0/733             |
| 50  | D4    | 0.31         | 0/527    | 0.76        | 0/709             |
| 51  | B5    | 0.36         | 0/473    | 1.02        | 6/639 (0.9%)      |
| 51  | D5    | 0.34         | 0/473    | 0.84        | 2/639 (0.3%)      |
| 52  | B6    | 0.34         | 0/396    | 0.76        | 0/529             |
| 52  | D6    | 0.34         | 0/396    | 0.89        | 2/529 (0.4%)      |
| 53  | B7    | 0.37         | 0/399    | 0.72        | 0/526             |
| 53  | D7    | 0.34         | 0/399    | 0.81        | 2/526 (0.4%)      |
| 54  | B8    | 0.42         | 0/486    | 0.90        | 1/638 (0.2%)      |
| 54  | D8    | 0.41         | 0/486    | 0.96        | 1/638 (0.2%)      |
| All | All   | 0.23         | 0/324157 | 0.50        | 129/485451 (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 |
|-----|-------|---------------------|---------------------|
| 31  | BH    | 0                   | 1                   |

There are no bond length outliers.

The worst 5 of 129 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 20  | CW    | 12  | ALA  | N-CA-C | -9.13 | 102.06      | 113.02   |
| 35  | BO    | 59  | LEU  | N-CA-C | -8.83 | 101.81      | 112.59   |
| 51  | B5    | 46  | CYS  | CA-C-N | 8.74  | 130.76      | 119.84   |
| 51  | B5    | 46  | CYS  | C-N-CA | 8.74  | 130.76      | 119.84   |
| 28  | BE    | 188 | VAL  | N-CA-C | 8.31  | 117.09      | 108.95   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 31  | BH    | 153 | LYS  | Peptide |

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

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    | 32284 | 0        | 16296    | 1132    | 1            |
| 1   | CA    | 32287 | 0        | 16295    | 1156    | 1            |
| 2   | AE    | 1924  | 0        | 1975     | 170     | 0            |
| 2   | CE    | 1924  | 0        | 1975     | 170     | 0            |
| 3   | AF    | 1605  | 0        | 1668     | 125     | 0            |
| 3   | CF    | 1612  | 0        | 1677     | 122     | 0            |
| 4   | AG    | 1703  | 0        | 1763     | 118     | 0            |
| 4   | CG    | 1703  | 0        | 1763     | 121     | 0            |
| 5   | AH    | 1155  | 0        | 1213     | 79      | 0            |
| 5   | CH    | 1155  | 0        | 1213     | 64      | 0            |
| 6   | AI    | 843   | 0        | 857      | 55      | 0            |
| 6   | CI    | 843   | 0        | 857      | 44      | 0            |
| 7   | AJ    | 1257  | 0        | 1296     | 68      | 0            |
| 7   | CJ    | 1257  | 0        | 1296     | 77      | 0            |
| 8   | AK    | 1116  | 0        | 1177     | 80      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | CK    | 1116  | 0        | 1177     | 48      | 0            |
| 9   | AL    | 1010  | 0        | 1037     | 83      | 0            |
| 9   | CL    | 1010  | 0        | 1037     | 119     | 0            |
| 10  | AM    | 801   | 0        | 849      | 78      | 0            |
| 10  | CM    | 801   | 0        | 849      | 86      | 0            |
| 11  | AN    | 885   | 0        | 904      | 59      | 0            |
| 11  | CN    | 885   | 0        | 904      | 40      | 0            |
| 12  | AO    | 975   | 0        | 1062     | 95      | 0            |
| 12  | CO    | 975   | 0        | 1062     | 67      | 0            |
| 13  | AP    | 928   | 0        | 987      | 83      | 0            |
| 13  | CP    | 933   | 0        | 992      | 87      | 0            |
| 14  | AQ    | 476   | 0        | 511      | 44      | 0            |
| 14  | CQ    | 476   | 0        | 511      | 45      | 0            |
| 15  | AR    | 734   | 0        | 771      | 35      | 0            |
| 15  | CR    | 734   | 0        | 771      | 34      | 0            |
| 16  | AS    | 705   | 0        | 725      | 58      | 0            |
| 16  | CS    | 705   | 0        | 725      | 26      | 0            |
| 17  | AT    | 834   | 0        | 904      | 46      | 0            |
| 17  | CT    | 834   | 0        | 904      | 43      | 0            |
| 18  | AU    | 591   | 0        | 662      | 31      | 0            |
| 18  | CU    | 591   | 0        | 662      | 39      | 0            |
| 19  | AV    | 624   | 0        | 636      | 56      | 0            |
| 19  | CV    | 624   | 0        | 636      | 71      | 0            |
| 20  | AW    | 763   | 0        | 861      | 64      | 0            |
| 20  | CW    | 763   | 0        | 861      | 62      | 0            |
| 21  | AX    | 217   | 0        | 234      | 19      | 0            |
| 21  | CX    | 217   | 0        | 234      | 19      | 0            |
| 22  | AB    | 1814  | 0        | 932      | 114     | 0            |
| 22  | AD    | 1814  | 0        | 932      | 109     | 0            |
| 22  | CB    | 1814  | 0        | 932      | 110     | 0            |
| 22  | CD    | 1814  | 0        | 932      | 99      | 0            |
| 23  | AC    | 1643  | 0        | 837      | 41      | 0            |
| 23  | CC    | 1643  | 0        | 837      | 38      | 0            |
| 24  | A1    | 346   | 0        | 174      | 20      | 0            |
| 24  | C1    | 346   | 0        | 174      | 17      | 0            |
| 25  | BA    | 62707 | 0        | 31614    | 1941    | 0            |
| 25  | DA    | 62607 | 0        | 31565    | 2101    | 1            |
| 26  | BB    | 2617  | 0        | 1328     | 89      | 0            |
| 26  | DB    | 2617  | 0        | 1328     | 111     | 0            |
| 27  | BD    | 2115  | 0        | 2195     | 202     | 0            |
| 27  | DD    | 2115  | 0        | 2195     | 193     | 0            |
| 28  | BE    | 1568  | 0        | 1634     | 151     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | DE    | 1568  | 0        | 1634     | 195     | 0            |
| 29  | BF    | 1585  | 0        | 1632     | 114     | 0            |
| 29  | DF    | 1627  | 0        | 1680     | 168     | 0            |
| 30  | BG    | 1474  | 0        | 1535     | 131     | 0            |
| 30  | DG    | 1474  | 0        | 1535     | 110     | 0            |
| 31  | BH    | 1307  | 0        | 1382     | 150     | 0            |
| 31  | DH    | 1307  | 0        | 1382     | 108     | 1            |
| 32  | BK    | 1136  | 0        | 1223     | 107     | 0            |
| 32  | DK    | 1136  | 0        | 1223     | 79      | 0            |
| 33  | BM    | 1104  | 0        | 1180     | 80      | 0            |
| 33  | DM    | 1104  | 0        | 1180     | 87      | 0            |
| 34  | BN    | 933   | 0        | 996      | 54      | 0            |
| 34  | DN    | 933   | 0        | 996      | 57      | 0            |
| 35  | BO    | 1145  | 0        | 1228     | 184     | 0            |
| 35  | DO    | 1145  | 0        | 1228     | 304     | 0            |
| 36  | BP    | 1122  | 0        | 1179     | 143     | 0            |
| 36  | DP    | 1122  | 0        | 1179     | 170     | 0            |
| 37  | B0    | 968   | 0        | 1033     | 80      | 0            |
| 37  | D0    | 960   | 0        | 1021     | 70      | 0            |
| 38  | BQ    | 882   | 0        | 943      | 89      | 0            |
| 38  | DQ    | 882   | 0        | 943      | 86      | 0            |
| 39  | BR    | 1141  | 0        | 1202     | 98      | 0            |
| 39  | DR    | 1141  | 0        | 1202     | 97      | 0            |
| 40  | B1    | 964   | 0        | 1022     | 81      | 0            |
| 40  | D1    | 964   | 0        | 1022     | 90      | 0            |
| 41  | B2    | 779   | 0        | 852      | 76      | 0            |
| 41  | D2    | 779   | 0        | 852      | 114     | 0            |
| 42  | BS    | 900   | 0        | 964      | 46      | 0            |
| 42  | DS    | 900   | 0        | 964      | 53      | 0            |
| 43  | BT    | 725   | 0        | 778      | 50      | 0            |
| 43  | DT    | 725   | 0        | 778      | 53      | 0            |
| 44  | BU    | 785   | 0        | 878      | 102     | 0            |
| 44  | DU    | 785   | 0        | 878      | 96      | 0            |
| 45  | BV    | 1397  | 0        | 1430     | 142     | 0            |
| 45  | DV    | 1428  | 0        | 1454     | 125     | 0            |
| 46  | B3    | 607   | 0        | 628      | 42      | 0            |
| 46  | D3    | 613   | 0        | 633      | 45      | 0            |
| 47  | BZ    | 763   | 0        | 848      | 52      | 0            |
| 47  | DZ    | 763   | 0        | 848      | 50      | 0            |
| 48  | BW    | 558   | 0        | 610      | 40      | 0            |
| 48  | DW    | 558   | 0        | 610      | 43      | 0            |
| 49  | BX    | 469   | 0        | 518      | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 49  | DX    | 469   | 0        | 518      | 25      | 0            |
| 50  | B4    | 533   | 0        | 522      | 131     | 0            |
| 50  | D4    | 515   | 0        | 510      | 82      | 0            |
| 51  | B5    | 459   | 0        | 480      | 92      | 0            |
| 51  | D5    | 459   | 0        | 476      | 40      | 0            |
| 52  | B6    | 389   | 0        | 404      | 86      | 0            |
| 52  | D6    | 389   | 0        | 404      | 51      | 0            |
| 53  | B7    | 391   | 0        | 432      | 18      | 0            |
| 53  | D7    | 391   | 0        | 432      | 26      | 0            |
| 54  | B8    | 480   | 0        | 549      | 119     | 0            |
| 54  | D8    | 480   | 0        | 549      | 86      | 0            |
| 55  | A1    | 1     | 0        | 0        | 0       | 0            |
| 55  | AA    | 220   | 0        | 0        | 0       | 0            |
| 55  | AB    | 4     | 0        | 0        | 0       | 0            |
| 55  | AC    | 8     | 0        | 0        | 0       | 0            |
| 55  | AD    | 3     | 0        | 0        | 0       | 0            |
| 55  | AG    | 2     | 0        | 0        | 0       | 0            |
| 55  | AN    | 1     | 0        | 0        | 0       | 0            |
| 55  | AR    | 1     | 0        | 0        | 0       | 0            |
| 55  | AS    | 1     | 0        | 0        | 0       | 0            |
| 55  | B0    | 1     | 0        | 0        | 0       | 0            |
| 55  | B1    | 2     | 0        | 0        | 0       | 0            |
| 55  | B2    | 1     | 0        | 0        | 0       | 0            |
| 55  | B3    | 3     | 0        | 0        | 0       | 0            |
| 55  | B5    | 1     | 0        | 0        | 0       | 0            |
| 55  | B6    | 1     | 0        | 0        | 0       | 0            |
| 55  | B7    | 1     | 0        | 0        | 0       | 0            |
| 55  | BA    | 568   | 0        | 0        | 0       | 0            |
| 55  | BB    | 18    | 0        | 0        | 0       | 0            |
| 55  | BD    | 1     | 0        | 0        | 0       | 0            |
| 55  | BE    | 3     | 0        | 0        | 0       | 0            |
| 55  | BF    | 3     | 0        | 0        | 0       | 0            |
| 55  | BO    | 2     | 0        | 0        | 0       | 0            |
| 55  | BW    | 1     | 0        | 0        | 0       | 0            |
| 55  | CA    | 219   | 0        | 0        | 0       | 0            |
| 55  | CB    | 4     | 0        | 0        | 0       | 0            |
| 55  | CC    | 9     | 0        | 0        | 0       | 0            |
| 55  | CD    | 1     | 0        | 0        | 0       | 0            |
| 55  | CG    | 2     | 0        | 0        | 0       | 0            |
| 55  | CK    | 1     | 0        | 0        | 0       | 0            |
| 55  | CR    | 1     | 0        | 0        | 0       | 0            |
| 55  | D0    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55  | D1    | 1      | 0        | 0        | 0       | 0            |
| 55  | D3    | 1      | 0        | 0        | 0       | 0            |
| 55  | D5    | 2      | 0        | 0        | 0       | 0            |
| 55  | D7    | 1      | 0        | 0        | 0       | 0            |
| 55  | D8    | 1      | 0        | 0        | 0       | 0            |
| 55  | DA    | 488    | 0        | 0        | 0       | 0            |
| 55  | DB    | 20     | 0        | 0        | 0       | 0            |
| 55  | DD    | 3      | 0        | 0        | 0       | 0            |
| 55  | DE    | 1      | 0        | 0        | 0       | 0            |
| 55  | DO    | 1      | 0        | 0        | 0       | 0            |
| 56  | AG    | 1      | 0        | 0        | 0       | 0            |
| 56  | AQ    | 1      | 0        | 0        | 0       | 0            |
| 56  | CG    | 1      | 0        | 0        | 0       | 0            |
| 56  | CQ    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 299676 | 0        | 200977   | 13727   | 2            |

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 28.

The worst 5 of 13727 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) |
|-------------------|------------------|--------------------------|-------------------|
| 35:DO:46:LYS:HD3  | 35:DO:51:PHE:CD1 | 1.38                     | 1.55              |
| 54:B8:34:TRP:CB   | 54:B8:35:GLN:HB2 | 1.34                     | 1.55              |
| 50:B4:37:SER:HB3  | 50:B4:42:PHE:CD1 | 1.40                     | 1.52              |
| 35:DO:71:VAL:HG13 | 35:DO:72:PRO:CD  | 1.44                     | 1.47              |
| 35:BO:19:VAL:HG23 | 35:BO:27:HIS:CB  | 1.45                     | 1.46              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:AA:85:U:O2' | 31:DH:100:GLY:O[3_555] | 1.97                     | 0.23              |
| 1:CA:86:U:O2' | 25:DA:276:A:OP2[3_545] | 2.19                     | 0.01              |



## 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   | AE    | 235/256 (92%) | 170 (72%) | 44 (19%) | 21 (9%)  | 0           | 3   |
| 2   | CE    | 235/256 (92%) | 161 (68%) | 48 (20%) | 26 (11%) | 0           | 1   |
| 3   | AF    | 203/239 (85%) | 157 (77%) | 36 (18%) | 10 (5%)  | 1           | 10  |
| 3   | CF    | 204/239 (85%) | 151 (74%) | 40 (20%) | 13 (6%)  | 1           | 6   |
| 4   | AG    | 206/208 (99%) | 169 (82%) | 29 (14%) | 8 (4%)   | 2           | 14  |
| 4   | CG    | 206/208 (99%) | 167 (81%) | 24 (12%) | 15 (7%)  | 1           | 4   |
| 5   | AH    | 149/162 (92%) | 128 (86%) | 16 (11%) | 5 (3%)   | 3           | 17  |
| 5   | CH    | 149/162 (92%) | 129 (87%) | 18 (12%) | 2 (1%)   | 9           | 38  |
| 6   | AI    | 99/101 (98%)  | 88 (89%)  | 8 (8%)   | 3 (3%)   | 3           | 19  |
| 6   | CI    | 99/101 (98%)  | 92 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 7   | AJ    | 153/156 (98%) | 127 (83%) | 21 (14%) | 5 (3%)   | 3           | 17  |
| 7   | CJ    | 153/156 (98%) | 131 (86%) | 16 (10%) | 6 (4%)   | 2           | 14  |
| 8   | AK    | 136/138 (99%) | 113 (83%) | 15 (11%) | 8 (6%)   | 1           | 7   |
| 8   | CK    | 136/138 (99%) | 116 (85%) | 17 (12%) | 3 (2%)   | 5           | 26  |
| 9   | AL    | 125/128 (98%) | 90 (72%)  | 26 (21%) | 9 (7%)   | 1           | 4   |
| 9   | CL    | 125/128 (98%) | 86 (69%)  | 30 (24%) | 9 (7%)   | 1           | 4   |
| 10  | AM    | 97/105 (92%)  | 77 (79%)  | 17 (18%) | 3 (3%)   | 3           | 19  |
| 10  | CM    | 97/105 (92%)  | 79 (81%)  | 13 (13%) | 5 (5%)   | 1           | 9   |
| 11  | AN    | 117/129 (91%) | 101 (86%) | 11 (9%)  | 5 (4%)   | 2           | 12  |
| 11  | CN    | 117/129 (91%) | 97 (83%)  | 16 (14%) | 4 (3%)   | 3           | 17  |
| 12  | AO    | 123/132 (93%) | 104 (85%) | 7 (6%)   | 12 (10%) | 0           | 2   |
| 12  | CO    | 123/132 (93%) | 96 (78%)  | 21 (17%) | 6 (5%)   | 1           | 10  |
| 13  | AP    | 114/126 (90%) | 76 (67%)  | 26 (23%) | 12 (10%) | 0           | 2   |
| 13  | CP    | 115/126 (91%) | 83 (72%)  | 18 (16%) | 14 (12%) | 0           | 1   |
| 14  | AQ    | 56/61 (92%)   | 37 (66%)  | 7 (12%)  | 12 (21%) | 0           | 0   |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 14  | CQ    | 56/61 (92%)   | 39 (70%)  | 9 (16%)  | 8 (14%)  | 0           | 1   |
| 15  | AR    | 86/89 (97%)   | 68 (79%)  | 14 (16%) | 4 (5%)   | 2           | 11  |
| 15  | CR    | 86/89 (97%)   | 82 (95%)  | 2 (2%)   | 2 (2%)   | 5           | 25  |
| 16  | AS    | 82/88 (93%)   | 64 (78%)  | 13 (16%) | 5 (6%)   | 1           | 7   |
| 16  | CS    | 82/88 (93%)   | 72 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 17  | AT    | 98/105 (93%)  | 83 (85%)  | 9 (9%)   | 6 (6%)   | 1           | 7   |
| 17  | CT    | 98/105 (93%)  | 85 (87%)  | 10 (10%) | 3 (3%)   | 3           | 19  |
| 18  | AU    | 70/88 (80%)   | 53 (76%)  | 13 (19%) | 4 (6%)   | 1           | 8   |
| 18  | CU    | 70/88 (80%)   | 60 (86%)  | 7 (10%)  | 3 (4%)   | 2           | 12  |
| 19  | AV    | 76/93 (82%)   | 56 (74%)  | 12 (16%) | 8 (10%)  | 0           | 2   |
| 19  | CV    | 76/93 (82%)   | 53 (70%)  | 16 (21%) | 7 (9%)   | 0           | 2   |
| 20  | AW    | 97/106 (92%)  | 75 (77%)  | 14 (14%) | 8 (8%)   | 0           | 3   |
| 20  | CW    | 97/106 (92%)  | 72 (74%)  | 16 (16%) | 9 (9%)   | 0           | 2   |
| 21  | AX    | 23/27 (85%)   | 19 (83%)  | 2 (9%)   | 2 (9%)   | 0           | 3   |
| 21  | CX    | 23/27 (85%)   | 18 (78%)  | 2 (9%)   | 3 (13%)  | 0           | 1   |
| 27  | BD    | 270/276 (98%) | 227 (84%) | 30 (11%) | 13 (5%)  | 2           | 11  |
| 27  | DD    | 270/276 (98%) | 226 (84%) | 32 (12%) | 12 (4%)  | 2           | 12  |
| 28  | BE    | 203/206 (98%) | 146 (72%) | 34 (17%) | 23 (11%) | 0           | 1   |
| 28  | DE    | 203/206 (98%) | 134 (66%) | 40 (20%) | 29 (14%) | 0           | 1   |
| 29  | BF    | 200/210 (95%) | 177 (88%) | 14 (7%)  | 9 (4%)   | 2           | 12  |
| 29  | DF    | 206/210 (98%) | 153 (74%) | 30 (15%) | 23 (11%) | 0           | 1   |
| 30  | BG    | 179/182 (98%) | 139 (78%) | 27 (15%) | 13 (7%)  | 1           | 4   |
| 30  | DG    | 179/182 (98%) | 140 (78%) | 28 (16%) | 11 (6%)  | 1           | 7   |
| 31  | BH    | 168/180 (93%) | 113 (67%) | 20 (12%) | 35 (21%) | 0           | 0   |
| 31  | DH    | 168/180 (93%) | 108 (64%) | 36 (21%) | 24 (14%) | 0           | 1   |
| 32  | BK    | 144/148 (97%) | 90 (62%)  | 39 (27%) | 15 (10%) | 0           | 2   |
| 32  | DK    | 144/148 (97%) | 98 (68%)  | 36 (25%) | 10 (7%)  | 1           | 5   |
| 33  | BM    | 136/140 (97%) | 107 (79%) | 21 (15%) | 8 (6%)   | 1           | 7   |
| 33  | DM    | 136/140 (97%) | 106 (78%) | 16 (12%) | 14 (10%) | 0           | 2   |
| 34  | BN    | 120/122 (98%) | 114 (95%) | 4 (3%)   | 2 (2%)   | 7           | 32  |
| 34  | DN    | 120/122 (98%) | 106 (88%) | 10 (8%)  | 4 (3%)   | 3           | 17  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 35  | BO    | 148/150 (99%) | 99 (67%)  | 29 (20%) | 20 (14%) | 0           | 1  |
| 35  | DO    | 148/150 (99%) | 92 (62%)  | 25 (17%) | 31 (21%) | 0           | 0  |
| 36  | BP    | 139/141 (99%) | 102 (73%) | 19 (14%) | 18 (13%) | 0           | 1  |
| 36  | DP    | 139/141 (99%) | 92 (66%)  | 31 (22%) | 16 (12%) | 0           | 1  |
| 37  | B0    | 116/118 (98%) | 97 (84%)  | 11 (10%) | 8 (7%)   | 1           | 5  |
| 37  | D0    | 115/118 (98%) | 95 (83%)  | 15 (13%) | 5 (4%)   | 2           | 12 |
| 38  | BQ    | 109/112 (97%) | 85 (78%)  | 17 (16%) | 7 (6%)   | 1           | 6  |
| 38  | DQ    | 109/112 (97%) | 73 (67%)  | 26 (24%) | 10 (9%)  | 0           | 2  |
| 39  | BR    | 135/146 (92%) | 105 (78%) | 21 (16%) | 9 (7%)   | 1           | 5  |
| 39  | DR    | 135/146 (92%) | 108 (80%) | 18 (13%) | 9 (7%)   | 1           | 5  |
| 40  | B1    | 115/118 (98%) | 102 (89%) | 8 (7%)   | 5 (4%)   | 2           | 12 |
| 40  | D1    | 115/118 (98%) | 91 (79%)  | 18 (16%) | 6 (5%)   | 1           | 9  |
| 41  | B2    | 99/101 (98%)  | 81 (82%)  | 12 (12%) | 6 (6%)   | 1           | 7  |
| 41  | D2    | 99/101 (98%)  | 68 (69%)  | 17 (17%) | 14 (14%) | 0           | 1  |
| 42  | BS    | 111/113 (98%) | 92 (83%)  | 13 (12%) | 6 (5%)   | 1           | 9  |
| 42  | DS    | 111/113 (98%) | 92 (83%)  | 15 (14%) | 4 (4%)   | 2           | 16 |
| 43  | BT    | 90/96 (94%)   | 81 (90%)  | 5 (6%)   | 4 (4%)   | 2           | 12 |
| 43  | DT    | 90/96 (94%)   | 72 (80%)  | 13 (14%) | 5 (6%)   | 1           | 8  |
| 44  | BU    | 100/110 (91%) | 65 (65%)  | 21 (21%) | 14 (14%) | 0           | 1  |
| 44  | DU    | 100/110 (91%) | 62 (62%)  | 19 (19%) | 19 (19%) | 0           | 0  |
| 45  | BV    | 173/206 (84%) | 112 (65%) | 32 (18%) | 29 (17%) | 0           | 0  |
| 45  | DV    | 177/206 (86%) | 109 (62%) | 39 (22%) | 29 (16%) | 0           | 0  |
| 46  | B3    | 74/85 (87%)   | 65 (88%)  | 6 (8%)   | 3 (4%)   | 2           | 13 |
| 46  | D3    | 75/85 (88%)   | 64 (85%)  | 8 (11%)  | 3 (4%)   | 2           | 14 |
| 47  | BZ    | 95/98 (97%)   | 79 (83%)  | 12 (13%) | 4 (4%)   | 2           | 13 |
| 47  | DZ    | 95/98 (97%)   | 76 (80%)  | 11 (12%) | 8 (8%)   | 0           | 3  |
| 48  | BW    | 64/72 (89%)   | 53 (83%)  | 6 (9%)   | 5 (8%)   | 1           | 4  |
| 48  | DW    | 64/72 (89%)   | 54 (84%)  | 6 (9%)   | 4 (6%)   | 1           | 6  |
| 49  | BX    | 57/60 (95%)   | 51 (90%)  | 5 (9%)   | 1 (2%)   | 6           | 31 |
| 49  | DX    | 57/60 (95%)   | 49 (86%)  | 5 (9%)   | 3 (5%)   | 1           | 9  |
| 50  | B4    | 64/71 (90%)   | 36 (56%)  | 12 (19%) | 16 (25%) | 0           | 0  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 50  | D4    | 61/71 (86%)       | 22 (36%)   | 22 (36%)   | 17 (28%) | 0           | 0   |
| 51  | B5    | 57/60 (95%)       | 44 (77%)   | 6 (10%)    | 7 (12%)  | 0           | 1   |
| 51  | D5    | 57/60 (95%)       | 46 (81%)   | 8 (14%)    | 3 (5%)   | 1           | 9   |
| 52  | B6    | 43/54 (80%)       | 24 (56%)   | 12 (28%)   | 7 (16%)  | 0           | 0   |
| 52  | D6    | 43/54 (80%)       | 26 (60%)   | 8 (19%)    | 9 (21%)  | 0           | 0   |
| 53  | B7    | 43/49 (88%)       | 42 (98%)   | 1 (2%)     | 0        | 100         | 100 |
| 53  | D7    | 43/49 (88%)       | 42 (98%)   | 1 (2%)     | 0        | 100         | 100 |
| 54  | B8    | 58/65 (89%)       | 42 (72%)   | 8 (14%)    | 8 (14%)  | 0           | 1   |
| 54  | D8    | 58/65 (89%)       | 37 (64%)   | 13 (22%)   | 8 (14%)  | 0           | 1   |
| All | All   | 11319/12052 (94%) | 8735 (77%) | 1671 (15%) | 913 (8%) | 1           | 3   |

