



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 08:14 AM UTC

PDB ID : 7LH5 / pdb\_00007lh5  
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with plazomicin, mRNA and tRNAs  
Authors : Golkar, T.; Berghuis, A.M.; Schmeing, T.M.  
Deposited on : 2021-01-21  
Resolution : 3.27 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  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

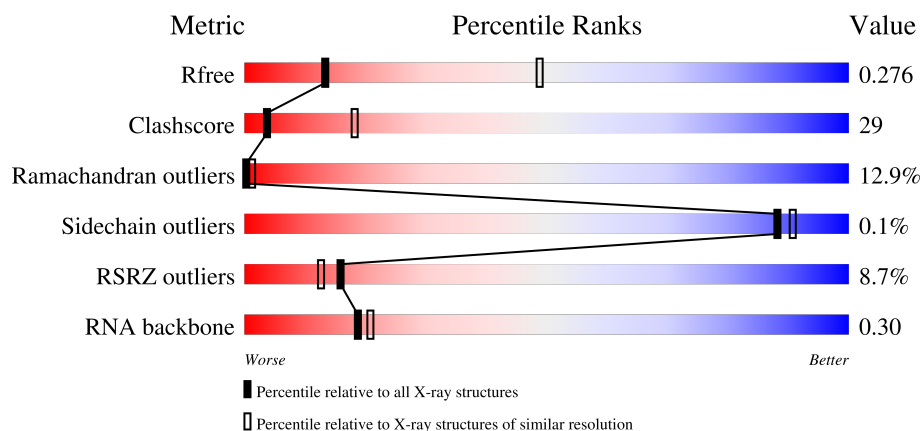
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.27 Å.

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



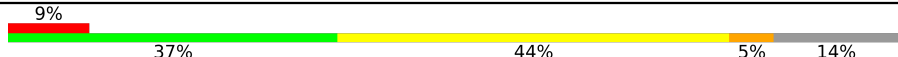
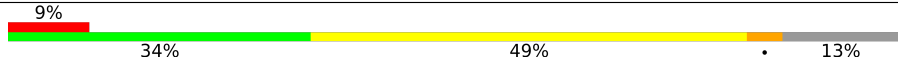
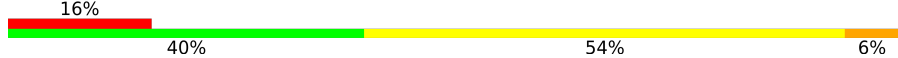
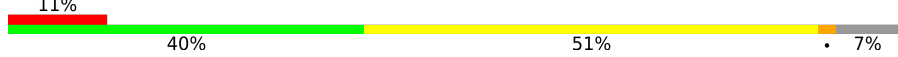
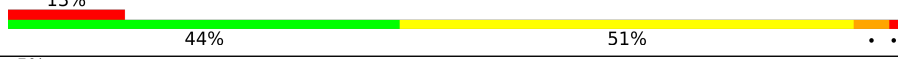
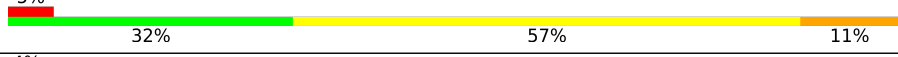
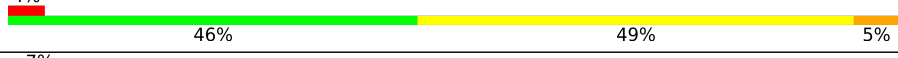
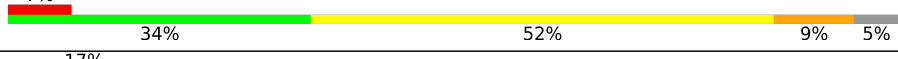
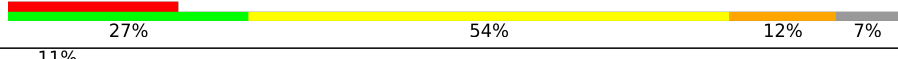
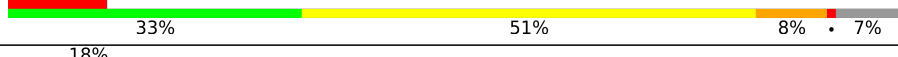
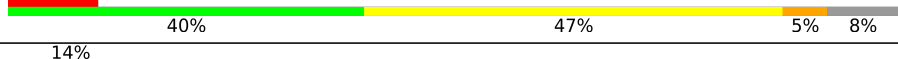
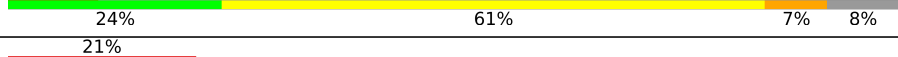
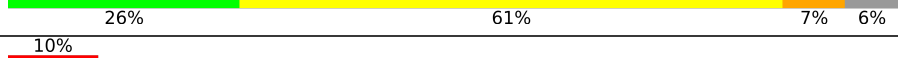
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1303 (3.30-3.26)                                      |
| Clashscore            | 190562                      | 1354 (3.30-3.26)                                      |
| Ramachandran outliers | 187476                      | 1334 (3.30-3.26)                                      |
| Sidechain outliers    | 187428                      | 1333 (3.30-3.26)                                      |
| RSRZ outliers         | 180081                      | 1303 (3.30-3.26)                                      |
| RNA backbone          | 3983                        | 1020 (3.58-2.98)                                      |

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    | 1520   | <div> <div>3%</div> <div>25%</div> <div>47%</div> <div>27%</div> <div>..</div> </div>  |
| 1   | CA    | 1520   | <div> <div>%</div> <div>25%</div> <div>52%</div> <div>22%</div> <div>.</div> </div>    |
| 2   | AB    | 256    | <div> <div>13%</div> <div>22%</div> <div>57%</div> <div>7%</div> <div>15%</div> </div> |
| 2   | CB    | 256    | <div> <div>5%</div> <div>27%</div> <div>59%</div> <div>5%</div> <div>9%</div> </div>   |

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | CO    | 89     |                  |
| 16  | AP    | 88     |                  |
| 16  | CP    | 88     |                  |
| 17  | AQ    | 105    |                  |
| 17  | CQ    | 105    |                  |
| 18  | AR    | 88     |                  |
| 18  | CR    | 88     |                  |
| 19  | AS    | 93     |                  |
| 19  | CS    | 93     |                  |
| 20  | AT    | 106    |                  |
| 20  | CT    | 106    |                  |
| 21  | AU    | 27     |                  |
| 21  | CU    | 27     |                  |
| 22  | AV    | 77     |                  |
| 22  | CV    | 77     |                  |
| 23  | AW    | 76     |                  |
| 23  | AY    | 76     |                  |
| 23  | CW    | 76     |                  |
| 23  | CY    | 76     |                  |
| 24  | AX    | 24     |                  |
| 24  | CX    | 24     |                  |
| 25  | B0    | 85     |                  |
| 25  | D0    | 85     |                  |
| 26  | B1    | 98     |                  |
| 26  | D1    | 98     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | B2    | 72     |                  |
| 27  | D2    | 72     |                  |
| 28  | B3    | 60     |                  |
| 28  | D3    | 60     |                  |
| 29  | B4    | 71     |                  |
| 29  | D4    | 71     |                  |
| 30  | B5    | 60     |                  |
| 30  | D5    | 60     |                  |
| 31  | B6    | 54     |                  |
| 31  | D6    | 54     |                  |
| 32  | B7    | 49     |                  |
| 32  | D7    | 49     |                  |
| 33  | B8    | 65     |                  |
| 33  | D8    | 65     |                  |
| 34  | B9    | 37     |                  |
| 34  | D9    | 37     |                  |
| 35  | BA    | 2839   |                  |
| 35  | DA    | 2839   |                  |
| 36  | BB    | 122    |                  |
| 36  | DB    | 122    |                  |
| 37  | BC    | 229    |                  |
| 37  | DC    | 229    |                  |
| 38  | BD    | 276    |                  |
| 38  | DD    | 276    |                  |
| 39  | BE    | 206    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | DE    | 206    |                  |
| 40  | BF    | 210    |                  |
| 40  | DF    | 210    |                  |
| 41  | BG    | 182    |                  |
| 41  | DG    | 182    |                  |
| 42  | BH    | 180    |                  |
| 42  | DH    | 180    |                  |
| 43  | BI    | 148    |                  |
| 43  | DI    | 148    |                  |
| 44  | BJ    | 173    |                  |
| 44  | DJ    | 173    |                  |
| 45  | BK    | 147    |                  |
| 45  | DK    | 147    |                  |
| 46  | BN    | 140    |                  |
| 46  | DN    | 140    |                  |
| 47  | BO    | 122    |                  |
| 47  | DO    | 122    |                  |
| 48  | BP    | 150    |                  |
| 48  | DP    | 150    |                  |
| 49  | BQ    | 141    |                  |
| 49  | DQ    | 141    |                  |
| 50  | BR    | 118    |                  |
| 50  | DR    | 118    |                  |
| 51  | BS    | 112    |                  |
| 51  | DS    | 112    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | BT    | 146    |                  |
| 52  | DT    | 146    |                  |
| 53  | BU    | 118    |                  |
| 53  | DU    | 118    |                  |
| 54  | BV    | 101    |                  |
| 54  | DV    | 101    |                  |
| 55  | BW    | 113    |                  |
| 55  | DW    | 113    |                  |
| 56  | BX    | 96     |                  |
| 56  | DX    | 96     |                  |
| 57  | BY    | 110    |                  |
| 57  | DY    | 110    |                  |
| 58  | BZ    | 206    |                  |
| 58  | DZ    | 206    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | AW    | 104  | -         | -        | -       | X                |
| 59  | MG   | BA    | 3453 | -         | -        | -       | X                |

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 296449 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    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32329 | 14390 | 5992 | 10444 | 1503 |         |         |       |
| 1   | CA    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32332 | 14390 | 5992 | 10446 | 1504 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1784  | 1139 | 321 | 319 | 5 |         |         |       |
| 2   | CB    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1213 | 341 | 341 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1612  | 1016 | 314 | 281 | 1 |         |         |       |
| 3   | CC    | 207      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1620  | 1021 | 315 | 282 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |
| 4   | CD    | 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   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 724 | 217 | 201 | 4 |         |         |       |
| 5   | CE    | 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   | AF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | CF    | 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   | AG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | CG    | 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   | AH    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 705 | 215 | 193 | 3 |         |         |       |
| 8   | CH    | 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   | AI    | 121      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 947   | 599 | 186 | 162 |  |         |         |       |
| 9   | CI    | 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  | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 499 | 156 | 138 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 794   | 499 | 156 | 138 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | CK    | 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  | AL    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 956   | 603 | 193 | 159 | 1 |         |         |       |
| 12  | CL    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 970   | 611 | 195 | 163 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 922   | 570 | 189 | 161 | 2 |         |         |       |
| 13  | CM    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 946   | 585 | 195 | 164 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | AN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 312 | 104 | 71 | 4 |         |         |       |
| 14  | CN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | CO    | 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  | AP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |
| 16  | CP    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 700   | 443 | 139 | 117 | 1 |         |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | AR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |
| 18  | CR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 629   | 403 | 114 | 110 | 2 |         |         |       |
| 19  | CS    | 78       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 629   | 403 | 114 | 110 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |
| 20  | CT    | 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  | AU    | 24       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 208   | 128 | 50 | 30 |         |         |       |
| 21  | CU    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 22 is a RNA chain called P-site tRNA fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AV    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1622  | 723 | 294 | 529 | 76 |         |         |       |
| 22  | CV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1643  | 732 | 297 | 537 | 77 |         |         |       |

- Molecule 23 is a RNA chain called E-Site tRNA Phe and A-site tRNA Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 23  | AW    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |         |       |
| 23  | AY    | 19       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 410   | 183 | 78  | 130 | 19 |         |         |       |
| 23  | CW    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |         |       |
| 23  | CY    | 21       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 453   | 202 | 86  | 144 | 21 |         |         |       |

- Molecule 24 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 24  | AX    | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 255   | 115 | 46 | 82 | 12 |         |         |       |
| 24  | CX    | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 255   | 115 | 46 | 82 | 12 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | B0    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 607   | 376 | 128 | 102 | 1 |         |         |       |
| 25  | D0    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 401 | 136 | 107 | 1 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | B1    | 88       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 692   | 435 | 139 | 118 |         |         |       |
| 26  | D1    | 88       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 692   | 435 | 139 | 118 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | B2    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 420   | 263 | 84 | 72 | 1 |         |         |       |
| 27  | D2    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 446   | 279 | 88 | 78 | 1 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | B3    | 58       | Total | C   | N  | O  |   | 0       | 0       | 0     |
|     |       |          | 459   | 293 | 89 | 77 |   |         |         |       |
| 28  | D3    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 476   | 303 | 91 | 81 | 1 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 29  | B4    | 45       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 222   | 132 | 45 | 45 |         |         |       |
| 29  | D4    | 49       | Total | C   | N  | O  |         | 0       | 0     |
|     |       |          | 241   | 143 | 49 | 49 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | B5    | 54       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 261 | 84 | 68 | 5 |         |         |       |
| 30  | D5    | 60       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 467   | 293 | 91 | 77 | 6 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | B6    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 398   | 247 | 81 | 66 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | D6    | 47       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 408   | 253 | 84 | 67 | 4 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32  | B7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 32  | D7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | B8    | 63       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 507   | 326 | 101 | 78 | 2 |         |         |       |
| 33  | D8    | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 495   | 317 | 100 | 76 | 2 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 34  | B9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 34  | D9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 35 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 35  | BA    | 2824     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60821 | 27070 | 11372 | 19556 | 2823 |         |         |       |
| 35  | DA    | 2824     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60821 | 27070 | 11372 | 19556 | 2823 |         |         |       |

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 36  | BB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2576  | 1146 | 476 | 834 | 120 |         |         |       |
| 36  | DB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2551  | 1136 | 471 | 826 | 118 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 37  | BC    | 190      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1141  | 691 | 220 | 230 |         |         |       |
| 37  | DC    | 190      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1141  | 691 | 220 | 230 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 38  | BD    | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2126  | 1341 | 424 | 358 | 3 |         |         |       |
| 38  | DD    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2144  | 1353 | 428 | 360 | 3 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |
| 39  | DE    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1563  | 988 | 299 | 270 | 6 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | BF    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1615  | 1030 | 302 | 281 | 2 |         |         |       |
| 40  | DF    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1627  | 1037 | 304 | 283 | 3 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BG    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1449  | 925 | 264 | 256 | 4 |         |         |       |
| 41  | DG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BH    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1222  | 773 | 228 | 220 | 1 |         |         |       |
| 42  | DH    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 806 | 237 | 226 | 1 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | BI    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1131  | 723 | 200 | 207 | 1 |         |         |       |
| 43  | DI    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1124  | 718 | 199 | 206 | 1 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44  | BJ    | 130      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 651   | 391 | 130 | 130 |         |         |       |
| 44  | DJ    | 130      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 651   | 391 | 130 | 130 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 45  | BK    | 140      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 700   | 420 | 140 | 140 |         |         |       |
| 45  | DK    | 140      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 700   | 420 | 140 | 140 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BN    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1096  | 707 | 205 | 181 | 3 |         |         |       |
| 46  | DN    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1120  | 722 | 208 | 186 | 4 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | BO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | DO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | BP    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1099  | 684 | 225 | 188 | 2 |         |         |       |
| 48  | DP    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1114  | 692 | 227 | 193 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | BQ    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 178 | 5 |         |         |       |
| 49  | DQ    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 691 | 206 | 181 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 50  | BR    | 116      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 949   | 593 | 198 | 158 |  |         |         |       |
| 50  | DR    | 117      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |  |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 51  | BS    | 102      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 813   | 512 | 164 | 137 |  |         |         |       |
| 51  | DS    | 99       | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 781   | 492 | 158 | 131 |  |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52  | BT    | 132      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1100  | 686 | 227 | 186 | 1 |         |         |       |
| 52  | DT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | BU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 53  | DU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | BV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 54  | DV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | BW    | 111      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 558 | 174 | 152 | 2 |         |         |       |
| 55  | DW    | 111      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 558 | 174 | 152 | 2 |         |         |       |

- Molecule 56 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | BX    | 89       | Total | C   | N   | O   |   | 0       | 0       | 0     |
|     |       |          | 704   | 458 | 128 | 118 |   |         |         |       |
| 56  | DX    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 742   | 482 | 134 | 125 | 1 |         |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | BY    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 500 | 148 | 123 | 4 |         |         |       |
| 57  | DY    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 835   | 534 | 157 | 139 | 5 |         |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58  | BZ    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1403  | 897 | 252 | 252 | 2 |         |         |       |
| 58  | DZ    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1403  | 897 | 252 | 252 | 2 |         |         |       |

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 59  | AA    | 209      | Total | Mg  | 0       | 0       |
|     |       |          | 209   | 209 |         |         |
| 59  | AC    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AD    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AE    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AL    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AT    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | AV    | 7        | Total | Mg  | 0       | 0       |
|     |       |          | 7     | 7   |         |         |
| 59  | AW    | 20       | Total | Mg  | 0       | 0       |
|     |       |          | 20    | 20  |         |         |
| 59  | AX    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 59  | B0    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | B1    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 59  | B2    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | B5    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | B7    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | B8    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 59  | BA    | 457      | Total | Mg  | 0       | 0       |
|     |       |          | 457   | 457 |         |         |
| 59  | BB    | 17       | Total | Mg  | 0       | 0       |
|     |       |          | 17    | 17  |         |         |
| 59  | BC    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 59  | BE    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | BF    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 59  | BQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BS    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BU    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 59  | BV    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | BX    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | CA    | 195      | Total<br>195 | Mg<br>195 | 0       | 0       |
| 59  | CE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CG    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CI    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CU    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | CV    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 59  | CW    | 13       | Total<br>13  | Mg<br>13  | 0       | 0       |
| 59  | CX    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | D2    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 59  | D5    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 59  | DA    | 392      | Total<br>392 | Mg<br>392 | 0       | 0       |
| 59  | DB    | 12       | Total<br>12  | Mg<br>12  | 0       | 0       |
| 59  | DE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59  | DF    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 59  | DN    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 59  | DO    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 59  | DV    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

- # EDS

| Mol | Chain | Residues | Atoms       |         |        |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 60  | AA    | 1        | Total<br>41 | C<br>25 | N<br>6 | O<br>10 | 0       | 0       |
| 60  | CA    | 1        | Total<br>41 | C<br>25 | N<br>6 | O<br>10 | 0       | 0       |

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 61  | AD    | 1        | Total Zn<br>1 1 | 0       | 0       |
| 61  | AN    | 1        | Total Zn<br>1 1 | 0       | 0       |



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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 61  | B9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 61  | CD    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 61  | CN    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 61  | D9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 62 is water.