5 of 913 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AE    | 195 | ASP  |
| 2   | AE    | 236 | TYR  |
| 2   | AE    | 237 | ALA  |
| 3   | AF    | 4   | LYS  |
| 3   | AF    | 12  | LEU  |

### 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   | AE    | 205/220 (93%)  | 167 (82%) | 38 (18%) | 1           | 9  |
| 2   | CE    | 205/220 (93%)  | 176 (86%) | 29 (14%) | 3           | 16 |
| 3   | AF    | 159/188 (85%)  | 139 (87%) | 20 (13%) | 4           | 20 |
| 3   | CF    | 160/188 (85%)  | 144 (90%) | 16 (10%) | 7           | 29 |
| 4   | AG    | 180/180 (100%) | 162 (90%) | 18 (10%) | 7           | 29 |
| 4   | CG    | 180/180 (100%) | 157 (87%) | 23 (13%) | 4           | 19 |
| 5   | AH    | 116/123 (94%)  | 95 (82%)  | 21 (18%) | 2           | 9  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5   | CH    | 116/123 (94%)  | 100 (86%) | 16 (14%) | 3           | 17 |
| 6   | AI    | 90/90 (100%)   | 82 (91%)  | 8 (9%)   | 9           | 34 |
| 6   | CI    | 90/90 (100%)   | 81 (90%)  | 9 (10%)  | 7           | 29 |
| 7   | AJ    | 126/127 (99%)  | 102 (81%) | 24 (19%) | 1           | 8  |
| 7   | CJ    | 126/127 (99%)  | 104 (82%) | 22 (18%) | 2           | 10 |
| 8   | AK    | 119/119 (100%) | 107 (90%) | 12 (10%) | 7           | 29 |
| 8   | CK    | 119/119 (100%) | 111 (93%) | 8 (7%)   | 15          | 46 |
| 9   | AL    | 98/99 (99%)    | 88 (90%)  | 10 (10%) | 7           | 29 |
| 9   | CL    | 98/99 (99%)    | 84 (86%)  | 14 (14%) | 3           | 16 |
| 10  | AM    | 89/92 (97%)    | 78 (88%)  | 11 (12%) | 4           | 20 |
| 10  | CM    | 89/92 (97%)    | 76 (85%)  | 13 (15%) | 3           | 15 |
| 11  | AN    | 90/99 (91%)    | 78 (87%)  | 12 (13%) | 4           | 18 |
| 11  | CN    | 90/99 (91%)    | 86 (96%)  | 4 (4%)   | 25          | 60 |
| 12  | AO    | 104/109 (95%)  | 93 (89%)  | 11 (11%) | 6           | 27 |
| 12  | CO    | 104/109 (95%)  | 92 (88%)  | 12 (12%) | 5           | 24 |
| 13  | AP    | 94/101 (93%)   | 84 (89%)  | 10 (11%) | 6           | 27 |
| 13  | CP    | 94/101 (93%)   | 84 (89%)  | 10 (11%) | 6           | 27 |
| 14  | AQ    | 48/50 (96%)    | 40 (83%)  | 8 (17%)  | 2           | 12 |
| 14  | CQ    | 48/50 (96%)    | 44 (92%)  | 4 (8%)   | 10          | 37 |
| 15  | AR    | 79/80 (99%)    | 74 (94%)  | 5 (6%)   | 16          | 48 |
| 15  | CR    | 79/80 (99%)    | 67 (85%)  | 12 (15%) | 3           | 14 |
| 16  | AS    | 72/74 (97%)    | 66 (92%)  | 6 (8%)   | 10          | 37 |
| 16  | CS    | 72/74 (97%)    | 64 (89%)  | 8 (11%)  | 6           | 25 |
| 17  | AT    | 95/97 (98%)    | 85 (90%)  | 10 (10%) | 6           | 27 |
| 17  | CT    | 95/97 (98%)    | 91 (96%)  | 4 (4%)   | 26          | 61 |
| 18  | AU    | 63/77 (82%)    | 56 (89%)  | 7 (11%)  | 6           | 25 |
| 18  | CU    | 63/77 (82%)    | 53 (84%)  | 10 (16%) | 2           | 13 |
| 19  | AV    | 67/80 (84%)    | 54 (81%)  | 13 (19%) | 1           | 8  |
| 19  | CV    | 67/80 (84%)    | 57 (85%)  | 10 (15%) | 3           | 15 |
| 20  | AW    | 76/82 (93%)    | 66 (87%)  | 10 (13%) | 4           | 18 |
| 20  | CW    | 76/82 (93%)    | 66 (87%)  | 10 (13%) | 4           | 18 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 21  | AX    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 21  | CX    | 20/22 (91%)    | 20 (100%) | 0        | 100         | 100 |
| 27  | BD    | 214/218 (98%)  | 177 (83%) | 37 (17%) | 2           | 10  |
| 27  | DD    | 214/218 (98%)  | 179 (84%) | 35 (16%) | 2           | 12  |
| 28  | BE    | 165/166 (99%)  | 130 (79%) | 35 (21%) | 1           | 6   |
| 28  | DE    | 165/166 (99%)  | 137 (83%) | 28 (17%) | 2           | 11  |
| 29  | BF    | 161/166 (97%)  | 133 (83%) | 28 (17%) | 2           | 10  |
| 29  | DF    | 165/166 (99%)  | 137 (83%) | 28 (17%) | 2           | 11  |
| 30  | BG    | 155/156 (99%)  | 137 (88%) | 18 (12%) | 5           | 23  |
| 30  | DG    | 155/156 (99%)  | 138 (89%) | 17 (11%) | 6           | 25  |
| 31  | BH    | 142/148 (96%)  | 116 (82%) | 26 (18%) | 2           | 9   |
| 31  | DH    | 142/148 (96%)  | 123 (87%) | 19 (13%) | 4           | 18  |
| 32  | BK    | 122/124 (98%)  | 102 (84%) | 20 (16%) | 2           | 12  |
| 32  | DK    | 122/124 (98%)  | 103 (84%) | 19 (16%) | 2           | 13  |
| 33  | BM    | 117/119 (98%)  | 97 (83%)  | 20 (17%) | 2           | 11  |
| 33  | DM    | 117/119 (98%)  | 95 (81%)  | 22 (19%) | 1           | 9   |
| 34  | BN    | 100/100 (100%) | 87 (87%)  | 13 (13%) | 4           | 19  |
| 34  | DN    | 100/100 (100%) | 86 (86%)  | 14 (14%) | 3           | 16  |
| 35  | BO    | 116/116 (100%) | 84 (72%)  | 32 (28%) | 0           | 2   |
| 35  | DO    | 116/116 (100%) | 76 (66%)  | 40 (34%) | 0           | 1   |
| 36  | BP    | 111/111 (100%) | 91 (82%)  | 20 (18%) | 2           | 10  |
| 36  | DP    | 111/111 (100%) | 89 (80%)  | 22 (20%) | 1           | 8   |
| 37  | B0    | 101/101 (100%) | 83 (82%)  | 18 (18%) | 2           | 10  |
| 37  | D0    | 100/101 (99%)  | 81 (81%)  | 19 (19%) | 1           | 8   |
| 38  | BQ    | 87/88 (99%)    | 71 (82%)  | 16 (18%) | 1           | 9   |
| 38  | DQ    | 87/88 (99%)    | 79 (91%)  | 8 (9%)   | 8           | 33  |
| 39  | BR    | 120/127 (94%)  | 96 (80%)  | 24 (20%) | 1           | 7   |
| 39  | DR    | 120/127 (94%)  | 100 (83%) | 20 (17%) | 2           | 12  |
| 40  | B1    | 93/94 (99%)    | 84 (90%)  | 9 (10%)  | 8           | 30  |
| 40  | D1    | 93/94 (99%)    | 84 (90%)  | 9 (10%)  | 8           | 30  |
| 41  | B2    | 82/82 (100%)   | 67 (82%)  | 15 (18%) | 2           | 9   |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 41  | D2    | 82/82 (100%)    | 67 (82%)   | 15 (18%)   | 2           | 9  |
| 42  | BS    | 92/92 (100%)    | 79 (86%)   | 13 (14%)   | 3           | 16 |
| 42  | DS    | 92/92 (100%)    | 78 (85%)   | 14 (15%)   | 3           | 14 |
| 43  | BT    | 74/78 (95%)     | 61 (82%)   | 13 (18%)   | 2           | 10 |
| 43  | DT    | 74/78 (95%)     | 64 (86%)   | 10 (14%)   | 4           | 18 |
| 44  | BU    | 85/91 (93%)     | 69 (81%)   | 16 (19%)   | 1           | 9  |
| 44  | DU    | 85/91 (93%)     | 65 (76%)   | 20 (24%)   | 1           | 4  |
| 45  | BV    | 154/179 (86%)   | 125 (81%)  | 29 (19%)   | 1           | 9  |
| 45  | DV    | 158/179 (88%)   | 141 (89%)  | 17 (11%)   | 6           | 26 |
| 46  | B3    | 61/67 (91%)     | 57 (93%)   | 4 (7%)     | 15          | 46 |
| 46  | D3    | 62/67 (92%)     | 55 (89%)   | 7 (11%)    | 5           | 24 |
| 47  | BZ    | 82/83 (99%)     | 68 (83%)   | 14 (17%)   | 2           | 11 |
| 47  | DZ    | 82/83 (99%)     | 68 (83%)   | 14 (17%)   | 2           | 11 |
| 48  | BW    | 62/67 (92%)     | 49 (79%)   | 13 (21%)   | 1           | 6  |
| 48  | DW    | 62/67 (92%)     | 49 (79%)   | 13 (21%)   | 1           | 6  |
| 49  | BX    | 51/52 (98%)     | 44 (86%)   | 7 (14%)    | 3           | 17 |
| 49  | DX    | 51/52 (98%)     | 45 (88%)   | 6 (12%)    | 5           | 22 |
| 50  | B4    | 59/63 (94%)     | 47 (80%)   | 12 (20%)   | 1           | 7  |
| 50  | D4    | 57/63 (90%)     | 47 (82%)   | 10 (18%)   | 2           | 10 |
| 51  | B5    | 51/52 (98%)     | 42 (82%)   | 9 (18%)    | 2           | 10 |
| 51  | D5    | 51/52 (98%)     | 42 (82%)   | 9 (18%)    | 2           | 10 |
| 52  | B6    | 44/52 (85%)     | 34 (77%)   | 10 (23%)   | 1           | 5  |
| 52  | D6    | 44/52 (85%)     | 39 (89%)   | 5 (11%)    | 5           | 24 |
| 53  | B7    | 38/42 (90%)     | 33 (87%)   | 5 (13%)    | 4           | 18 |
| 53  | D7    | 38/42 (90%)     | 32 (84%)   | 6 (16%)    | 2           | 13 |
| 54  | B8    | 50/55 (91%)     | 37 (74%)   | 13 (26%)   | 0           | 3  |
| 54  | D8    | 50/55 (91%)     | 39 (78%)   | 11 (22%)   | 1           | 5  |
| All | All   | 9565/9996 (96%) | 8131 (85%) | 1434 (15%) | 3           | 14 |

5 of 1434 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | CR    | 17  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DN    | 10  | VAL  |
| 18  | CU    | 54  | ARG  |
| 15  | CR    | 6   | GLU  |
| 29  | DF    | 7   | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 303 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | DM    | 101 | HIS  |
| 48  | DW    | 65  | ASN  |
| 35  | DO    | 38  | GLN  |
| 40  | D1    | 81  | HIS  |
| 53  | D7    | 8   | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1501/1506 (99%) | 295 (19%)         | 43 (2%)         |
| 1   | CA    | 1501/1506 (99%) | 296 (19%)         | 49 (3%)         |
| 22  | AB    | 84/85 (98%)     | 38 (45%)          | 8 (9%)          |
| 22  | AD    | 84/85 (98%)     | 27 (32%)          | 5 (5%)          |
| 22  | CB    | 84/85 (98%)     | 38 (45%)          | 9 (10%)         |
| 22  | CD    | 84/85 (98%)     | 25 (29%)          | 4 (4%)          |
| 23  | AC    | 76/77 (98%)     | 11 (14%)          | 1 (1%)          |
| 23  | CC    | 76/77 (98%)     | 13 (17%)          | 3 (3%)          |
| 24  | A1    | 15/16 (93%)     | 6 (40%)           | 2 (13%)         |
| 24  | C1    | 15/16 (93%)     | 6 (40%)           | 3 (20%)         |
| 25  | BA    | 2911/2912 (99%) | 542 (18%)         | 51 (1%)         |
| 25  | DA    | 2905/2912 (99%) | 569 (19%)         | 53 (1%)         |
| 26  | BB    | 121/122 (99%)   | 17 (14%)          | 0               |
| 26  | DB    | 121/122 (99%)   | 27 (22%)          | 1 (0%)          |
| All | All   | 9578/9606 (99%) | 1910 (19%)        | 232 (2%)        |

5 of 1910 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 7   | G    |
| 1   | AA    | 8   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 13  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 32  | A    |

5 of 232 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 115  | G    |
| 25  | DA    | 2447 | G    |
| 1   | CA    | 1053 | G    |
| 25  | DA    | 2402 | C    |
| 25  | DA    | 1379 | A    |

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

4 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$ |
| 22  | MIA  | CD    | 38  | 22   | 28,31,32     | 1.96 | 2 (7%)      | 38,44,47    | 2.80 | 13 (34%)    |
| 22  | MIA  | AB    | 38  | 22   | 28,31,32     | 1.91 | 3 (10%)     | 38,44,47    | 2.61 | 13 (34%)    |
| 22  | MIA  | CB    | 38  | 22   | 28,31,32     | 2.01 | 2 (7%)      | 38,44,47    | 2.59 | 13 (34%)    |
| 22  | MIA  | AD    | 38  | 22   | 28,31,32     | 1.95 | 2 (7%)      | 38,44,47    | 2.79 | 12 (31%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 22  | MIA  | CD    | 38  | 22   | -       | 7/15/33/34 | 0/3/3/3 |
| 22  | MIA  | AB    | 38  | 22   | -       | 4/15/33/34 | 0/3/3/3 |
| 22  | MIA  | CB    | 38  | 22   | -       | 4/15/33/34 | 0/3/3/3 |
| 22  | MIA  | AD    | 38  | 22   | -       | 8/15/33/34 | 0/3/3/3 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | CB    | 38  | MIA  | C6-N6   | 7.81 | 1.46        | 1.34     |
| 22  | CD    | 38  | MIA  | C6-N6   | 7.48 | 1.46        | 1.34     |
| 22  | AD    | 38  | MIA  | C6-N6   | 7.37 | 1.45        | 1.34     |
| 22  | AB    | 38  | MIA  | C6-N6   | 7.22 | 1.45        | 1.34     |
| 22  | CB    | 38  | MIA  | C13-C14 | 6.08 | 1.50        | 1.32     |

The worst 5 of 51 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 22  | CD    | 38  | MIA  | C11-S10-C2 | 10.16 | 109.88      | 102.25   |
| 22  | AD    | 38  | MIA  | C11-S10-C2 | 9.68  | 109.51      | 102.25   |
| 22  | CB    | 38  | MIA  | C11-S10-C2 | 7.56  | 107.92      | 102.25   |
| 22  | AB    | 38  | MIA  | C5-C4-N3   | -7.51 | 119.27      | 127.18   |
| 22  | CB    | 38  | MIA  | C5-C4-N3   | -7.50 | 119.28      | 127.18   |

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | AB    | 38  | MIA  | N1-C2-S10-C11   |
| 22  | AB    | 38  | MIA  | N3-C2-S10-C11   |
| 22  | AB    | 38  | MIA  | C12-C13-C14-C15 |
| 22  | AB    | 38  | MIA  | C12-C13-C14-C16 |
| 22  | AD    | 38  | MIA  | O4'-C4'-C5'-O5' |

There are no ring outliers.

4 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | CD    | 38  | MIA  | 4       | 0            |
| 22  | AB    | 38  | MIA  | 2       | 0            |
| 22  | CB    | 38  | MIA  | 3       | 0            |
| 22  | AD    | 38  | MIA  | 2       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 1608 ligands modelled in this entry, 1608 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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    | 1502/1506 (99%) | -0.24  | 5 (0%) 90 79  | 54, 99, 183, 246      | 0     |
| 1   | CA    | 1502/1506 (99%) | -0.20  | 13 (0%) 81 61 | 59, 100, 182, 245     | 0     |
| 2   | AE    | 237/256 (92%)   | 0.46   | 11 (4%) 37 20 | 98, 139, 177, 190     | 0     |
| 2   | CE    | 237/256 (92%)   | 0.63   | 11 (4%) 37 20 | 106, 152, 189, 209    | 0     |
| 3   | AF    | 205/239 (85%)   | 0.48   | 7 (3%) 48 27  | 88, 113, 149, 158     | 0     |
| 3   | CF    | 206/239 (86%)   | 0.66   | 15 (7%) 21 11 | 101, 135, 165, 180    | 0     |
| 4   | AG    | 208/208 (100%)  | 0.40   | 6 (2%) 53 31  | 81, 107, 131, 143     | 0     |
| 4   | CG    | 208/208 (100%)  | 0.39   | 9 (4%) 40 21  | 75, 95, 123, 135      | 0     |
| 5   | AH    | 151/162 (93%)   | 0.13   | 2 (1%) 75 53  | 78, 99, 125, 164      | 0     |
| 5   | CH    | 151/162 (93%)   | 0.47   | 8 (5%) 32 16  | 84, 106, 131, 167     | 0     |
| 6   | AI    | 101/101 (100%)  | -0.11  | 0 100 100     | 67, 99, 115, 141      | 0     |
| 6   | CI    | 101/101 (100%)  | -0.24  | 0 100 100     | 76, 96, 115, 153      | 0     |
| 7   | AJ    | 155/156 (99%)   | 0.56   | 15 (9%) 13 7  | 96, 114, 143, 161     | 0     |
| 7   | CJ    | 155/156 (99%)   | 0.66   | 13 (8%) 17 9  | 100, 119, 147, 158    | 0     |
| 8   | AK    | 138/138 (100%)  | 0.24   | 0 100 100     | 81, 103, 117, 132     | 0     |
| 8   | CK    | 138/138 (100%)  | 0.08   | 2 (1%) 73 51  | 81, 108, 125, 136     | 0     |
| 9   | AL    | 127/128 (99%)   | 0.55   | 3 (2%) 59 36  | 83, 138, 159, 166     | 0     |
| 9   | CL    | 127/128 (99%)   | 0.60   | 10 (7%) 18 10 | 95, 147, 165, 171     | 0     |
| 10  | AM    | 99/105 (94%)    | 0.66   | 1 (1%) 79 59  | 81, 140, 167, 178     | 0     |
| 10  | CM    | 99/105 (94%)    | 0.70   | 7 (7%) 22 11  | 103, 154, 174, 180    | 0     |
| 11  | AN    | 119/129 (92%)   | 0.49   | 7 (5%) 28 14  | 62, 95, 130, 161      | 0     |
| 11  | CN    | 119/129 (92%)   | 0.37   | 3 (2%) 58 35  | 74, 99, 133, 164      | 0     |
| 12  | AO    | 125/132 (94%)   | 0.20   | 6 (4%) 35 19  | 59, 75, 107, 162      | 0     |
| 12  | CO    | 125/132 (94%)   | 0.56   | 13 (10%) 11 6 | 63, 91, 126, 166      | 0     |

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| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 13  | AP    | 116/126 (92%)    | 0.45   | 5 (4%) 40 21  | 75, 124, 143, 155     | 0     |
| 13  | CP    | 117/126 (92%)    | 0.74   | 12 (10%) 12 6 | 91, 145, 161, 169     | 0     |
| 14  | AQ    | 58/61 (95%)      | 0.56   | 3 (5%) 33 17  | 87, 103, 120, 127     | 0     |
| 14  | CQ    | 58/61 (95%)      | 0.95   | 3 (5%) 33 17  | 108, 125, 150, 154    | 0     |
| 15  | AR    | 88/89 (98%)      | 0.13   | 1 (1%) 78 57  | 70, 94, 116, 120      | 0     |
| 15  | CR    | 88/89 (98%)      | 0.11   | 1 (1%) 78 57  | 67, 96, 124, 136      | 0     |
| 16  | AS    | 84/88 (95%)      | 0.52   | 4 (4%) 35 19  | 87, 109, 134, 174     | 0     |
| 16  | CS    | 84/88 (95%)      | 0.25   | 1 (1%) 76 55  | 76, 91, 118, 157      | 0     |
| 17  | AT    | 100/105 (95%)    | 0.54   | 8 (8%) 18 9   | 80, 102, 118, 129     | 0     |
| 17  | CT    | 100/105 (95%)    | 0.52   | 6 (6%) 27 14  | 75, 100, 126, 144     | 0     |
| 18  | AU    | 72/88 (81%)      | 0.02   | 0 100 100     | 77, 97, 135, 164      | 0     |
| 18  | CU    | 72/88 (81%)      | -0.16  | 0 100 100     | 85, 103, 149, 172     | 0     |
| 19  | AV    | 78/93 (83%)      | 0.48   | 5 (6%) 25 13  | 97, 120, 145, 156     | 0     |
| 19  | CV    | 78/93 (83%)      | 0.89   | 9 (11%) 9 6   | 128, 152, 178, 186    | 0     |
| 20  | AW    | 99/106 (93%)     | 0.54   | 7 (7%) 22 11  | 96, 121, 148, 153     | 0     |
| 20  | CW    | 99/106 (93%)     | 0.43   | 3 (3%) 52 30  | 86, 106, 141, 153     | 0     |
| 21  | AX    | 25/27 (92%)      | 0.71   | 2 (8%) 18 9   | 97, 107, 121, 153     | 0     |
| 21  | CX    | 25/27 (92%)      | 1.00   | 3 (12%) 9 5   | 101, 129, 150, 171    | 0     |
| 22  | AB    | 84/85 (98%)      | 0.40   | 5 (5%) 27 14  | 76, 148, 167, 178     | 0     |
| 22  | AD    | 84/85 (98%)      | 0.22   | 3 (3%) 46 26  | 70, 147, 206, 218     | 0     |
| 22  | CB    | 84/85 (98%)      | 0.53   | 3 (3%) 46 26  | 92, 155, 171, 179     | 0     |
| 22  | CD    | 84/85 (98%)      | 0.06   | 2 (2%) 59 36  | 74, 147, 207, 212     | 0     |
| 23  | AC    | 77/77 (100%)     | -0.12  | 1 (1%) 75 53  | 66, 91, 135, 155      | 0     |
| 23  | CC    | 77/77 (100%)     | -0.08  | 1 (1%) 75 53  | 79, 104, 143, 165     | 0     |
| 24  | A1    | 16/16 (100%)     | 0.71   | 3 (18%) 3 2   | 66, 97, 168, 177      | 0     |
| 24  | C1    | 16/16 (100%)     | 0.79   | 3 (18%) 3 2   | 75, 107, 176, 183     | 0     |
| 25  | BA    | 2912/2912 (100%) | -0.58  | 12 (0%) 88 76 | 39, 68, 206, 243      | 0     |
| 25  | DA    | 2907/2912 (99%)  | -0.36  | 15 (0%) 87 72 | 49, 82, 226, 247      | 0     |
| 26  | BB    | 122/122 (100%)   | -0.51  | 0 100 100     | 65, 92, 113, 183      | 0     |
| 26  | DB    | 122/122 (100%)   | -0.19  | 2 (1%) 70 47  | 78, 110, 139, 198     | 0     |
| 27  | BD    | 272/276 (98%)    | 0.03   | 7 (2%) 57 34  | 39, 59, 82, 104       | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 27  | DD    | 272/276 (98%)  | 0.07   | 7 (2%) 57 34  | 45, 67, 87, 120       | 0     |
| 28  | BE    | 205/206 (99%)  | 0.45   | 15 (7%) 21 11 | 44, 77, 125, 150      | 0     |
| 28  | DE    | 205/206 (99%)  | 0.38   | 12 (5%) 28 14 | 56, 92, 144, 157      | 0     |
| 29  | BF    | 202/210 (96%)  | -0.10  | 4 (1%) 65 41  | 42, 75, 110, 127      | 0     |
| 29  | DF    | 208/210 (99%)  | 0.22   | 3 (1%) 73 51  | 53, 93, 155, 185      | 0     |
| 30  | BG    | 181/182 (99%)  | 0.27   | 3 (1%) 69 45  | 79, 105, 136, 146     | 0     |
| 30  | DG    | 181/182 (99%)  | 0.67   | 15 (8%) 17 9  | 96, 128, 157, 168     | 0     |
| 31  | BH    | 170/180 (94%)  | 0.29   | 6 (3%) 47 27  | 71, 105, 126, 151     | 0     |
| 31  | DH    | 170/180 (94%)  | 1.09   | 23 (13%) 7 4  | 143, 193, 217, 231    | 0     |
| 32  | BK    | 146/148 (98%)  | 0.44   | 6 (4%) 41 23  | 72, 120, 141, 153     | 0     |
| 32  | DK    | 146/148 (98%)  | 0.42   | 9 (6%) 26 14  | 73, 120, 147, 151     | 0     |
| 33  | BM    | 138/140 (98%)  | 0.34   | 5 (3%) 46 26  | 58, 79, 115, 136      | 0     |
| 33  | DM    | 138/140 (98%)  | 0.49   | 4 (2%) 53 31  | 72, 104, 137, 147     | 0     |
| 34  | BN    | 122/122 (100%) | -0.08  | 0 100 100     | 55, 71, 87, 93        | 0     |
| 34  | DN    | 122/122 (100%) | 0.32   | 2 (1%) 70 47  | 66, 85, 103, 110      | 0     |
| 35  | BO    | 150/150 (100%) | 0.45   | 11 (7%) 21 11 | 45, 82, 109, 167      | 0     |
| 35  | DO    | 150/150 (100%) | 0.94   | 24 (16%) 5 3  | 45, 93, 136, 174      | 0     |
| 36  | BP    | 141/141 (100%) | 0.66   | 19 (13%) 7 4  | 55, 77, 105, 140      | 0     |
| 36  | DP    | 141/141 (100%) | 1.02   | 25 (17%) 4 2  | 58, 100, 130, 154     | 0     |
| 37  | B0    | 118/118 (100%) | -0.04  | 2 (1%) 69 45  | 53, 74, 96, 106       | 0     |
| 37  | D0    | 117/118 (99%)  | 0.03   | 2 (1%) 69 45  | 62, 81, 100, 117      | 0     |
| 38  | BQ    | 111/112 (99%)  | 0.02   | 3 (2%) 56 33  | 71, 91, 116, 130      | 0     |
| 38  | DQ    | 111/112 (99%)  | 0.23   | 4 (3%) 46 26  | 73, 109, 135, 157     | 0     |
| 39  | BR    | 137/146 (93%)  | 0.46   | 9 (6%) 24 12  | 66, 85, 135, 167      | 0     |
| 39  | DR    | 137/146 (93%)  | 0.49   | 6 (4%) 39 21  | 73, 94, 154, 184      | 0     |
| 40  | B1    | 117/118 (99%)  | 0.02   | 2 (1%) 69 45  | 50, 70, 98, 140       | 0     |
| 40  | D1    | 117/118 (99%)  | 0.08   | 1 (0%) 81 61  | 60, 99, 137, 155      | 0     |
| 41  | B2    | 101/101 (100%) | 0.40   | 6 (5%) 28 14  | 46, 91, 116, 128      | 0     |
| 41  | D2    | 101/101 (100%) | 0.32   | 3 (2%) 52 30  | 63, 122, 139, 150     | 0     |
| 42  | BS    | 113/113 (100%) | -0.10  | 2 (1%) 67 44  | 44, 67, 99, 152       | 0     |
| 42  | DS    | 113/113 (100%) | 0.18   | 4 (3%) 47 27  | 61, 75, 109, 161      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 43  | BT    | 92/96 (95%)       | 0.10   | 2 (2%) 62 39   | 54, 69, 95, 112       | 0     |
| 43  | DT    | 92/96 (95%)       | 0.33   | 4 (4%) 40 21   | 65, 81, 109, 122      | 0     |
| 44  | BU    | 102/110 (92%)     | 0.68   | 12 (11%) 9 5   | 70, 94, 144, 165      | 0     |
| 44  | DU    | 102/110 (92%)     | 1.40   | 27 (26%) 1 1   | 78, 111, 162, 172     | 0     |
| 45  | BV    | 175/206 (84%)     | 0.72   | 9 (5%) 33 17   | 79, 120, 189, 194     | 0     |
| 45  | DV    | 179/206 (86%)     | 0.81   | 11 (6%) 27 14  | 111, 152, 207, 219    | 0     |
| 46  | B3    | 76/85 (89%)       | 0.19   | 5 (6%) 24 12   | 51, 72, 92, 125       | 0     |
| 46  | D3    | 77/85 (90%)       | 0.55   | 6 (7%) 19 10   | 64, 87, 110, 151      | 0     |
| 47  | BZ    | 97/98 (98%)       | 0.43   | 7 (7%) 21 11   | 48, 71, 115, 155      | 0     |
| 47  | DZ    | 97/98 (98%)       | 0.56   | 6 (6%) 26 14   | 54, 74, 126, 152      | 0     |
| 48  | BW    | 66/72 (91%)       | 0.26   | 6 (9%) 15 8    | 59, 79, 95, 127       | 0     |
| 48  | DW    | 66/72 (91%)       | 0.22   | 3 (4%) 38 20   | 75, 99, 121, 134      | 0     |
| 49  | BX    | 59/60 (98%)       | -0.07  | 0 100 100      | 61, 77, 112, 131      | 0     |
| 49  | DX    | 59/60 (98%)       | 0.19   | 1 (1%) 69 45   | 76, 103, 136, 159     | 0     |
| 50  | B4    | 66/71 (92%)       | 0.56   | 3 (4%) 38 20   | 112, 153, 176, 181    | 0     |
| 50  | D4    | 63/71 (88%)       | 0.73   | 6 (9%) 14 7    | 141, 181, 191, 201    | 0     |
| 51  | B5    | 59/60 (98%)       | 0.70   | 8 (13%) 7 4    | 43, 81, 156, 165      | 0     |
| 51  | D5    | 59/60 (98%)       | 0.53   | 6 (10%) 12 6   | 61, 84, 169, 188      | 0     |
| 52  | B6    | 45/54 (83%)       | 1.54   | 11 (24%) 2 1   | 117, 148, 164, 173    | 0     |
| 52  | D6    | 45/54 (83%)       | 2.04   | 20 (44%) 0 1   | 131, 164, 181, 185    | 0     |
| 53  | B7    | 45/49 (91%)       | -0.30  | 1 (2%) 62 39   | 38, 48, 68, 85        | 0     |
| 53  | D7    | 45/49 (91%)       | 0.06   | 1 (2%) 62 39   | 52, 59, 74, 94        | 0     |
| 54  | B8    | 60/65 (92%)       | 0.49   | 8 (13%) 7 4    | 51, 68, 88, 115       | 0     |
| 54  | D8    | 60/65 (92%)       | 1.26   | 11 (18%) 3 2   | 64, 80, 106, 132      | 0     |
| All | All   | 21100/21658 (97%) | 0.07   | 708 (3%) 48 27 | 38, 95, 177, 247      | 0     |