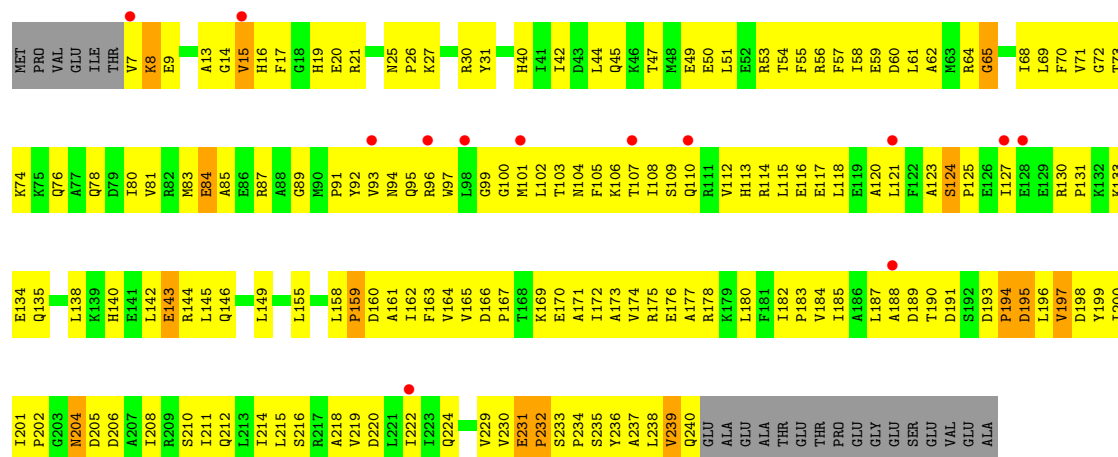
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 62  | AA    | 2        | Total<br>2 | O<br>2 | 0       | 0       |



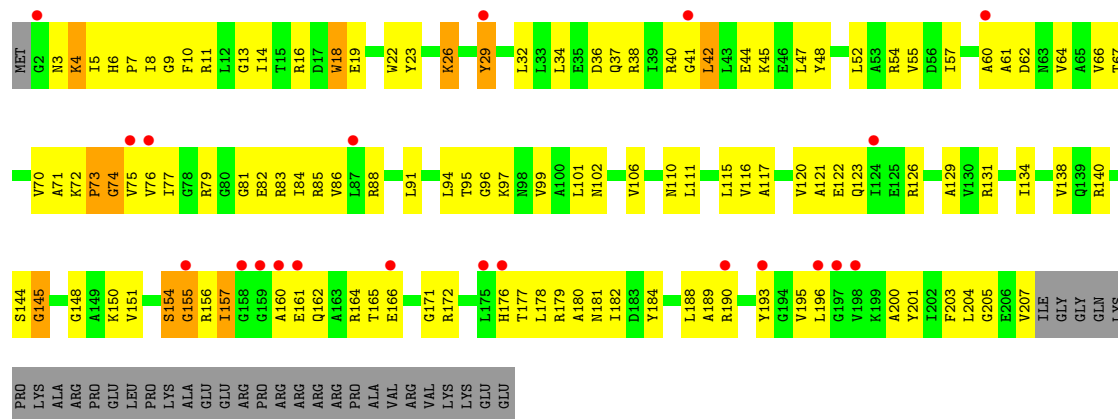


|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |        |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G963 | G964 | G965 | G966 | G967 | G968 | G969 | G970 | G971 | G972 | G973 | G974 | G975 | G976 | G977 | G978 | G979 | G980 | G981 | G982 | G983 | G984 | G985 | G986 | G987 | G988 | G989 | G990 | G991 | G992 | G993 | G994 | G995 | G1001A | G1002 | G1003 | A1004 | A1005 | C1006 | C1007 | C1008 | G1009 | G1010 | G1011 | G1012 | G1013 | A1014 | A1015 | A1016 | G1017 | G1020 | G1021 | G1022 | G1023 | G1024 | G1025 | G1026 | C1027 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| U891 | A892 | C893 | G894 | G895 | C896 | C897 | A898 | A899 | G900 | G901 | G902 | G903 | C904 | C905 | C906 | C907 | C908 | C909 | C910 | C911 | C912 | C913 | C914 | C915 | C916 | C917 | C918 | C919 | C920 | C921 | C922 | C923 | C924   | C925  | C926  | C927  | C928  | C929  | C930  | C931  | C932  | C933  | C934  | C935  | C936  | C937  | C938  | C939  | C940  | C941  | C942  | C943  | C944  | C945  | C946  | C947  | C948  | C949 | C950 | C951 | C952 | C953 | C954 | C955 | C956 | C957 | C958 | C959 | C960 | C961 | C962 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C748 | C749 | C750 | C751 | C752 | C753 | C754 | C755 | C756 | C757 | C758 | C759 | C760 | C761 | C762 | C763 | C764 | C765 | C766 | C767 | C768 | C769 | C770 | C771 | C772 | C773 | C774 | C775 | C776 | C777 | C778 | C779 | C780 | C781   | C782  | C783  | C784  | C785  | C786  | C787  | C788  | C789  | C790  | C791  | C792  | C793  | C794  | C795  | C796  | C797  | C798  | C799  | C800  | C801  | C802  | C803  | C804  | C805  | C806 | C807 | C808 | C809 | C810 | C811 | C812 | C813 | C814 | C815 | C816 | C817 | C818 | C819 | C820 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
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| G537 | G538 | A539 | G540 | G541 | G542 | G543 | G544 | G545 | G546 | G547 | G548 | U549 | U550 | U551 | U552 | U553 | U554 | U555 | U556 | U557 | U558 | U559 | U560 | U561 | U562 | U563 | U564 | U565 | U566 | U567 | U568 | U569 | U570   | U571  | U572  | U573  | U574  | U575  | U576  | U577  | U578  | U579  | U580  | U581  | U582  | U583  | U584  | U585  | U586  | U587  | U588  | U589  | U590  | U591  | U592  | U593  | U594  | U595 | U596 | U597 | U598 | U599 | U600 | U601 | U602 | U603 | U604 | U605 | U606 | U607 | U608 | U609 | U610 | U611 | U612 | U613 | U614 | U615 | U616 | U617 | U618 | U619 | U620 | U621 | U622 | U623 | U624 | U625 | U626 | U627 | U628 | U629 | U630 | U631 | U632 | U633 | U634 | U635 | U636 | U637 | U638 | U639 | U640 | U641 | U642 | U643 | U644 | U645 | U646 | U647 | U648 | U649 | U650 | U651 | U652 | U653 | U654 | U655 | U656 | U657 | U658 | U659 | U660 | U661 | U662 | U663 | U664 | U665 | U666 | U667 | U668 | U669 | U670 | U671 | U672 | U673 | U674 | U675 | U676 | U677 | U678 | U679 | U680 | U681 | U682 | U683 | U684 | U685 | U686 | U687 | U688 | U689 | U690 | U691 | U692 | U693 | U694 | U695 | U696 | U697 | U698 | U699 | U700 | U701 | U702 | U703 | U704 | U705 | U706 | U707 | U708 | U709 | U710 | U711 | U712 | U713 | U714 | U715 | U716 | U717  | U718  | U719  | U720  | U721  | U722  | U723  | U724  | U725  | U726  | U727  | U728  | U729  | U730  | U731  | U732  | U733  | U734  | U735  | U736  | U737  | U738  | U739  | U740  | U741  | U742  | U743  | U744  | U745 | U746 | U747 | U748 | U749 | U750 | U751 | U752 | U753 | U754 | U755 | U756 | U757 | U758 | U759 | U760 | U761 | U762 | U763 | U764 | U765 | U766 | U767 | U768 | U769 | U770 | U771 | U772 | U773 | U774 | U775 | U776 | U777 | U778 | U779 | U780 | U781 | U782 | U783 | U784 | U785 | U786 | U787 | U788 | U789 | U790 | U791 | U792 | U793 | U794 | U795 | U796 | U797 | U798 | U799 | U800 | U801 | U802 | U803 | U804 | U805 | U806 | U807 | U808 | U809 | U810 | U811 | U812 | U813 | U814 | U815 | U816 | U817 | U818 | U819 | U820 | U821 | U822 | U823 | U824 | U825 | U826 | U827 | U828 | U829 | U830 | U831 | U832 | U833 | U834 | U835 | U836 | U837 | U838 | U839 | U840 | U841 | U842 | U843 | U844 | U845 | U846 | U847 | U848 | U849 | U850 | U851 | U852 | U853 | U854 | U855 | U856 | U857 | U858 | U859 | U860 | U861 | U862  | U863  | U864  | U865  | U866  | U867  | U868  | U869  | U870  | U871  | U872  | U873  | U874  | U875  | U876  | U877  | U878  | U879  | U880  | U881  | U882  | U883  | U884  | U885  | U886  | U887  | U888  | U889  | U890 | U891 | U892 | U893 | U894 | U895 | U896 | U897 | U898 | U899 | U900 | U901 | U902 | U903 | U904 | U905 | U906 | U907 | U908 | U909 | U910 | U911 | U912 | U913 | U914 | U915 | U916 | U917 | U918 | U919 | U920 | U921 | U922 | U923 | U924 | U925 | U926 | U927 | U928 | U929 | U930 | U931 | U932 | U933 | U934 | U935 | U936 | U937 | U938 | U939 | U940 | U941 | U942 | U943 | U944 | U945 | U946 | U947 | U948 | U949 | U950 | U951 | U952 | U953 | U954 | U955 | U956 | U957 | U958 | U959 | U960 | U961 | U962 | U963 | U964 | U965 | U966 | U967 | U968 | U969 | U970 | U971 | U972 | U973 | U974 | U975 | U976 | U977 | U978 | U979 | U980 | U981 | U982 | U983 | U984 | U985 | U986 | U987 | U988 | U989 | U990 | U991 | U992 | U993 | U994 | U995 | U996 | U997 | U998 | U999 | G1000 | G1001 | G1002 | G1003 | G1004 | G1005 | G1006 | G1007 | G1008 | G1009 | G1010 | G1011 | G1012 | G1013 | G1014 | G1015 | G1016 | G1017 | G1018 | G1019 | G1020 | G1021 | G1022 | G1023 | G1024 | G1025 | G1026 | C1027 |
| C63  | G64  | U65  | G66  | C67  | G68  | G69  | C70  | C71  | C72  | C73  | C74  | C75  | C76  | C77  | C78  | C79  | C80  | C81  | C82  | C83  | C84  | C85  | C86  | C87  | C88  | C89  | C90  | C91  | C92  | C93  | C94  | C95  | C96    | C97   | C98   | C99   | C100  | C101  | C102  | C103  | C104  | C105  | C106  | C107  | C108  | C109  | C110  | C111  | C112  | C113  | C114  | C115  | C116  | C117  | C118  | C119  | C120  | C121 | C122 | C123 | C124 | C125 | C126 | C127 | C128 | C129 | C130 | C131 | C132 | C133 | C134 | C135 | C136 | C137 | C138 | C139 | C140 | C141 | C142 | C143 | C144 | C145 | C146 | C147 | C148 | C149 | C150 | C151 | C152 | C153 | C154 | C155 | C156 | C157 | C158 | C159 | C160 | C161 | C162 | C163 | C164 | C165 | C166 | C167 | C168 | C169 | C170 | C171 | C172 | C173 | C174 | C175 | C176 | C177 | C178 | C179 | C180 | C181 | C182 | C183 | C184 | C185 | C186 | C187 | C188 | C189 | C190 | C191 | C192 | C193 | C194 | C195 | C196 | C197 | C198 | C199 | C200 | C201 | C202 | C203 | C204 | C205 | C206 | C207 | C208 | C209 | C210 | C211 | C212 | C213 | C214 | C215 | C216 | C217 | C218 | C219 | C220 | C221 | C222 | C223 | C224 | C225 | C226 | C227 | C228 | C229 | C230 | C231 | C232 | C233 | C234 | C235 | C236 | C237 | C238 | C239 | C240 | C241 | C242 | C243  | C244  | C245  | C246  | C247  | C248  | C249  | C250  | C251  | C252  | C253  | C254  | C255  | C256  | C257  | C258  | C259  | C260  | C261  | C262  | C263  | C264  | C265  | C266  | C267  | C268  | C269  | C270  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

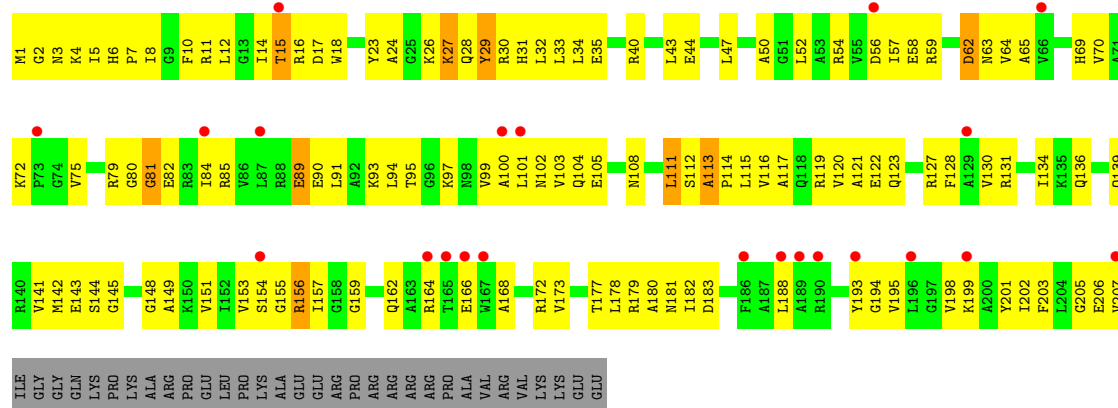




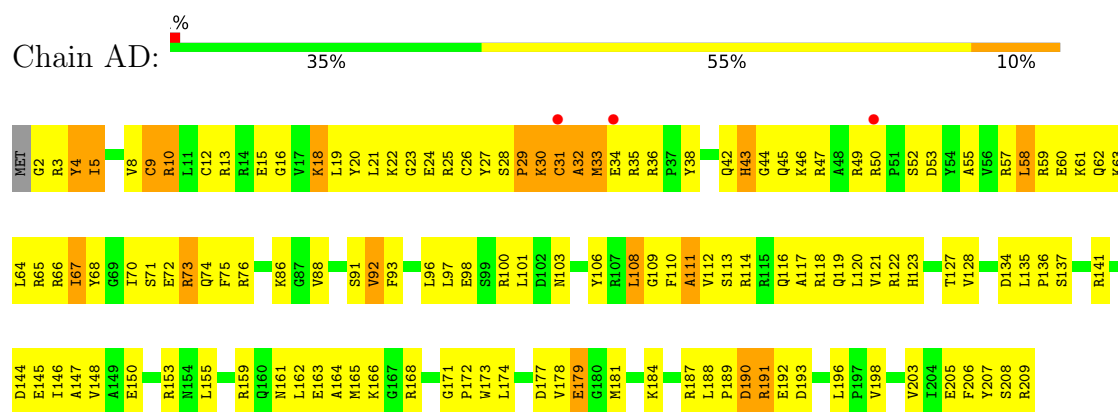
• Molecule 3: 30S ribosomal protein S3



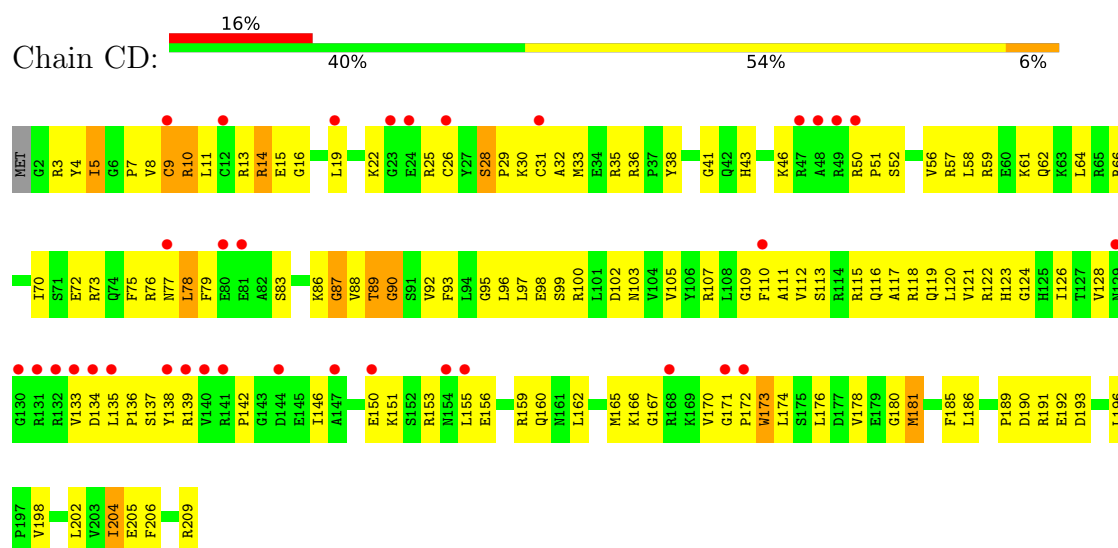
• Molecule 3: 30S ribosomal protein S3



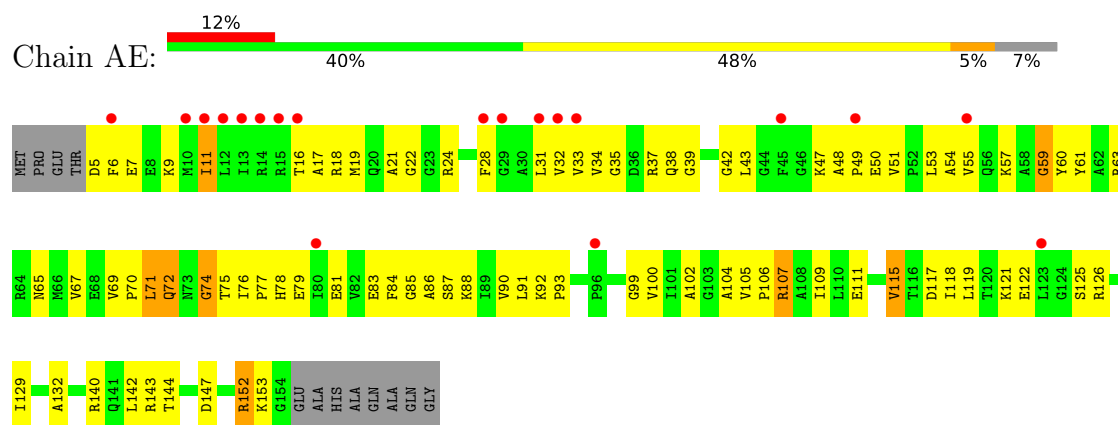
• Molecule 4: 30S ribosomal protein S4



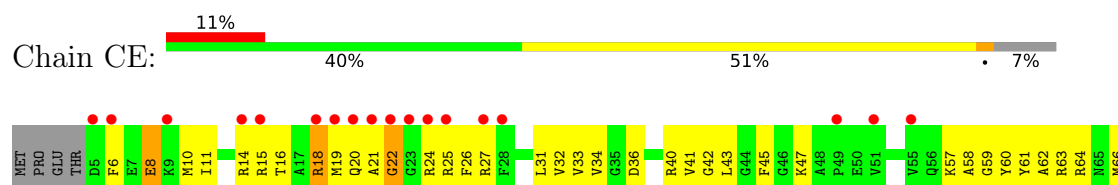
• Molecule 4: 30S ribosomal protein S4

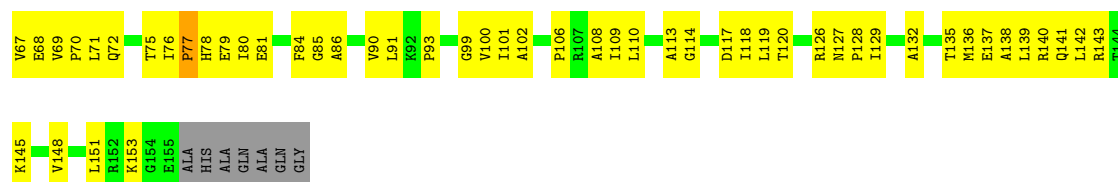


• Molecule 5: 30S ribosomal protein S5

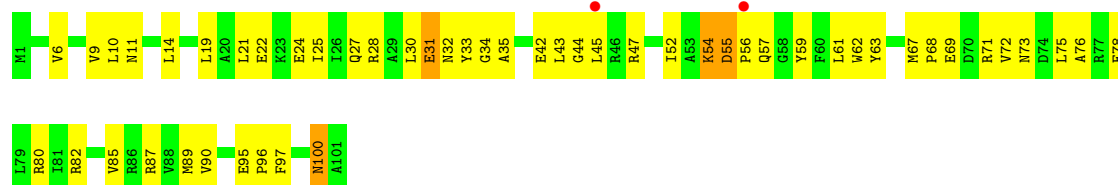


• Molecule 5: 30S ribosomal protein S5

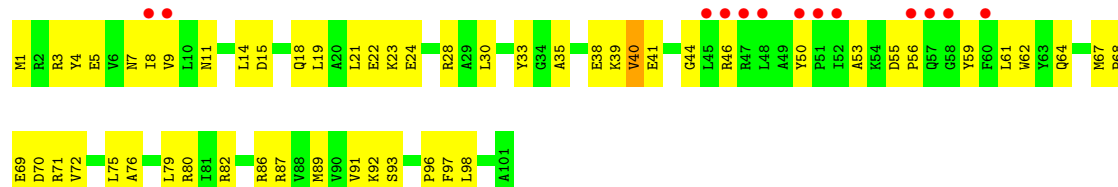




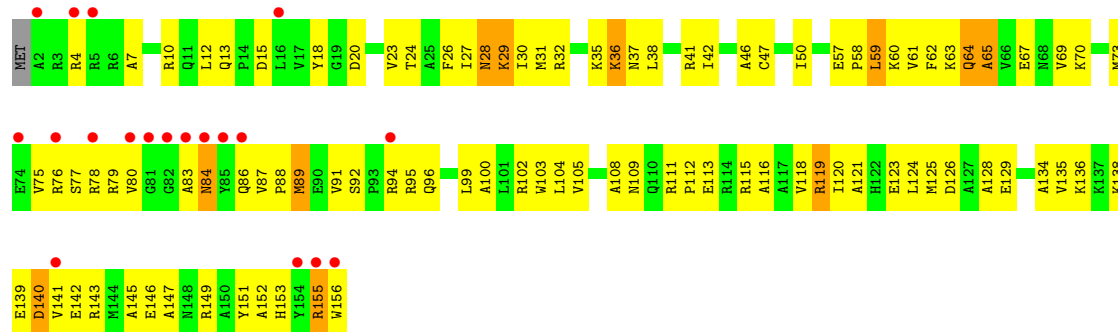
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

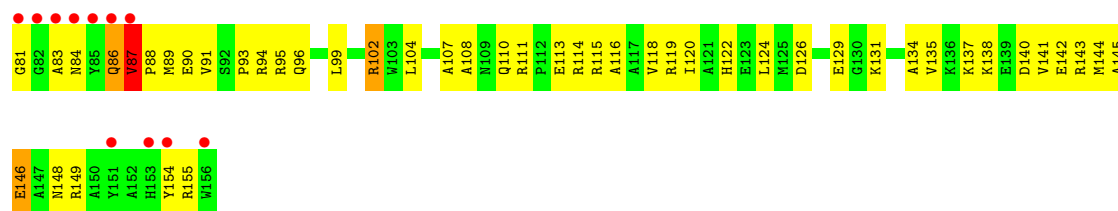


• Molecule 7: 30S ribosomal protein S7

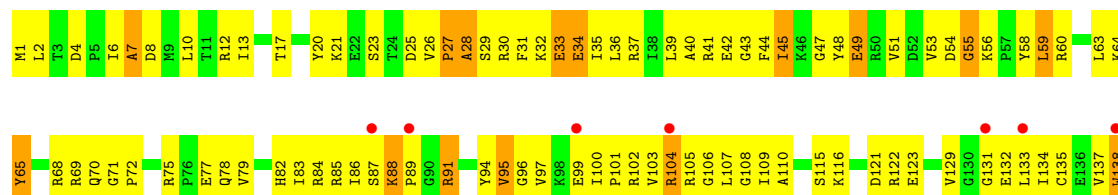


• Molecule 7: 30S ribosomal protein S7

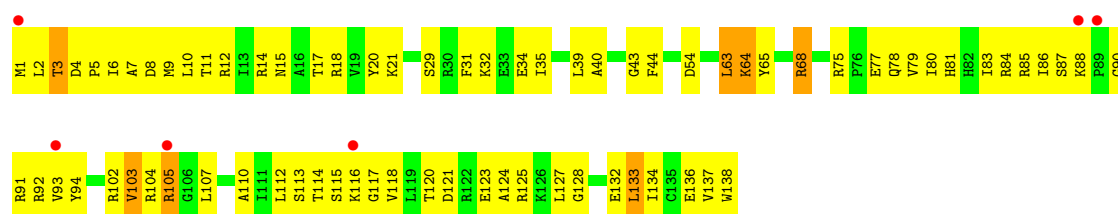




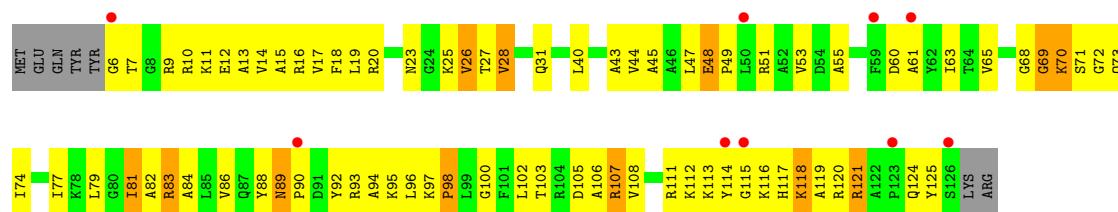
• Molecule 8: 30S ribosomal protein S8



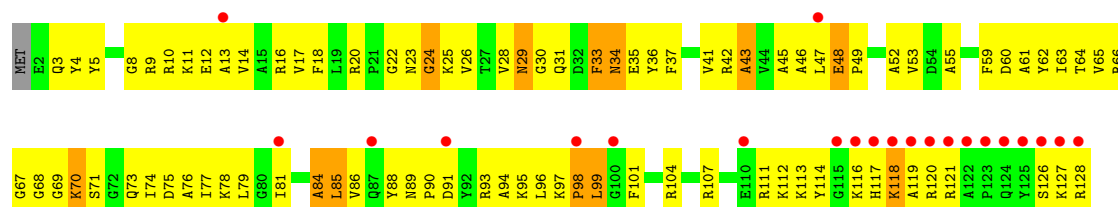
• Molecule 8: 30S ribosomal protein S8



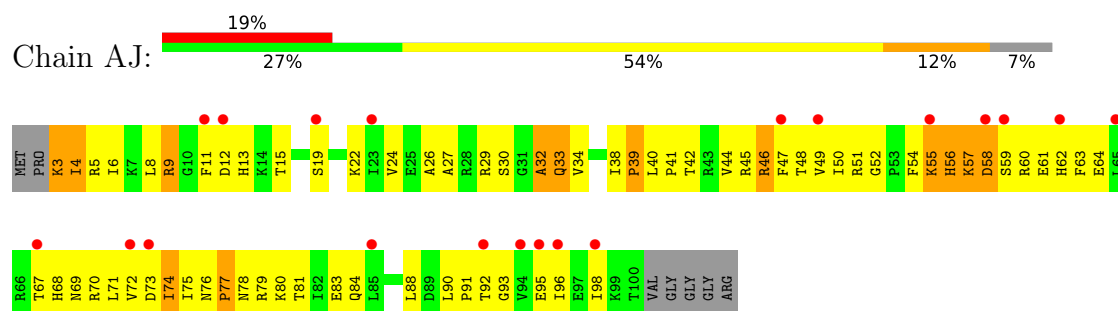
• Molecule 9: 30S ribosomal protein S9



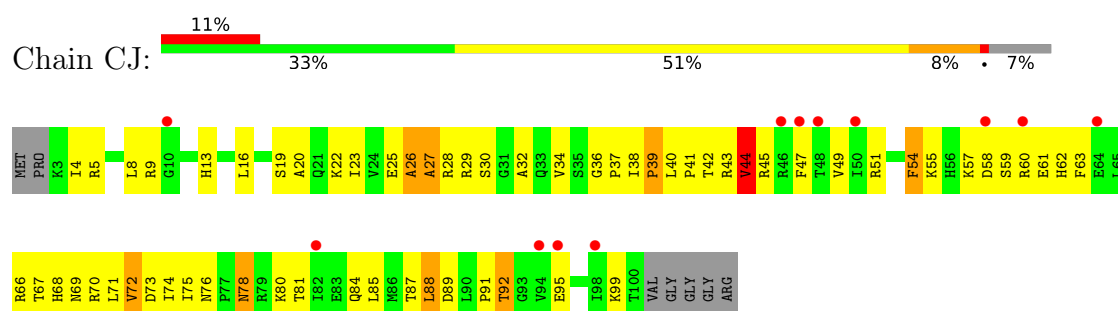
• Molecule 9: 30S ribosomal protein S9



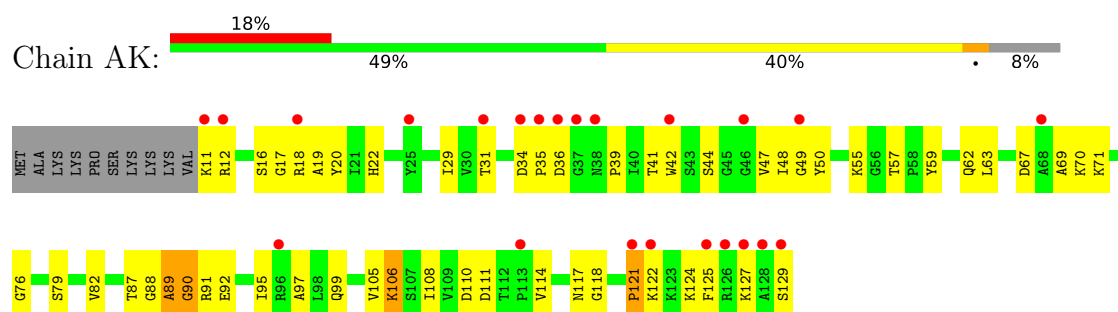
- Molecule 10: 30S ribosomal protein S10



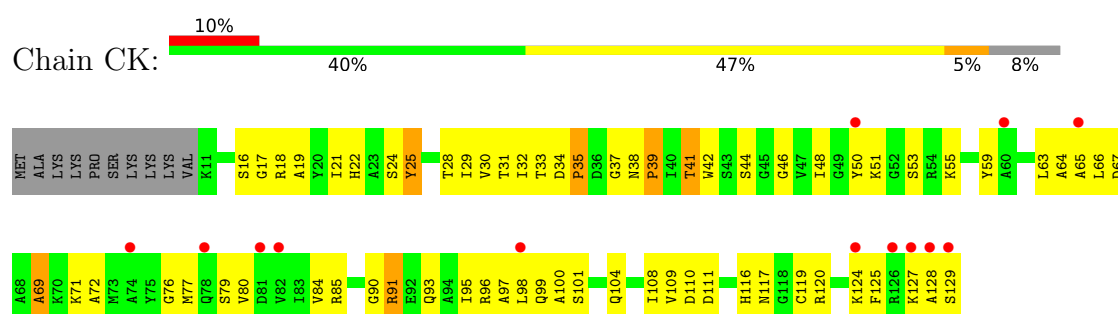
- Molecule 10: 30S ribosomal protein S10



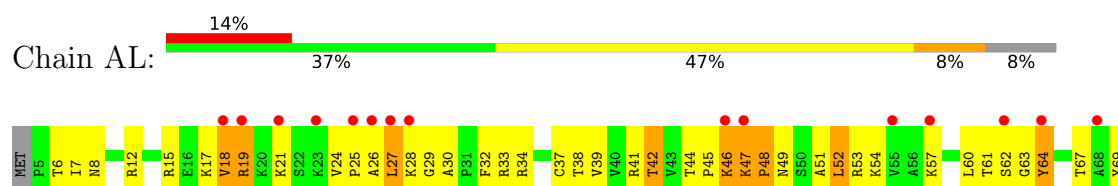
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

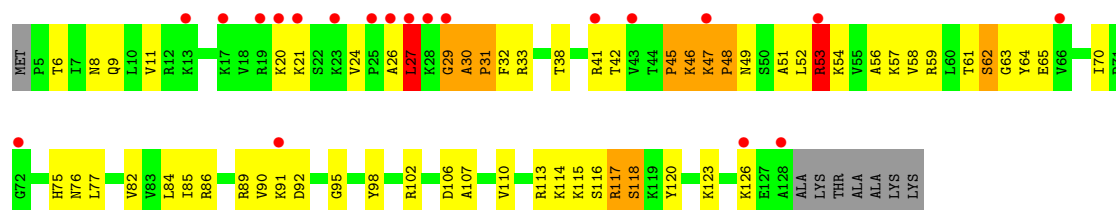


- Molecule 12: 30S ribosomal protein S12

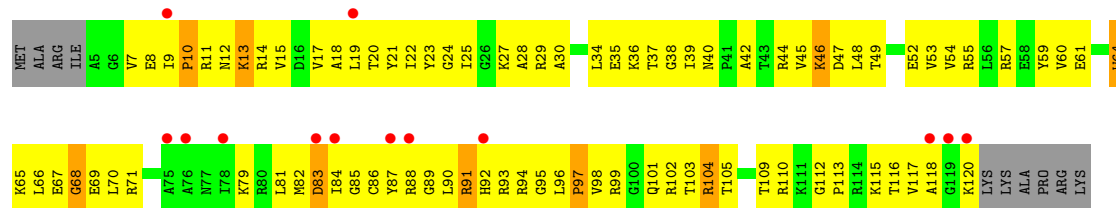




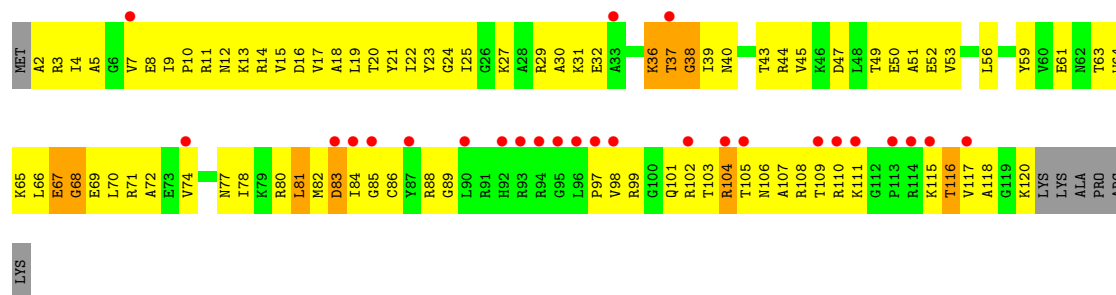
• Molecule 12: 30S ribosomal protein S12



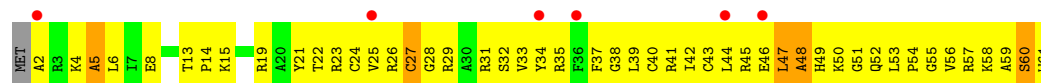
• Molecule 13: 30S ribosomal protein S13



• Molecule 13: 30S ribosomal protein S13

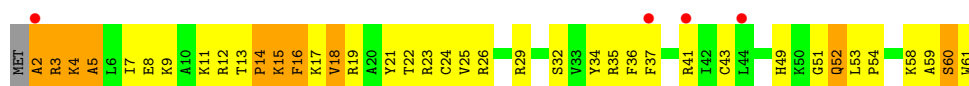


• Molecule 14: 30S ribosomal protein S14 type Z

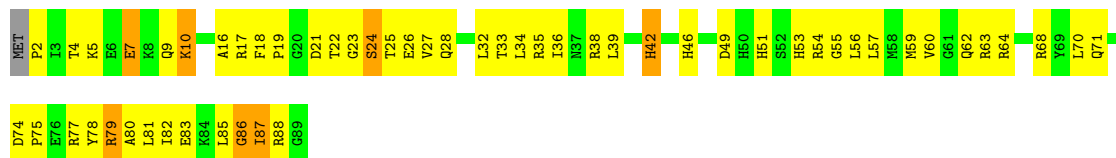


• Molecule 14: 30S ribosomal protein S14 type Z

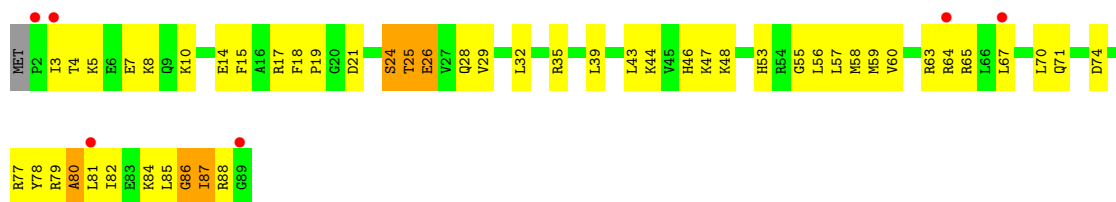
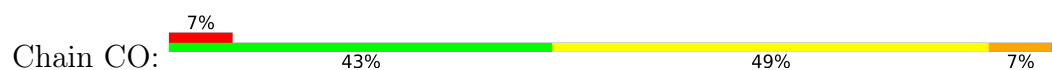




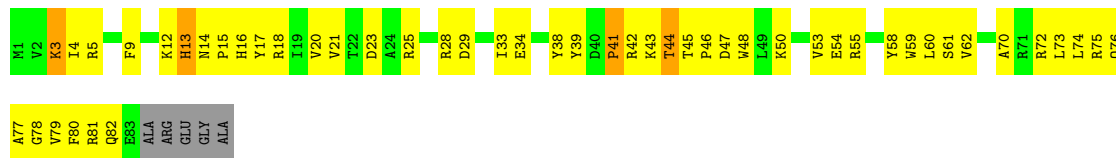
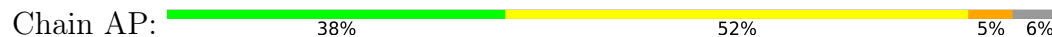
- Molecule 15: 30S ribosomal protein S15



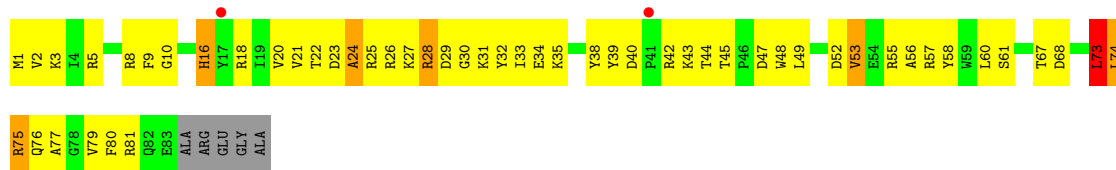
- Molecule 15: 30S ribosomal protein S15



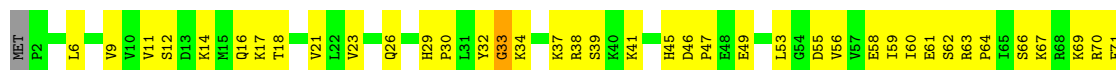
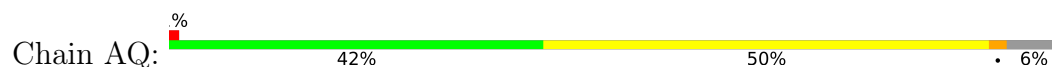
- Molecule 16: 30S ribosomal protein S16

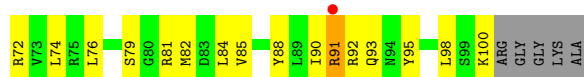


- Molecule 16: 30S ribosomal protein S16

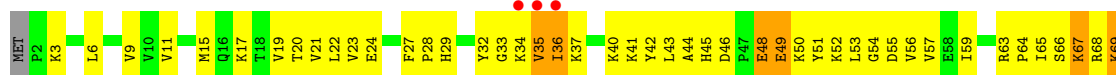


- Molecule 17: 30S ribosomal protein S17

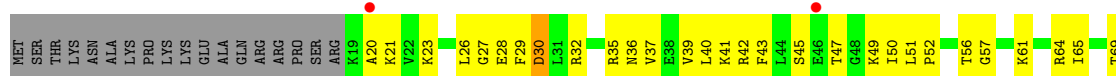




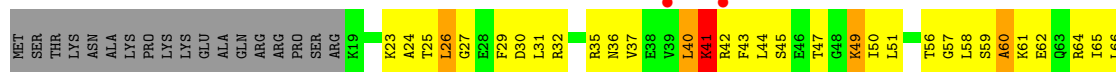
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

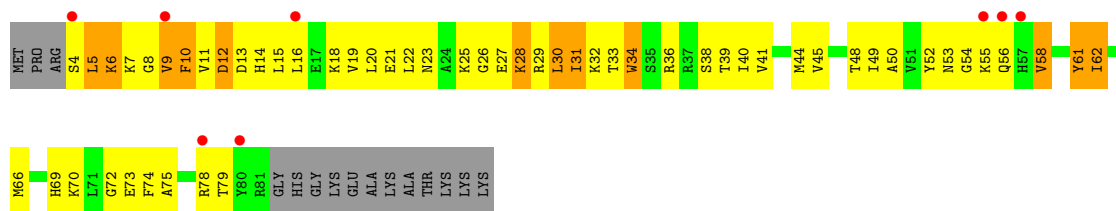


- Molecule 19: 30S ribosomal protein S19

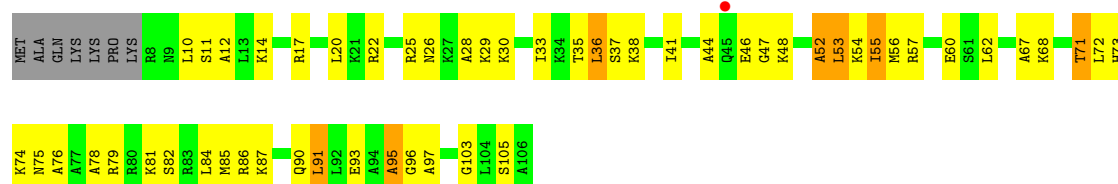


- Molecule 19: 30S ribosomal protein S19

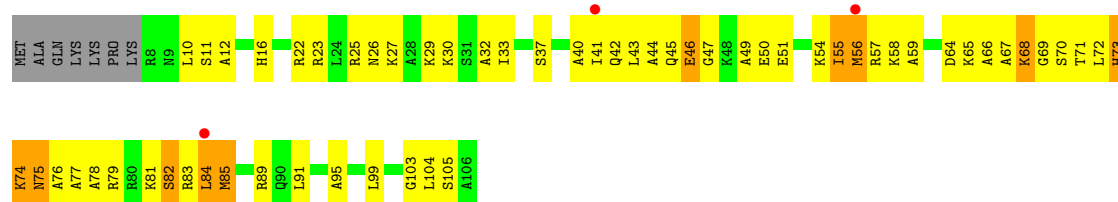




• Molecule 20: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S20



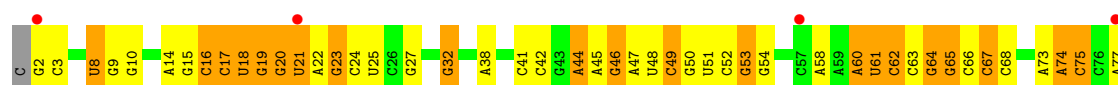
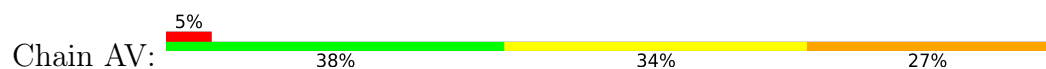
• Molecule 21: 30S ribosomal protein Thx