The worst 5 of 708 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 51  | B5    | 2   | ALA  | 9.7  |
| 7   | CJ    | 81  | GLY  | 9.6  |
| 51  | D5    | 2   | ALA  | 9.3  |
| 31  | DH    | 150 | ALA  | 8.3  |
| 9   | CL    | 115 | GLY  | 8.1  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 22  | MIA  | CD    | 38  | 29/30 | 0.90 | 0.14 | 101,121,146,154            | 0     |
| 22  | MIA  | CB    | 38  | 29/30 | 0.91 | 0.12 | 63,95,112,126              | 0     |
| 22  | MIA  | AD    | 38  | 29/30 | 0.93 | 0.12 | 98,122,141,145             | 0     |
| 22  | MIA  | AB    | 38  | 29/30 | 0.95 | 0.10 | 65,78,90,93                | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 55  | MG   | CA    | 1745 | 1/1   | -0.22 | 0.20 | 159,159,159,159            | 0     |
| 55  | MG   | CA    | 1781 | 1/1   | -0.18 | 0.21 | 172,172,172,172            | 0     |
| 55  | MG   | BA    | 3456 | 1/1   | -0.12 | 0.16 | 168,168,168,168            | 0     |
| 55  | MG   | AA    | 1750 | 1/1   | -0.10 | 0.28 | 134,134,134,134            | 0     |
| 55  | MG   | AA    | 1805 | 1/1   | -0.08 | 0.28 | 152,152,152,152            | 0     |
| 55  | MG   | AA    | 1765 | 1/1   | -0.08 | 0.21 | 149,149,149,149            | 0     |
| 55  | MG   | BA    | 3406 | 1/1   | -0.05 | 0.11 | 182,182,182,182            | 0     |
| 55  | MG   | CB    | 104  | 1/1   | 0.01  | 0.27 | 147,147,147,147            | 0     |
| 55  | MG   | AA    | 1764 | 1/1   | 0.03  | 0.18 | 146,146,146,146            | 0     |
| 55  | MG   | AA    | 1809 | 1/1   | 0.05  | 0.19 | 204,204,204,204            | 0     |
| 55  | MG   | AA    | 1783 | 1/1   | 0.05  | 0.16 | 167,167,167,167            | 0     |
| 55  | MG   | DA    | 3362 | 1/1   | 0.05  | 0.28 | 150,150,150,150            | 0     |
| 55  | MG   | CA    | 1812 | 1/1   | 0.06  | 0.15 | 176,176,176,176            | 0     |
| 55  | MG   | AD    | 101  | 1/1   | 0.08  | 0.27 | 154,154,154,154            | 0     |
| 55  | MG   | BA    | 3397 | 1/1   | 0.09  | 0.21 | 131,131,131,131            | 0     |
| 55  | MG   | BA    | 3429 | 1/1   | 0.10  | 0.34 | 146,146,146,146            | 0     |
| 55  | MG   | BA    | 3475 | 1/1   | 0.14  | 0.10 | 212,212,212,212            | 0     |
| 55  | MG   | BA    | 3550 | 1/1   | 0.15  | 0.11 | 131,131,131,131            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3479 | 1/1   | 0.16 | 0.30 | 146,146,146,146             | 0     |
| 55  | MG   | CA    | 1785 | 1/1   | 0.22 | 0.42 | 155,155,155,155             | 0     |
| 55  | MG   | DA    | 3417 | 1/1   | 0.22 | 0.14 | 135,135,135,135             | 0     |
| 55  | MG   | DB    | 212  | 1/1   | 0.24 | 0.35 | 120,120,120,120             | 0     |
| 55  | MG   | BA    | 3420 | 1/1   | 0.26 | 0.19 | 114,114,114,114             | 0     |
| 55  | MG   | AA    | 1758 | 1/1   | 0.27 | 0.19 | 165,165,165,165             | 0     |
| 55  | MG   | BA    | 3446 | 1/1   | 0.28 | 0.35 | 121,121,121,121             | 0     |
| 55  | MG   | CA    | 1627 | 1/1   | 0.29 | 0.19 | 140,140,140,140             | 0     |
| 55  | MG   | CA    | 1808 | 1/1   | 0.32 | 0.46 | 153,153,153,153             | 0     |
| 55  | MG   | BA    | 3488 | 1/1   | 0.32 | 0.32 | 137,137,137,137             | 0     |
| 55  | MG   | DA    | 3388 | 1/1   | 0.33 | 0.26 | 138,138,138,138             | 0     |
| 55  | MG   | DA    | 3411 | 1/1   | 0.33 | 0.27 | 144,144,144,144             | 0     |
| 55  | MG   | DA    | 3035 | 1/1   | 0.33 | 0.33 | 124,124,124,124             | 0     |
| 55  | MG   | CB    | 103  | 1/1   | 0.33 | 0.17 | 147,147,147,147             | 0     |
| 55  | MG   | DA    | 3229 | 1/1   | 0.34 | 0.29 | 118,118,118,118             | 0     |
| 55  | MG   | DA    | 3219 | 1/1   | 0.36 | 0.20 | 128,128,128,128             | 0     |
| 55  | MG   | CA    | 1796 | 1/1   | 0.36 | 0.21 | 146,146,146,146             | 0     |
| 55  | MG   | DA    | 3351 | 1/1   | 0.36 | 0.24 | 151,151,151,151             | 0     |
| 55  | MG   | CA    | 1675 | 1/1   | 0.36 | 0.42 | 111,111,111,111             | 0     |
| 55  | MG   | BA    | 3469 | 1/1   | 0.37 | 0.28 | 124,124,124,124             | 0     |
| 55  | MG   | AA    | 1810 | 1/1   | 0.37 | 0.40 | 148,148,148,148             | 0     |
| 55  | MG   | CA    | 1737 | 1/1   | 0.38 | 0.24 | 122,122,122,122             | 0     |
| 55  | MG   | CA    | 1630 | 1/1   | 0.38 | 0.20 | 149,149,149,149             | 0     |
| 55  | MG   | CA    | 1778 | 1/1   | 0.39 | 0.34 | 133,133,133,133             | 0     |
| 55  | MG   | DA    | 3405 | 1/1   | 0.40 | 0.23 | 135,135,135,135             | 0     |
| 55  | MG   | BA    | 3202 | 1/1   | 0.40 | 0.35 | 97,97,97,97                 | 0     |
| 55  | MG   | CD    | 101  | 1/1   | 0.41 | 0.27 | 145,145,145,145             | 0     |
| 55  | MG   | CA    | 1776 | 1/1   | 0.42 | 0.44 | 118,118,118,118             | 0     |
| 55  | MG   | AA    | 1773 | 1/1   | 0.42 | 0.31 | 130,130,130,130             | 0     |
| 55  | MG   | CA    | 1672 | 1/1   | 0.43 | 0.21 | 119,119,119,119             | 0     |
| 55  | MG   | CA    | 1749 | 1/1   | 0.43 | 0.25 | 117,117,117,117             | 0     |
| 55  | MG   | CA    | 1761 | 1/1   | 0.43 | 0.15 | 143,143,143,143             | 0     |
| 55  | MG   | CA    | 1773 | 1/1   | 0.43 | 0.19 | 139,139,139,139             | 0     |
| 55  | MG   | AA    | 1613 | 1/1   | 0.45 | 0.15 | 116,116,116,116             | 0     |
| 55  | MG   | DA    | 3172 | 1/1   | 0.45 | 0.30 | 122,122,122,122             | 0     |
| 55  | MG   | DA    | 3188 | 1/1   | 0.45 | 0.31 | 113,113,113,113             | 0     |
| 55  | MG   | AC    | 107  | 1/1   | 0.45 | 0.21 | 124,124,124,124             | 0     |
| 55  | MG   | AA    | 1694 | 1/1   | 0.46 | 0.21 | 142,142,142,142             | 0     |
| 55  | MG   | AA    | 1730 | 1/1   | 0.46 | 0.12 | 113,113,113,113             | 0     |
| 55  | MG   | DA    | 3342 | 1/1   | 0.47 | 0.23 | 122,122,122,122             | 0     |
| 55  | MG   | CA    | 1768 | 1/1   | 0.48 | 0.26 | 138,138,138,138             | 0     |
| 55  | MG   | CA    | 1692 | 1/1   | 0.48 | 0.17 | 157,157,157,157             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3407 | 1/1   | 0.48 | 0.28 | 103,103,103,103             | 0     |
| 55  | MG   | DB    | 220  | 1/1   | 0.48 | 0.15 | 121,121,121,121             | 0     |
| 55  | MG   | BA    | 3378 | 1/1   | 0.49 | 0.15 | 140,140,140,140             | 0     |
| 55  | MG   | AA    | 1757 | 1/1   | 0.49 | 0.43 | 101,101,101,101             | 0     |
| 55  | MG   | DD    | 303  | 1/1   | 0.49 | 0.21 | 69,69,69,69                 | 0     |
| 55  | MG   | BB    | 208  | 1/1   | 0.50 | 0.27 | 117,117,117,117             | 0     |
| 55  | MG   | AA    | 1800 | 1/1   | 0.50 | 0.28 | 131,131,131,131             | 0     |
| 55  | MG   | DA    | 3221 | 1/1   | 0.50 | 0.14 | 154,154,154,154             | 0     |
| 55  | MG   | BB    | 211  | 1/1   | 0.51 | 0.21 | 109,109,109,109             | 0     |
| 55  | MG   | DA    | 3194 | 1/1   | 0.52 | 0.29 | 104,104,104,104             | 0     |
| 55  | MG   | BA    | 3245 | 1/1   | 0.52 | 0.26 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1785 | 1/1   | 0.52 | 0.17 | 125,125,125,125             | 0     |
| 55  | MG   | DA    | 3177 | 1/1   | 0.52 | 0.13 | 129,129,129,129             | 0     |
| 55  | MG   | CA    | 1764 | 1/1   | 0.52 | 0.23 | 117,117,117,117             | 0     |
| 55  | MG   | DA    | 3321 | 1/1   | 0.53 | 0.24 | 112,112,112,112             | 0     |
| 55  | MG   | AD    | 102  | 1/1   | 0.53 | 0.21 | 125,125,125,125             | 0     |
| 55  | MG   | BA    | 3343 | 1/1   | 0.53 | 0.27 | 114,114,114,114             | 0     |
| 55  | MG   | AA    | 1819 | 1/1   | 0.54 | 0.20 | 126,126,126,126             | 0     |
| 55  | MG   | BA    | 3439 | 1/1   | 0.54 | 0.24 | 115,115,115,115             | 0     |
| 55  | MG   | DA    | 3414 | 1/1   | 0.54 | 0.28 | 111,111,111,111             | 0     |
| 55  | MG   | AA    | 1703 | 1/1   | 0.54 | 0.22 | 106,106,106,106             | 0     |
| 55  | MG   | DB    | 209  | 1/1   | 0.54 | 0.32 | 130,130,130,130             | 0     |
| 55  | MG   | DA    | 3366 | 1/1   | 0.54 | 0.54 | 105,105,105,105             | 0     |
| 55  | MG   | BD    | 301  | 1/1   | 0.54 | 0.34 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3393 | 1/1   | 0.54 | 0.28 | 118,118,118,118             | 0     |
| 55  | MG   | DA    | 3372 | 1/1   | 0.55 | 0.21 | 125,125,125,125             | 0     |
| 55  | MG   | DB    | 215  | 1/1   | 0.55 | 0.37 | 129,129,129,129             | 0     |
| 55  | MG   | DA    | 3383 | 1/1   | 0.55 | 0.21 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1772 | 1/1   | 0.55 | 0.29 | 131,131,131,131             | 0     |
| 55  | MG   | BA    | 3546 | 1/1   | 0.56 | 0.28 | 101,101,101,101             | 0     |
| 55  | MG   | AA    | 1626 | 1/1   | 0.56 | 0.30 | 91,91,91,91                 | 0     |
| 55  | MG   | CA    | 1813 | 1/1   | 0.56 | 0.34 | 108,108,108,108             | 0     |
| 55  | MG   | CA    | 1819 | 1/1   | 0.56 | 0.39 | 134,134,134,134             | 0     |
| 55  | MG   | DA    | 3406 | 1/1   | 0.56 | 0.49 | 129,129,129,129             | 0     |
| 55  | MG   | CA    | 1806 | 1/1   | 0.56 | 0.41 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3369 | 1/1   | 0.56 | 0.40 | 108,108,108,108             | 0     |
| 55  | MG   | DA    | 3409 | 1/1   | 0.57 | 0.38 | 124,124,124,124             | 0     |
| 55  | MG   | DA    | 3371 | 1/1   | 0.57 | 0.48 | 122,122,122,122             | 0     |
| 55  | MG   | BA    | 3411 | 1/1   | 0.57 | 0.33 | 102,102,102,102             | 0     |
| 55  | MG   | CA    | 1766 | 1/1   | 0.57 | 0.23 | 114,114,114,114             | 0     |
| 55  | MG   | DA    | 3439 | 1/1   | 0.57 | 0.42 | 107,107,107,107             | 0     |
| 55  | MG   | DA    | 3386 | 1/1   | 0.57 | 0.27 | 130,130,130,130             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3318 | 1/1   | 0.57 | 0.22 | 102,102,102,102             | 0     |
| 55  | MG   | AA    | 1748 | 1/1   | 0.57 | 0.22 | 116,116,116,116             | 0     |
| 55  | MG   | BA    | 3189 | 1/1   | 0.57 | 0.14 | 108,108,108,108             | 0     |
| 55  | MG   | DA    | 3279 | 1/1   | 0.57 | 0.55 | 135,135,135,135             | 0     |
| 55  | MG   | CA    | 1771 | 1/1   | 0.58 | 0.22 | 117,117,117,117             | 0     |
| 55  | MG   | CA    | 1683 | 1/1   | 0.58 | 0.27 | 121,121,121,121             | 0     |
| 55  | MG   | BA    | 3210 | 1/1   | 0.58 | 0.23 | 99,99,99,99                 | 0     |
| 55  | MG   | CA    | 1732 | 1/1   | 0.58 | 0.30 | 105,105,105,105             | 0     |
| 55  | MG   | AA    | 1682 | 1/1   | 0.58 | 0.18 | 93,93,93,93                 | 0     |
| 55  | MG   | AA    | 1648 | 1/1   | 0.58 | 0.21 | 115,115,115,115             | 0     |
| 55  | MG   | CA    | 1788 | 1/1   | 0.58 | 0.25 | 132,132,132,132             | 0     |
| 55  | MG   | AA    | 1801 | 1/1   | 0.59 | 0.19 | 130,130,130,130             | 0     |
| 55  | MG   | CA    | 1736 | 1/1   | 0.59 | 0.14 | 143,143,143,143             | 0     |
| 55  | MG   | AG    | 302  | 1/1   | 0.59 | 0.28 | 109,109,109,109             | 0     |
| 55  | MG   | DA    | 3365 | 1/1   | 0.59 | 0.11 | 112,112,112,112             | 0     |
| 55  | MG   | BA    | 3122 | 1/1   | 0.59 | 0.27 | 106,106,106,106             | 0     |
| 55  | MG   | BA    | 3163 | 1/1   | 0.59 | 0.34 | 86,86,86,86                 | 0     |
| 55  | MG   | AA    | 1781 | 1/1   | 0.59 | 0.29 | 87,87,87,87                 | 0     |
| 55  | MG   | CA    | 1707 | 1/1   | 0.59 | 0.26 | 109,109,109,109             | 0     |
| 55  | MG   | AA    | 1722 | 1/1   | -    | -    | 62,62,62,62                 | 1     |
| 55  | MG   | DA    | 3465 | 1/1   | 0.60 | 0.24 | 112,112,112,112             | 0     |
| 55  | MG   | BA    | 3563 | 1/1   | 0.60 | 0.28 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3398 | 1/1   | 0.60 | 0.27 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3040 | 1/1   | 0.60 | 0.21 | 118,118,118,118             | 0     |
| 55  | MG   | BA    | 3472 | 1/1   | 0.60 | 0.58 | 133,133,133,133             | 0     |
| 55  | MG   | DA    | 3238 | 1/1   | 0.60 | 0.29 | 105,105,105,105             | 0     |
| 55  | MG   | AA    | 1778 | 1/1   | 0.61 | 0.18 | 143,143,143,143             | 0     |
| 55  | MG   | DA    | 3359 | 1/1   | 0.61 | 0.25 | 111,111,111,111             | 0     |
| 55  | MG   | AA    | 1713 | 1/1   | 0.61 | 0.20 | 98,98,98,98                 | 0     |
| 55  | MG   | DA    | 3227 | 1/1   | 0.61 | 0.21 | 118,118,118,118             | 0     |
| 55  | MG   | DB    | 218  | 1/1   | 0.61 | 0.19 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1700 | 1/1   | 0.61 | 0.17 | 136,136,136,136             | 0     |
| 55  | MG   | DA    | 3445 | 1/1   | 0.61 | 0.34 | 118,118,118,118             | 0     |
| 55  | MG   | AA    | 1818 | 1/1   | 0.62 | 0.26 | 124,124,124,124             | 0     |
| 55  | MG   | AA    | 1782 | 1/1   | 0.62 | 0.26 | 118,118,118,118             | 0     |
| 55  | MG   | AA    | 1775 | 1/1   | 0.62 | 0.23 | 129,129,129,129             | 0     |
| 55  | MG   | B6    | 101  | 1/1   | 0.62 | 0.22 | 102,102,102,102             | 0     |
| 55  | MG   | BA    | 3271 | 1/1   | 0.62 | 0.36 | 92,92,92,92                 | 0     |
| 55  | MG   | DB    | 217  | 1/1   | 0.62 | 0.36 | 97,97,97,97                 | 0     |
| 55  | MG   | DA    | 3278 | 1/1   | 0.62 | 0.30 | 100,100,100,100             | 0     |
| 55  | MG   | BA    | 3568 | 1/1   | 0.62 | 0.26 | 106,106,106,106             | 0     |
| 55  | MG   | DA    | 3399 | 1/1   | 0.62 | 0.15 | 117,117,117,117             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3514 | 1/1   | 0.63 | 0.26 | 113,113,113,113             | 0     |
| 55  | MG   | CA    | 1758 | 1/1   | 0.63 | 0.28 | 107,107,107,107             | 0     |
| 55  | MG   | DA    | 3478 | 1/1   | 0.63 | 0.17 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1637 | 1/1   | 0.63 | 0.22 | 112,112,112,112             | 0     |
| 55  | MG   | DA    | 3350 | 1/1   | 0.63 | 0.32 | 120,120,120,120             | 0     |
| 55  | MG   | DA    | 3166 | 1/1   | 0.63 | 0.37 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1790 | 1/1   | 0.63 | 0.17 | 142,142,142,142             | 0     |
| 55  | MG   | AA    | 1784 | 1/1   | 0.63 | 0.30 | 112,112,112,112             | 0     |
| 55  | MG   | DA    | 3394 | 1/1   | 0.63 | 0.30 | 101,101,101,101             | 0     |
| 55  | MG   | BA    | 3270 | 1/1   | 0.63 | 0.45 | 96,96,96,96                 | 0     |
| 55  | MG   | BA    | 3335 | 1/1   | 0.64 | 0.17 | 102,102,102,102             | 0     |
| 55  | MG   | BA    | 3069 | 1/1   | 0.64 | 0.14 | 93,93,93,93                 | 0     |
| 55  | MG   | DA    | 3100 | 1/1   | 0.64 | 0.30 | 116,116,116,116             | 0     |
| 55  | MG   | DA    | 3423 | 1/1   | 0.64 | 0.17 | 118,118,118,118             | 0     |
| 55  | MG   | DA    | 3382 | 1/1   | 0.64 | 0.13 | 121,121,121,121             | 0     |
| 55  | MG   | CA    | 1809 | 1/1   | 0.64 | 0.28 | 93,93,93,93                 | 0     |
| 55  | MG   | CA    | 1708 | 1/1   | 0.64 | 0.16 | 124,124,124,124             | 0     |
| 55  | MG   | DA    | 3323 | 1/1   | 0.64 | 0.24 | 104,104,104,104             | 0     |
| 55  | MG   | CA    | 1729 | 1/1   | 0.64 | 0.41 | 102,102,102,102             | 0     |
| 55  | MG   | DB    | 211  | 1/1   | 0.64 | 0.20 | 111,111,111,111             | 0     |
| 55  | MG   | AA    | 1696 | 1/1   | 0.64 | 0.26 | 112,112,112,112             | 0     |
| 55  | MG   | CB    | 102  | 1/1   | 0.64 | 0.34 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3212 | 1/1   | 0.64 | 0.25 | 121,121,121,121             | 0     |
| 55  | MG   | BA    | 3443 | 1/1   | 0.64 | 0.14 | 125,125,125,125             | 0     |
| 55  | MG   | BA    | 3386 | 1/1   | 0.64 | 0.18 | 115,115,115,115             | 0     |
| 55  | MG   | CA    | 1740 | 1/1   | 0.64 | 0.23 | 122,122,122,122             | 0     |
| 55  | MG   | DA    | 3206 | 1/1   | 0.65 | 0.29 | 109,109,109,109             | 0     |
| 55  | MG   | AA    | 1788 | 1/1   | 0.65 | 0.23 | 98,98,98,98                 | 0     |
| 55  | MG   | DA    | 3308 | 1/1   | 0.65 | 0.24 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 3513 | 1/1   | 0.65 | 0.23 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3373 | 1/1   | 0.65 | 0.40 | 92,92,92,92                 | 0     |
| 55  | MG   | CA    | 1610 | 1/1   | 0.65 | 0.16 | 118,118,118,118             | 0     |
| 55  | MG   | DA    | 3402 | 1/1   | 0.65 | 0.14 | 124,124,124,124             | 0     |
| 55  | MG   | DA    | 3039 | 1/1   | 0.65 | 0.21 | 101,101,101,101             | 0     |
| 55  | MG   | AA    | 1799 | 1/1   | 0.65 | 0.23 | 101,101,101,101             | 0     |
| 55  | MG   | CA    | 1629 | 1/1   | 0.66 | 0.22 | 115,115,115,115             | 0     |
| 55  | MG   | AB    | 104  | 1/1   | 0.66 | 0.22 | 97,97,97,97                 | 0     |
| 55  | MG   | AC    | 102  | 1/1   | 0.66 | 0.37 | 106,106,106,106             | 0     |
| 55  | MG   | AA    | 1795 | 1/1   | 0.66 | 0.25 | 113,113,113,113             | 0     |
| 55  | MG   | AA    | 1687 | 1/1   | 0.66 | 0.19 | 108,108,108,108             | 0     |
| 55  | MG   | BA    | 3445 | 1/1   | 0.66 | 0.27 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3414 | 1/1   | 0.66 | 0.28 | 100,100,100,100             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | CA    | 1710 | 1/1   | 0.67 | 0.27 | 118,118,118,118             | 0     |
| 55  | MG   | DA    | 3448 | 1/1   | 0.67 | 0.24 | 129,129,129,129             | 0     |
| 55  | MG   | AA    | 1678 | 1/1   | 0.67 | 0.26 | 115,115,115,115             | 0     |
| 55  | MG   | CA    | 1673 | 1/1   | 0.67 | 0.26 | 136,136,136,136             | 0     |
| 55  | MG   | CA    | 1815 | 1/1   | 0.67 | 0.12 | 95,95,95,95                 | 0     |
| 55  | MG   | AA    | 1736 | 1/1   | 0.67 | 0.32 | 108,108,108,108             | 0     |
| 55  | MG   | AA    | 1631 | 1/1   | 0.67 | 0.21 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3449 | 1/1   | 0.67 | 0.29 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3239 | 1/1   | 0.67 | 0.43 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3125 | 1/1   | 0.67 | 0.30 | 107,107,107,107             | 0     |
| 55  | MG   | DA    | 3426 | 1/1   | 0.67 | 0.38 | 103,103,103,103             | 0     |
| 55  | MG   | AA    | 1724 | 1/1   | 0.67 | 0.16 | 78,78,78,78                 | 0     |
| 55  | MG   | BB    | 217  | 1/1   | 0.68 | 0.18 | 104,104,104,104             | 0     |
| 55  | MG   | CA    | 1687 | 1/1   | 0.68 | 0.14 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 3391 | 1/1   | 0.68 | 0.26 | 112,112,112,112             | 0     |
| 55  | MG   | AA    | 1621 | 1/1   | 0.68 | 0.26 | 102,102,102,102             | 0     |
| 55  | MG   | CA    | 1765 | 1/1   | 0.68 | 0.29 | 115,115,115,115             | 0     |
| 55  | MG   | AA    | 1815 | 1/1   | 0.68 | 0.34 | 114,114,114,114             | 0     |
| 55  | MG   | CA    | 1767 | 1/1   | 0.68 | 0.31 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3324 | 1/1   | 0.68 | 0.33 | 105,105,105,105             | 0     |
| 55  | MG   | AA    | 1680 | 1/1   | 0.68 | 0.39 | 97,97,97,97                 | 0     |
| 55  | MG   | AA    | 1780 | 1/1   | 0.68 | 0.39 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3352 | 1/1   | 0.68 | 0.33 | 122,122,122,122             | 0     |
| 55  | MG   | CA    | 1653 | 1/1   | 0.68 | 0.16 | 97,97,97,97                 | 0     |
| 55  | MG   | AA    | 1728 | 1/1   | 0.68 | 0.32 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 3082 | 1/1   | 0.68 | 0.09 | 100,100,100,100             | 0     |
| 55  | MG   | CC    | 109  | 1/1   | 0.68 | 0.30 | 114,114,114,114             | 0     |
| 55  | MG   | AA    | 1762 | 1/1   | 0.68 | 0.17 | 121,121,121,121             | 0     |
| 55  | MG   | AA    | 1777 | 1/1   | 0.69 | 0.41 | 115,115,115,115             | 0     |
| 55  | MG   | CC    | 103  | 1/1   | 0.69 | 0.20 | 114,114,114,114             | 0     |
| 55  | MG   | DA    | 3336 | 1/1   | 0.69 | 0.10 | 115,115,115,115             | 0     |
| 55  | MG   | AC    | 106  | 1/1   | 0.69 | 0.35 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3393 | 1/1   | 0.69 | 0.14 | 116,116,116,116             | 0     |
| 55  | MG   | DA    | 3446 | 1/1   | 0.69 | 0.24 | 166,166,166,166             | 0     |
| 55  | MG   | BA    | 3252 | 1/1   | 0.69 | 0.17 | 107,107,107,107             | 0     |
| 55  | MG   | BA    | 3425 | 1/1   | 0.69 | 0.20 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3467 | 1/1   | 0.69 | 0.15 | 103,103,103,103             | 0     |
| 55  | MG   | CA    | 1618 | 1/1   | 0.69 | 0.22 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3480 | 1/1   | 0.69 | 0.27 | 109,109,109,109             | 0     |
| 55  | MG   | BA    | 3462 | 1/1   | 0.69 | 0.34 | 116,116,116,116             | 0     |
| 55  | MG   | DA    | 3404 | 1/1   | 0.69 | 0.21 | 119,119,119,119             | 0     |
| 55  | MG   | AA    | 1726 | 1/1   | 0.69 | 0.38 | 94,94,94,94                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3432 | 1/1   | 0.69 | 0.12 | 106,106,106,106             | 0     |
| 55  | MG   | DA    | 3264 | 1/1   | 0.69 | 0.39 | 88,88,88,88                 | 0     |
| 55  | MG   | CB    | 101  | 1/1   | 0.69 | 0.17 | 106,106,106,106             | 0     |
| 55  | MG   | BA    | 3348 | 1/1   | 0.69 | 0.16 | 96,96,96,96                 | 0     |
| 55  | MG   | AA    | 1756 | 1/1   | 0.69 | 0.24 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3309 | 1/1   | 0.70 | 0.34 | 116,116,116,116             | 0     |
| 55  | MG   | AA    | 1751 | 1/1   | 0.70 | 0.45 | 105,105,105,105             | 0     |
| 55  | MG   | AA    | 1625 | 1/1   | 0.70 | 0.27 | 68,68,68,68                 | 0     |
| 55  | MG   | CA    | 1803 | 1/1   | 0.70 | 0.19 | 103,103,103,103             | 0     |
| 55  | MG   | BE    | 303  | 1/1   | 0.70 | 0.27 | 105,105,105,105             | 0     |
| 55  | MG   | BA    | 3331 | 1/1   | 0.70 | 0.25 | 106,106,106,106             | 0     |
| 55  | MG   | AA    | 1690 | 1/1   | 0.70 | 0.13 | 98,98,98,98                 | 0     |
| 55  | MG   | A1    | 101  | 1/1   | 0.70 | 0.30 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3356 | 1/1   | 0.70 | 0.27 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3053 | 1/1   | 0.70 | 0.15 | 106,106,106,106             | 0     |
| 55  | MG   | DB    | 210  | 1/1   | 0.70 | 0.17 | 128,128,128,128             | 0     |
| 55  | MG   | CA    | 1814 | 1/1   | 0.70 | 0.28 | 83,83,83,83                 | 0     |
| 55  | MG   | BB    | 207  | 1/1   | 0.70 | 0.23 | 109,109,109,109             | 0     |
| 55  | MG   | DA    | 3263 | 1/1   | 0.70 | 0.22 | 96,96,96,96                 | 0     |
| 55  | MG   | DB    | 216  | 1/1   | 0.70 | 0.25 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3125 | 1/1   | 0.70 | 0.51 | 74,74,74,74                 | 0     |
| 55  | MG   | CA    | 1817 | 1/1   | 0.70 | 0.19 | 106,106,106,106             | 0     |
| 55  | MG   | BA    | 3358 | 1/1   | 0.70 | 0.27 | 98,98,98,98                 | 0     |
| 55  | MG   | BA    | 3066 | 1/1   | 0.70 | 0.17 | 99,99,99,99                 | 0     |
| 55  | MG   | DO    | 201  | 1/1   | 0.70 | 0.28 | 98,98,98,98                 | 0     |
| 55  | MG   | CA    | 1677 | 1/1   | 0.71 | 0.26 | 107,107,107,107             | 0     |
| 55  | MG   | DA    | 3307 | 1/1   | 0.71 | 0.28 | 99,99,99,99                 | 0     |
| 55  | MG   | DA    | 3451 | 1/1   | 0.71 | 0.31 | 92,92,92,92                 | 0     |
| 55  | MG   | AA    | 1643 | 1/1   | 0.71 | 0.53 | 127,127,127,127             | 0     |
| 55  | MG   | BA    | 3437 | 1/1   | 0.71 | 0.28 | 97,97,97,97                 | 0     |
| 55  | MG   | AA    | 1779 | 1/1   | 0.71 | 0.12 | 119,119,119,119             | 0     |
| 55  | MG   | CA    | 1777 | 1/1   | 0.71 | 0.22 | 112,112,112,112             | 0     |
| 55  | MG   | AA    | 1688 | 1/1   | 0.71 | 0.20 | 93,93,93,93                 | 0     |
| 55  | MG   | DA    | 3225 | 1/1   | 0.71 | 0.40 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3192 | 1/1   | 0.72 | 0.21 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3087 | 1/1   | 0.72 | 0.33 | 85,85,85,85                 | 0     |
| 55  | MG   | CA    | 1786 | 1/1   | 0.72 | 0.24 | 111,111,111,111             | 0     |
| 55  | MG   | CA    | 1733 | 1/1   | 0.72 | 0.41 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3400 | 1/1   | 0.72 | 0.23 | 115,115,115,115             | 0     |
| 55  | MG   | DA    | 3134 | 1/1   | 0.72 | 0.20 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3510 | 1/1   | 0.72 | 0.34 | 108,108,108,108             | 0     |
| 55  | MG   | BA    | 3290 | 1/1   | 0.72 | 0.23 | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3353 | 1/1   | 0.72 | 0.29 | 102,102,102,102             | 0     |
| 55  | MG   | BA    | 3487 | 1/1   | 0.72 | 0.29 | 100,100,100,100             | 0     |
| 55  | MG   | BA    | 3242 | 1/1   | 0.72 | 0.09 | 116,116,116,116             | 0     |
| 55  | MG   | DA    | 3392 | 1/1   | 0.72 | 0.22 | 126,126,126,126             | 0     |
| 55  | MG   | DA    | 3486 | 1/1   | 0.73 | 0.24 | 101,101,101,101             | 0     |
| 55  | MG   | DB    | 204  | 1/1   | 0.73 | 0.27 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3284 | 1/1   | 0.73 | 0.16 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3299 | 1/1   | 0.73 | 0.22 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3403 | 1/1   | 0.73 | 0.57 | 107,107,107,107             | 0     |
| 55  | MG   | CA    | 1688 | 1/1   | 0.73 | 0.33 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3024 | 1/1   | 0.73 | 0.34 | 104,104,104,104             | 0     |
| 55  | MG   | BA    | 3380 | 1/1   | 0.73 | 0.26 | 98,98,98,98                 | 0     |
| 55  | MG   | DA    | 3258 | 1/1   | 0.73 | 0.20 | 87,87,87,87                 | 0     |
| 55  | MG   | CA    | 1804 | 1/1   | 0.73 | 0.25 | 108,108,108,108             | 0     |
| 55  | MG   | AA    | 1767 | 1/1   | 0.73 | 0.25 | 116,116,116,116             | 0     |
| 55  | MG   | B2    | 201  | 1/1   | 0.73 | 0.34 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3396 | 1/1   | 0.73 | 0.32 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3121 | 1/1   | 0.74 | 0.12 | 104,104,104,104             | 0     |
| 55  | MG   | CA    | 1702 | 1/1   | 0.74 | 0.19 | 106,106,106,106             | 0     |
| 55  | MG   | DA    | 3444 | 1/1   | 0.74 | 0.27 | 109,109,109,109             | 0     |
| 55  | MG   | AR    | 101  | 1/1   | 0.74 | 0.15 | 114,114,114,114             | 0     |
| 55  | MG   | DA    | 3287 | 1/1   | 0.74 | 0.13 | 120,120,120,120             | 0     |
| 55  | MG   | AB    | 101  | 1/1   | 0.74 | 0.12 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3544 | 1/1   | 0.74 | 0.31 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3448 | 1/1   | 0.74 | 0.24 | 104,104,104,104             | 0     |
| 55  | MG   | CA    | 1731 | 1/1   | 0.74 | 0.37 | 97,97,97,97                 | 0     |
| 55  | MG   | CK    | 201  | 1/1   | 0.74 | 0.14 | 124,124,124,124             | 0     |
| 55  | MG   | BA    | 3338 | 1/1   | 0.74 | 0.32 | 91,91,91,91                 | 0     |
| 55  | MG   | AA    | 1727 | 1/1   | 0.74 | 0.19 | 95,95,95,95                 | 0     |
| 55  | MG   | AA    | 1741 | 1/1   | 0.74 | 0.19 | 98,98,98,98                 | 0     |
| 55  | MG   | DA    | 3346 | 1/1   | 0.74 | 0.26 | 102,102,102,102             | 0     |
| 55  | MG   | AA    | 1704 | 1/1   | 0.74 | 0.20 | 110,110,110,110             | 0     |
| 55  | MG   | BA    | 3121 | 1/1   | 0.74 | 0.31 | 72,72,72,72                 | 0     |