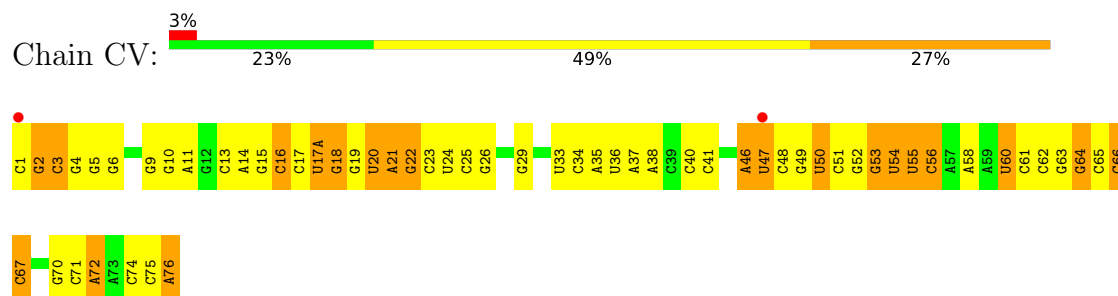
• Molecule 21: 30S ribosomal protein Thx



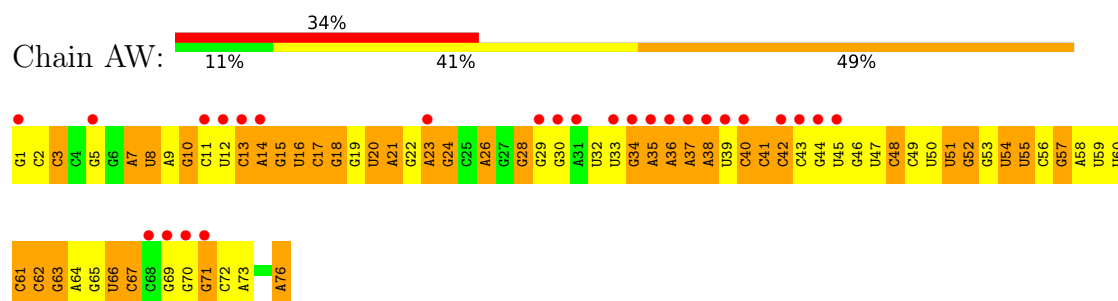
• Molecule 22: P-site tRNA fMet



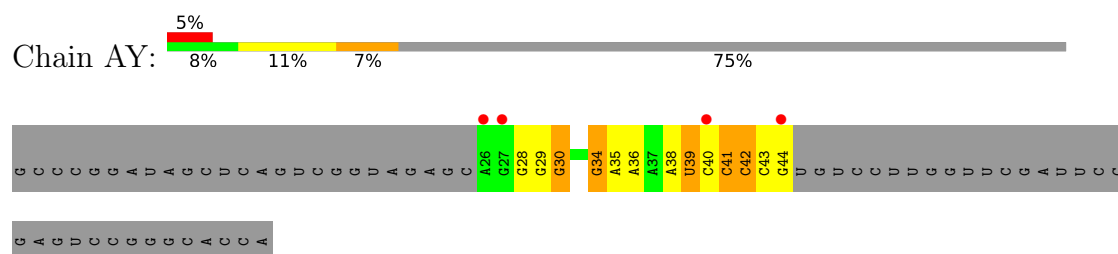
- Molecule 22: P-site tRNA fMet



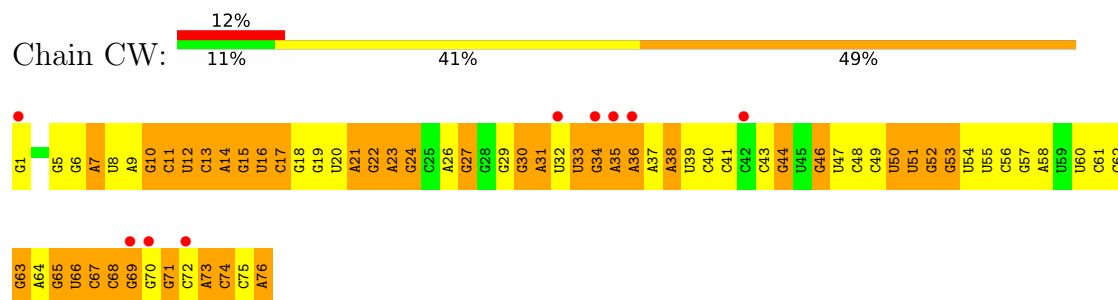
- Molecule 23: E-Site tRNA Phe and A-site tRNA Phe



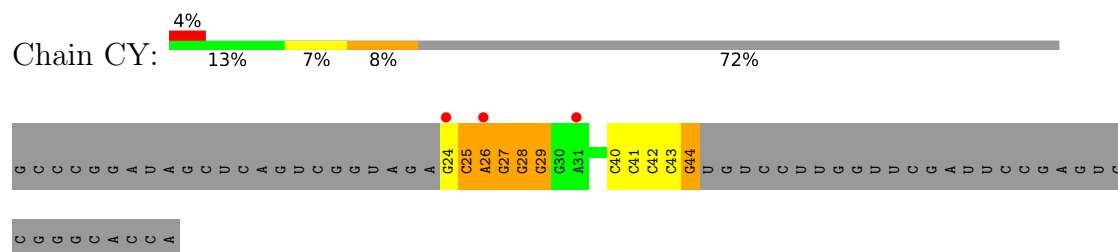
- Molecule 23: E-Site tRNA Phe and A-site tRNA Phe



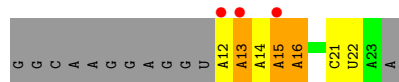
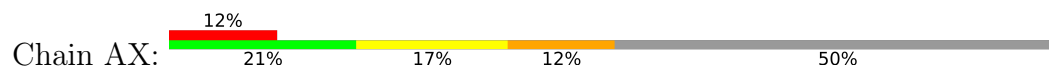
- Molecule 23: E-Site tRNA Phe and A-site tRNA Phe



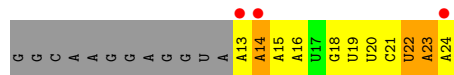
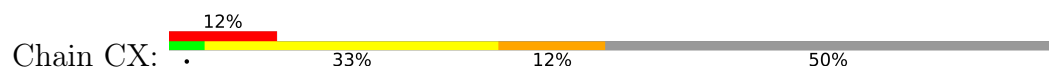
- Molecule 23: E-Site tRNA Phe and A-site tRNA Phe



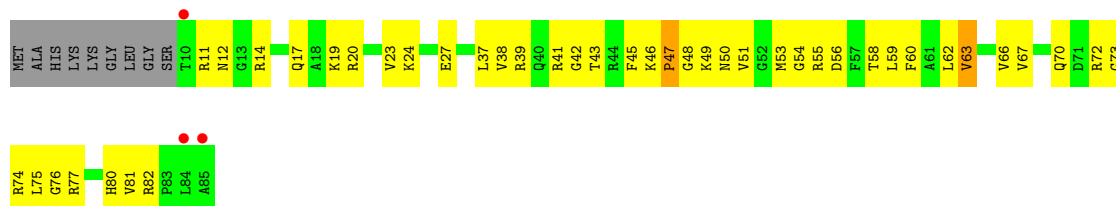
- Molecule 24: mRNA



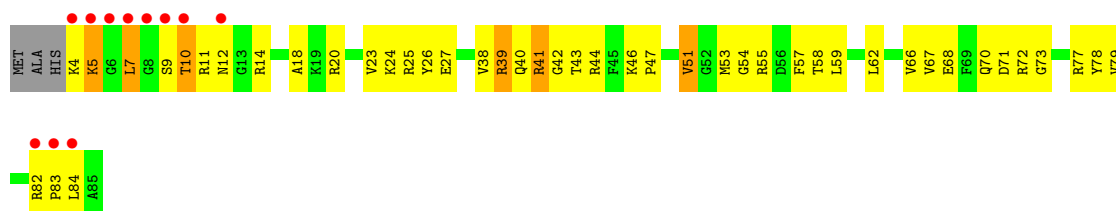
- Molecule 24: mRNA



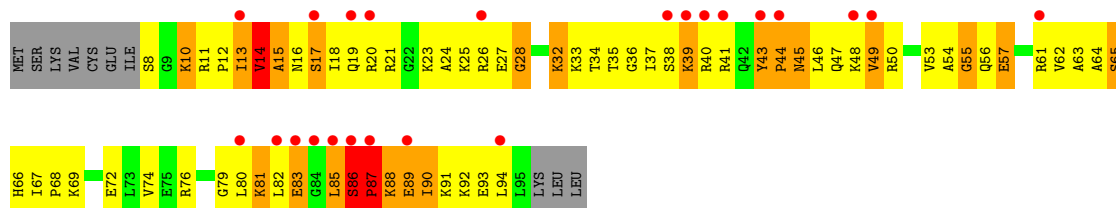
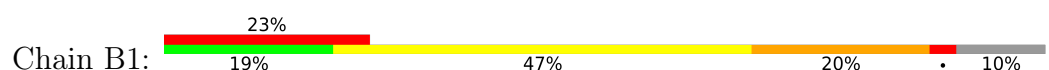
- Molecule 25: 50S ribosomal protein L27



- Molecule 25: 50S ribosomal protein L27



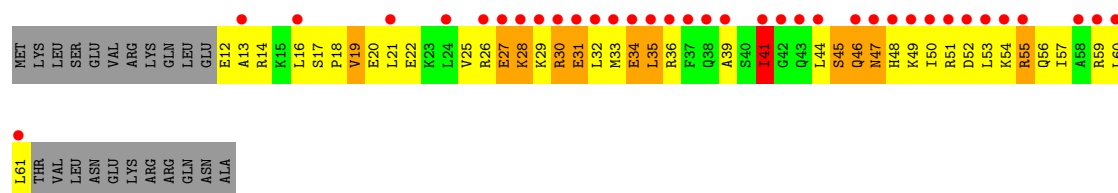
- Molecule 26: 50S ribosomal protein L28



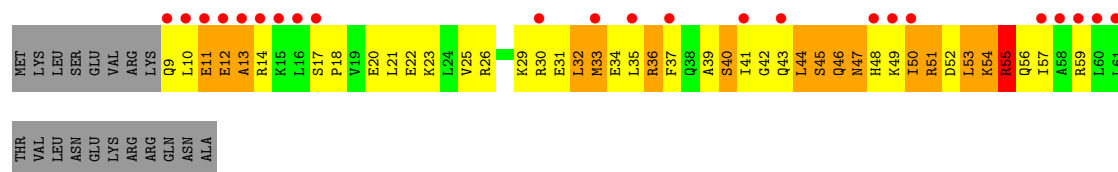
- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L29



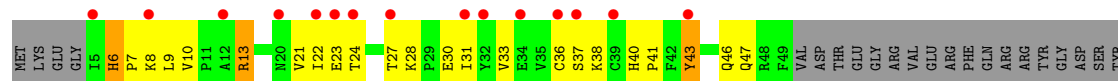
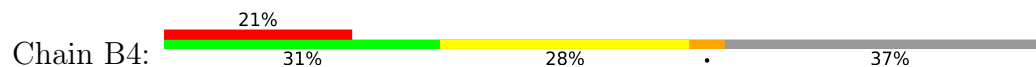
- Molecule 28: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L31



ARG  
LYS  
GLY  
ARG

- Molecule 29: 50S ribosomal protein L31

Chain D4: 15% 30% 31% 8% 31%

M1 K2 E3 G4 I5 H6 P7 V10 R13 I14 I15 C16 G17 C18 G19 N20 E23 T24 Y25 K28 P29 E30 I31 Y32 V33 E34 V35 C36 C39 H40 P41 F42 Y43 T44 Q45 Q46 Q47 R48 F49 VAL ASP THR GLY ARG VAL GLU ARG PHE GLN ARG TYR GLY ASP

SER  
TYR  
ARG  
LYS  
GLY  
ARG

- Molecule 30: 50S ribosomal protein L32

Chain B5: 12% 30% 48% 8% 10%

MET A2 K3 H4 V5 P6 V7 K8 K9 R10 T11 A14 R15 R19 R20 S21 H22 H23 A24 L25 T29 L30 V31 P32 C33 P34 E35 C36 K37 K40 P41 P42 H43 T44 V45 C46 P47 F48 C49 G50 Y51 Y52 G54 H55 LYS VAL LEU VAL

- Molecule 30: 50S ribosomal protein L32

Chain D5: 18% 55% 38% 5%

M1 A2 K3 H4 V5 P6 V7 T11 A14 R18 R19 R20 H23 A24 L25 C33 P34 E35 C36 K37 K40 P41 T44 V45 C46 E48 L36 G50 A53 G54 R55 K56 V57 L58 E59 V60

- Molecule 31: 50S ribosomal protein L33

Chain B6: 19% 6% 48% 28% 15%

MET ALA SER GLU VAL ARG ILE K8 L9 L10 L11 L12 C13 T14 E15 C16 K17 R18 R19 R20 N21 Y21 A22 T23 E24 K25 N26 K27 R28 N29 T30 P31 N32 K33 L34 E35 L36 L37 K38 Y39 C40 P41 W42 C43 R44 K45 V46 T47 V48 H49 R50 E51 V52 K53 ILE

- Molecule 31: 50S ribosomal protein L33

Chain D6: 15% 17% 43% 19% 9% 13%

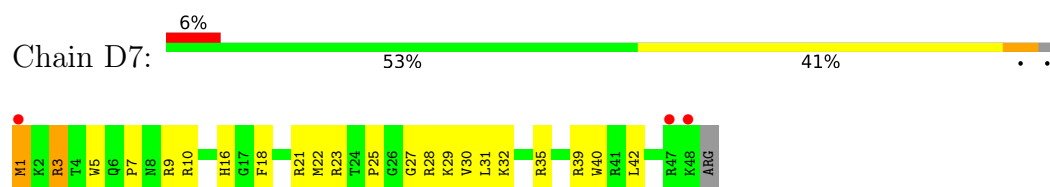
MET ALA SER GLU VAL R6 I7 K8 L9 L10 L11 L12 C13 T14 E15 C16 K17 R18 R19 R20 N21 Y21 A22 T23 E24 K25 N26 K27 R28 N29 T30 P31 N32 K33 L34 E35 L36 L37 K38 Y39 C40 P41 W42 C43 R44 K45 V46 T47 V48 H49 R50 E51 V52 LYS ILE

- Molecule 32: 50S ribosomal protein L34

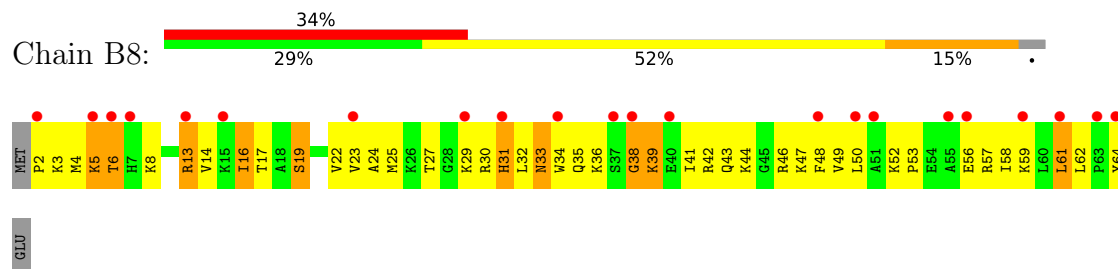
Chain B7: 10% 35% 51% 10%

M1 K2 R3 T4 W5 Q6 P7 H8 R9 R10 R11 R12 A13 K14 F18 R19 M22 G26 G27 R28 K29 V30 L31 R32 R33 R34 R35 R36 K37 G38 R39 W40 R41 L42 A45 V46 R47 K48 ARG

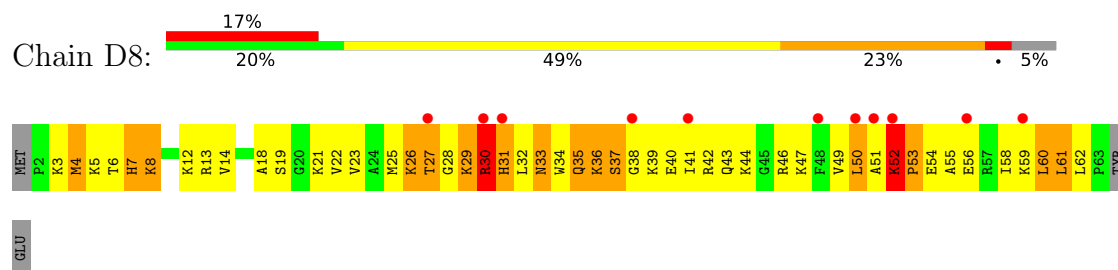
- Molecule 32: 50S ribosomal protein L34



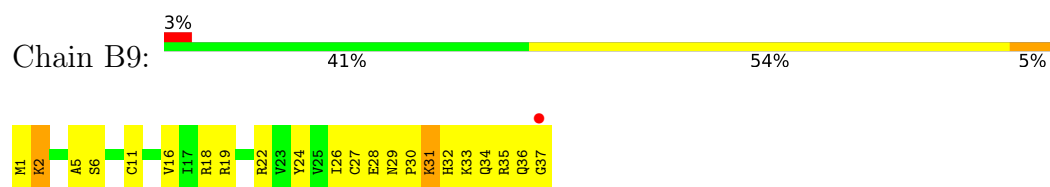
• Molecule 33: 50S ribosomal protein L35



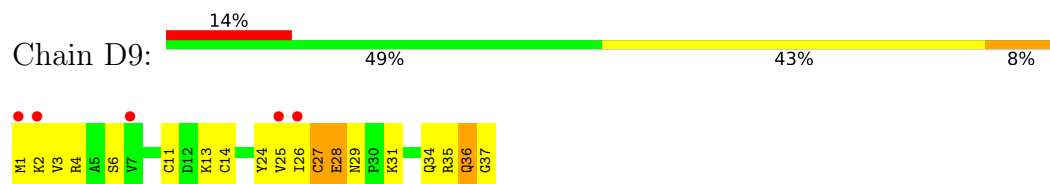
• Molecule 33: 50S ribosomal protein L35



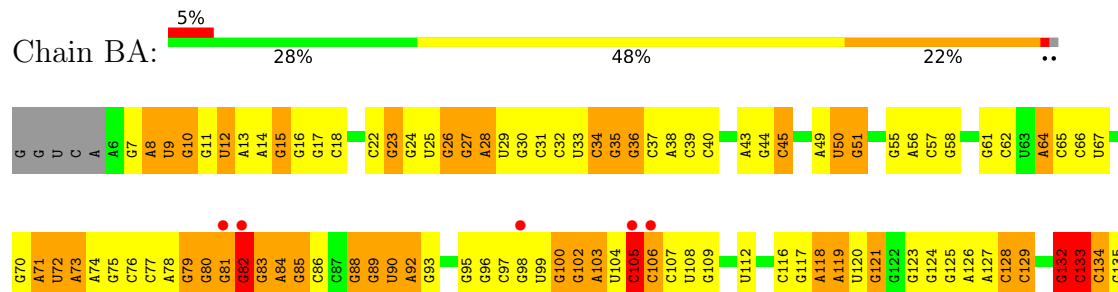
• Molecule 34: 50S ribosomal protein L36