| 55  | MG   | CA    | 1742 | 1/1   | 0.74 | 0.20 | 108,108,108,108             | 0     |
| 55  | MG   | BB    | 210  | 1/1   | 0.74 | 0.19 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 1633 | 1/1   | 0.74 | 0.52 | 102,102,102,102             | 0     |
| 55  | MG   | AA    | 1804 | 1/1   | 0.74 | 0.48 | 113,113,113,113             | 0     |
| 55  | MG   | AA    | 1735 | 1/1   | 0.74 | 0.12 | 102,102,102,102             | 0     |
| 55  | MG   | CA    | 1763 | 1/1   | 0.74 | 0.23 | 100,100,100,100             | 0     |
| 55  | MG   | BA    | 3178 | 1/1   | 0.74 | 0.17 | 96,96,96,96                 | 0     |
| 55  | MG   | BA    | 3181 | 1/1   | 0.74 | 0.28 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3243 | 1/1   | 0.75 | 0.41 | 97,97,97,97                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3246 | 1/1   | 0.75 | 0.33 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1636 | 1/1   | 0.75 | 0.35 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3195 | 1/1   | 0.75 | 0.17 | 97,97,97,97                 | 0     |
| 55  | MG   | CA    | 1792 | 1/1   | 0.75 | 0.16 | 104,104,104,104             | 0     |
| 55  | MG   | BA    | 3257 | 1/1   | 0.75 | 0.28 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3424 | 1/1   | 0.75 | 0.42 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3334 | 1/1   | 0.75 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | BA    | 3262 | 1/1   | 0.75 | 0.27 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3037 | 1/1   | 0.75 | 0.35 | 105,105,105,105             | 0     |
| 55  | MG   | CA    | 1738 | 1/1   | 0.75 | 0.24 | 113,113,113,113             | 0     |
| 55  | MG   | CA    | 1810 | 1/1   | 0.75 | 0.22 | 101,101,101,101             | 0     |
| 55  | MG   | AA    | 1796 | 1/1   | 0.75 | 0.30 | 102,102,102,102             | 0     |
| 55  | MG   | CA    | 1616 | 1/1   | 0.75 | 0.26 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3322 | 1/1   | 0.75 | 0.39 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 3438 | 1/1   | 0.75 | 0.33 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1621 | 1/1   | 0.75 | 0.29 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3289 | 1/1   | 0.75 | 0.27 | 95,95,95,95                 | 0     |
| 55  | MG   | AA    | 1749 | 1/1   | 0.75 | 0.37 | 110,110,110,110             | 0     |
| 55  | MG   | AA    | 1695 | 1/1   | 0.76 | 0.19 | 128,128,128,128             | 0     |
| 55  | MG   | DA    | 3319 | 1/1   | 0.76 | 0.17 | 95,95,95,95                 | 0     |
| 55  | MG   | AB    | 103  | 1/1   | 0.76 | 0.19 | 104,104,104,104             | 0     |
| 55  | MG   | DA    | 3468 | 1/1   | 0.76 | 0.28 | 101,101,101,101             | 0     |
| 55  | MG   | BA    | 3301 | 1/1   | 0.76 | 0.16 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1684 | 1/1   | 0.76 | 0.41 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3330 | 1/1   | 0.76 | 0.20 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3334 | 1/1   | 0.76 | 0.27 | 87,87,87,87                 | 0     |
| 55  | MG   | CA    | 1743 | 1/1   | 0.76 | 0.29 | 106,106,106,106             | 0     |
| 55  | MG   | BA    | 3098 | 1/1   | 0.76 | 0.29 | 88,88,88,88                 | 0     |
| 55  | MG   | AA    | 1797 | 1/1   | 0.76 | 0.18 | 79,79,79,79                 | 0     |
| 55  | MG   | CA    | 1791 | 1/1   | 0.76 | 0.28 | 80,80,80,80                 | 0     |
| 55  | MG   | CC    | 105  | 1/1   | 0.76 | 0.18 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3296 | 1/1   | 0.76 | 0.16 | 93,93,93,93                 | 0     |
| 55  | MG   | DA    | 3443 | 1/1   | 0.76 | 0.25 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3397 | 1/1   | 0.76 | 0.20 | 105,105,105,105             | 0     |
| 55  | MG   | CC    | 107  | 1/1   | 0.76 | 0.19 | 123,123,123,123             | 0     |
| 55  | MG   | BA    | 3400 | 1/1   | 0.76 | 0.24 | 108,108,108,108             | 0     |
| 55  | MG   | BA    | 3556 | 1/1   | 0.76 | 0.30 | 98,98,98,98                 | 0     |
| 55  | MG   | D1    | 201  | 1/1   | 0.76 | 0.12 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1638 | 1/1   | 0.77 | 0.27 | 105,105,105,105             | 0     |
| 55  | MG   | BA    | 3234 | 1/1   | 0.77 | 0.34 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1723 | 1/1   | 0.77 | 0.17 | 93,93,93,93                 | 0     |
| 55  | MG   | CR    | 101  | 1/1   | 0.77 | 0.11 | 135,135,135,135             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3370 | 1/1   | 0.77 | 0.47 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3187 | 1/1   | 0.77 | 0.28 | 101,101,101,101             | 0     |
| 55  | MG   | BA    | 3079 | 1/1   | 0.77 | 0.20 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3189 | 1/1   | 0.77 | 0.14 | 86,86,86,86                 | 0     |
| 55  | MG   | BA    | 3404 | 1/1   | 0.77 | 0.36 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3460 | 1/1   | 0.77 | 0.31 | 116,116,116,116             | 0     |
| 55  | MG   | DA    | 3462 | 1/1   | 0.77 | 0.21 | 98,98,98,98                 | 0     |
| 55  | MG   | AD    | 103  | 1/1   | 0.77 | 0.15 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3311 | 1/1   | 0.77 | 0.36 | 109,109,109,109             | 0     |
| 55  | MG   | BA    | 3410 | 1/1   | 0.77 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3477 | 1/1   | 0.77 | 0.34 | 88,88,88,88                 | 0     |
| 55  | MG   | AA    | 1624 | 1/1   | 0.77 | 0.24 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3479 | 1/1   | 0.77 | 0.18 | 97,97,97,97                 | 0     |
| 55  | MG   | DA    | 3217 | 1/1   | 0.77 | 0.14 | 125,125,125,125             | 0     |
| 55  | MG   | DA    | 3484 | 1/1   | 0.77 | 0.25 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1762 | 1/1   | 0.77 | 0.10 | 108,108,108,108             | 0     |
| 55  | MG   | DA    | 3327 | 1/1   | 0.77 | 0.12 | 93,93,93,93                 | 0     |
| 55  | MG   | CA    | 1797 | 1/1   | 0.77 | 0.30 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3540 | 1/1   | 0.77 | 0.40 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3259 | 1/1   | 0.77 | 0.07 | 109,109,109,109             | 0     |
| 55  | MG   | BA    | 3382 | 1/1   | 0.77 | 0.48 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3421 | 1/1   | 0.77 | 0.12 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3461 | 1/1   | 0.77 | 0.26 | 98,98,98,98                 | 0     |
| 55  | MG   | AA    | 1629 | 1/1   | 0.77 | 0.17 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3464 | 1/1   | 0.77 | 0.18 | 91,91,91,91                 | 0     |
| 55  | MG   | BB    | 201  | 1/1   | 0.77 | 0.25 | 97,97,97,97                 | 0     |
| 55  | MG   | CA    | 1661 | 1/1   | 0.77 | 0.25 | 92,92,92,92                 | 0     |
| 55  | MG   | AA    | 1803 | 1/1   | 0.77 | 0.28 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3360 | 1/1   | 0.77 | 0.19 | 97,97,97,97                 | 0     |
| 55  | MG   | AA    | 1706 | 1/1   | 0.78 | 0.17 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3251 | 1/1   | 0.78 | 0.35 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3191 | 1/1   | 0.78 | 0.13 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3358 | 1/1   | 0.78 | 0.45 | 90,90,90,90                 | 0     |
| 55  | MG   | AA    | 1711 | 1/1   | 0.78 | 0.18 | 97,97,97,97                 | 0     |
| 55  | MG   | CA    | 1625 | 1/1   | 0.78 | 0.20 | 104,104,104,104             | 0     |
| 55  | MG   | DA    | 3273 | 1/1   | 0.78 | 0.15 | 77,77,77,77                 | 0     |
| 55  | MG   | CA    | 1711 | 1/1   | 0.78 | 0.35 | 101,101,101,101             | 0     |
| 55  | MG   | CA    | 1719 | 1/1   | 0.78 | 0.31 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3565 | 1/1   | 0.78 | 0.33 | 105,105,105,105             | 0     |
| 55  | MG   | BA    | 3065 | 1/1   | 0.78 | 0.27 | 82,82,82,82                 | 0     |
| 55  | MG   | DA    | 3288 | 1/1   | 0.78 | 0.14 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3290 | 1/1   | 0.78 | 0.33 | 99,99,99,99                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3374 | 1/1   | 0.78 | 0.15 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3276 | 1/1   | 0.78 | 0.10 | 92,92,92,92                 | 0     |
| 55  | MG   | CA    | 1648 | 1/1   | 0.78 | 0.32 | 113,113,113,113             | 0     |
| 55  | MG   | BA    | 3483 | 1/1   | 0.78 | 0.16 | 120,120,120,120             | 0     |
| 55  | MG   | AA    | 1743 | 1/1   | 0.78 | 0.14 | 107,107,107,107             | 0     |
| 55  | MG   | DA    | 3390 | 1/1   | 0.78 | 0.23 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3224 | 1/1   | 0.78 | 0.29 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3495 | 1/1   | 0.78 | 0.37 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3126 | 1/1   | 0.78 | 0.49 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3209 | 1/1   | 0.78 | 0.36 | 96,96,96,96                 | 0     |
| 55  | MG   | BA    | 3128 | 1/1   | 0.78 | 0.27 | 71,71,71,71                 | 0     |
| 55  | MG   | AA    | 1747 | 1/1   | 0.78 | 0.21 | 98,98,98,98                 | 0     |
| 55  | MG   | AA    | 1725 | 1/1   | 0.78 | 0.26 | 100,100,100,100             | 0     |
| 55  | MG   | CC    | 108  | 1/1   | 0.78 | 0.20 | 95,95,95,95                 | 0     |
| 55  | MG   | CA    | 1685 | 1/1   | 0.78 | 0.33 | 91,91,91,91                 | 0     |
| 55  | MG   | B3    | 102  | 1/1   | 0.78 | 0.19 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1649 | 1/1   | 0.78 | 0.24 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3344 | 1/1   | 0.78 | 0.17 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3029 | 1/1   | 0.78 | 0.30 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3427 | 1/1   | 0.78 | 0.35 | 97,97,97,97                 | 0     |
| 55  | MG   | CA    | 1807 | 1/1   | 0.78 | 0.27 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3412 | 1/1   | 0.78 | 0.35 | 92,92,92,92                 | 0     |
| 55  | MG   | D5    | 102  | 1/1   | 0.78 | 0.16 | 104,104,104,104             | 0     |
| 55  | MG   | BA    | 3285 | 1/1   | 0.79 | 0.23 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3420 | 1/1   | 0.79 | 0.17 | 108,108,108,108             | 0     |
| 55  | MG   | BA    | 3355 | 1/1   | 0.79 | 0.31 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3452 | 1/1   | 0.79 | 0.24 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3270 | 1/1   | 0.79 | 0.49 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3547 | 1/1   | 0.79 | 0.35 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3133 | 1/1   | 0.79 | 0.29 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3453 | 1/1   | 0.79 | 0.20 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3281 | 1/1   | 0.79 | 0.32 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3148 | 1/1   | 0.79 | 0.14 | 111,111,111,111             | 0     |
| 55  | MG   | AA    | 1615 | 1/1   | 0.79 | 0.24 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1716 | 1/1   | 0.79 | 0.40 | 103,103,103,103             | 0     |
| 55  | MG   | BA    | 3369 | 1/1   | 0.79 | 0.20 | 92,92,92,92                 | 0     |
| 55  | MG   | CA    | 1722 | 1/1   | 0.79 | 0.32 | 106,106,106,106             | 0     |
| 55  | MG   | AA    | 1733 | 1/1   | 0.79 | 0.20 | 101,101,101,101             | 0     |
| 55  | MG   | CA    | 1645 | 1/1   | 0.79 | 0.33 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3198 | 1/1   | 0.79 | 0.24 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3305 | 1/1   | 0.79 | 0.36 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3310 | 1/1   | 0.79 | 0.54 | 105,105,105,105             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3205 | 1/1   | 0.79 | 0.29 | 110,110,110,110             | 0     |
| 55  | MG   | DA    | 3482 | 1/1   | 0.79 | 0.33 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3318 | 1/1   | 0.79 | 0.28 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3426 | 1/1   | 0.79 | 0.30 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3320 | 1/1   | 0.79 | 0.48 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3314 | 1/1   | 0.79 | 0.28 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1786 | 1/1   | 0.79 | 0.12 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1689 | 1/1   | 0.79 | 0.23 | 107,107,107,107             | 0     |
| 55  | MG   | BA    | 3043 | 1/1   | 0.79 | 0.26 | 78,78,78,78                 | 0     |
| 55  | MG   | CA    | 1681 | 1/1   | 0.79 | 0.33 | 89,89,89,89                 | 0     |
| 55  | MG   | BA    | 3333 | 1/1   | 0.79 | 0.31 | 80,80,80,80                 | 0     |
| 55  | MG   | AA    | 1630 | 1/1   | 0.79 | 0.29 | 112,112,112,112             | 0     |
| 55  | MG   | BA    | 3274 | 1/1   | 0.79 | 0.33 | 108,108,108,108             | 0     |
| 55  | MG   | CA    | 1759 | 1/1   | 0.79 | 0.25 | 99,99,99,99                 | 0     |
| 55  | MG   | AA    | 1814 | 1/1   | 0.79 | 0.13 | 107,107,107,107             | 0     |
| 55  | MG   | BA    | 3278 | 1/1   | 0.79 | 0.14 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3050 | 1/1   | 0.79 | 0.22 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3054 | 1/1   | 0.79 | 0.09 | 108,108,108,108             | 0     |
| 55  | MG   | CA    | 1617 | 1/1   | 0.80 | 0.40 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1787 | 1/1   | 0.80 | 0.25 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3442 | 1/1   | 0.80 | 0.30 | 98,98,98,98                 | 0     |
| 55  | MG   | BA    | 3482 | 1/1   | 0.80 | 0.22 | 82,82,82,82                 | 0     |
| 55  | MG   | CA    | 1746 | 1/1   | 0.80 | 0.17 | 87,87,87,87                 | 0     |
| 55  | MG   | CA    | 1747 | 1/1   | 0.80 | 0.34 | 109,109,109,109             | 0     |
| 55  | MG   | CA    | 1624 | 1/1   | 0.80 | 0.20 | 93,93,93,93                 | 0     |
| 55  | MG   | AA    | 1729 | 1/1   | 0.80 | 0.25 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3374 | 1/1   | 0.80 | 0.25 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3033 | 1/1   | 0.80 | 0.31 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3213 | 1/1   | 0.80 | 0.20 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3384 | 1/1   | 0.80 | 0.33 | 97,97,97,97                 | 0     |
| 55  | MG   | AG    | 301  | 1/1   | 0.80 | 0.24 | 98,98,98,98                 | 0     |
| 55  | MG   | DA    | 3034 | 1/1   | 0.80 | 0.30 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3473 | 1/1   | 0.80 | 0.19 | 56,56,56,56                 | 0     |
| 55  | MG   | AC    | 105  | 1/1   | 0.80 | 0.38 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3036 | 1/1   | 0.80 | 0.24 | 100,100,100,100             | 0     |
| 55  | MG   | BA    | 3045 | 1/1   | 0.80 | 0.48 | 105,105,105,105             | 0     |
| 55  | MG   | AA    | 1644 | 1/1   | 0.80 | 0.45 | 94,94,94,94                 | 0     |
| 55  | MG   | BA    | 3064 | 1/1   | 0.80 | 0.29 | 87,87,87,87                 | 0     |
| 55  | MG   | CA    | 1667 | 1/1   | 0.80 | 0.16 | 98,98,98,98                 | 0     |
| 55  | MG   | DA    | 3333 | 1/1   | 0.80 | 0.13 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3242 | 1/1   | 0.80 | 0.14 | 81,81,81,81                 | 0     |
| 55  | MG   | DB    | 208  | 1/1   | 0.80 | 0.09 | 99,99,99,99                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | CA    | 1671 | 1/1   | 0.80 | 0.23 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3339 | 1/1   | 0.80 | 0.43 | 104,104,104,104             | 0     |
| 55  | MG   | BA    | 3543 | 1/1   | 0.80 | 0.18 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3114 | 1/1   | 0.80 | 0.40 | 91,91,91,91                 | 0     |
| 55  | MG   | AA    | 1746 | 1/1   | 0.80 | 0.36 | 93,93,93,93                 | 0     |
| 55  | MG   | CA    | 1816 | 1/1   | 0.80 | 0.28 | 102,102,102,102             | 0     |
| 55  | MG   | AA    | 1732 | 1/1   | 0.80 | 0.29 | 95,95,95,95                 | 0     |
| 55  | MG   | CA    | 1676 | 1/1   | 0.80 | 0.35 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3250 | 1/1   | 0.80 | 0.24 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3163 | 1/1   | 0.80 | 0.36 | 75,75,75,75                 | 0     |
| 55  | MG   | CA    | 1780 | 1/1   | 0.80 | 0.24 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3295 | 1/1   | 0.80 | 0.21 | 92,92,92,92                 | 0     |
| 55  | MG   | AB    | 102  | 1/1   | 0.80 | 0.35 | 96,96,96,96                 | 0     |
| 55  | MG   | CA    | 1696 | 1/1   | 0.81 | 0.17 | 104,104,104,104             | 0     |
| 55  | MG   | DA    | 3314 | 1/1   | 0.81 | 0.27 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3422 | 1/1   | 0.81 | 0.22 | 110,110,110,110             | 0     |
| 55  | MG   | CA    | 1704 | 1/1   | 0.81 | 0.33 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3458 | 1/1   | 0.81 | 0.42 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3350 | 1/1   | 0.81 | 0.39 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3074 | 1/1   | 0.81 | 0.17 | 91,91,91,91                 | 0     |
| 55  | MG   | CA    | 1640 | 1/1   | 0.81 | 0.48 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3079 | 1/1   | 0.81 | 0.17 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3082 | 1/1   | 0.81 | 0.32 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3489 | 1/1   | 0.81 | 0.30 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3474 | 1/1   | 0.81 | 0.29 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3061 | 1/1   | 0.81 | 0.34 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3081 | 1/1   | 0.81 | 0.10 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3428 | 1/1   | 0.81 | 0.27 | 91,91,91,91                 | 0     |
| 55  | MG   | BB    | 218  | 1/1   | 0.81 | 0.22 | 98,98,98,98                 | 0     |
| 55  | MG   | CA    | 1669 | 1/1   | 0.81 | 0.36 | 85,85,85,85                 | 0     |
| 55  | MG   | AA    | 1737 | 1/1   | 0.81 | 0.20 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 1816 | 1/1   | 0.81 | 0.25 | 95,95,95,95                 | 0     |
| 55  | MG   | BO    | 202  | 1/1   | 0.81 | 0.26 | 98,98,98,98                 | 0     |
| 55  | MG   | DB    | 207  | 1/1   | 0.81 | 0.27 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3218 | 1/1   | 0.81 | 0.24 | 64,64,64,64                 | 0     |
| 55  | MG   | CA    | 1784 | 1/1   | 0.81 | 0.13 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3176 | 1/1   | 0.81 | 0.07 | 105,105,105,105             | 0     |
| 55  | MG   | BA    | 3467 | 1/1   | 0.81 | 0.22 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 1709 | 1/1   | 0.81 | 0.21 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3299 | 1/1   | 0.81 | 0.27 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3473 | 1/1   | 0.81 | 0.24 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3440 | 1/1   | 0.81 | 0.51 | 96,96,96,96                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3562 | 1/1   | 0.81 | 0.13 | 91,91,91,91                 | 0     |
| 55  | MG   | DB    | 219  | 1/1   | 0.81 | 0.17 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3199 | 1/1   | 0.81 | 0.16 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3225 | 1/1   | 0.81 | 0.27 | 68,68,68,68                 | 0     |
| 55  | MG   | AA    | 1808 | 1/1   | 0.81 | 0.31 | 88,88,88,88                 | 0     |
| 55  | MG   | CA    | 1755 | 1/1   | 0.81 | 0.46 | 104,104,104,104             | 0     |
| 55  | MG   | BA    | 3567 | 1/1   | 0.81 | 0.26 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 3371 | 1/1   | 0.82 | 0.33 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3185 | 1/1   | 0.82 | 0.15 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3291 | 1/1   | -    | -    | 56,56,56,56                 | 1     |
| 55  | MG   | BA    | 3564 | 1/1   | 0.82 | 0.22 | 112,112,112,112             | 0     |
| 55  | MG   | BA    | 3481 | 1/1   | 0.82 | 0.23 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3095 | 1/1   | 0.82 | 0.25 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3298 | 1/1   | 0.82 | 0.28 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3041 | 1/1   | 0.82 | 0.26 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3304 | 1/1   | 0.82 | 0.21 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3373 | 1/1   | 0.82 | 0.41 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3021 | 1/1   | 0.82 | 0.31 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3183 | 1/1   | 0.82 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1751 | 1/1   | 0.82 | 0.25 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1753 | 1/1   | 0.82 | 0.15 | 103,103,103,103             | 0     |
| 55  | MG   | AS    | 101  | 1/1   | 0.82 | 0.34 | 96,96,96,96                 | 0     |
| 55  | MG   | DA    | 3387 | 1/1   | 0.82 | 0.21 | 102,102,102,102             | 0     |
| 55  | MG   | AA    | 1609 | 1/1   | 0.82 | 0.36 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3249 | 1/1   | 0.82 | 0.17 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3503 | 1/1   | 0.82 | 0.33 | 111,111,111,111             | 0     |
| 55  | MG   | BA    | 3455 | 1/1   | 0.82 | 0.15 | 89,89,89,89                 | 0     |
| 55  | MG   | BA    | 3390 | 1/1   | 0.82 | 0.28 | 98,98,98,98                 | 0     |
| 55  | MG   | CA    | 1713 | 1/1   | 0.82 | 0.22 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3458 | 1/1   | 0.82 | 0.24 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3312 | 1/1   | -    | -    | 62,62,62,62                 | 1     |
| 55  | MG   | AA    | 1699 | 1/1   | 0.82 | 0.19 | 99,99,99,99                 | 0     |
| 55  | MG   | AA    | 1655 | 1/1   | 0.82 | 0.32 | 78,78,78,78                 | 0     |
| 55  | MG   | CA    | 1726 | 1/1   | 0.82 | 0.22 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3253 | 1/1   | 0.82 | 0.45 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3335 | 1/1   | 0.82 | 0.18 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3062 | 1/1   | 0.82 | 0.19 | 79,79,79,79                 | 0     |
| 55  | MG   | AA    | 1670 | 1/1   | 0.82 | 0.29 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3357 | 1/1   | 0.82 | 0.27 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3252 | 1/1   | 0.82 | 0.21 | 99,99,99,99                 | 0     |
| 55  | MG   | CA    | 1735 | 1/1   | 0.82 | 0.22 | 119,119,119,119             | 0     |
| 55  | MG   | DA    | 3159 | 1/1   | 0.82 | 0.39 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | CA    | 1615 | 1/1   | 0.82 | 0.27 | 106,106,106,106             | 0     |
| 55  | MG   | DA    | 3165 | 1/1   | 0.82 | 0.43 | 73,73,73,73                 | 0     |
| 55  | MG   | CA    | 1680 | 1/1   | 0.82 | 0.22 | 99,99,99,99                 | 0     |
| 55  | MG   | DA    | 3168 | 1/1   | 0.82 | 0.35 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3176 | 1/1   | 0.82 | 0.21 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3267 | 1/1   | 0.82 | 0.29 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3256 | 1/1   | 0.83 | 0.25 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3248 | 1/1   | 0.83 | 0.24 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3464 | 1/1   | 0.83 | 0.37 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3102 | 1/1   | 0.83 | 0.24 | 72,72,72,72                 | 0     |
| 55  | MG   | CA    | 1650 | 1/1   | 0.83 | 0.22 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3351 | 1/1   | 0.83 | 0.22 | 88,88,88,88                 | 0     |
| 55  | MG   | CA    | 1656 | 1/1   | 0.83 | 0.33 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3511 | 1/1   | 0.83 | 0.15 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3476 | 1/1   | 0.83 | 0.22 | 104,104,104,104             | 0     |
| 55  | MG   | CA    | 1769 | 1/1   | 0.83 | 0.28 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3208 | 1/1   | 0.83 | 0.37 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3030 | 1/1   | 0.83 | 0.23 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3444 | 1/1   | 0.83 | 0.10 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3293 | 1/1   | 0.83 | 0.26 | 96,96,96,96                 | 0     |
| 55  | MG   | BA    | 3316 | 1/1   | 0.83 | 0.36 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3485 | 1/1   | 0.83 | 0.33 | 84,84,84,84                 | 0     |
| 55  | MG   | AA    | 1635 | 1/1   | 0.83 | 0.18 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3488 | 1/1   | 0.83 | 0.19 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3376 | 1/1   | 0.83 | 0.16 | 107,107,107,107             | 0     |
| 55  | MG   | DB    | 206  | 1/1   | 0.83 | 0.30 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3167 | 1/1   | 0.83 | 0.15 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3403 | 1/1   | 0.83 | 0.25 | 71,71,71,71                 | 0     |
| 55  | MG   | DA    | 3424 | 1/1   | 0.83 | 0.24 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1666 | 1/1   | 0.83 | 0.23 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3434 | 1/1   | 0.83 | 0.26 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3173 | 1/1   | 0.83 | 0.32 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3441 | 1/1   | 0.83 | 0.10 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3343 | 1/1   | 0.83 | 0.39 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3471 | 1/1   | 0.83 | 0.26 | 126,126,126,126             | 0     |
| 55  | MG   | DA    | 3389 | 1/1   | 0.83 | 0.31 | 97,97,97,97                 | 0     |
| 55  | MG   | CA    | 1644 | 1/1   | 0.83 | 0.14 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3391 | 1/1   | 0.83 | 0.31 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3306 | 1/1   | 0.83 | 0.37 | 96,96,96,96                 | 0     |
| 55  | MG   | CC    | 106  | 1/1   | 0.83 | 0.43 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3453 | 1/1   | 0.83 | 0.38 | 65,65,65,65                 | 0     |
| 55  | MG   | D3    | 101  | 1/1   | 0.83 | 0.19 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1611 | 1/1   | 0.83 | 0.26 | 94,94,94,94                 | 0     |
| 55  | MG   | BA    | 3306 | 1/1   | 0.84 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3200 | 1/1   | 0.84 | 0.24 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 1820 | 1/1   | 0.84 | 0.19 | 82,82,82,82                 | 0     |
| 55  | MG   | CA    | 1705 | 1/1   | 0.84 | 0.22 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3216 | 1/1   | 0.84 | 0.23 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3265 | 1/1   | 0.84 | 0.14 | 89,89,89,89                 | 0     |
| 55  | MG   | BA    | 3320 | 1/1   | 0.84 | 0.31 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3338 | 1/1   | 0.84 | 0.28 | 69,69,69,69                 | 0     |
| 55  | MG   | CA    | 1709 | 1/1   | 0.84 | 0.15 | 110,110,110,110             | 0     |
| 55  | MG   | DA    | 3340 | 1/1   | 0.84 | 0.25 | 75,75,75,75                 | 0     |
| 55  | MG   | AA    | 1614 | 1/1   | 0.84 | 0.29 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3329 | 1/1   | 0.84 | 0.47 | 67,67,67,67                 | 0     |
| 55  | MG   | CA    | 1782 | 1/1   | 0.84 | 0.15 | 113,113,113,113             | 0     |
| 55  | MG   | BA    | 3451 | 1/1   | 0.84 | 0.40 | 101,101,101,101             | 0     |
| 55  | MG   | AA    | 1753 | 1/1   | 0.84 | 0.09 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3223 | 1/1   | 0.84 | 0.47 | 56,56,56,56                 | 0     |
| 55  | MG   | AA    | 1738 | 1/1   | 0.84 | 0.20 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3245 | 1/1   | 0.84 | 0.25 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3354 | 1/1   | 0.84 | 0.23 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3138 | 1/1   | 0.84 | 0.35 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3076 | 1/1   | 0.84 | 0.14 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1616 | 1/1   | 0.84 | 0.15 | 110,110,110,110             | 0     |