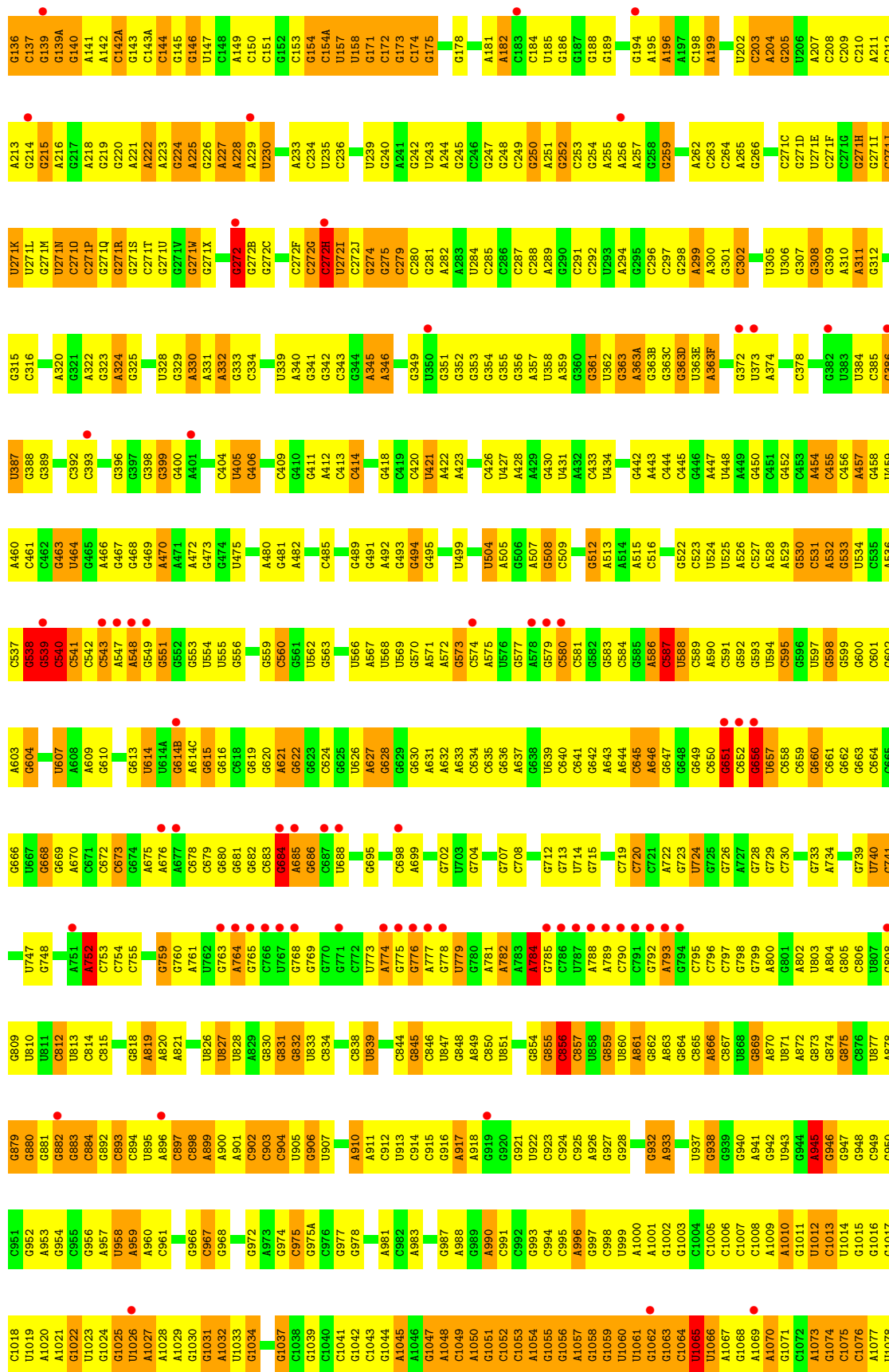


• Molecule 34: 50S ribosomal protein L36

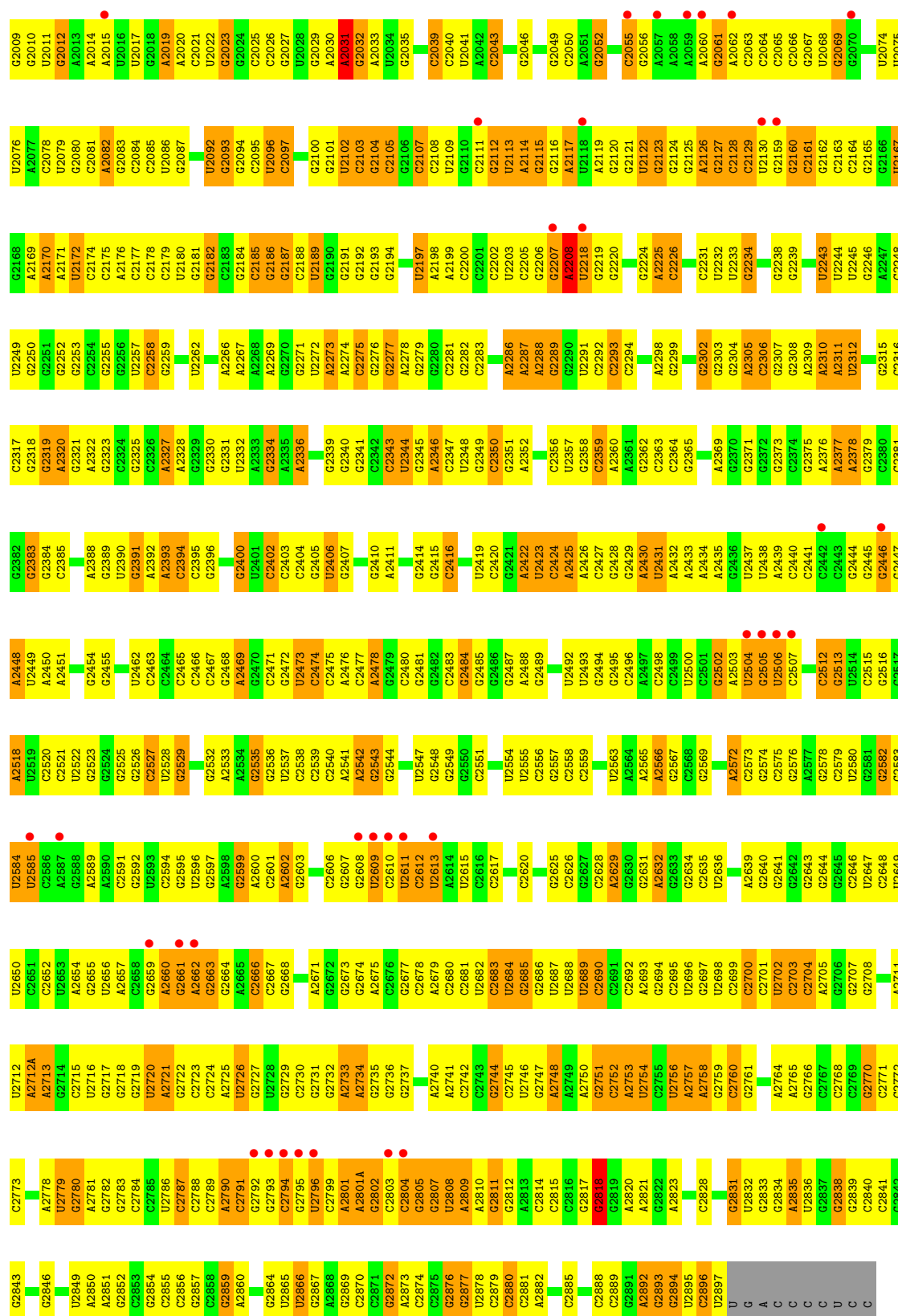


• Molecule 35: 23S ribosomal RNA



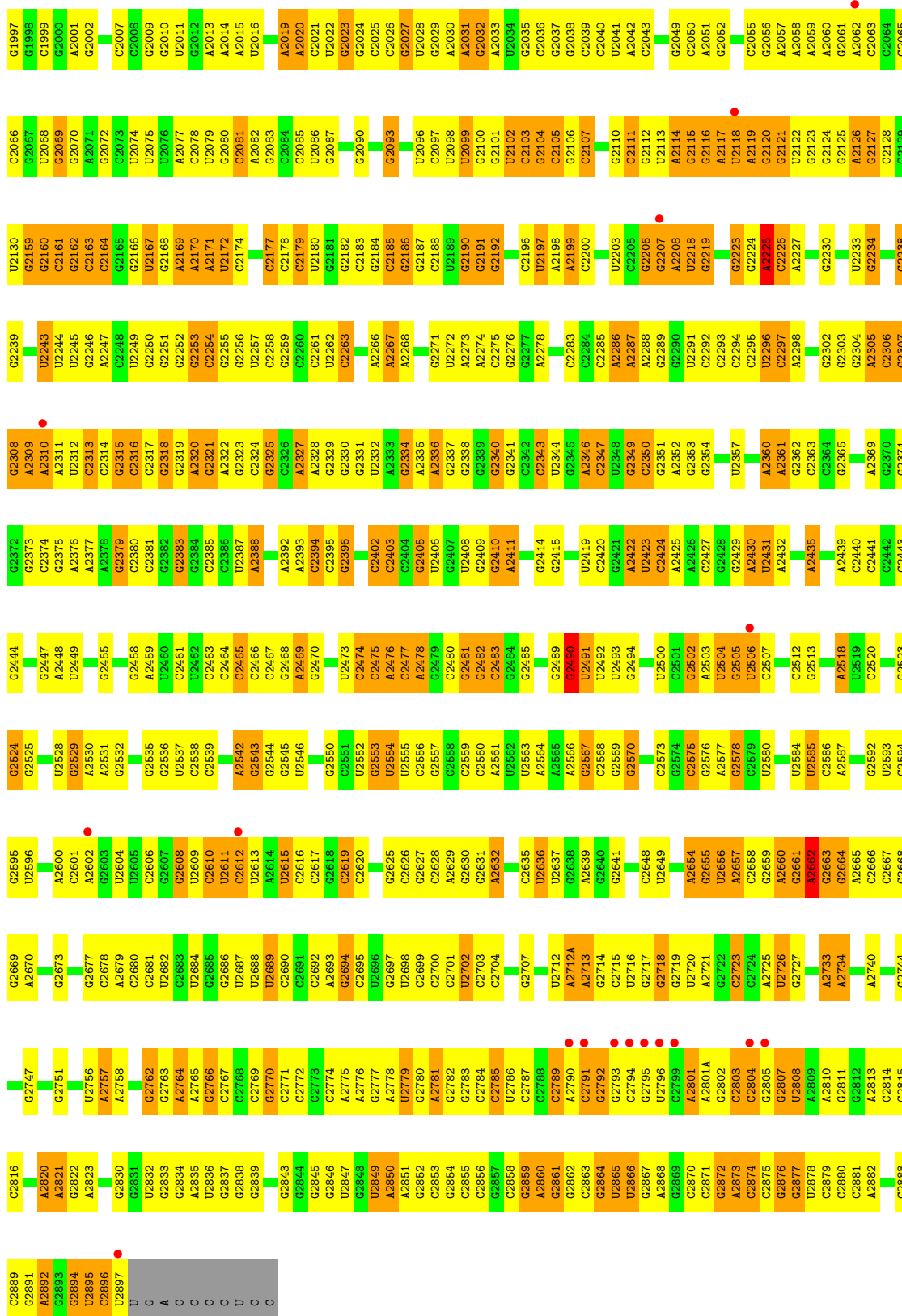


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A1848 | A1849 | A1850 | A1851 | A1852 | A1853 | A1854 | A1855 | A1856 | A1857 | A1858 | A1859 | A1860 | A1861 | A1862 | A1863 | A1864 | A1865 | A1866 | A1867 | A1868 | A1869 | A1870 | A1871 | A1872 | A1873 | A1874 | A1875 | A1876 | A1877 | A1878 | A1879 | A1880 | A1881 | A1882 | A1883 | A1884 | A1885 | A1886 | A1887 | A1888 | A1889 | A1890 | A1891 | A1892 | A1893 | A1894 | A1895 | A1896 | A1897 | A1898 | A1899 | A1900 | A1901 | A1902 | A1903 | A1904 | A1905 | A1906 | A1907 | A1908 | A1909 | A1910 | A1911 | A1912 | A1913 | A1914 | A1915 | A1916 | A1917 | A1918 | A1919 | A1920 | A1921 | A1922 | A1923 | A1924 | A1925 | A1926 | A1927 | A1928 | A1929 | A1930 | A1931 | A1932 | A1933 |
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| U1142 | U1143 | U1144 | U1145 | U1146 | U1147 | U1148 | U1149 | U1150 | U1151 | U1152 | U1153 | U1154 | U1155 | U1156 | U1157 | U1158 | U1159 | U1160 | U1161 | U1162 | U1163 | U1164 | U1165 | U1166 | U1167 | U1168 | U1169 | U1170 | U1171 | U1172 | U1173 | U1174 | U1175 | U1176 | U1177 | U1178 | U1179 | U1180 | U1181 | U1182 | U1183 | U1184 | U1185 | U1186 | U1187 | U1188 | U1189 | U1190 | U1191 | U1192 | U1193 | U1194 | U1195 | U1196 | U1197 | U1198 | U1199 | U1200 | U1201 | U1202 | U1203 | U1204 | U1205 | U1206 | U1207 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C1079 | C1080 | C1081 | C1082 | C1083 | U1084 | U1085 | U1086 | U1087 | U1088 | U1089 | U1090 | U1091 | U1092 | U1093 | U1094 | U1095 | U1096 | U1097 | U1098 | U1099 | U1100 | U1101 | U1102 | U1103 | U1104 | U1105 | U1106 | U1107 | U1108 | U1109 | U1110 | U1111 | U1112 | U1113 | U1114 | U1115 | U1116 | U1117 | U1118 | U1119 | U1120 | U1121 | U1122 | U1123 | U1124 | U1125 | U1126 | U1127 | U1128 | U1129 | U1130 | U1131 | U1132 | U1133 | U1134 | U1135 | U1136 | U1137 | U1138 | U1139 | U1140 | U1141 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