| 55  | MG   | BA    | 3279 | 1/1   | 0.84 | 0.29 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3344 | 1/1   | 0.84 | 0.27 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3466 | 1/1   | 0.84 | 0.26 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3261 | 1/1   | 0.84 | 0.14 | 78,78,78,78                 | 0     |
| 55  | MG   | CA    | 1652 | 1/1   | 0.84 | 0.21 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3469 | 1/1   | 0.84 | 0.32 | 109,109,109,109             | 0     |
| 55  | MG   | CA    | 1799 | 1/1   | 0.84 | 0.18 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 1794 | 1/1   | 0.84 | 0.33 | 112,112,112,112             | 0     |
| 55  | MG   | CA    | 1655 | 1/1   | 0.84 | 0.16 | 85,85,85,85                 | 0     |
| 55  | MG   | CA    | 1805 | 1/1   | 0.84 | 0.30 | 102,102,102,102             | 0     |
| 55  | MG   | BA    | 3566 | 1/1   | 0.84 | 0.27 | 83,83,83,83                 | 0     |
| 55  | MG   | CA    | 1658 | 1/1   | 0.84 | 0.39 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3466 | 1/1   | 0.84 | 0.44 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3379 | 1/1   | 0.84 | 0.35 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3416 | 1/1   | 0.84 | 0.24 | 98,98,98,98                 | 0     |
| 55  | MG   | BA    | 3349 | 1/1   | 0.84 | 0.26 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3470 | 1/1   | 0.84 | 0.30 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3293 | 1/1   | 0.84 | 0.41 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3294 | 1/1   | 0.84 | 0.38 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3288 | 1/1   | 0.84 | 0.26 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3078 | 1/1   | 0.84 | 0.31 | 101,101,101,101             | 0     |
| 55  | MG   | AA    | 1715 | 1/1   | 0.84 | 0.32 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3301 | 1/1   | 0.84 | 0.34 | 90,90,90,90                 | 0     |
| 55  | MG   | AA    | 1720 | 1/1   | 0.84 | 0.44 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1617 | 1/1   | 0.84 | 0.29 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1678 | 1/1   | 0.84 | 0.46 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3366 | 1/1   | 0.84 | 0.22 | 91,91,91,91                 | 0     |
| 55  | MG   | AA    | 1673 | 1/1   | 0.84 | 0.27 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3300 | 1/1   | 0.84 | 0.38 | 80,80,80,80                 | 0     |
| 55  | MG   | AA    | 1708 | 1/1   | 0.84 | 0.12 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3304 | 1/1   | 0.84 | 0.24 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3316 | 1/1   | 0.84 | 0.23 | 102,102,102,102             | 0     |
| 55  | MG   | BA    | 3375 | 1/1   | 0.84 | 0.16 | 87,87,87,87                 | 0     |
| 55  | MG   | AA    | 1639 | 1/1   | 0.84 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | CC    | 104  | 1/1   | 0.84 | 0.24 | 98,98,98,98                 | 0     |
| 55  | MG   | CA    | 1691 | 1/1   | 0.84 | 0.21 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1614 | 1/1   | 0.84 | 0.32 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3557 | 1/1   | 0.85 | 0.17 | 94,94,94,94                 | 0     |
| 55  | MG   | DA    | 3052 | 1/1   | 0.85 | 0.18 | 78,78,78,78                 | 0     |
| 55  | MG   | AA    | 1705 | 1/1   | 0.85 | 0.23 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3387 | 1/1   | 0.85 | 0.12 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3184 | 1/1   | 0.85 | 0.35 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3238 | 1/1   | 0.85 | 0.24 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3084 | 1/1   | 0.85 | 0.31 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 3436 | 1/1   | 0.85 | 0.11 | 107,107,107,107             | 0     |
| 55  | MG   | AA    | 1640 | 1/1   | 0.85 | 0.27 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3395 | 1/1   | 0.85 | 0.23 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1651 | 1/1   | 0.85 | 0.43 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3051 | 1/1   | 0.85 | 0.15 | 103,103,103,103             | 0     |
| 55  | MG   | CG    | 301  | 1/1   | 0.85 | 0.45 | 107,107,107,107             | 0     |
| 55  | MG   | DA    | 3126 | 1/1   | 0.85 | 0.22 | 63,63,63,63                 | 0     |
| 55  | MG   | DA    | 3324 | 1/1   | 0.85 | 0.26 | 91,91,91,91                 | 0     |
| 55  | MG   | AA    | 1771 | 1/1   | 0.85 | 0.41 | 108,108,108,108             | 0     |
| 55  | MG   | DA    | 3329 | 1/1   | 0.85 | 0.24 | 71,71,71,71                 | 0     |
| 55  | MG   | AA    | 1676 | 1/1   | 0.85 | 0.34 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3332 | 1/1   | 0.85 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3319 | 1/1   | 0.85 | 0.35 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3362 | 1/1   | 0.85 | 0.26 | 84,84,84,84                 | 0     |
| 55  | MG   | BB    | 214  | 1/1   | 0.85 | 0.18 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3154 | 1/1   | 0.85 | 0.41 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3481 | 1/1   | 0.85 | 0.24 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3408 | 1/1   | 0.85 | 0.09 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3158 | 1/1   | 0.85 | 0.29 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3508 | 1/1   | 0.85 | 0.30 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3254 | 1/1   | 0.85 | 0.32 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3277 | 1/1   | 0.85 | 0.17 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3412 | 1/1   | 0.85 | 0.29 | 89,89,89,89                 | 0     |
| 55  | MG   | BA    | 3413 | 1/1   | 0.85 | 0.33 | 83,83,83,83                 | 0     |
| 55  | MG   | B3    | 103  | 1/1   | 0.85 | 0.19 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3410 | 1/1   | 0.85 | 0.49 | 103,103,103,103             | 0     |
| 55  | MG   | BA    | 3206 | 1/1   | 0.85 | 0.17 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3008 | 1/1   | 0.85 | 0.36 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3413 | 1/1   | 0.85 | 0.28 | 86,86,86,86                 | 0     |
| 55  | MG   | AA    | 1702 | 1/1   | 0.85 | 0.28 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1761 | 1/1   | 0.85 | 0.30 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3419 | 1/1   | 0.85 | 0.19 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3376 | 1/1   | 0.85 | 0.24 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3357 | 1/1   | 0.85 | 0.17 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3298 | 1/1   | 0.85 | 0.33 | 66,66,66,66                 | 0     |
| 55  | MG   | AA    | 1620 | 1/1   | 0.85 | 0.25 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3548 | 1/1   | 0.85 | 0.25 | 95,95,95,95                 | 0     |
| 55  | MG   | AA    | 1697 | 1/1   | 0.85 | 0.09 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3440 | 1/1   | 0.85 | 0.14 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3553 | 1/1   | 0.85 | 0.23 | 49,49,49,49                 | 0     |
| 55  | MG   | BA    | 3385 | 1/1   | 0.85 | 0.15 | 86,86,86,86                 | 0     |
| 55  | MG   | CA    | 1772 | 1/1   | 0.86 | 0.17 | 107,107,107,107             | 0     |
| 55  | MG   | BA    | 3430 | 1/1   | 0.86 | 0.18 | 105,105,105,105             | 0     |
| 55  | MG   | BA    | 3112 | 1/1   | 0.86 | 0.50 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3035 | 1/1   | 0.86 | 0.35 | 61,61,61,61                 | 0     |
| 55  | MG   | DA    | 3179 | 1/1   | 0.86 | 0.28 | 88,88,88,88                 | 0     |
| 55  | MG   | AA    | 1701 | 1/1   | 0.86 | 0.27 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3190 | 1/1   | 0.86 | 0.34 | 86,86,86,86                 | 0     |
| 55  | MG   | BB    | 202  | 1/1   | 0.86 | 0.24 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3399 | 1/1   | 0.86 | 0.23 | 99,99,99,99                 | 0     |
| 55  | MG   | AA    | 1656 | 1/1   | 0.86 | 0.36 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3017 | 1/1   | 0.86 | 0.12 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3401 | 1/1   | 0.86 | 0.23 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3203 | 1/1   | 0.86 | 0.33 | 74,74,74,74                 | 0     |
| 55  | MG   | AA    | 1768 | 1/1   | 0.86 | 0.38 | 71,71,71,71                 | 0     |
| 55  | MG   | DA    | 3025 | 1/1   | 0.86 | 0.22 | 70,70,70,70                 | 0     |
| 55  | MG   | DA    | 3207 | 1/1   | 0.86 | 0.39 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3196 | 1/1   | 0.86 | 0.15 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3331 | 1/1   | 0.86 | 0.45 | 91,91,91,91                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1769 | 1/1   | 0.86 | 0.15 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3032 | 1/1   | 0.86 | 0.35 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3507 | 1/1   | 0.86 | 0.28 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3132 | 1/1   | 0.86 | 0.25 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1793 | 1/1   | 0.86 | 0.34 | 110,110,110,110             | 0     |
| 55  | MG   | BA    | 3409 | 1/1   | 0.86 | 0.55 | 98,98,98,98                 | 0     |
| 55  | MG   | BF    | 302  | 1/1   | 0.86 | 0.13 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3043 | 1/1   | 0.86 | 0.23 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3047 | 1/1   | 0.86 | 0.28 | 67,67,67,67                 | 0     |
| 55  | MG   | BA    | 3135 | 1/1   | 0.86 | 0.31 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3231 | 1/1   | 0.86 | 0.55 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3234 | 1/1   | 0.86 | 0.33 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3459 | 1/1   | 0.86 | 0.33 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1744 | 1/1   | 0.86 | 0.35 | 73,73,73,73                 | 0     |
| 55  | MG   | AA    | 1605 | 1/1   | 0.86 | 0.27 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3066 | 1/1   | 0.86 | 0.30 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3074 | 1/1   | 0.86 | 0.26 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3141 | 1/1   | 0.86 | 0.29 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3525 | 1/1   | 0.86 | 0.25 | 51,51,51,51                 | 0     |
| 55  | MG   | BA    | 3537 | 1/1   | 0.86 | 0.43 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3080 | 1/1   | 0.86 | 0.20 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3155 | 1/1   | 0.86 | 0.24 | 114,114,114,114             | 0     |
| 55  | MG   | DA    | 3253 | 1/1   | 0.86 | 0.25 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3256 | 1/1   | 0.86 | 0.20 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3363 | 1/1   | 0.86 | 0.24 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3092 | 1/1   | 0.86 | 0.19 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3259 | 1/1   | 0.86 | 0.34 | 92,92,92,92                 | 0     |
| 55  | MG   | CA    | 1754 | 1/1   | 0.86 | 0.32 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3262 | 1/1   | 0.86 | 0.20 | 99,99,99,99                 | 0     |
| 55  | MG   | AA    | 1622 | 1/1   | 0.86 | 0.22 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3107 | 1/1   | 0.86 | 0.24 | 55,55,55,55                 | 0     |
| 55  | MG   | CA    | 1757 | 1/1   | 0.86 | 0.34 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3115 | 1/1   | 0.86 | 0.46 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3460 | 1/1   | 0.86 | 0.46 | 97,97,97,97                 | 0     |
| 55  | MG   | DA    | 3377 | 1/1   | 0.86 | 0.22 | 87,87,87,87                 | 0     |
| 55  | MG   | AA    | 1731 | 1/1   | 0.86 | 0.15 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3233 | 1/1   | 0.86 | 0.34 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3280 | 1/1   | 0.86 | 0.29 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3383 | 1/1   | 0.86 | 0.23 | 94,94,94,94                 | 0     |
| 55  | MG   | CA    | 1622 | 1/1   | 0.86 | 0.15 | 110,110,110,110             | 0     |
| 55  | MG   | DA    | 3135 | 1/1   | 0.86 | 0.28 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3146 | 1/1   | 0.86 | 0.10 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DB    | 213  | 1/1   | 0.86 | 0.18 | 99,99,99,99                 | 0     |
| 55  | MG   | DA    | 3147 | 1/1   | 0.86 | 0.13 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3291 | 1/1   | 0.86 | 0.09 | 149,149,149,149             | 0     |
| 55  | MG   | DA    | 3292 | 1/1   | 0.86 | 0.34 | 98,98,98,98                 | 0     |
| 55  | MG   | BA    | 3384 | 1/1   | 0.86 | 0.42 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3151 | 1/1   | 0.86 | 0.26 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3171 | 1/1   | 0.86 | 0.27 | 96,96,96,96                 | 0     |
| 55  | MG   | DD    | 302  | 1/1   | 0.86 | 0.20 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3026 | 1/1   | 0.86 | 0.22 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3561 | 1/1   | 0.86 | 0.19 | 84,84,84,84                 | 0     |
| 55  | MG   | AA    | 1754 | 1/1   | 0.86 | 0.26 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3180 | 1/1   | 0.86 | 0.27 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3099 | 1/1   | 0.86 | 0.23 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3295 | 1/1   | 0.87 | 0.56 | 76,76,76,76                 | 0     |
| 55  | MG   | AA    | 1698 | 1/1   | 0.87 | 0.49 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3048 | 1/1   | 0.87 | 0.25 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3049 | 1/1   | 0.87 | 0.16 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3300 | 1/1   | 0.87 | 0.21 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3317 | 1/1   | 0.87 | 0.32 | 70,70,70,70                 | 0     |
| 55  | MG   | CA    | 1760 | 1/1   | 0.87 | 0.18 | 105,105,105,105             | 0     |
| 55  | MG   | DA    | 3305 | 1/1   | 0.87 | 0.29 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3433 | 1/1   | 0.87 | 0.22 | 99,99,99,99                 | 0     |
| 55  | MG   | AA    | 1813 | 1/1   | 0.87 | 0.24 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3504 | 1/1   | 0.87 | 0.32 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3178 | 1/1   | 0.87 | 0.27 | 88,88,88,88                 | 0     |
| 55  | MG   | B1    | 202  | 1/1   | 0.87 | 0.13 | 86,86,86,86                 | 0     |
| 55  | MG   | AA    | 1755 | 1/1   | 0.87 | 0.26 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3054 | 1/1   | 0.87 | 0.23 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3509 | 1/1   | 0.87 | 0.28 | 97,97,97,97                 | 0     |
| 55  | MG   | DA    | 3415 | 1/1   | 0.87 | 0.36 | 85,85,85,85                 | 0     |
| 55  | MG   | CA    | 1690 | 1/1   | 0.87 | 0.19 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3418 | 1/1   | 0.87 | 0.17 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3321 | 1/1   | 0.87 | 0.23 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3322 | 1/1   | 0.87 | 0.17 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3198 | 1/1   | 0.87 | 0.31 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3192 | 1/1   | 0.87 | 0.33 | 92,92,92,92                 | 0     |
| 55  | MG   | CA    | 1700 | 1/1   | 0.87 | 0.27 | 96,96,96,96                 | 0     |
| 55  | MG   | CA    | 1701 | 1/1   | 0.87 | 0.29 | 108,108,108,108             | 0     |
| 55  | MG   | DA    | 3325 | 1/1   | 0.87 | 0.34 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3326 | 1/1   | 0.87 | 0.28 | 67,67,67,67                 | 0     |
| 55  | MG   | AA    | 1685 | 1/1   | 0.87 | 0.29 | 85,85,85,85                 | 0     |
| 55  | MG   | AA    | 1798 | 1/1   | 0.87 | 0.29 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3129 | 1/1   | 0.87 | 0.31 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3268 | 1/1   | 0.87 | 0.13 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1783 | 1/1   | 0.87 | 0.08 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3450 | 1/1   | 0.87 | 0.25 | 82,82,82,82                 | 0     |
| 55  | MG   | DA    | 3447 | 1/1   | 0.87 | 0.36 | 92,92,92,92                 | 0     |
| 55  | MG   | DA    | 3046 | 1/1   | 0.87 | 0.27 | 100,100,100,100             | 0     |
| 55  | MG   | DA    | 3449 | 1/1   | 0.87 | 0.32 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3199 | 1/1   | 0.87 | 0.22 | 65,65,65,65                 | 0     |
| 55  | MG   | DA    | 3337 | 1/1   | 0.87 | 0.31 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3048 | 1/1   | 0.87 | 0.27 | 76,76,76,76                 | 0     |
| 55  | MG   | AA    | 1734 | 1/1   | 0.87 | 0.34 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3342 | 1/1   | 0.87 | 0.14 | 66,66,66,66                 | 0     |
| 55  | MG   | CA    | 1628 | 1/1   | 0.87 | 0.16 | 123,123,123,123             | 0     |
| 55  | MG   | AA    | 1770 | 1/1   | 0.87 | 0.22 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3137 | 1/1   | 0.87 | 0.15 | 88,88,88,88                 | 0     |
| 55  | MG   | CA    | 1725 | 1/1   | 0.87 | 0.45 | 86,86,86,86                 | 0     |
| 55  | MG   | CA    | 1633 | 1/1   | 0.87 | 0.32 | 61,61,61,61                 | 0     |
| 55  | MG   | CA    | 1727 | 1/1   | 0.87 | 0.17 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1639 | 1/1   | 0.87 | 0.38 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3085 | 1/1   | 0.87 | 0.48 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3554 | 1/1   | 0.87 | 0.24 | 48,48,48,48                 | 0     |
| 55  | MG   | DA    | 3355 | 1/1   | 0.87 | 0.30 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1742 | 1/1   | 0.87 | 0.23 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3095 | 1/1   | 0.87 | 0.32 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1802 | 1/1   | 0.87 | 0.11 | 75,75,75,75                 | 0     |
| 55  | MG   | CA    | 1647 | 1/1   | 0.87 | 0.38 | 96,96,96,96                 | 0     |
| 55  | MG   | DA    | 3106 | 1/1   | 0.87 | 0.27 | 57,57,57,57                 | 0     |
| 55  | MG   | AA    | 1760 | 1/1   | 0.87 | 0.35 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3110 | 1/1   | 0.87 | 0.18 | 61,61,61,61                 | 0     |
| 55  | MG   | AA    | 1681 | 1/1   | 0.87 | 0.39 | 72,72,72,72                 | 0     |
| 55  | MG   | AA    | 1752 | 1/1   | 0.87 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3119 | 1/1   | 0.87 | 0.37 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3162 | 1/1   | 0.87 | 0.30 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3265 | 1/1   | 0.87 | 0.34 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3267 | 1/1   | 0.87 | 0.28 | 80,80,80,80                 | 0     |
| 55  | MG   | AA    | 1806 | 1/1   | 0.87 | 0.37 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3237 | 1/1   | 0.87 | 0.37 | 102,102,102,102             | 0     |
| 55  | MG   | DA    | 3274 | 1/1   | 0.87 | 0.22 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3275 | 1/1   | 0.87 | 0.35 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3365 | 1/1   | 0.87 | 0.17 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3381 | 1/1   | 0.87 | 0.23 | 90,90,90,90                 | 0     |
| 55  | MG   | DB    | 214  | 1/1   | 0.87 | 0.14 | 95,95,95,95                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1763 | 1/1   | 0.87 | 0.19 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3042 | 1/1   | 0.87 | 0.40 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3142 | 1/1   | 0.87 | 0.17 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3243 | 1/1   | 0.87 | 0.13 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3372 | 1/1   | 0.87 | 0.32 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1750 | 1/1   | 0.87 | 0.23 | 86,86,86,86                 | 0     |
| 55  | MG   | AA    | 1683 | 1/1   | 0.87 | 0.38 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3153 | 1/1   | 0.87 | 0.18 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3246 | 1/1   | 0.87 | 0.28 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3160 | 1/1   | 0.87 | 0.38 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3162 | 1/1   | 0.87 | 0.33 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3097 | 1/1   | 0.87 | 0.16 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3271 | 1/1   | 0.88 | 0.20 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3541 | 1/1   | 0.88 | 0.24 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3308 | 1/1   | 0.88 | 0.15 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3389 | 1/1   | 0.88 | 0.25 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3050 | 1/1   | 0.88 | 0.21 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3468 | 1/1   | 0.88 | 0.29 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3353 | 1/1   | 0.88 | 0.33 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3354 | 1/1   | 0.88 | 0.26 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3068 | 1/1   | 0.88 | 0.29 | 54,54,54,54                 | 0     |
| 55  | MG   | CA    | 1619 | 1/1   | 0.88 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | AA    | 1790 | 1/1   | 0.88 | 0.24 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3190 | 1/1   | 0.88 | 0.38 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3356 | 1/1   | 0.88 | 0.18 | 60,60,60,60                 | 0     |
| 55  | MG   | DA    | 3361 | 1/1   | 0.88 | 0.13 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3081 | 1/1   | 0.88 | 0.27 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3195 | 1/1   | 0.88 | 0.26 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3076 | 1/1   | 0.88 | 0.35 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3474 | 1/1   | 0.88 | 0.22 | 72,72,72,72                 | 0     |
| 55  | MG   | DA    | 3367 | 1/1   | 0.88 | 0.21 | 82,82,82,82                 | 0     |
| 55  | MG   | DA    | 3368 | 1/1   | 0.88 | 0.18 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3052 | 1/1   | 0.88 | 0.29 | 66,66,66,66                 | 0     |
| 55  | MG   | AA    | 1651 | 1/1   | 0.88 | 0.40 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3297 | 1/1   | 0.88 | 0.37 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3281 | 1/1   | 0.88 | 0.20 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3203 | 1/1   | 0.88 | 0.18 | 106,106,106,106             | 0     |
| 55  | MG   | BA    | 3205 | 1/1   | 0.88 | 0.22 | 59,59,59,59                 | 0     |
| 55  | MG   | AA    | 1686 | 1/1   | 0.88 | 0.19 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3104 | 1/1   | 0.88 | 0.26 | 62,62,62,62                 | 0     |
| 55  | MG   | DA    | 3378 | 1/1   | 0.88 | 0.38 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3058 | 1/1   | 0.88 | 0.23 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | CA    | 1643 | 1/1   | 0.88 | 0.38 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3108 | 1/1   | 0.88 | 0.30 | 54,54,54,54                 | 0     |
| 55  | MG   | AA    | 1691 | 1/1   | 0.88 | 0.36 | 88,88,88,88                 | 0     |
| 55  | MG   | CC    | 102  | 1/1   | 0.88 | 0.40 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3222 | 1/1   | 0.88 | 0.18 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3294 | 1/1   | 0.88 | 0.19 | 61,61,61,61                 | 0     |
| 55  | MG   | CA    | 1646 | 1/1   | 0.88 | 0.29 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3315 | 1/1   | 0.88 | 0.16 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3501 | 1/1   | 0.88 | 0.44 | 86,86,86,86                 | 0     |
| 55  | MG   | BA    | 3220 | 1/1   | 0.88 | 0.25 | 70,70,70,70                 | 0     |
| 55  | MG   | BA    | 3013 | 1/1   | 0.88 | 0.20 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3505 | 1/1   | 0.88 | 0.28 | 61,61,61,61                 | 0     |
| 55  | MG   | BA    | 3063 | 1/1   | 0.88 | 0.16 | 80,80,80,80                 | 0     |
| 55  | MG   | BB    | 213  | 1/1   | 0.88 | 0.22 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3140 | 1/1   | 0.88 | 0.33 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3141 | 1/1   | 0.88 | 0.35 | 101,101,101,101             | 0     |
| 55  | MG   | BA    | 3017 | 1/1   | 0.88 | 0.28 | 58,58,58,58                 | 0     |
| 55  | MG   | DA    | 3326 | 1/1   | 0.88 | 0.25 | 109,109,109,109             | 0     |
| 55  | MG   | BB    | 215  | 1/1   | 0.88 | 0.21 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3381 | 1/1   | 0.88 | 0.36 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3230 | 1/1   | 0.88 | 0.29 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3302 | 1/1   | 0.88 | 0.22 | 83,83,83,83                 | 0     |
| 55  | MG   | DA    | 3255 | 1/1   | 0.88 | 0.15 | 82,82,82,82                 | 0     |
| 55  | MG   | AA    | 1672 | 1/1   | 0.88 | 0.44 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3156 | 1/1   | 0.88 | 0.21 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3459 | 1/1   | 0.88 | 0.23 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3423 | 1/1   | 0.88 | 0.09 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3530 | 1/1   | 0.88 | 0.28 | 71,71,71,71                 | 0     |
| 55  | MG   | CA    | 1741 | 1/1   | 0.88 | 0.23 | 85,85,85,85                 | 0     |
| 55  | MG   | CA    | 1674 | 1/1   | 0.88 | 0.39 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3535 | 1/1   | 0.88 | 0.26 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3100 | 1/1   | 0.88 | 0.31 | 93,93,93,93                 | 0     |
| 55  | MG   | AA    | 1610 | 1/1   | 0.88 | 0.30 | 58,58,58,58                 | 0     |
| 55  | MG   | BB    | 204  | 1/1   | 0.89 | 0.27 | 91,91,91,91                 | 0     |
| 55  | MG   | AA    | 1650 | 1/1   | 0.89 | 0.23 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3080 | 1/1   | 0.89 | 0.22 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3090 | 1/1   | 0.89 | 0.11 | 40,40,40,40                 | 0     |
| 55  | MG   | DA    | 3210 | 1/1   | 0.89 | 0.27 | 77,77,77,77                 | 0     |
| 55  | MG   | AA    | 1671 | 1/1   | 0.89 | 0.13 | 95,95,95,95                 | 0     |
| 55  | MG   | BA    | 3347 | 1/1   | 0.89 | 0.22 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3214 | 1/1   | 0.89 | 0.32 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3215 | 1/1   | 0.89 | 0.27 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AC    | 108  | 1/1   | 0.89 | 0.16 | 82,82,82,82                 | 0     |
| 55  | MG   | CA    | 1739 | 1/1   | 0.89 | 0.22 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3247 | 1/1   | 0.89 | 0.37 | 97,97,97,97                 | 0     |
| 55  | MG   | CA    | 1662 | 1/1   | 0.89 | 0.45 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3098 | 1/1   | 0.89 | 0.25 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3398 | 1/1   | 0.89 | 0.14 | 57,57,57,57                 | 0     |
| 55  | MG   | CA    | 1668 | 1/1   | 0.89 | 0.35 | 72,72,72,72                 | 0     |
| 55  | MG   | DA    | 3228 | 1/1   | 0.89 | 0.15 | 103,103,103,103             | 0     |
| 55  | MG   | AA    | 1714 | 1/1   | 0.89 | 0.20 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1601 | 1/1   | 0.89 | 0.31 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3156 | 1/1   | 0.89 | 0.24 | 61,61,61,61                 | 0     |
| 55  | MG   | DA    | 3425 | 1/1   | 0.89 | 0.40 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3236 | 1/1   | 0.89 | 0.40 | 62,62,62,62                 | 0     |
| 55  | MG   | AA    | 1744 | 1/1   | 0.89 | 0.24 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3435 | 1/1   | 0.89 | 0.21 | 51,51,51,51                 | 0     |