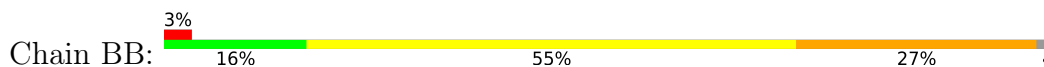


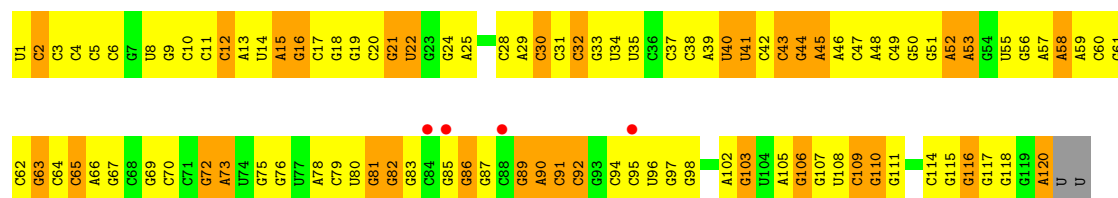




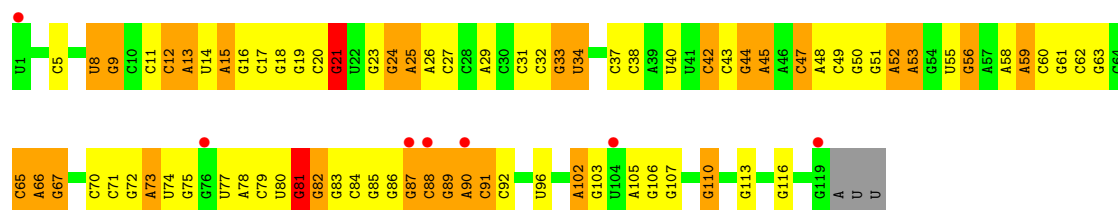


- Molecule 36: 5S ribosomal RNA

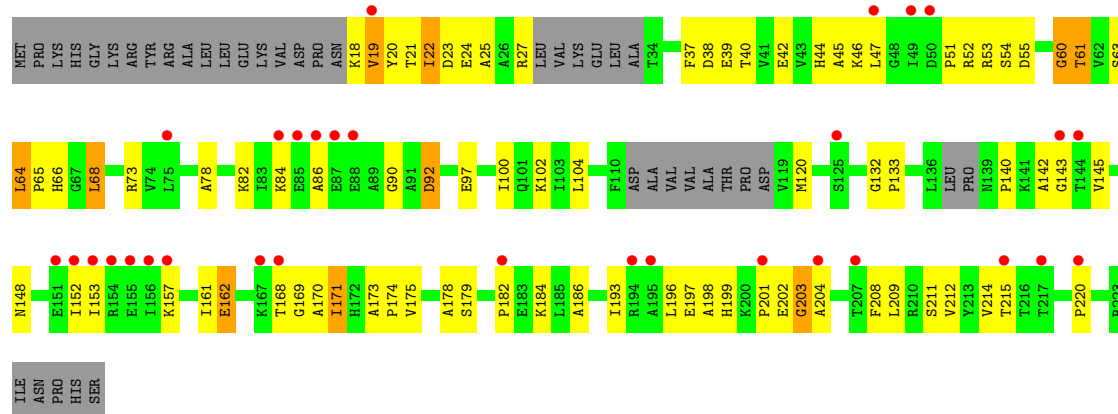




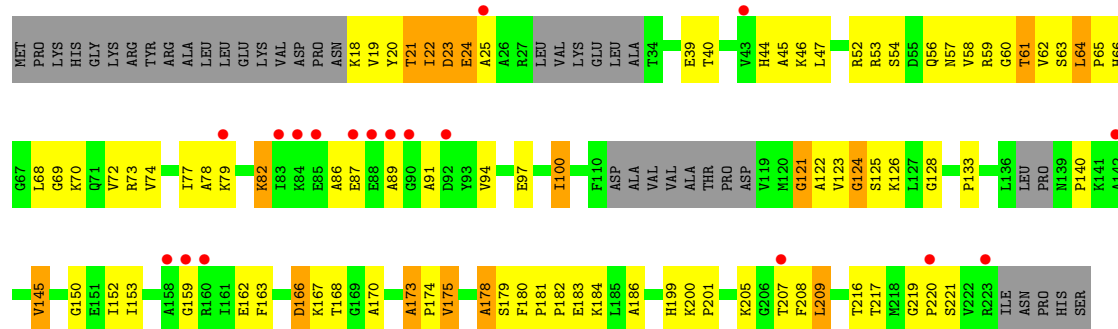
• Molecule 36: 5S ribosomal RNA



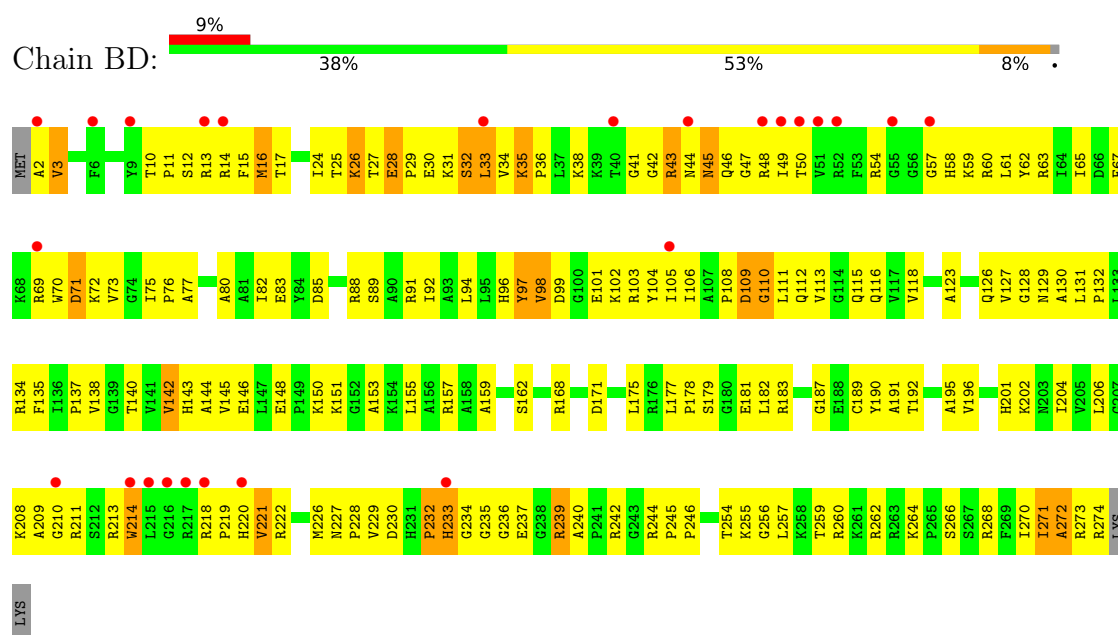
• Molecule 37: 50S ribosomal protein L1



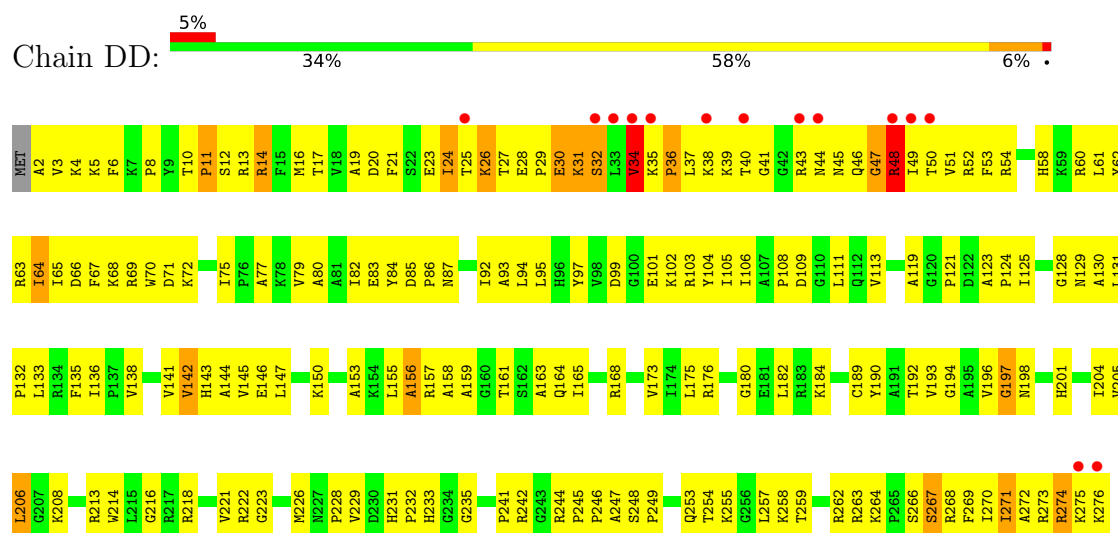
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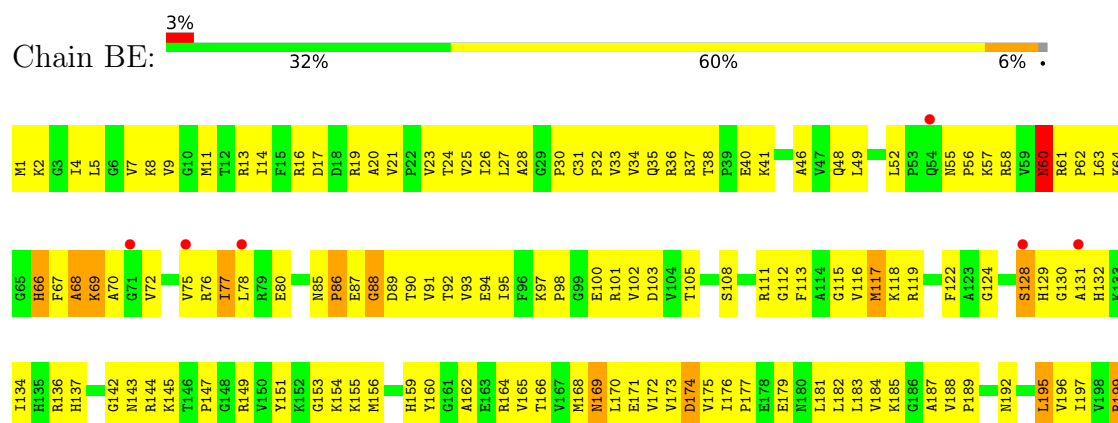
• Molecule 38: 50S ribosomal protein L2

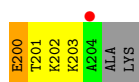


• Molecule 38: 50S ribosomal protein L2

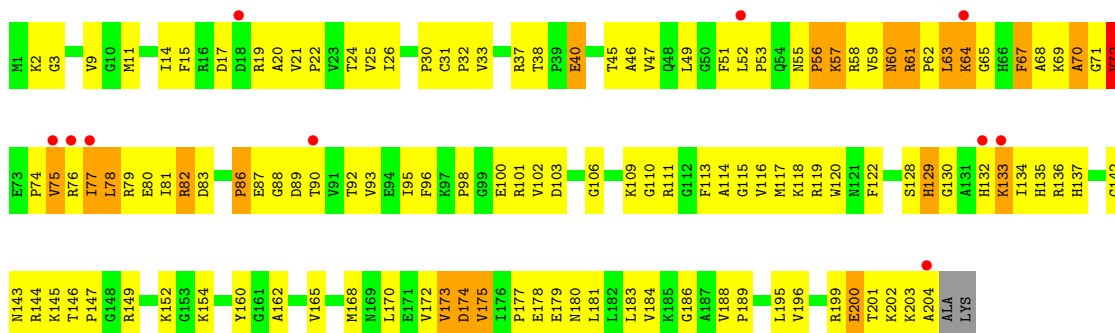


• Molecule 39: 50S ribosomal protein L3

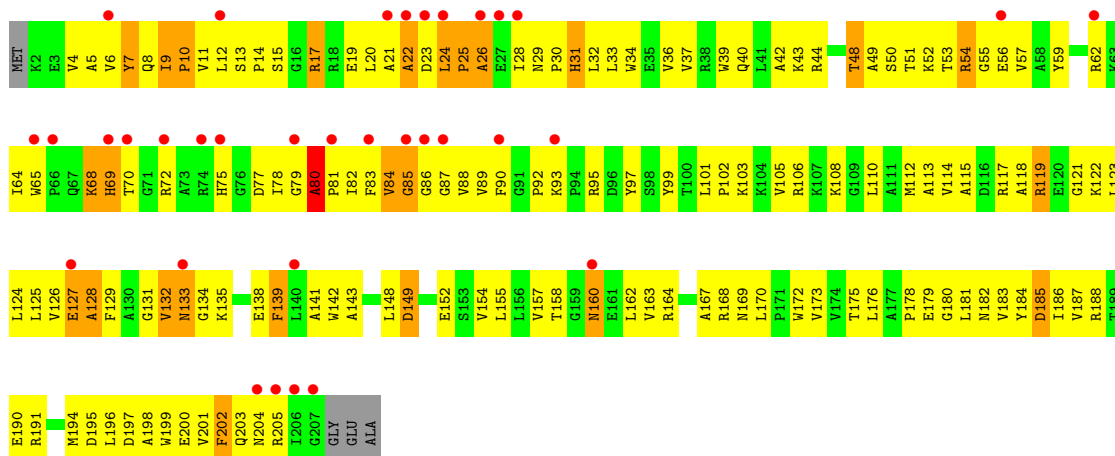




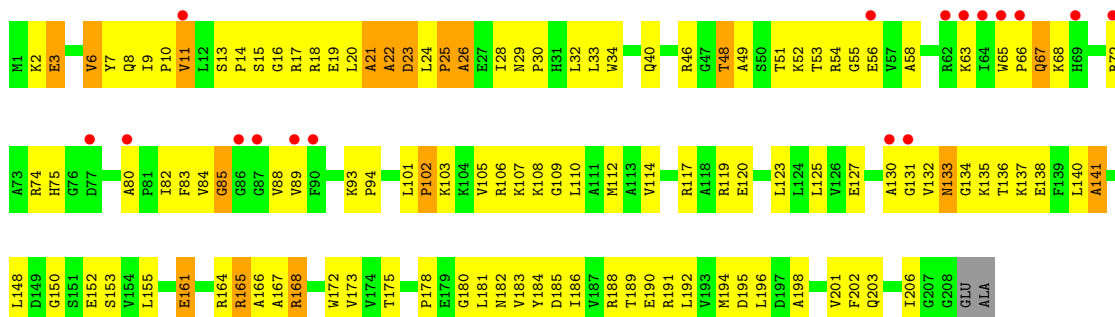
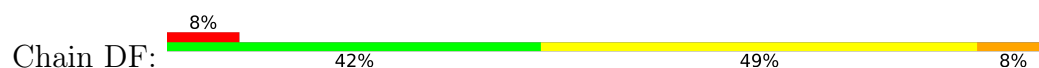
• Molecule 39: 50S ribosomal protein L3



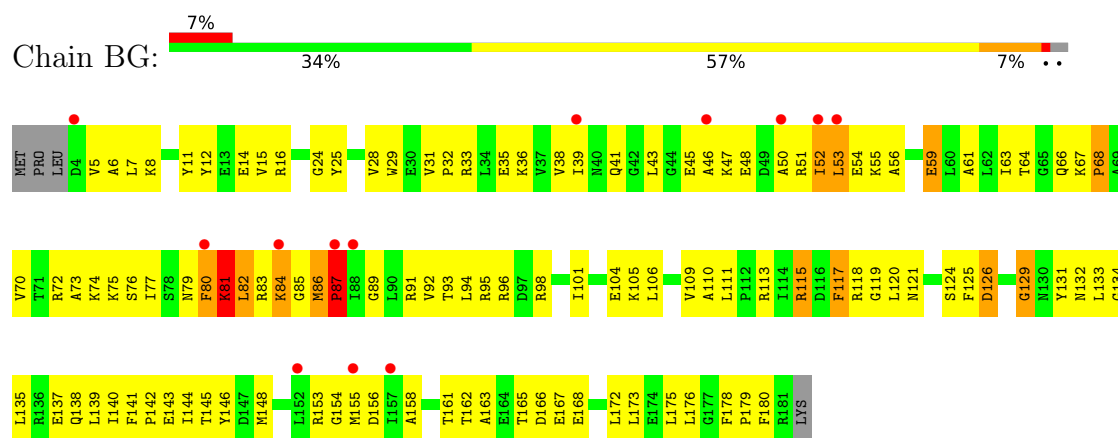
• Molecule 40: 50S ribosomal protein L4



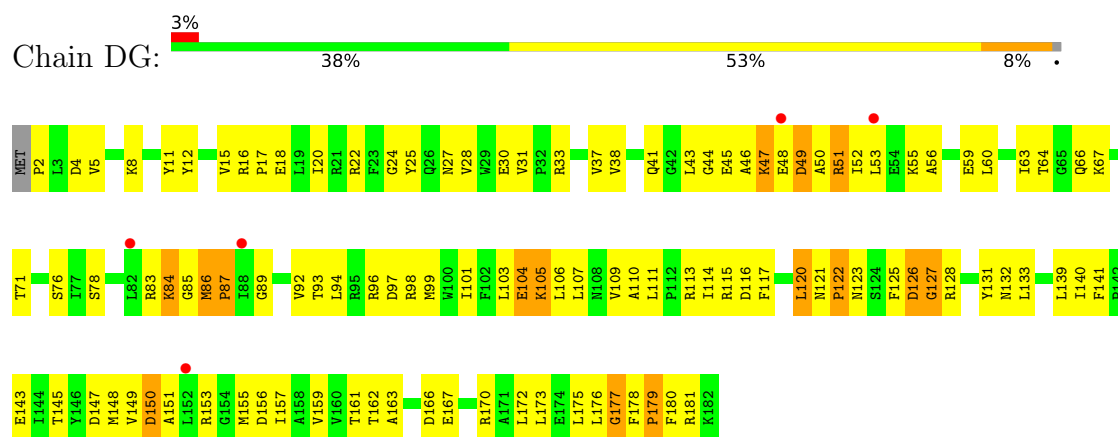
• Molecule 40: 50S ribosomal protein L4



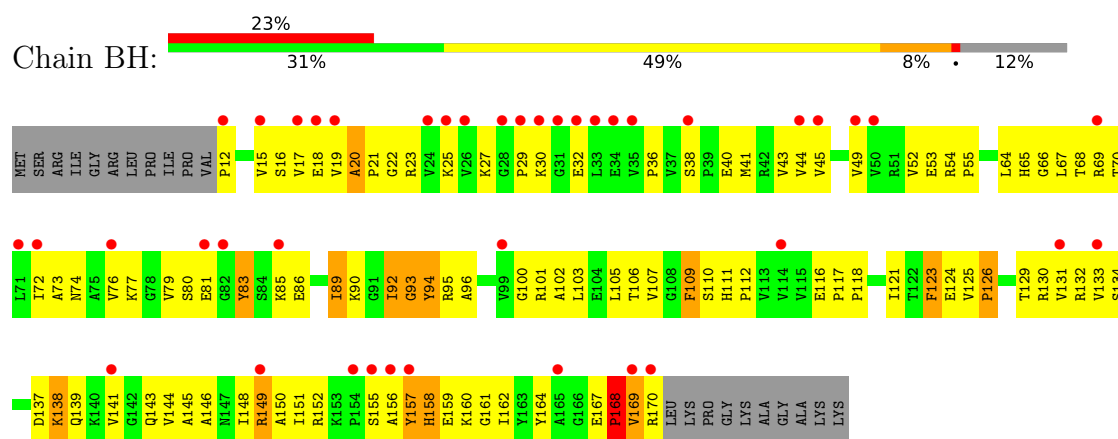
## • Molecule 41: 50S ribosomal protein L5



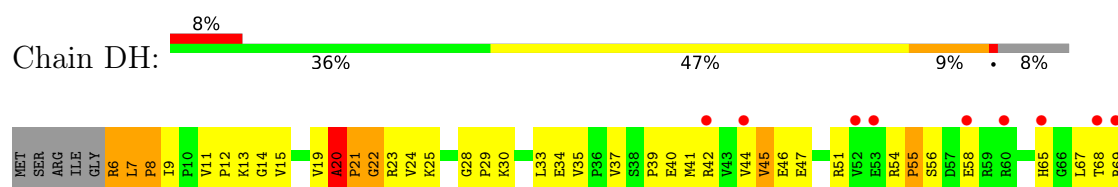
## • Molecule 41: 50S ribosomal protein L5

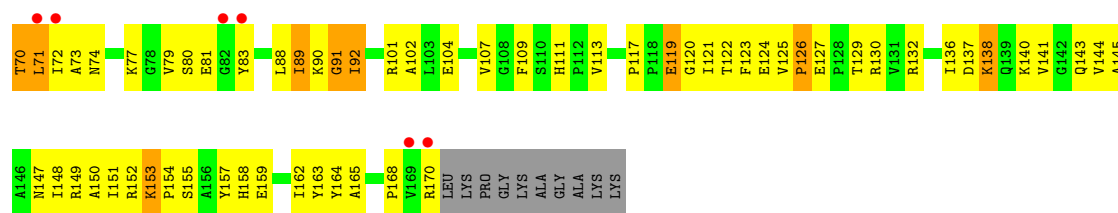


## • Molecule 42: 50S ribosomal protein L6

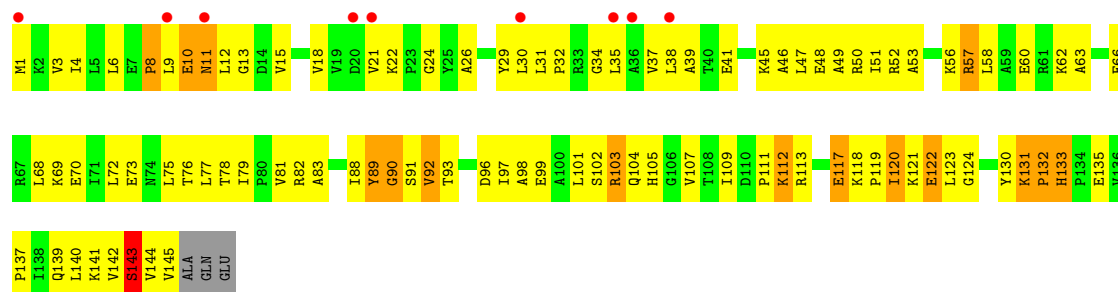


## • Molecule 42: 50S ribosomal protein L6

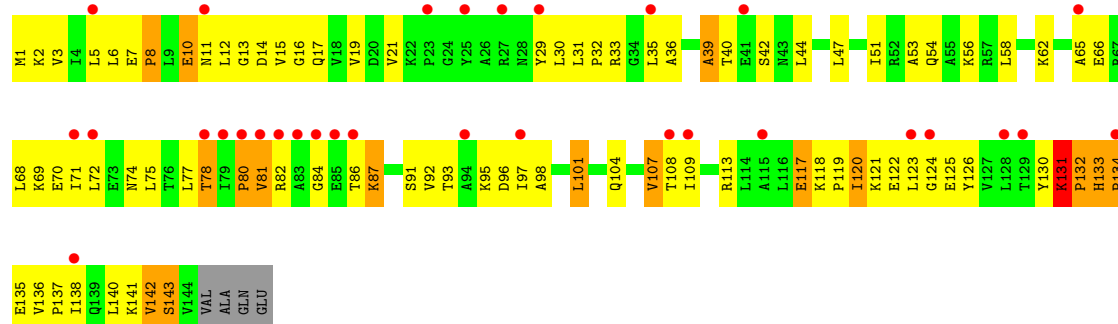




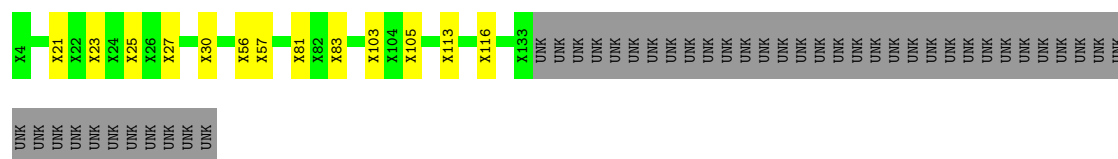
• Molecule 43: 50S ribosomal protein L9



• Molecule 43: 50S ribosomal protein L9

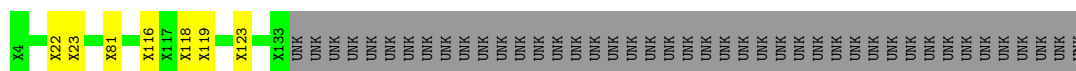


• Molecule 44: 50S ribosomal protein L10



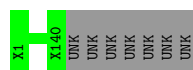
• Molecule 44: 50S ribosomal protein L10





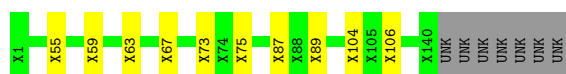
- Molecule 45: 50S ribosomal protein L11

Chain BK: 95% 5%



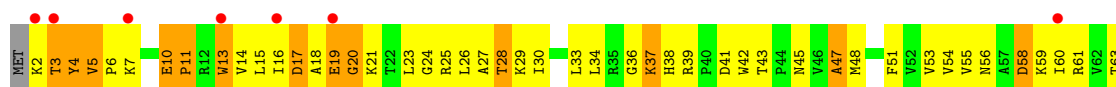
- Molecule 45: 50S ribosomal protein L11

Chain DK: 88% 7% 5%



- Molecule 46: 50S ribosomal protein L13

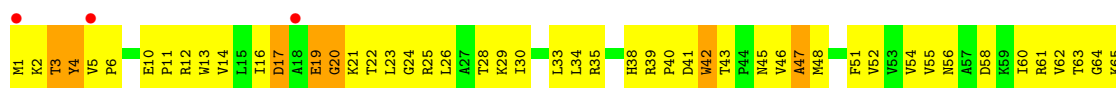
Chain BN: 10% 32% 54% 11% ..



VAL

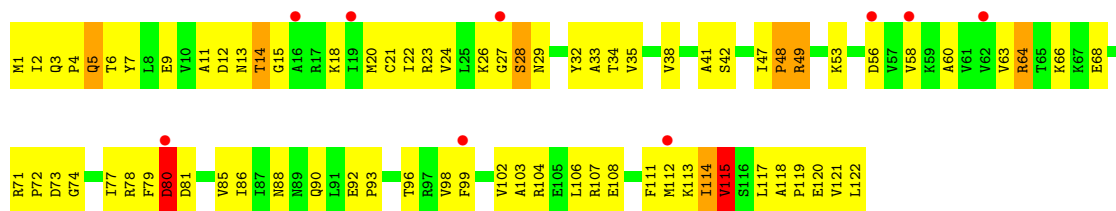
- Molecule 46: 50S ribosomal protein L13

Chain DN: 10% 25% 58% 16% .