| 55  | MG   | CA    | 1748 | 1/1   | 0.89 | 0.35 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3241 | 1/1   | 0.89 | 0.26 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3113 | 1/1   | 0.89 | 0.19 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3106 | 1/1   | 0.89 | 0.24 | 89,89,89,89                 | 0     |
| 55  | MG   | BA    | 3107 | 1/1   | 0.89 | 0.25 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3521 | 1/1   | 0.89 | 0.18 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3120 | 1/1   | 0.89 | 0.32 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3407 | 1/1   | 0.89 | 0.31 | 73,73,73,73                 | 0     |
| 55  | MG   | B3    | 101  | 1/1   | 0.89 | 0.52 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3347 | 1/1   | 0.89 | 0.13 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3209 | 1/1   | 0.89 | 0.34 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3129 | 1/1   | 0.89 | 0.36 | 65,65,65,65                 | 0     |
| 55  | MG   | CA    | 1756 | 1/1   | 0.89 | 0.27 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3457 | 1/1   | 0.89 | 0.17 | 85,85,85,85                 | 0     |
| 55  | MG   | CA    | 1682 | 1/1   | 0.89 | 0.20 | 100,100,100,100             | 0     |
| 55  | MG   | BA    | 3258 | 1/1   | 0.89 | 0.38 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1604 | 1/1   | 0.89 | 0.18 | 60,60,60,60                 | 0     |
| 55  | MG   | DA    | 3463 | 1/1   | 0.89 | 0.41 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3538 | 1/1   | 0.89 | 0.17 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3539 | 1/1   | 0.89 | 0.25 | 35,35,35,35                 | 0     |
| 55  | MG   | BA    | 3361 | 1/1   | 0.89 | 0.16 | 70,70,70,70                 | 0     |
| 55  | MG   | BA    | 3067 | 1/1   | 0.89 | 0.17 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3315 | 1/1   | 0.89 | 0.40 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3216 | 1/1   | 0.89 | 0.26 | 53,53,53,53                 | 0     |
| 55  | MG   | DA    | 3272 | 1/1   | 0.89 | 0.42 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3364 | 1/1   | 0.89 | 0.12 | 93,93,93,93                 | 0     |
| 55  | MG   | DA    | 3155 | 1/1   | 0.89 | 0.09 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3113 | 1/1   | 0.89 | 0.20 | 47,47,47,47                 | 0     |
| 55  | MG   | CA    | 1697 | 1/1   | 0.89 | 0.12 | 84,84,84,84                 | 0     |
| 55  | MG   | AA    | 1791 | 1/1   | 0.89 | 0.40 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3222 | 1/1   | 0.89 | 0.41 | 68,68,68,68                 | 0     |
| 55  | MG   | AA    | 1792 | 1/1   | 0.89 | 0.19 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3551 | 1/1   | 0.89 | 0.28 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3123 | 1/1   | 0.89 | 0.29 | 81,81,81,81                 | 0     |
| 55  | MG   | AA    | 1653 | 1/1   | 0.89 | 0.42 | 95,95,95,95                 | 0     |
| 55  | MG   | DA    | 3285 | 1/1   | 0.89 | 0.34 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3375 | 1/1   | 0.89 | 0.14 | 86,86,86,86                 | 0     |
| 55  | MG   | DB    | 202  | 1/1   | 0.89 | 0.18 | 91,91,91,91                 | 0     |
| 55  | MG   | BA    | 3323 | 1/1   | 0.89 | 0.19 | 73,73,73,73                 | 0     |
| 55  | MG   | DB    | 205  | 1/1   | 0.89 | 0.27 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3169 | 1/1   | 0.89 | 0.23 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3023 | 1/1   | 0.89 | 0.38 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3325 | 1/1   | 0.89 | 0.16 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3380 | 1/1   | 0.89 | 0.28 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3038 | 1/1   | 0.89 | 0.28 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3231 | 1/1   | 0.89 | 0.30 | 46,46,46,46                 | 0     |
| 55  | MG   | CA    | 1712 | 1/1   | 0.89 | 0.41 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3187 | 1/1   | 0.89 | 0.39 | 73,73,73,73                 | 0     |
| 55  | MG   | CA    | 1641 | 1/1   | 0.89 | 0.18 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3478 | 1/1   | 0.89 | 0.28 | 61,61,61,61                 | 0     |
| 55  | MG   | AA    | 1774 | 1/1   | 0.89 | 0.36 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3284 | 1/1   | 0.89 | 0.38 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3236 | 1/1   | 0.89 | 0.33 | 67,67,67,67                 | 0     |
| 55  | MG   | AC    | 103  | 1/1   | 0.89 | 0.27 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3057 | 1/1   | 0.89 | 0.33 | 56,56,56,56                 | 0     |
| 55  | MG   | DA    | 3064 | 1/1   | 0.89 | 0.28 | 70,70,70,70                 | 0     |
| 55  | MG   | AA    | 1759 | 1/1   | 0.89 | 0.07 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3396 | 1/1   | 0.89 | 0.26 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1794 | 1/1   | 0.89 | 0.09 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3072 | 1/1   | 0.89 | 0.32 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3341 | 1/1   | 0.89 | 0.34 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3149 | 1/1   | 0.90 | 0.20 | 93,93,93,93                 | 0     |
| 55  | MG   | BA    | 3512 | 1/1   | 0.90 | 0.36 | 90,90,90,90                 | 0     |
| 55  | MG   | AA    | 1664 | 1/1   | 0.90 | 0.18 | 53,53,53,53                 | 0     |
| 55  | MG   | AA    | 1665 | 1/1   | 0.90 | 0.10 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3520 | 1/1   | 0.90 | 0.30 | 40,40,40,40                 | 0     |
| 55  | MG   | DA    | 3421 | 1/1   | 0.90 | 0.12 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3042 | 1/1   | 0.90 | 0.32 | 51,51,51,51                 | 0     |
| 55  | MG   | BB    | 206  | 1/1   | 0.90 | 0.15 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3161 | 1/1   | 0.90 | 0.20 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3044 | 1/1   | 0.90 | 0.39 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3431 | 1/1   | 0.90 | 0.19 | 69,69,69,69                 | 0     |
| 55  | MG   | CA    | 1802 | 1/1   | 0.90 | 0.22 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3219 | 1/1   | 0.90 | 0.30 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3438 | 1/1   | 0.90 | 0.26 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3131 | 1/1   | 0.90 | 0.25 | 41,41,41,41                 | 0     |
| 55  | MG   | BB    | 209  | 1/1   | 0.90 | 0.21 | 96,96,96,96                 | 0     |
| 55  | MG   | DA    | 3051 | 1/1   | 0.90 | 0.17 | 87,87,87,87                 | 0     |
| 55  | MG   | AA    | 1679 | 1/1   | 0.90 | 0.33 | 83,83,83,83                 | 0     |
| 55  | MG   | CA    | 1693 | 1/1   | 0.90 | 0.31 | 103,103,103,103             | 0     |
| 55  | MG   | AA    | 1618 | 1/1   | 0.90 | 0.16 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3060 | 1/1   | 0.90 | 0.27 | 67,67,67,67                 | 0     |
| 55  | MG   | AA    | 1652 | 1/1   | 0.90 | 0.47 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3332 | 1/1   | 0.90 | 0.31 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3297 | 1/1   | 0.90 | 0.25 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3181 | 1/1   | 0.90 | 0.14 | 50,50,50,50                 | 0     |
| 55  | MG   | AA    | 1807 | 1/1   | 0.90 | 0.15 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3282 | 1/1   | 0.90 | 0.23 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3283 | 1/1   | 0.90 | 0.20 | 88,88,88,88                 | 0     |
| 55  | MG   | BA    | 3229 | 1/1   | 0.90 | 0.28 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3542 | 1/1   | 0.90 | 0.31 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3336 | 1/1   | 0.90 | 0.09 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3480 | 1/1   | 0.90 | 0.23 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3289 | 1/1   | 0.90 | 0.28 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3075 | 1/1   | 0.90 | 0.23 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3263 | 1/1   | 0.90 | 0.28 | 80,80,80,80                 | 0     |
| 55  | MG   | CG    | 302  | 1/1   | 0.90 | 0.12 | 89,89,89,89                 | 0     |
| 55  | MG   | AA    | 1634 | 1/1   | 0.90 | 0.31 | 67,67,67,67                 | 0     |
| 55  | MG   | AA    | 1776 | 1/1   | 0.90 | 0.26 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3091 | 1/1   | 0.90 | 0.23 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3039 | 1/1   | 0.90 | 0.23 | 55,55,55,55                 | 0     |
| 55  | MG   | CA    | 1714 | 1/1   | 0.90 | 0.21 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3269 | 1/1   | 0.90 | 0.23 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3099 | 1/1   | 0.90 | 0.48 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3119 | 1/1   | 0.90 | 0.31 | 61,61,61,61                 | 0     |
| 55  | MG   | CA    | 1601 | 1/1   | 0.90 | 0.28 | 67,67,67,67                 | 0     |
| 55  | MG   | CA    | 1665 | 1/1   | 0.90 | 0.32 | 70,70,70,70                 | 0     |
| 55  | MG   | CA    | 1774 | 1/1   | 0.90 | 0.20 | 75,75,75,75                 | 0     |
| 55  | MG   | CA    | 1775 | 1/1   | 0.90 | 0.33 | 69,69,69,69                 | 0     |
| 55  | MG   | CA    | 1666 | 1/1   | 0.90 | 0.20 | 90,90,90,90                 | 0     |
| 55  | MG   | CA    | 1603 | 1/1   | 0.90 | 0.27 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3487 | 1/1   | 0.90 | 0.27 | 85,85,85,85                 | 0     |
| 55  | MG   | BA    | 3161 | 1/1   | 0.90 | 0.33 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3218 | 1/1   | 0.90 | 0.25 | 86,86,86,86                 | 0     |
| 55  | MG   | DB    | 203  | 1/1   | 0.90 | 0.17 | 111,111,111,111             | 0     |
| 55  | MG   | CA    | 1779 | 1/1   | 0.90 | 0.13 | 109,109,109,109             | 0     |
| 55  | MG   | CA    | 1606 | 1/1   | 0.90 | 0.22 | 65,65,65,65                 | 0     |
| 55  | MG   | DA    | 3005 | 1/1   | 0.90 | 0.22 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 1712 | 1/1   | 0.90 | 0.16 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3226 | 1/1   | 0.90 | 0.30 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3395 | 1/1   | 0.90 | 0.22 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3016 | 1/1   | 0.90 | 0.31 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3124 | 1/1   | 0.90 | 0.24 | 47,47,47,47                 | 0     |
| 55  | MG   | CA    | 1612 | 1/1   | 0.90 | 0.27 | 75,75,75,75                 | 0     |
| 55  | MG   | AA    | 1642 | 1/1   | 0.90 | 0.36 | 70,70,70,70                 | 0     |
| 55  | MG   | DA    | 3127 | 1/1   | 0.90 | 0.41 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3235 | 1/1   | 0.90 | 0.29 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 1607 | 1/1   | 0.90 | 0.20 | 86,86,86,86                 | 0     |
| 55  | MG   | BA    | 3124 | 1/1   | 0.90 | 0.27 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3028 | 1/1   | 0.90 | 0.36 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3328 | 1/1   | 0.90 | 0.28 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3083 | 1/1   | 0.90 | 0.43 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3282 | 1/1   | 0.90 | 0.38 | 103,103,103,103             | 0     |
| 55  | MG   | DA    | 3031 | 1/1   | 0.90 | 0.17 | 70,70,70,70                 | 0     |
| 55  | MG   | DE    | 301  | 1/1   | 0.90 | 0.34 | 59,59,59,59                 | 0     |
| 55  | MG   | BA    | 3463 | 1/1   | 0.90 | 0.10 | 101,101,101,101             | 0     |
| 55  | MG   | DA    | 3033 | 1/1   | 0.90 | 0.34 | 83,83,83,83                 | 0     |
| 55  | MG   | CA    | 1620 | 1/1   | 0.90 | 0.17 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3089 | 1/1   | 0.90 | 0.28 | 61,61,61,61                 | 0     |
| 55  | MG   | D8    | 101  | 1/1   | 0.90 | 0.14 | 88,88,88,88                 | 0     |
| 55  | MG   | CA    | 1723 | 1/1   | 0.91 | 0.31 | 90,90,90,90                 | 0     |
| 55  | MG   | AA    | 1674 | 1/1   | 0.91 | 0.19 | 56,56,56,56                 | 0     |
| 55  | MG   | AA    | 1619 | 1/1   | 0.91 | 0.28 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3201 | 1/1   | 0.91 | 0.31 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3250 | 1/1   | 0.91 | 0.17 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3352 | 1/1   | 0.91 | 0.30 | 75,75,75,75                 | 0     |
| 55  | MG   | BF    | 303  | 1/1   | 0.91 | 0.12 | 78,78,78,78                 | 0     |
| 55  | MG   | CA    | 1657 | 1/1   | 0.91 | 0.31 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3154 | 1/1   | 0.91 | 0.19 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3432 | 1/1   | 0.91 | 0.28 | 64,64,64,64                 | 0     |
| 55  | MG   | BO    | 201  | 1/1   | 0.91 | 0.12 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3345 | 1/1   | 0.91 | 0.22 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3436 | 1/1   | 0.91 | 0.28 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3437 | 1/1   | 0.91 | 0.31 | 66,66,66,66                 | 0     |
| 55  | MG   | CA    | 1659 | 1/1   | 0.91 | 0.37 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3022 | 1/1   | 0.91 | 0.16 | 46,46,46,46                 | 0     |
| 55  | MG   | B1    | 201  | 1/1   | 0.91 | 0.34 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3240 | 1/1   | 0.91 | 0.33 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3086 | 1/1   | 0.91 | 0.17 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3477 | 1/1   | 0.91 | 0.33 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3545 | 1/1   | 0.91 | 0.15 | 82,82,82,82                 | 0     |
| 55  | MG   | AA    | 1812 | 1/1   | 0.91 | 0.34 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3268 | 1/1   | 0.91 | 0.31 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3053 | 1/1   | 0.91 | 0.26 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3024 | 1/1   | 0.91 | 0.31 | 44,44,44,44                 | 0     |
| 55  | MG   | DA    | 3056 | 1/1   | 0.91 | 0.44 | 52,52,52,52                 | 0     |
| 55  | MG   | DA    | 3171 | 1/1   | 0.91 | 0.17 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3442 | 1/1   | 0.91 | 0.30 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3549 | 1/1   | 0.91 | 0.34 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3174 | 1/1   | 0.91 | 0.32 | 63,63,63,63                 | 0     |
| 55  | MG   | AA    | 1645 | 1/1   | 0.91 | 0.17 | 65,65,65,65                 | 0     |
| 55  | MG   | CA    | 1605 | 1/1   | 0.91 | 0.29 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3027 | 1/1   | 0.91 | 0.16 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3070 | 1/1   | 0.91 | 0.32 | 68,68,68,68                 | 0     |
| 55  | MG   | CA    | 1611 | 1/1   | 0.91 | 0.38 | 82,82,82,82                 | 0     |
| 55  | MG   | DA    | 3183 | 1/1   | 0.91 | 0.23 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3184 | 1/1   | 0.91 | 0.32 | 78,78,78,78                 | 0     |
| 55  | MG   | CA    | 1679 | 1/1   | 0.91 | 0.20 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3077 | 1/1   | 0.91 | 0.30 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3485 | 1/1   | 0.91 | 0.18 | 98,98,98,98                 | 0     |
| 55  | MG   | BA    | 3555 | 1/1   | 0.91 | 0.15 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3287 | 1/1   | 0.91 | 0.21 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3447 | 1/1   | 0.91 | 0.35 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3559 | 1/1   | 0.91 | 0.31 | 86,86,86,86                 | 0     |
| 55  | MG   | BA    | 3182 | 1/1   | 0.91 | 0.37 | 45,45,45,45                 | 0     |
| 55  | MG   | AA    | 1716 | 1/1   | 0.91 | 0.12 | 82,82,82,82                 | 0     |
| 55  | MG   | AA    | 1654 | 1/1   | 0.91 | 0.23 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3330 | 1/1   | 0.91 | 0.17 | 61,61,61,61                 | 0     |
| 55  | MG   | BA    | 3292 | 1/1   | 0.91 | 0.25 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3101 | 1/1   | 0.91 | 0.21 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3105 | 1/1   | 0.91 | 0.13 | 71,71,71,71                 | 0     |
| 55  | MG   | CA    | 1626 | 1/1   | 0.91 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3101 | 1/1   | 0.91 | 0.28 | 76,76,76,76                 | 0     |
| 55  | MG   | DB    | 201  | 1/1   | 0.91 | 0.13 | 92,92,92,92                 | 0     |
| 55  | MG   | AA    | 1745 | 1/1   | 0.91 | 0.18 | 83,83,83,83                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3211 | 1/1   | 0.91 | 0.31 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3056 | 1/1   | 0.91 | 0.28 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 3418 | 1/1   | 0.91 | 0.28 | 82,82,82,82                 | 0     |
| 55  | MG   | BB    | 203  | 1/1   | 0.91 | 0.31 | 71,71,71,71                 | 0     |
| 55  | MG   | CA    | 1632 | 1/1   | 0.91 | 0.18 | 53,53,53,53                 | 0     |
| 55  | MG   | BA    | 3228 | 1/1   | 0.91 | 0.38 | 82,82,82,82                 | 0     |
| 55  | MG   | CA    | 1638 | 1/1   | 0.91 | 0.26 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3007 | 1/1   | 0.91 | 0.18 | 55,55,55,55                 | 0     |
| 55  | MG   | BA    | 3260 | 1/1   | 0.91 | 0.31 | 65,65,65,65                 | 0     |
| 55  | MG   | DA    | 3220 | 1/1   | 0.91 | 0.23 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3012 | 1/1   | 0.91 | 0.26 | 50,50,50,50                 | 0     |
| 55  | MG   | DA    | 3013 | 1/1   | 0.91 | 0.22 | 51,51,51,51                 | 0     |
| 55  | MG   | DA    | 3015 | 1/1   | 0.91 | 0.30 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3339 | 1/1   | 0.91 | 0.23 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3146 | 1/1   | 0.91 | 0.25 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3517 | 1/1   | 0.91 | 0.30 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3001 | 1/1   | 0.91 | 0.42 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3128 | 1/1   | 0.91 | 0.28 | 47,47,47,47                 | 0     |
| 55  | MG   | DD    | 301  | 1/1   | 0.91 | 0.38 | 51,51,51,51                 | 0     |
| 55  | MG   | BA    | 3003 | 1/1   | 0.91 | 0.20 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3524 | 1/1   | 0.91 | 0.22 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3266 | 1/1   | 0.91 | 0.32 | 71,71,71,71                 | 0     |
| 55  | MG   | DA    | 3237 | 1/1   | 0.91 | 0.20 | 79,79,79,79                 | 0     |
| 55  | MG   | D0    | 201  | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3232 | 1/1   | 0.91 | 0.26 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3139 | 1/1   | 0.91 | 0.26 | 53,53,53,53                 | 0     |
| 55  | MG   | CA    | 1720 | 1/1   | 0.91 | 0.36 | 68,68,68,68                 | 0     |
| 55  | MG   | BA    | 3115 | 1/1   | 0.91 | 0.30 | 41,41,41,41                 | 0     |
| 55  | MG   | DA    | 3103 | 1/1   | 0.92 | 0.25 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3493 | 1/1   | 0.92 | 0.22 | 51,51,51,51                 | 0     |
| 55  | MG   | AA    | 1663 | 1/1   | 0.92 | 0.35 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3046 | 1/1   | 0.92 | 0.30 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3502 | 1/1   | 0.92 | 0.33 | 78,78,78,78                 | 0     |
| 55  | MG   | AA    | 1739 | 1/1   | 0.92 | 0.29 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3226 | 1/1   | 0.92 | 0.23 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3223 | 1/1   | 0.92 | 0.28 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3109 | 1/1   | 0.92 | 0.29 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3422 | 1/1   | 0.92 | 0.25 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3001 | 1/1   | 0.92 | 0.27 | 46,46,46,46                 | 0     |
| 55  | MG   | DA    | 3117 | 1/1   | 0.92 | 0.17 | 61,61,61,61                 | 0     |
| 55  | MG   | CA    | 1698 | 1/1   | 0.92 | 0.23 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3310 | 1/1   | 0.92 | 0.24 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3402 | 1/1   | 0.92 | 0.21 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3233 | 1/1   | 0.92 | 0.30 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3009 | 1/1   | 0.92 | 0.27 | 53,53,53,53                 | 0     |
| 55  | MG   | DA    | 3011 | 1/1   | 0.92 | 0.29 | 50,50,50,50                 | 0     |
| 55  | MG   | CA    | 1770 | 1/1   | 0.92 | 0.32 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3028 | 1/1   | 0.92 | 0.25 | 52,52,52,52                 | 0     |
| 55  | MG   | DA    | 3014 | 1/1   | 0.92 | 0.27 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1703 | 1/1   | 0.92 | 0.32 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3029 | 1/1   | 0.92 | 0.21 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3341 | 1/1   | 0.92 | 0.29 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3405 | 1/1   | 0.92 | 0.18 | 82,82,82,82                 | 0     |
| 55  | MG   | CA    | 1706 | 1/1   | 0.92 | 0.44 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3136 | 1/1   | 0.92 | 0.47 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3137 | 1/1   | 0.92 | 0.23 | 53,53,53,53                 | 0     |
| 55  | MG   | DA    | 3022 | 1/1   | 0.92 | 0.27 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3148 | 1/1   | 0.92 | 0.09 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3149 | 1/1   | 0.92 | 0.22 | 41,41,41,41                 | 0     |
| 55  | MG   | DA    | 3026 | 1/1   | 0.92 | 0.24 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3272 | 1/1   | 0.92 | 0.16 | 59,59,59,59                 | 0     |
| 55  | MG   | CA    | 1642 | 1/1   | 0.92 | 0.23 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3516 | 1/1   | 0.92 | 0.20 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3257 | 1/1   | 0.92 | 0.36 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3194 | 1/1   | 0.92 | 0.16 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3087 | 1/1   | 0.92 | 0.19 | 38,38,38,38                 | 0     |
| 55  | MG   | BA    | 3277 | 1/1   | 0.92 | 0.26 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3522 | 1/1   | 0.92 | 0.32 | 45,45,45,45                 | 0     |
| 55  | MG   | AA    | 1604 | 1/1   | 0.92 | 0.21 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3367 | 1/1   | 0.92 | 0.39 | 72,72,72,72                 | 0     |
| 55  | MG   | CA    | 1787 | 1/1   | 0.92 | 0.17 | 84,84,84,84                 | 0     |
| 55  | MG   | BA    | 3526 | 1/1   | 0.92 | 0.25 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3368 | 1/1   | 0.92 | 0.21 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3471 | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3532 | 1/1   | 0.92 | 0.29 | 54,54,54,54                 | 0     |
| 55  | MG   | BA    | 3534 | 1/1   | 0.92 | 0.21 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3164 | 1/1   | 0.92 | 0.18 | 67,67,67,67                 | 0     |
| 55  | MG   | BA    | 3012 | 1/1   | 0.92 | 0.26 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3280 | 1/1   | 0.92 | 0.21 | 80,80,80,80                 | 0     |
| 55  | MG   | CA    | 1730 | 1/1   | 0.92 | 0.16 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3093 | 1/1   | 0.92 | 0.33 | 57,57,57,57                 | 0     |
| 55  | MG   | AA    | 1766 | 1/1   | 0.92 | 0.12 | 98,98,98,98                 | 0     |
| 55  | MG   | CA    | 1800 | 1/1   | 0.92 | 0.25 | 99,99,99,99                 | 0     |
| 55  | MG   | CA    | 1660 | 1/1   | 0.92 | 0.12 | 85,85,85,85                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1628 | 1/1   | 0.92 | 0.44 | 77,77,77,77                 | 0     |
| 55  | MG   | AA    | 1646 | 1/1   | 0.92 | 0.35 | 60,60,60,60                 | 0     |
| 55  | MG   | DA    | 3055 | 1/1   | 0.92 | 0.32 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3168 | 1/1   | 0.92 | 0.25 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3204 | 1/1   | 0.92 | 0.11 | 56,56,56,56                 | 0     |
| 55  | MG   | DA    | 3286 | 1/1   | 0.92 | 0.42 | 78,78,78,78                 | 0     |
| 55  | MG   | B5    | 101  | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 55  | MG   | DA    | 3180 | 1/1   | 0.92 | 0.18 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3379 | 1/1   | 0.92 | 0.32 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3169 | 1/1   | 0.92 | 0.23 | 45,45,45,45                 | 0     |
| 55  | MG   | CA    | 1670 | 1/1   | 0.92 | 0.32 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3069 | 1/1   | 0.92 | 0.49 | 76,76,76,76                 | 0     |
| 55  | MG   | CA    | 1811 | 1/1   | 0.92 | 0.32 | 69,69,69,69                 | 0     |
| 55  | MG   | AC    | 101  | 1/1   | 0.92 | 0.21 | 55,55,55,55                 | 0     |
| 55  | MG   | BA    | 3172 | 1/1   | 0.92 | 0.38 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3173 | 1/1   | 0.92 | 0.27 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3211 | 1/1   | 0.92 | 0.21 | 55,55,55,55                 | 0     |
| 55  | MG   | CA    | 1609 | 1/1   | 0.92 | 0.23 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3175 | 1/1   | 0.92 | 0.20 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3217 | 1/1   | 0.92 | 0.24 | 40,40,40,40                 | 0     |
| 55  | MG   | BA    | 3127 | 1/1   | 0.92 | 0.08 | 73,73,73,73                 | 0     |
| 55  | MG   | CA    | 1613 | 1/1   | 0.92 | 0.22 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1752 | 1/1   | 0.92 | 0.47 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3088 | 1/1   | 0.92 | 0.18 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3059 | 1/1   | 0.92 | 0.36 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3484 | 1/1   | 0.92 | 0.40 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3094 | 1/1   | 0.92 | 0.21 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 1623 | 1/1   | 0.92 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3345 | 1/1   | 0.92 | 0.14 | 46,46,46,46                 | 0     |
| 55  | MG   | DA    | 3312 | 1/1   | 0.92 | 0.29 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3346 | 1/1   | 0.92 | 0.34 | 69,69,69,69                 | 0     |
| 55  | MG   | CC    | 101  | 1/1   | 0.92 | 0.32 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3560 | 1/1   | 0.92 | 0.28 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3103 | 1/1   | 0.92 | 0.32 | 76,76,76,76                 | 0     |
| 56  | ZN   | AG    | 303  | 1/1   | 0.92 | 0.26 | 100,100,100,100             | 0     |
| 56  | ZN   | AQ    | 101  | 1/1   | 0.92 | 0.14 | 142,142,142,142             | 0     |
| 55  | MG   | DA    | 3232 | 1/1   | 0.93 | 0.09 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3283 | 1/1   | 0.93 | 0.18 | 56,56,56,56                 | 0     |
| 55  | MG   | AA    | 1717 | 1/1   | 0.93 | 0.30 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3364 | 1/1   | 0.93 | 0.21 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3019 | 1/1   | 0.93 | 0.20 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3045 | 1/1   | 0.93 | 0.39 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3143 | 1/1   | 0.93 | 0.30 | 74,74,74,74                 | 0     |
| 55  | MG   | AA    | 1793 | 1/1   | 0.93 | 0.16 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3328 | 1/1   | 0.93 | 0.17 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3047 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 55  | MG   | DA    | 3428 | 1/1   | 0.93 | 0.34 | 59,59,59,59                 | 0     |
| 55  | MG   | CA    | 1623 | 1/1   | 0.93 | 0.30 | 75,75,75,75                 | 0     |