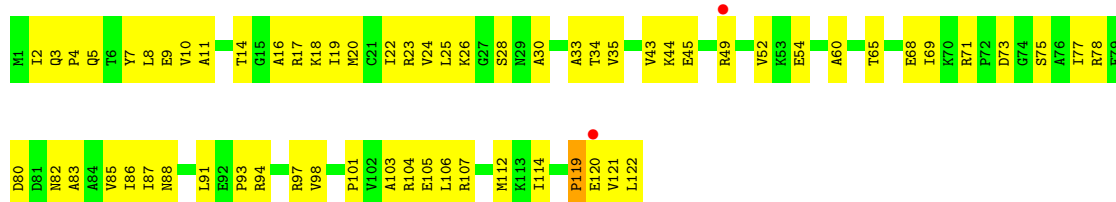


- Molecule 47: 50S ribosomal protein L14

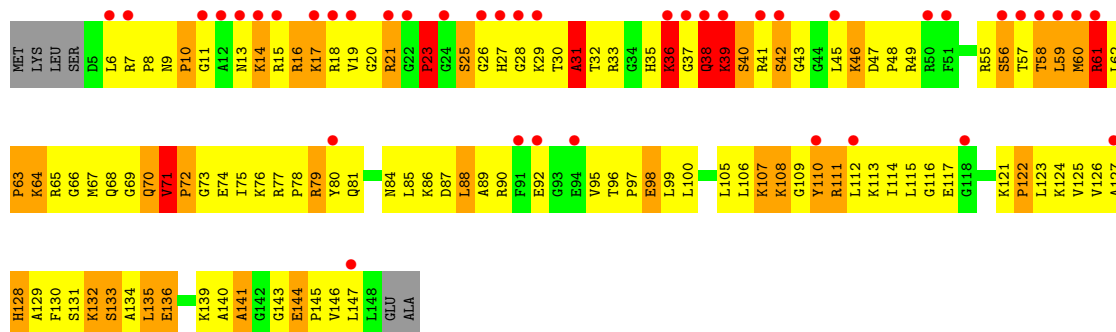
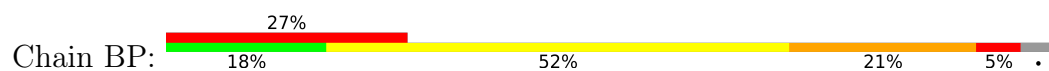
Chain BO: 7% 38% 55% 6% .



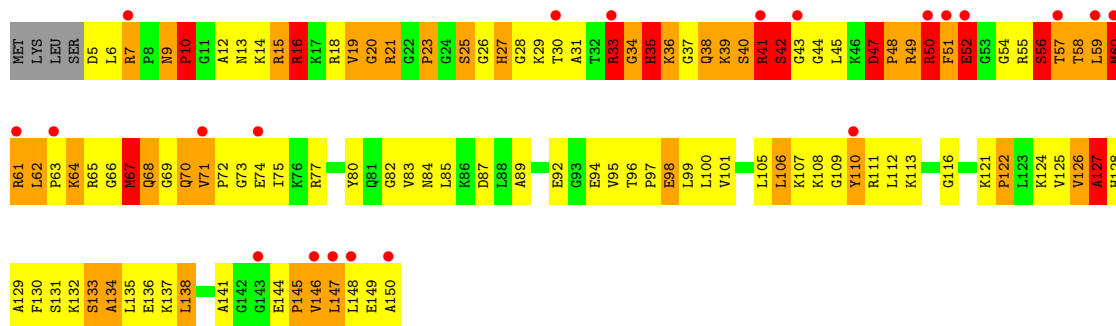
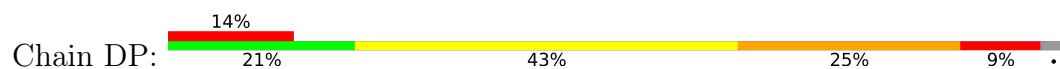
• Molecule 47: 50S ribosomal protein L14



• Molecule 48: 50S ribosomal protein L15

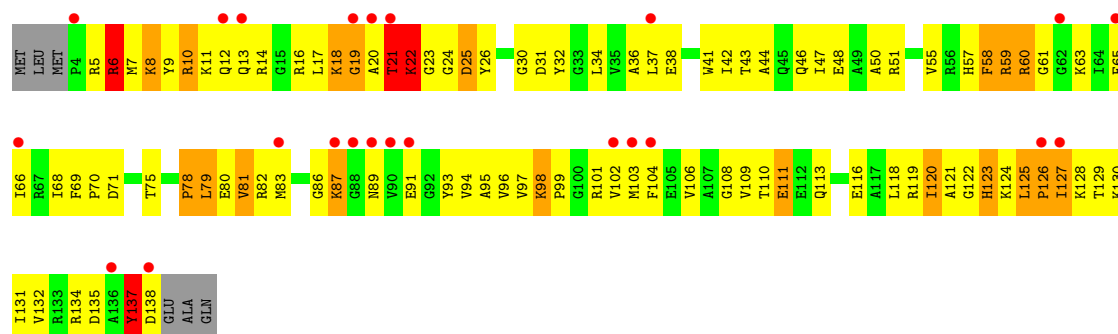


• Molecule 48: 50S ribosomal protein L15

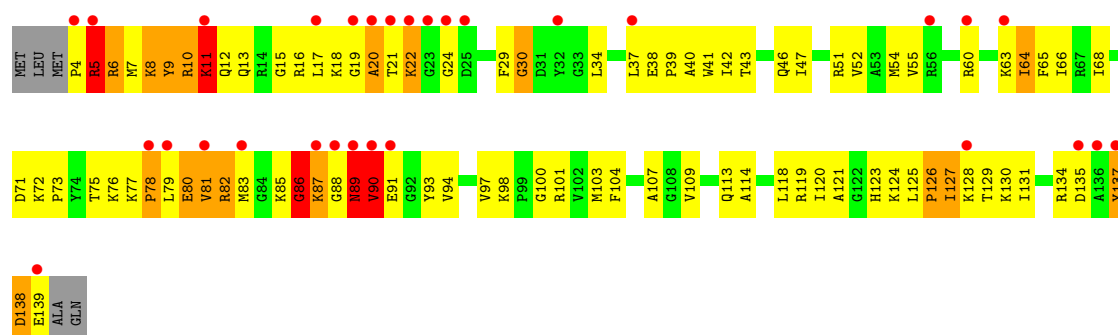


• Molecule 49: 50S ribosomal protein L16

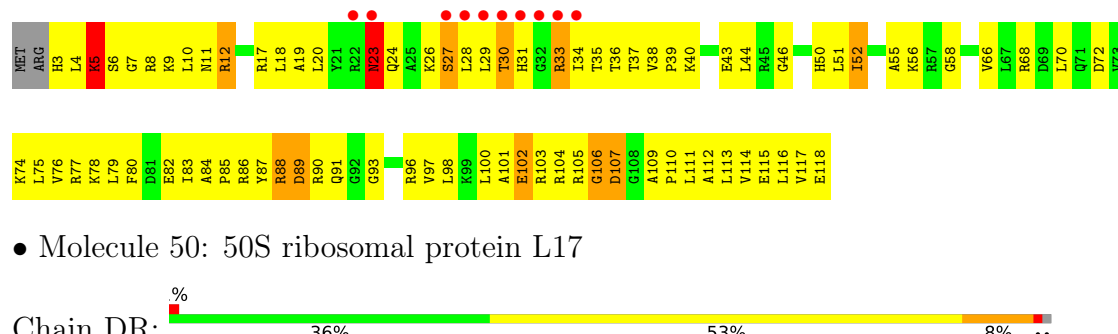




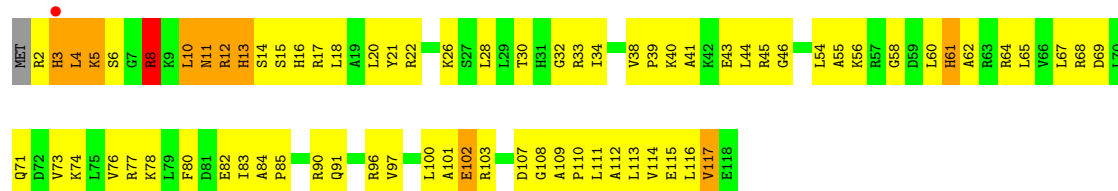
• Molecule 49: 50S ribosomal protein L16



• Molecule 50: 50S ribosomal protein L17

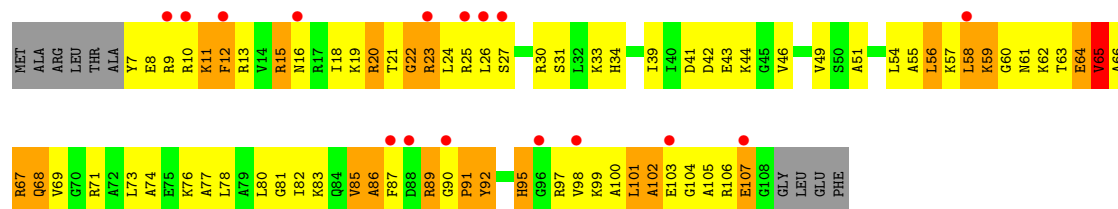


• Molecule 50: 50S ribosomal protein L17

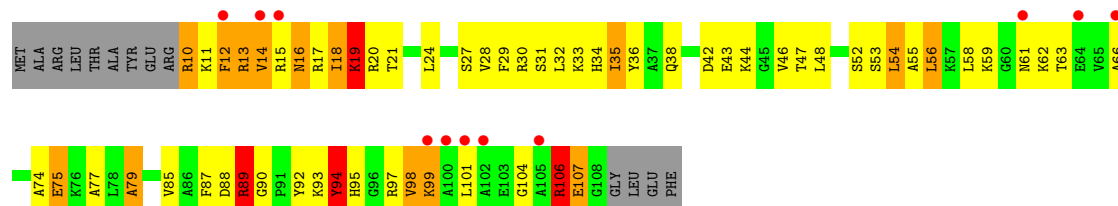


• Molecule 51: 50S ribosomal protein L18

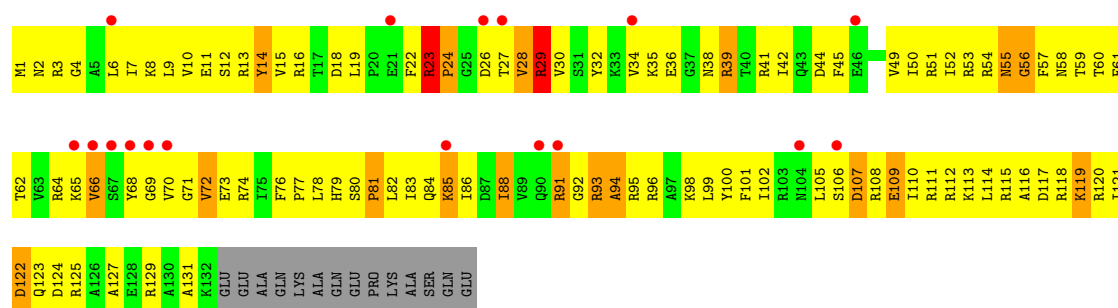




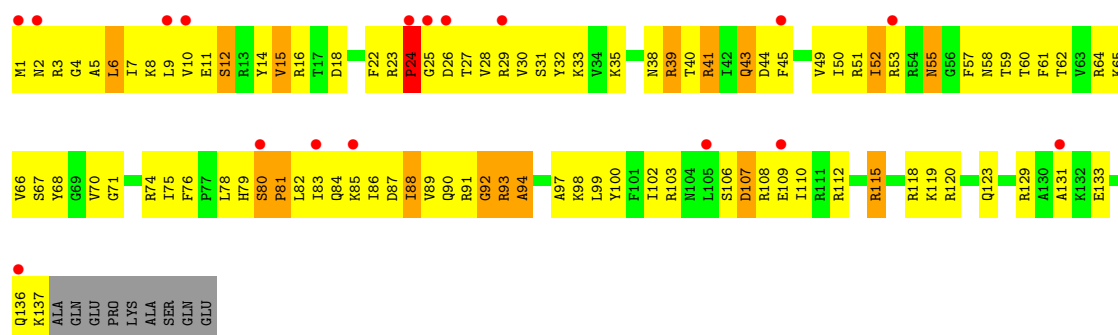
• Molecule 51: 50S ribosomal protein L18



• Molecule 52: 50S ribosomal protein L19

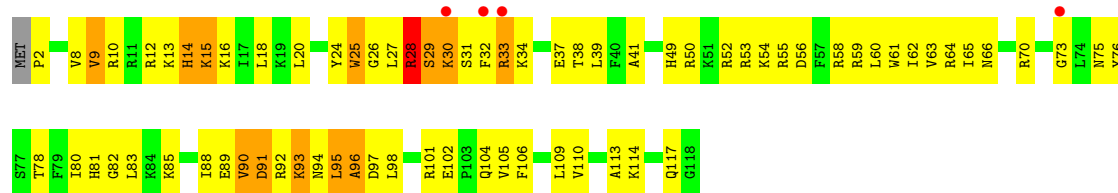


• Molecule 52: 50S ribosomal protein L19

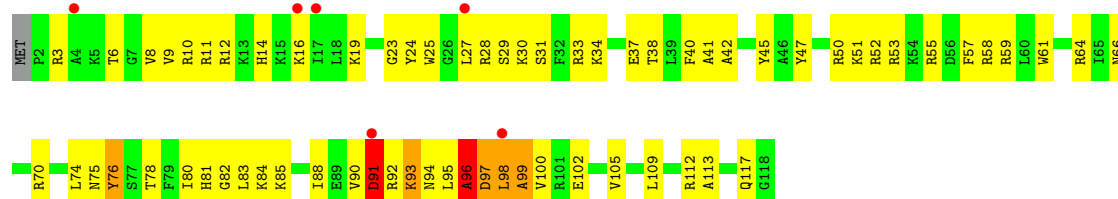
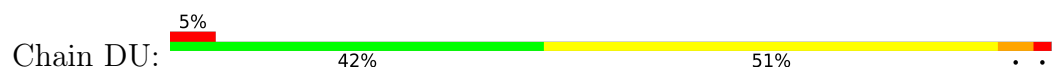


• Molecule 53: 50S ribosomal protein L20

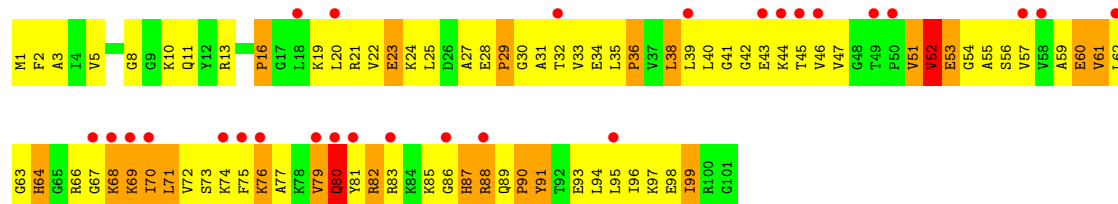




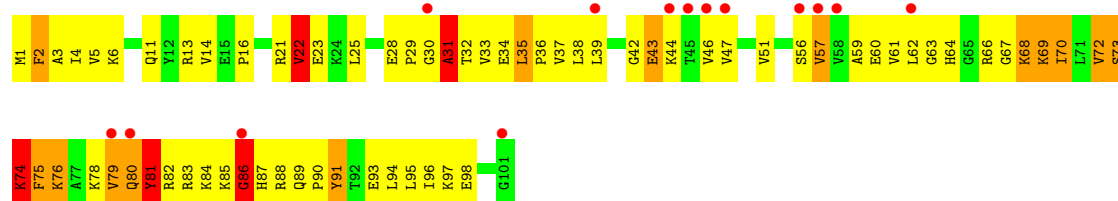
• Molecule 53: 50S ribosomal protein L20



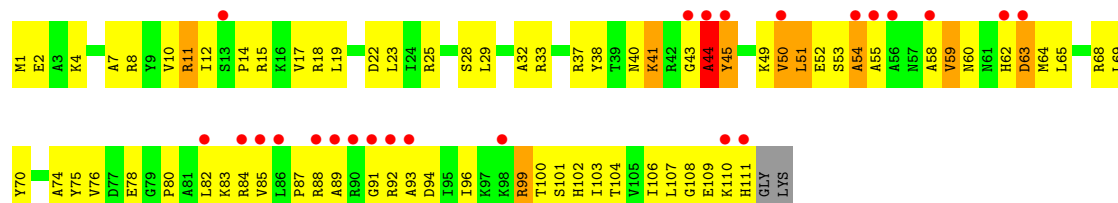
• Molecule 54: 50S ribosomal protein L21



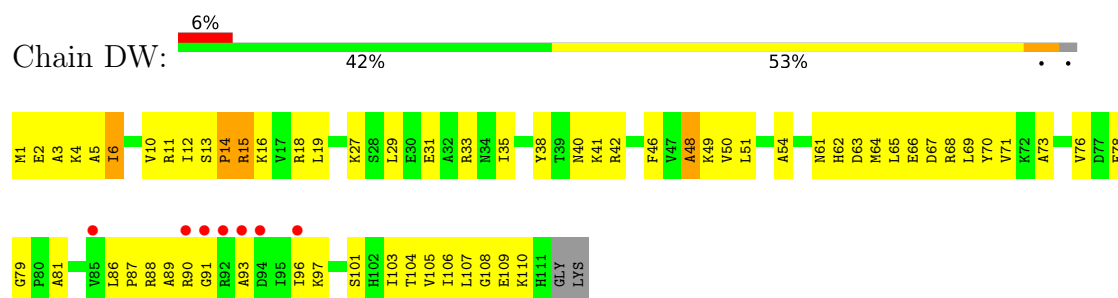
• Molecule 54: 50S ribosomal protein L21



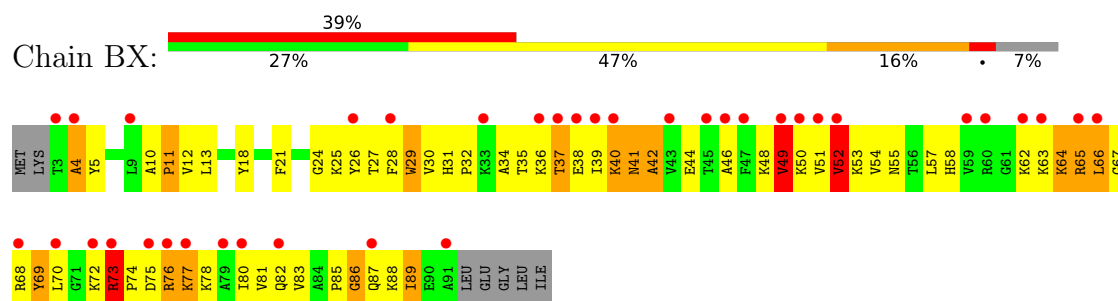
• Molecule 55: 50S ribosomal protein L22



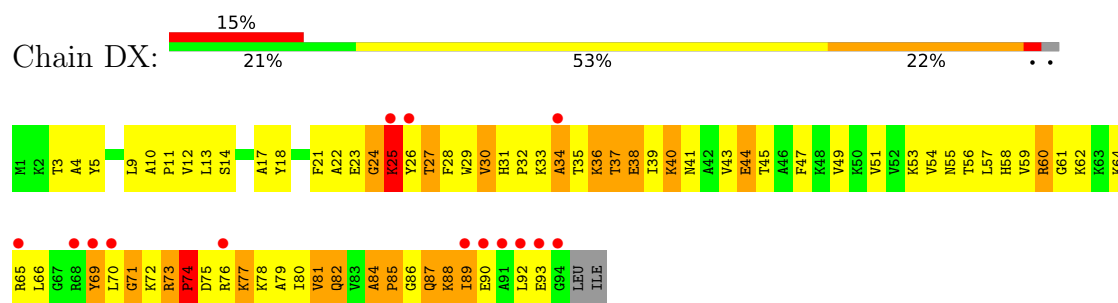
- Molecule 55: 50S ribosomal protein L22



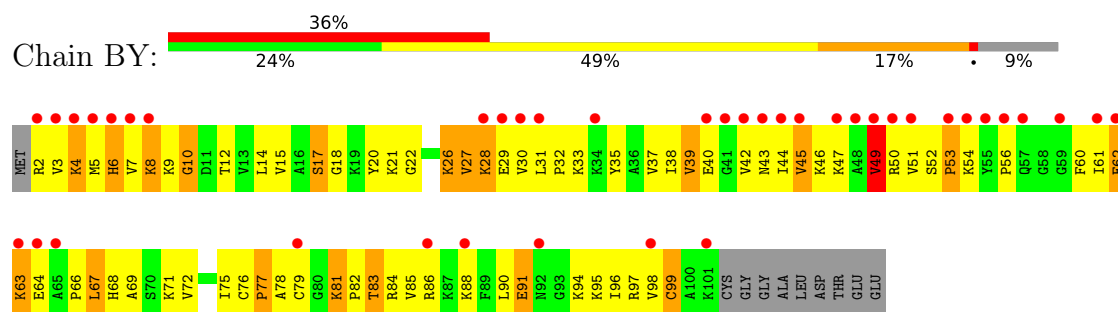
- Molecule 56: 50S ribosomal protein L23