| 55  | MG   | CA    | 1686 | 1/1   | 0.93 | 0.27 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3152 | 1/1   | 0.93 | 0.24 | 63,63,63,63                 | 0     |
| 55  | MG   | AA    | 1710 | 1/1   | 0.93 | 0.16 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3071 | 1/1   | 0.93 | 0.15 | 63,63,63,63                 | 0     |
| 55  | MG   | AA    | 1669 | 1/1   | 0.93 | 0.25 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3136 | 1/1   | 0.93 | 0.10 | 53,53,53,53                 | 0     |
| 55  | MG   | DA    | 3157 | 1/1   | 0.93 | 0.18 | 51,51,51,51                 | 0     |
| 55  | MG   | BA    | 3104 | 1/1   | 0.93 | 0.15 | 82,82,82,82                 | 0     |
| 55  | MG   | AA    | 1740 | 1/1   | 0.93 | 0.44 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3059 | 1/1   | 0.93 | 0.33 | 61,61,61,61                 | 0     |
| 55  | MG   | DA    | 3348 | 1/1   | 0.93 | 0.19 | 56,56,56,56                 | 0     |
| 55  | MG   | DA    | 3349 | 1/1   | 0.93 | 0.18 | 78,78,78,78                 | 0     |
| 55  | MG   | CA    | 1694 | 1/1   | 0.93 | 0.18 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3061 | 1/1   | 0.93 | 0.30 | 53,53,53,53                 | 0     |
| 55  | MG   | BA    | 3415 | 1/1   | 0.93 | 0.17 | 65,65,65,65                 | 0     |
| 55  | MG   | AA    | 1608 | 1/1   | 0.93 | 0.22 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3417 | 1/1   | 0.93 | 0.34 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3450 | 1/1   | 0.93 | 0.26 | 54,54,54,54                 | 0     |
| 55  | MG   | CA    | 1699 | 1/1   | 0.93 | 0.54 | 87,87,87,87                 | 0     |
| 55  | MG   | DA    | 3071 | 1/1   | 0.93 | 0.43 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3266 | 1/1   | 0.93 | 0.35 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3188 | 1/1   | 0.93 | 0.24 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3170 | 1/1   | 0.93 | 0.31 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3461 | 1/1   | 0.93 | 0.35 | 97,97,97,97                 | 0     |
| 55  | MG   | AA    | 1693 | 1/1   | 0.93 | 0.22 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3340 | 1/1   | 0.93 | 0.24 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3528 | 1/1   | 0.93 | 0.21 | 32,32,32,32                 | 0     |
| 55  | MG   | BA    | 3529 | 1/1   | 0.93 | 0.30 | 42,42,42,42                 | 0     |
| 55  | MG   | DA    | 3175 | 1/1   | 0.93 | 0.33 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3227 | 1/1   | 0.93 | 0.30 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3276 | 1/1   | 0.93 | 0.14 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3108 | 1/1   | 0.93 | 0.28 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3533 | 1/1   | 0.93 | 0.37 | 91,91,91,91                 | 0     |
| 55  | MG   | DA    | 3472 | 1/1   | 0.93 | 0.20 | 53,53,53,53                 | 0     |
| 55  | MG   | DA    | 3083 | 1/1   | 0.93 | 0.16 | 65,65,65,65                 | 0     |
| 55  | MG   | AA    | 1675 | 1/1   | 0.93 | 0.15 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BF    | 301  | 1/1   | 0.93 | 0.16 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3151 | 1/1   | 0.93 | 0.48 | 97,97,97,97                 | 0     |
| 55  | MG   | BA    | 3536 | 1/1   | 0.93 | 0.07 | 37,37,37,37                 | 0     |
| 55  | MG   | DA    | 3090 | 1/1   | 0.93 | 0.30 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3153 | 1/1   | 0.93 | 0.33 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3110 | 1/1   | 0.93 | 0.22 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3093 | 1/1   | 0.93 | 0.26 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3004 | 1/1   | 0.93 | 0.21 | 36,36,36,36                 | 0     |
| 55  | MG   | BA    | 3388 | 1/1   | 0.93 | 0.23 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3097 | 1/1   | 0.93 | 0.30 | 53,53,53,53                 | 0     |
| 55  | MG   | BA    | 3055 | 1/1   | 0.93 | 0.48 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3010 | 1/1   | 0.93 | 0.23 | 53,53,53,53                 | 0     |
| 55  | MG   | BA    | 3431 | 1/1   | 0.93 | 0.17 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3200 | 1/1   | 0.93 | 0.37 | 55,55,55,55                 | 0     |
| 55  | MG   | CA    | 1721 | 1/1   | 0.93 | 0.30 | 82,82,82,82                 | 0     |
| 55  | MG   | DA    | 3204 | 1/1   | 0.93 | 0.17 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3311 | 1/1   | 0.93 | 0.28 | 68,68,68,68                 | 0     |
| 55  | MG   | BA    | 3157 | 1/1   | 0.93 | 0.31 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3434 | 1/1   | 0.93 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3435 | 1/1   | 0.93 | 0.29 | 49,49,49,49                 | 0     |
| 55  | MG   | BA    | 3392 | 1/1   | 0.93 | 0.35 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3019 | 1/1   | 0.93 | 0.24 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3020 | 1/1   | 0.93 | 0.20 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3275 | 1/1   | 0.93 | 0.24 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3394 | 1/1   | 0.93 | 0.26 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3486 | 1/1   | 0.93 | 0.23 | 42,42,42,42                 | 0     |
| 55  | MG   | BA    | 3034 | 1/1   | 0.93 | 0.23 | 40,40,40,40                 | 0     |
| 55  | MG   | CA    | 1607 | 1/1   | 0.93 | 0.14 | 70,70,70,70                 | 0     |
| 55  | MG   | DA    | 3027 | 1/1   | 0.93 | 0.11 | 47,47,47,47                 | 0     |
| 55  | MG   | CA    | 1734 | 1/1   | 0.93 | 0.19 | 80,80,80,80                 | 0     |
| 55  | MG   | CA    | 1608 | 1/1   | 0.93 | 0.17 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3009 | 1/1   | 0.93 | 0.23 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3036 | 1/1   | 0.93 | 0.22 | 58,58,58,58                 | 0     |
| 55  | MG   | CA    | 1798 | 1/1   | 0.93 | 0.34 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3010 | 1/1   | 0.93 | 0.26 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3408 | 1/1   | 0.93 | 0.17 | 66,66,66,66                 | 0     |
| 55  | MG   | DA    | 3224 | 1/1   | 0.93 | 0.15 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3011 | 1/1   | 0.93 | 0.29 | 40,40,40,40                 | 0     |
| 55  | MG   | DA    | 3130 | 1/1   | 0.93 | 0.25 | 49,49,49,49                 | 0     |
| 55  | MG   | CA    | 1801 | 1/1   | 0.93 | 0.27 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3498 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 55  | MG   | AA    | 1662 | 1/1   | 0.93 | 0.15 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1647 | 1/1   | 0.93 | 0.31 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3416 | 1/1   | 0.93 | 0.48 | 77,77,77,77                 | 0     |
| 55  | MG   | CA    | 1649 | 1/1   | 0.94 | 0.50 | 77,77,77,77                 | 0     |
| 55  | MG   | AA    | 1627 | 1/1   | 0.94 | 0.21 | 62,62,62,62                 | 0     |
| 55  | MG   | DA    | 3006 | 1/1   | 0.94 | 0.26 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3094 | 1/1   | 0.94 | 0.30 | 68,68,68,68                 | 0     |
| 55  | MG   | BA    | 3018 | 1/1   | 0.94 | 0.30 | 44,44,44,44                 | 0     |
| 55  | MG   | B0    | 201  | 1/1   | 0.94 | 0.23 | 46,46,46,46                 | 0     |
| 55  | MG   | DA    | 3433 | 1/1   | 0.94 | 0.44 | 50,50,50,50                 | 0     |
| 55  | MG   | DA    | 3086 | 1/1   | 0.94 | 0.46 | 75,75,75,75                 | 0     |
| 55  | MG   | CA    | 1654 | 1/1   | 0.94 | 0.25 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3260 | 1/1   | 0.94 | 0.27 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3174 | 1/1   | 0.94 | 0.27 | 46,46,46,46                 | 0     |
| 55  | MG   | DA    | 3089 | 1/1   | 0.94 | 0.45 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3044 | 1/1   | 0.94 | 0.17 | 68,68,68,68                 | 0     |
| 55  | MG   | AA    | 1684 | 1/1   | 0.94 | 0.27 | 83,83,83,83                 | 0     |
| 55  | MG   | BA    | 3307 | 1/1   | 0.94 | 0.39 | 79,79,79,79                 | 0     |
| 55  | MG   | CA    | 1724 | 1/1   | 0.94 | 0.13 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3177 | 1/1   | 0.94 | 0.17 | 34,34,34,34                 | 0     |
| 55  | MG   | BA    | 3309 | 1/1   | 0.94 | 0.40 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3269 | 1/1   | 0.94 | 0.29 | 78,78,78,78                 | 0     |
| 55  | MG   | DA    | 3018 | 1/1   | 0.94 | 0.22 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3130 | 1/1   | 0.94 | 0.36 | 50,50,50,50                 | 0     |
| 55  | MG   | CA    | 1789 | 1/1   | 0.94 | 0.17 | 71,71,71,71                 | 0     |
| 55  | MG   | AA    | 1718 | 1/1   | 0.94 | 0.09 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3441 | 1/1   | 0.94 | 0.22 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3186 | 1/1   | 0.94 | 0.20 | 60,60,60,60                 | 0     |
| 55  | MG   | CA    | 1602 | 1/1   | 0.94 | 0.32 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3455 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 55  | MG   | BA    | 3313 | 1/1   | 0.94 | 0.20 | 74,74,74,74                 | 0     |
| 55  | MG   | AA    | 1719 | 1/1   | 0.94 | 0.24 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3105 | 1/1   | 0.94 | 0.20 | 37,37,37,37                 | 0     |
| 55  | MG   | BA    | 3133 | 1/1   | 0.94 | 0.16 | 42,42,42,42                 | 0     |
| 55  | MG   | AA    | 1667 | 1/1   | 0.94 | 0.51 | 78,78,78,78                 | 0     |
| 55  | MG   | BA    | 3496 | 1/1   | 0.94 | 0.17 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3197 | 1/1   | 0.94 | 0.21 | 48,48,48,48                 | 0     |
| 55  | MG   | DA    | 3109 | 1/1   | 0.94 | 0.29 | 55,55,55,55                 | 0     |
| 55  | MG   | BA    | 3497 | 1/1   | 0.94 | 0.12 | 30,30,30,30                 | 0     |
| 55  | MG   | BA    | 3102 | 1/1   | 0.94 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3201 | 1/1   | 0.94 | 0.24 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3202 | 1/1   | 0.94 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3470 | 1/1   | 0.94 | 0.32 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3500 | 1/1   | 0.94 | 0.45 | 64,64,64,64                 | 0     |
| 55  | MG   | BA    | 3360 | 1/1   | 0.94 | 0.26 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3116 | 1/1   | 0.94 | 0.28 | 61,61,61,61                 | 0     |
| 55  | MG   | BA    | 3558 | 1/1   | 0.94 | 0.31 | 85,85,85,85                 | 0     |
| 55  | MG   | DA    | 3475 | 1/1   | 0.94 | 0.25 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3072 | 1/1   | 0.94 | 0.33 | 67,67,67,67                 | 0     |
| 55  | MG   | BA    | 3073 | 1/1   | 0.94 | 0.26 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3025 | 1/1   | 0.94 | 0.34 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3145 | 1/1   | 0.94 | 0.16 | 54,54,54,54                 | 0     |
| 55  | MG   | BA    | 3506 | 1/1   | 0.94 | 0.27 | 73,73,73,73                 | 0     |
| 55  | MG   | AA    | 1817 | 1/1   | 0.94 | 0.14 | 61,61,61,61                 | 0     |
| 55  | MG   | DA    | 3385 | 1/1   | 0.94 | 0.29 | 86,86,86,86                 | 0     |
| 55  | MG   | DA    | 3483 | 1/1   | 0.94 | 0.42 | 82,82,82,82                 | 0     |
| 55  | MG   | BA    | 3147 | 1/1   | 0.94 | 0.23 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3454 | 1/1   | 0.94 | 0.41 | 80,80,80,80                 | 0     |
| 55  | MG   | AA    | 1602 | 1/1   | 0.94 | 0.19 | 71,71,71,71                 | 0     |
| 55  | MG   | DA    | 3302 | 1/1   | 0.94 | 0.33 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3005 | 1/1   | 0.94 | 0.25 | 40,40,40,40                 | 0     |
| 55  | MG   | DA    | 3132 | 1/1   | 0.94 | 0.24 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3239 | 1/1   | 0.94 | 0.12 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3327 | 1/1   | 0.94 | 0.21 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3006 | 1/1   | 0.94 | 0.36 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3241 | 1/1   | 0.94 | 0.25 | 62,62,62,62                 | 0     |
| 55  | MG   | BA    | 3032 | 1/1   | 0.94 | 0.22 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3518 | 1/1   | 0.94 | 0.35 | 36,36,36,36                 | 0     |
| 55  | MG   | BA    | 3008 | 1/1   | 0.94 | 0.25 | 44,44,44,44                 | 0     |
| 55  | MG   | DA    | 3313 | 1/1   | 0.94 | 0.06 | 84,84,84,84                 | 0     |
| 55  | MG   | CA    | 1695 | 1/1   | 0.94 | 0.35 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3419 | 1/1   | 0.94 | 0.34 | 80,80,80,80                 | 0     |
| 55  | MG   | AA    | 1657 | 1/1   | 0.94 | 0.26 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3145 | 1/1   | 0.94 | 0.22 | 54,54,54,54                 | 0     |
| 55  | MG   | DA    | 3058 | 1/1   | 0.94 | 0.24 | 53,53,53,53                 | 0     |
| 55  | MG   | DA    | 3230 | 1/1   | 0.94 | 0.40 | 74,74,74,74                 | 0     |
| 55  | MG   | BA    | 3465 | 1/1   | 0.94 | 0.35 | 61,61,61,61                 | 0     |
| 55  | MG   | CA    | 1635 | 1/1   | 0.94 | 0.33 | 72,72,72,72                 | 0     |
| 55  | MG   | BB    | 212  | 1/1   | 0.94 | 0.40 | 74,74,74,74                 | 0     |
| 55  | MG   | AA    | 1707 | 1/1   | 0.94 | 0.14 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3065 | 1/1   | 0.94 | 0.33 | 75,75,75,75                 | 0     |
| 55  | MG   | BA    | 3117 | 1/1   | 0.94 | 0.28 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3118 | 1/1   | 0.94 | 0.31 | 49,49,49,49                 | 0     |
| 55  | MG   | BB    | 216  | 1/1   | 0.94 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3084 | 1/1   | 0.94 | 0.26 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3240 | 1/1   | 0.94 | 0.20 | 55,55,55,55                 | 0     |
| 55  | MG   | AA    | 1789 | 1/1   | 0.94 | 0.23 | 63,63,63,63                 | 0     |
| 55  | MG   | DA    | 3158 | 1/1   | 0.94 | 0.27 | 80,80,80,80                 | 0     |
| 55  | MG   | AA    | 1658 | 1/1   | 0.94 | 0.24 | 56,56,56,56                 | 0     |
| 55  | MG   | D5    | 101  | 1/1   | 0.94 | 0.28 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3165 | 1/1   | 0.94 | 0.24 | 60,60,60,60                 | 0     |
| 55  | MG   | D7    | 101  | 1/1   | 0.94 | 0.35 | 86,86,86,86                 | 0     |
| 55  | MG   | AA    | 1811 | 1/1   | 0.94 | 0.33 | 65,65,65,65                 | 0     |
| 55  | MG   | DA    | 3078 | 1/1   | 0.94 | 0.37 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3015 | 1/1   | 0.94 | 0.25 | 35,35,35,35                 | 0     |
| 55  | MG   | BA    | 3016 | 1/1   | 0.95 | 0.30 | 48,48,48,48                 | 0     |
| 55  | MG   | DA    | 3131 | 1/1   | 0.95 | 0.26 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3160 | 1/1   | 0.95 | 0.21 | 44,44,44,44                 | 0     |
| 55  | MG   | BA    | 3264 | 1/1   | 0.95 | 0.32 | 61,61,61,61                 | 0     |
| 55  | MG   | AA    | 1668 | 1/1   | 0.95 | 0.33 | 68,68,68,68                 | 0     |
| 55  | MG   | CA    | 1728 | 1/1   | 0.95 | 0.32 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3120 | 1/1   | 0.95 | 0.26 | 42,42,42,42                 | 0     |
| 55  | MG   | BA    | 3212 | 1/1   | 0.95 | 0.30 | 68,68,68,68                 | 0     |
| 55  | MG   | DA    | 3138 | 1/1   | 0.95 | 0.32 | 54,54,54,54                 | 0     |
| 55  | MG   | DA    | 3247 | 1/1   | 0.95 | 0.27 | 58,58,58,58                 | 0     |
| 55  | MG   | CA    | 1818 | 1/1   | 0.95 | 0.32 | 81,81,81,81                 | 0     |
| 55  | MG   | DA    | 3249 | 1/1   | 0.95 | 0.10 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3214 | 1/1   | 0.95 | 0.33 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3296 | 1/1   | 0.95 | 0.24 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3215 | 1/1   | 0.95 | 0.22 | 44,44,44,44                 | 0     |
| 55  | MG   | CA    | 1689 | 1/1   | 0.95 | 0.24 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3254 | 1/1   | 0.95 | 0.34 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3144 | 1/1   | 0.95 | 0.40 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3030 | 1/1   | 0.95 | 0.23 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3140 | 1/1   | 0.95 | 0.33 | 67,67,67,67                 | 0     |
| 55  | MG   | BA    | 3167 | 1/1   | 0.95 | 0.27 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3085 | 1/1   | 0.95 | 0.23 | 38,38,38,38                 | 0     |
| 55  | MG   | AN    | 201  | 1/1   | 0.95 | 0.11 | 67,67,67,67                 | 0     |
| 55  | MG   | AA    | 1612 | 1/1   | 0.95 | 0.07 | 88,88,88,88                 | 0     |
| 55  | MG   | DA    | 3041 | 1/1   | 0.95 | 0.37 | 47,47,47,47                 | 0     |
| 55  | MG   | DA    | 3429 | 1/1   | 0.95 | 0.30 | 54,54,54,54                 | 0     |
| 55  | MG   | BA    | 3359 | 1/1   | 0.95 | 0.40 | 78,78,78,78                 | 0     |
| 55  | MG   | AA    | 1721 | 1/1   | 0.95 | 0.26 | 60,60,60,60                 | 0     |
| 55  | MG   | AC    | 104  | 1/1   | 0.95 | 0.26 | 64,64,64,64                 | 0     |
| 55  | MG   | AA    | 1659 | 1/1   | 0.95 | 0.29 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3077 | 1/1   | 0.95 | 0.06 | 83,83,83,83                 | 0     |
| 55  | MG   | BE    | 301  | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BE    | 302  | 1/1   | 0.95 | 0.29 | 40,40,40,40                 | 0     |
| 55  | MG   | BA    | 3002 | 1/1   | 0.95 | 0.25 | 40,40,40,40                 | 0     |
| 55  | MG   | BA    | 3519 | 1/1   | 0.95 | 0.23 | 24,24,24,24                 | 0     |
| 55  | MG   | CA    | 1664 | 1/1   | 0.95 | 0.28 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3003 | 1/1   | 0.95 | 0.19 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3337 | 1/1   | 0.95 | 0.29 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3096 | 1/1   | 0.95 | 0.31 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3038 | 1/1   | 0.95 | 0.14 | 33,33,33,33                 | 0     |
| 55  | MG   | BA    | 3179 | 1/1   | 0.95 | 0.26 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3370 | 1/1   | 0.95 | 0.33 | 78,78,78,78                 | 0     |
| 55  | MG   | AA    | 1692 | 1/1   | 0.95 | 0.26 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3527 | 1/1   | 0.95 | 0.05 | 40,40,40,40                 | 0     |
| 55  | MG   | BA    | 3490 | 1/1   | 0.95 | 0.23 | 36,36,36,36                 | 0     |
| 55  | MG   | CA    | 1631 | 1/1   | 0.95 | 0.22 | 65,65,65,65                 | 0     |
| 55  | MG   | CA    | 1715 | 1/1   | 0.95 | 0.32 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3452 | 1/1   | 0.95 | 0.25 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3286 | 1/1   | 0.95 | 0.32 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3494 | 1/1   | 0.95 | 0.30 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3456 | 1/1   | 0.95 | 0.32 | 57,57,57,57                 | 0     |
| 55  | MG   | AA    | 1661 | 1/1   | 0.95 | 0.26 | 56,56,56,56                 | 0     |
| 55  | MG   | CA    | 1636 | 1/1   | 0.95 | 0.21 | 53,53,53,53                 | 0     |
| 55  | MG   | CA    | 1637 | 1/1   | 0.95 | 0.14 | 70,70,70,70                 | 0     |
| 55  | MG   | DA    | 3073 | 1/1   | 0.95 | 0.35 | 84,84,84,84                 | 0     |
| 55  | MG   | BW    | 101  | 1/1   | 0.95 | 0.15 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3401 | 1/1   | 0.95 | 0.10 | 75,75,75,75                 | 0     |
| 55  | MG   | DA    | 3075 | 1/1   | 0.95 | 0.23 | 57,57,57,57                 | 0     |
| 56  | ZN   | CG    | 303  | 1/1   | 0.95 | 0.23 | 109,109,109,109             | 0     |
| 55  | MG   | DA    | 3303 | 1/1   | 0.96 | 0.19 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3023 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3492 | 1/1   | 0.96 | 0.49 | 54,54,54,54                 | 0     |
| 55  | MG   | DA    | 3096 | 1/1   | 0.96 | 0.30 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3255 | 1/1   | 0.96 | 0.26 | 50,50,50,50                 | 0     |
| 55  | MG   | CA    | 1634 | 1/1   | 0.96 | 0.35 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3007 | 1/1   | 0.96 | 0.14 | 36,36,36,36                 | 0     |
| 55  | MG   | DA    | 3063 | 1/1   | 0.96 | 0.20 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3273 | 1/1   | 0.96 | 0.29 | 73,73,73,73                 | 0     |
| 55  | MG   | CA    | 1717 | 1/1   | 0.96 | 0.36 | 73,73,73,73                 | 0     |
| 55  | MG   | CA    | 1718 | 1/1   | 0.96 | 0.14 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3067 | 1/1   | 0.96 | 0.17 | 50,50,50,50                 | 0     |
| 55  | MG   | CA    | 1663 | 1/1   | 0.96 | 0.32 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3185 | 1/1   | 0.96 | 0.10 | 46,46,46,46                 | 0     |
| 55  | MG   | DA    | 3317 | 1/1   | 0.96 | 0.26 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3070 | 1/1   | 0.96 | 0.30 | 49,49,49,49                 | 0     |
| 55  | MG   | DA    | 3150 | 1/1   | 0.96 | 0.39 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3193 | 1/1   | 0.96 | 0.35 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3476 | 1/1   | 0.96 | 0.24 | 47,47,47,47                 | 0     |
| 55  | MG   | DA    | 3002 | 1/1   | 0.96 | 0.31 | 48,48,48,48                 | 0     |
| 55  | MG   | BA    | 3213 | 1/1   | 0.96 | 0.24 | 41,41,41,41                 | 0     |
| 55  | MG   | DA    | 3004 | 1/1   | 0.96 | 0.10 | 39,39,39,39                 | 0     |
| 55  | MG   | BA    | 3164 | 1/1   | 0.96 | 0.25 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3523 | 1/1   | 0.96 | 0.30 | 36,36,36,36                 | 0     |
| 55  | MG   | BA    | 3088 | 1/1   | 0.96 | 0.27 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 3261 | 1/1   | 0.96 | 0.32 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3118 | 1/1   | 0.96 | 0.30 | 55,55,55,55                 | 0     |
| 55  | MG   | BB    | 205  | 1/1   | 0.96 | 0.17 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3111 | 1/1   | 0.96 | 0.16 | 55,55,55,55                 | 0     |
| 55  | MG   | AA    | 1641 | 1/1   | 0.96 | 0.19 | 56,56,56,56                 | 0     |
| 55  | MG   | DA    | 3122 | 1/1   | 0.96 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | AA    | 1603 | 1/1   | 0.96 | 0.20 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3552 | 1/1   | 0.96 | 0.22 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3170 | 1/1   | 0.96 | 0.19 | 54,54,54,54                 | 0     |
| 55  | MG   | BA    | 3114 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 55  | MG   | DA    | 3049 | 1/1   | 0.96 | 0.32 | 55,55,55,55                 | 0     |
| 55  | MG   | BA    | 3531 | 1/1   | 0.96 | 0.18 | 31,31,31,31                 | 0     |
| 55  | MG   | BA    | 3251 | 1/1   | 0.96 | 0.38 | 80,80,80,80                 | 0     |
| 55  | MG   | DA    | 3427 | 1/1   | 0.96 | 0.24 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3303 | 1/1   | 0.96 | 0.34 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3207 | 1/1   | 0.96 | 0.48 | 70,70,70,70                 | 0     |
| 55  | MG   | BA    | 3152 | 1/1   | 0.96 | 0.27 | 58,58,58,58                 | 0     |
| 55  | MG   | BA    | 3142 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 55  | MG   | BA    | 3491 | 1/1   | 0.96 | 0.21 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3014 | 1/1   | 0.97 | 0.34 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3193 | 1/1   | 0.97 | 0.04 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3040 | 1/1   | 0.97 | 0.29 | 74,74,74,74                 | 0     |
| 55  | MG   | DA    | 3430 | 1/1   | 0.97 | 0.35 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3092 | 1/1   | 0.97 | 0.20 | 67,67,67,67                 | 0     |
| 55  | MG   | DA    | 3191 | 1/1   | 0.97 | 0.41 | 55,55,55,55                 | 0     |
| 55  | MG   | BA    | 3363 | 1/1   | 0.97 | 0.26 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 3134 | 1/1   | 0.97 | 0.15 | 59,59,59,59                 | 0     |
| 55  | MG   | AA    | 1632 | 1/1   | 0.97 | 0.16 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3111 | 1/1   | 0.97 | 0.17 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3112 | 1/1   | 0.97 | 0.26 | 63,63,63,63                 | 0     |
| 55  | MG   | BA    | 3150 | 1/1   | 0.97 | 0.35 | 49,49,49,49                 | 0     |
| 55  | MG   | AA    | 1677 | 1/1   | 0.97 | 0.26 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3057 | 1/1   | 0.97 | 0.09 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3020 | 1/1   | 0.97 | 0.15 | 29,29,29,29                 | 0     |
| 55  | MG   | BA    | 3221 | 1/1   | 0.97 | 0.38 | 59,59,59,59                 | 0     |
| 55  | MG   | B7    | 101  | 1/1   | 0.97 | 0.24 | 72,72,72,72                 | 0     |
| 55  | MG   | BA    | 3068 | 1/1   | 0.97 | 0.31 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3186 | 1/1   | 0.97 | 0.16 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3244 | 1/1   | 0.97 | 0.11 | 34,34,34,34                 | 0     |
| 55  | MG   | BA    | 3031 | 1/1   | 0.97 | 0.30 | 54,54,54,54                 | 0     |
| 55  | MG   | BA    | 3021 | 1/1   | 0.97 | 0.20 | 42,42,42,42                 | 0     |
| 55  | MG   | BA    | 3515 | 1/1   | 0.97 | 0.20 | 81,81,81,81                 | 0     |
| 55  | MG   | BA    | 3143 | 1/1   | 0.97 | 0.13 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3377 | 1/1   | 0.97 | 0.37 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3182 | 1/1   | 0.97 | 0.14 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3248 | 1/1   | 0.97 | 0.10 | 34,34,34,34                 | 0     |
| 55  | MG   | DA    | 3454 | 1/1   | 0.97 | 0.27 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3208 | 1/1   | 0.97 | 0.36 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3244 | 1/1   | 0.97 | 0.40 | 80,80,80,80                 | 0     |
| 55  | MG   | BA    | 3144 | 1/1   | 0.97 | 0.32 | 39,39,39,39                 | 0     |
| 55  | MG   | BA    | 3159 | 1/1   | 0.97 | 0.23 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3062 | 1/1   | 0.98 | 0.16 | 39,39,39,39                 | 0     |
| 55  | MG   | DA    | 3123 | 1/1   | 0.98 | 0.39 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3139 | 1/1   | 0.98 | 0.31 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3091 | 1/1   | 0.98 | 0.35 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3166 | 1/1   | 0.98 | 0.15 | 28,28,28,28                 | 0     |
| 55  | MG   | BA    | 3197 | 1/1   | 0.98 | 0.33 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 3499 | 1/1   | 0.98 | 0.32 | 38,38,38,38                 | 0     |
| 55  | MG   | BA    | 3116 | 1/1   | 0.98 | 0.38 | 50,50,50,50                 | 0     |
| 55  | MG   | AA    | 1606 | 1/1   | 0.98 | 0.04 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3196 | 1/1   | 0.98 | 0.12 | 45,45,45,45                 | 0     |
| 55  | MG   | BA    | 3235 | 1/1   | 0.98 | 0.31 | 39,39,39,39                 | 0     |
| 55  | MG   | DA    | 3037 | 1/1   | 0.98 | 0.09 | 71,71,71,71                 | 0     |
| 55  | MG   | BA    | 3060 | 1/1   | 0.98 | 0.17 | 51,51,51,51                 | 0     |
| 55  | MG   | CA    | 1795 | 1/1   | 0.98 | 0.35 | 73,73,73,73                 | 0     |
| 56  | ZN   | CQ    | 101  | 1/1   | 0.98 | 0.06 | 118,118,118,118             | 0     |
| 55  | MG   | DA    | 3457 | 1/1   | 0.99 | 0.24 | 48,48,48,48                 | 0     |
| 55  | MG   | AA    | 1660 | 1/1   | 0.99 | 0.41 | 77,77,77,77                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.