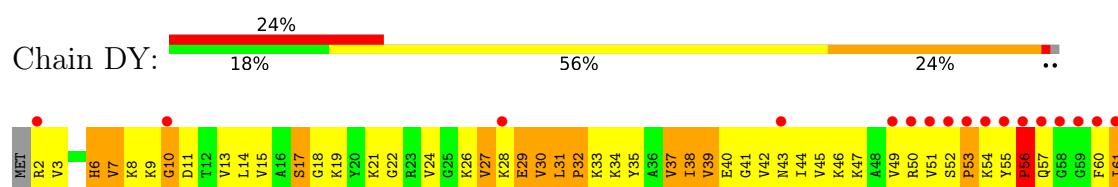
- Molecule 56: 50S ribosomal protein L23

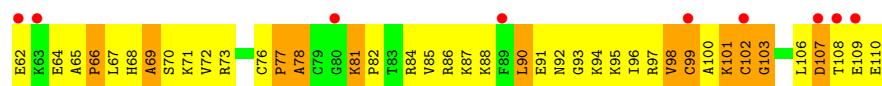


- Molecule 57: 50S ribosomal protein L24

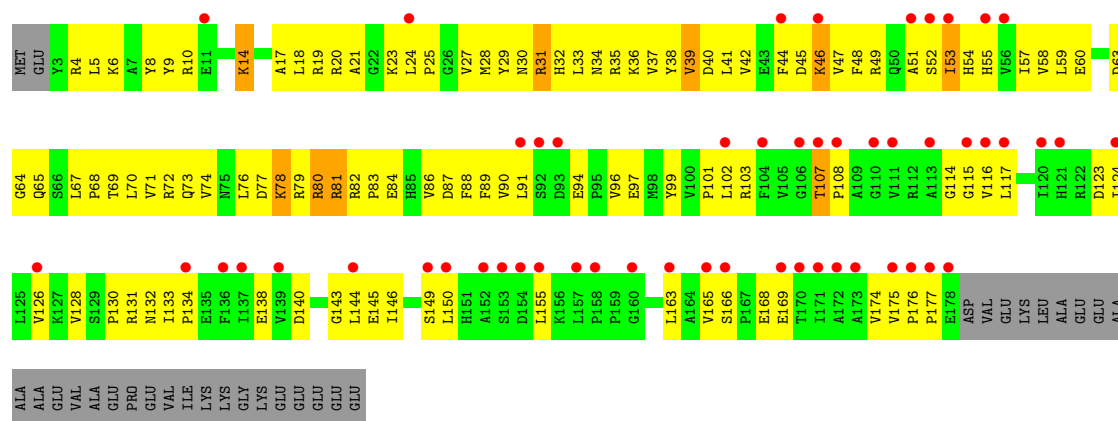


- Molecule 57: 50S ribosomal protein L24

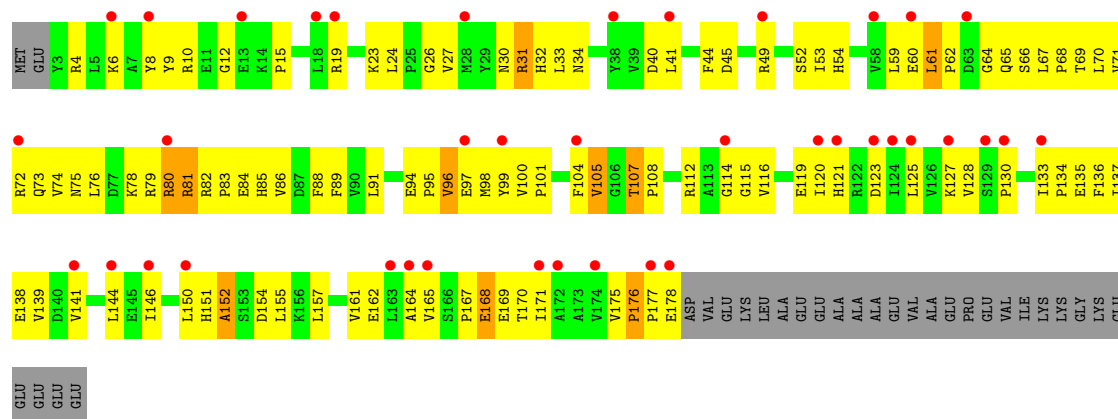




• Molecule 58: 50S ribosomal protein L25



• Molecule 58: 50S ribosomal protein L25



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.45Å 449.38Å 619.59Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 147.06 – 3.27<br>147.06 – 3.27                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (147.06-3.27)<br>99.8 (147.06-3.27)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.40 (at 3.26Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.16_3549                                            | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.277<br>0.215 , 0.276                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 44321 reflections (4.96%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.091                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.25 , 59.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 296449                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5         |
| 1   | AA    | 0.51         | 0/36190       | 0.78        | 18/56486 (0.0%) |
| 1   | CA    | 0.49         | 0/36193       | 0.72        | 9/56490 (0.0%)  |
| 2   | AB    | 0.49         | 1/1816 (0.1%) | 0.89        | 4/2445 (0.2%)   |
| 2   | CB    | 0.41         | 0/1935        | 0.71        | 0/2609          |
| 3   | AC    | 0.41         | 0/1636        | 0.71        | 0/2205          |
| 3   | CC    | 0.44         | 0/1644        | 0.74        | 0/2215          |
| 4   | AD    | 0.56         | 0/1733        | 0.89        | 2/2318 (0.1%)   |
| 4   | CD    | 0.48         | 0/1733        | 0.79        | 0/2318          |
| 5   | AE    | 0.47         | 0/1162        | 0.80        | 3/1564 (0.2%)   |
| 5   | CE    | 0.54         | 0/1171        | 0.83        | 0/1576          |
| 6   | AF    | 0.47         | 0/856         | 0.71        | 0/1154          |
| 6   | CF    | 0.48         | 0/856         | 0.68        | 0/1154          |
| 7   | AG    | 0.44         | 0/1276        | 0.80        | 0/1709          |
| 7   | CG    | 0.50         | 0/1276        | 0.81        | 4/1709 (0.2%)   |
| 8   | AH    | 0.89         | 6/1136 (0.5%) | 1.07        | 3/1527 (0.2%)   |
| 8   | CH    | 0.50         | 0/1136        | 0.76        | 0/1527          |
| 9   | AI    | 0.39         | 0/964         | 0.69        | 0/1294          |
| 9   | CI    | 0.39         | 0/1029        | 0.74        | 0/1379          |
| 10  | AJ    | 0.43         | 0/807         | 0.79        | 1/1085 (0.1%)   |
| 10  | CJ    | 0.43         | 0/807         | 0.76        | 1/1085 (0.1%)   |
| 11  | AK    | 0.51         | 0/900         | 0.82        | 0/1213          |
| 11  | CK    | 0.52         | 0/900         | 0.78        | 0/1213          |
| 12  | AL    | 0.62         | 0/972         | 0.97        | 0/1301          |
| 12  | CL    | 0.70         | 0/986         | 1.05        | 2/1320 (0.2%)   |
| 13  | AM    | 0.42         | 0/932         | 0.75        | 0/1249          |
| 13  | CM    | 0.44         | 0/956         | 0.75        | 0/1281          |
| 14  | AN    | 0.49         | 0/500         | 0.91        | 0/664           |
| 14  | CN    | 0.51         | 0/501         | 0.97        | 0/664           |
| 15  | AO    | 0.48         | 0/745         | 0.79        | 2/992 (0.2%)    |
| 15  | CO    | 0.52         | 0/745         | 0.79        | 0/992           |
| 16  | AP    | 0.55         | 0/716         | 0.91        | 0/963           |
| 16  | CP    | 0.51         | 0/716         | 0.84        | 1/963 (0.1%)    |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 17  | AQ    | 0.51         | 0/836           | 0.80        | 0/1117           |
| 17  | CQ    | 0.52         | 0/836           | 0.91        | 0/1117           |
| 18  | AR    | 0.47         | 0/579           | 0.82        | 0/768            |
| 18  | CR    | 0.54         | 0/579           | 0.86        | 0/768            |
| 19  | AS    | 0.41         | 0/642           | 0.82        | 0/865            |
| 19  | CS    | 0.49         | 0/642           | 0.85        | 0/865            |
| 20  | AT    | 0.49         | 0/765           | 0.81        | 0/1007           |
| 20  | CT    | 0.48         | 0/765           | 0.91        | 1/1007 (0.1%)    |
| 21  | AU    | 0.44         | 0/212           | 0.82        | 0/277            |
| 21  | CU    | 0.58         | 0/221           | 0.83        | 0/288            |
| 22  | AV    | 0.48         | 0/1812          | 0.76        | 0/2823           |
| 22  | CV    | 0.52         | 0/1835          | 0.81        | 0/2857           |
| 23  | AW    | 0.39         | 0/1813          | 0.76        | 0/2823           |
| 23  | AY    | 0.60         | 0/459           | 0.77        | 0/714            |
| 23  | CW    | 0.40         | 0/1813          | 0.74        | 0/2823           |
| 23  | CY    | 0.48         | 0/507           | 0.71        | 0/789            |
| 24  | AX    | 0.48         | 0/285           | 0.83        | 0/441            |
| 24  | CX    | 0.60         | 0/285           | 0.97        | 0/441            |
| 25  | B0    | 0.61         | 0/615           | 0.94        | 0/819            |
| 25  | D0    | 0.80         | 0/653           | 1.15        | 3/869 (0.3%)     |
| 26  | B1    | 1.02         | 0/699           | 1.42        | 7/929 (0.8%)     |
| 26  | D1    | 1.07         | 3/699 (0.4%)    | 1.56        | 7/929 (0.8%)     |
| 27  | B2    | 0.75         | 0/422           | 1.27        | 0/558            |
| 27  | D2    | 1.13         | 0/448           | 1.61        | 5/593 (0.8%)     |
| 28  | B3    | 0.54         | 0/464           | 0.78        | 0/623            |
| 28  | D3    | 0.65         | 0/481           | 0.95        | 0/646            |
| 29  | B4    | 0.67         | 1/221 (0.5%)    | 1.21        | 2/306 (0.7%)     |
| 29  | D4    | 0.47         | 0/240           | 1.23        | 1/332 (0.3%)     |
| 30  | B5    | 0.70         | 0/432           | 1.18        | 5/585 (0.9%)     |
| 30  | D5    | 0.79         | 0/481           | 1.14        | 3/649 (0.5%)     |
| 31  | B6    | 0.85         | 0/405           | 1.40        | 1/540 (0.2%)     |
| 31  | D6    | 0.98         | 0/415           | 1.48        | 8/554 (1.4%)     |
| 32  | B7    | 0.85         | 0/426           | 1.20        | 3/561 (0.5%)     |
| 32  | D7    | 0.82         | 0/426           | 0.98        | 1/561 (0.2%)     |
| 33  | B8    | 1.00         | 1/515 (0.2%)    | 1.51        | 6/679 (0.9%)     |
| 33  | D8    | 1.04         | 1/502 (0.2%)    | 1.51        | 8/661 (1.2%)     |
| 34  | B9    | 0.52         | 0/310           | 0.88        | 0/407            |
| 34  | D9    | 0.66         | 0/310           | 1.00        | 0/407            |
| 35  | BA    | 0.63         | 10/68122 (0.0%) | 0.85        | 56/106350 (0.1%) |
| 35  | DA    | 0.70         | 8/68122 (0.0%)  | 0.90        | 40/106350 (0.0%) |
| 36  | BB    | 0.45         | 0/2881          | 0.75        | 1/4494 (0.0%)    |
| 36  | DB    | 0.55         | 0/2853          | 0.82        | 3/4451 (0.1%)    |
| 37  | BC    | 0.35         | 0/1144          | 0.76        | 2/1554 (0.1%)    |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 37  | DC    | 0.42         | 1/1144 (0.1%)    | 0.62        | 0/1554            |
| 38  | BD    | 0.77         | 0/2176           | 1.10        | 3/2933 (0.1%)     |
| 38  | DD    | 0.79         | 0/2194           | 1.14        | 8/2955 (0.3%)     |
| 39  | BE    | 0.68         | 0/1596           | 1.04        | 2/2153 (0.1%)     |
| 39  | DE    | 0.76         | 0/1596           | 1.09        | 1/2153 (0.0%)     |
| 40  | BF    | 0.65         | 0/1650           | 0.99        | 1/2234 (0.0%)     |
| 40  | DF    | 0.73         | 0/1662           | 1.08        | 8/2249 (0.4%)     |
| 41  | BG    | 0.43         | 0/1473           | 0.84        | 1/1983 (0.1%)     |
| 41  | DG    | 0.49         | 0/1499           | 0.88        | 3/2016 (0.1%)     |
| 42  | BH    | 0.39         | 0/1245           | 0.73        | 1/1682 (0.1%)     |
| 42  | DH    | 0.62         | 0/1295           | 0.94        | 0/1753            |
| 43  | BI    | 0.48         | 0/1146           | 0.85        | 1/1551 (0.1%)     |
| 43  | DI    | 0.50         | 0/1139           | 0.93        | 1/1541 (0.1%)     |
| 46  | BN    | 0.65         | 0/1123           | 0.97        | 2/1515 (0.1%)     |
| 46  | DN    | 0.79         | 1/1147 (0.1%)    | 1.07        | 2/1547 (0.1%)     |
| 47  | BO    | 0.64         | 0/943            | 1.00        | 2/1269 (0.2%)     |
| 47  | DO    | 0.74         | 0/943            | 0.96        | 0/1269            |
| 48  | BP    | 0.93         | 0/1116           | 1.47        | 8/1485 (0.5%)     |
| 48  | DP    | 1.15         | 6/1131 (0.5%)    | 1.66        | 23/1504 (1.5%)    |
| 49  | BQ    | 0.74         | 0/1095           | 1.15        | 8/1464 (0.5%)     |
| 49  | DQ    | 0.87         | 0/1104           | 1.39        | 16/1476 (1.1%)    |
| 50  | BR    | 0.81         | 0/963            | 1.15        | 2/1288 (0.2%)     |
| 50  | DR    | 0.79         | 0/974            | 1.13        | 4/1302 (0.3%)     |
| 51  | BS    | 0.73         | 3/822 (0.4%)     | 1.14        | 4/1094 (0.4%)     |
| 51  | DS    | 0.74         | 1/789 (0.1%)     | 1.26        | 10/1050 (1.0%)    |
| 52  | BT    | 0.69         | 0/1114           | 1.07        | 0/1488            |
| 52  | DT    | 0.82         | 0/1155           | 1.15        | 2/1542 (0.1%)     |
| 53  | BU    | 0.71         | 0/982            | 0.92        | 1/1306 (0.1%)     |
| 53  | DU    | 0.81         | 1/982 (0.1%)     | 1.05        | 2/1306 (0.2%)     |
| 54  | BV    | 0.71         | 0/790            | 1.31        | 3/1057 (0.3%)     |
| 54  | DV    | 0.85         | 1/790 (0.1%)     | 1.41        | 12/1057 (1.1%)    |
| 55  | BW    | 0.76         | 0/897            | 1.18        | 3/1204 (0.2%)     |
| 55  | DW    | 0.70         | 0/897            | 0.96        | 1/1204 (0.1%)     |
| 56  | BX    | 0.81         | 0/718            | 1.32        | 8/965 (0.8%)      |
| 56  | DX    | 0.99         | 0/756            | 1.52        | 11/1014 (1.1%)    |
| 57  | BY    | 0.66         | 0/788            | 1.09        | 2/1051 (0.2%)     |
| 57  | DY    | 0.79         | 0/848            | 1.30        | 6/1132 (0.5%)     |
| 58  | BZ    | 0.46         | 0/1435           | 0.80        | 0/1949            |
| 58  | DZ    | 0.49         | 0/1435           | 0.87        | 0/1949            |
| All | All   | 0.62         | 45/317649 (0.0%) | 0.88        | 375/475105 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | AB    | 0                   | 1                   |
| 2   | CB    | 0                   | 1                   |
| 3   | AC    | 0                   | 1                   |
| 3   | CC    | 0                   | 1                   |
| 4   | AD    | 0                   | 2                   |
| 4   | CD    | 0                   | 2                   |
| 7   | CG    | 0                   | 1                   |
| 8   | AH    | 0                   | 2                   |
| 9   | CI    | 0                   | 1                   |
| 10  | AJ    | 0                   | 3                   |
| 10  | CJ    | 0                   | 2                   |
| 12  | AL    | 0                   | 3                   |
| 12  | CL    | 0                   | 4                   |
| 14  | CN    | 0                   | 2                   |
| 16  | AP    | 0                   | 2                   |
| 16  | CP    | 0                   | 1                   |
| 17  | AQ    | 0                   | 1                   |
| 17  | CQ    | 0                   | 2                   |
| 18  | AR    | 0                   | 1                   |
| 18  | CR    | 0                   | 1                   |
| 19  | CS    | 0                   | 1                   |
| 20  | AT    | 0                   | 1                   |
| 20  | CT    | 0                   | 2                   |
| 26  | B1    | 0                   | 5                   |
| 26  | D1    | 0                   | 4                   |
| 27  | B2    | 0                   | 3                   |
| 27  | D2    | 0                   | 5                   |
| 29  | D4    | 0                   | 2                   |
| 30  | B5    | 0                   | 2                   |
| 31  | B6    | 0                   | 4                   |
| 31  | D6    | 0                   | 4                   |
| 32  | B7    | 0                   | 4                   |
| 32  | D7    | 0                   | 1                   |
| 33  | B8    | 0                   | 2                   |
| 33  | D8    | 0                   | 1                   |
| 37  | DC    | 0                   | 1                   |
| 38  | BD    | 0                   | 4                   |
| 38  | DD    | 0                   | 6                   |
| 39  | BE    | 0                   | 3                   |
| 39  | DE    | 0                   | 4                   |
| 40  | BF    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 40  | DF    | 0                   | 1                   |
| 41  | BG    | 0                   | 4                   |
| 41  | DG    | 0                   | 1                   |
| 42  | BH    | 0                   | 1                   |
| 42  | DH    | 0                   | 2                   |
| 43  | BI    | 0                   | 2                   |
| 43  | DI    | 0                   | 3                   |
| 46  | BN    | 0                   | 3                   |
| 46  | DN    | 0                   | 5                   |
| 47  | BO    | 0                   | 3                   |
| 47  | DO    | 0                   | 1                   |
| 48  | BP    | 0                   | 10                  |
| 48  | DP    | 0                   | 12                  |
| 49  | BQ    | 0                   | 6                   |
| 49  | DQ    | 0                   | 5                   |
| 50  | BR    | 0                   | 3                   |
| 50  | DR    | 0                   | 1                   |
| 51  | BS    | 0                   | 3                   |
| 51  | DS    | 0                   | 5                   |
| 52  | BT    | 0                   | 4                   |
| 52  | DT    | 0                   | 6                   |
| 53  | BU    | 0                   | 3                   |
| 53  | DU    | 0                   | 3                   |
| 54  | BV    | 0                   | 5                   |
| 54  | DV    | 0                   | 5                   |
| 55  | BW    | 0                   | 2                   |
| 56  | BX    | 0                   | 4                   |
| 56  | DX    | 0                   | 5                   |
| 57  | BY    | 0                   | 2                   |
| 57  | DY    | 0                   | 3                   |
| 58  | DZ    | 0                   | 1                   |
| All | All   | 0                   | 209                 |

The worst 5 of 45 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 8   | AH    | 104 | ARG  | CG-CD  | 14.23  | 1.95        | 1.52     |
| 48  | DP    | 16  | ARG  | CZ-NH1 | -10.68 | 1.17        | 1.32     |
| 37  | DC    | 163 | PHE  | CA-C   | -10.64 | 1.47        | 1.53     |
| 8   | AH    | 65  | TYR  | CA-C   | -10.21 | 1.47        | 1.52     |
| 8   | AH    | 104 | ARG  | CZ-NH1 | -8.82  | 1.20        | 1.32     |

The worst 5 of 375 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 8   | AH    | 104 | ARG  | CG-CD-NE  | 20.20  | 156.44      | 112.00   |
| 54  | BV    | 38  | LEU  | CB-CG-CD2 | -15.70 | 63.60       | 110.70   |
| 54  | BV    | 38  | LEU  | CB-CG-CD1 | 11.78  | 146.03      | 110.70   |
| 2   | AB    | 142 | LEU  | CA-CB-CG  | 11.45  | 156.36      | 116.30   |
| 48  | DP    | 16  | ARG  | CD-NE-CZ  | 11.06  | 139.88      | 124.40   |

There are no chirality outliers.

5 of 209 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | AB    | 109 | SER  | Peptide |
| 3   | AC    | 161 | GLU  | Peptide |
| 4   | AD    | 31  | CYS  | Peptide |
| 4   | AD    | 32  | ALA  | Peptide |
| 8   | AH    | 7   | ALA  | 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    | 32329 | 0        | 16318    | 1281    | 0            |
| 1   | CA    | 32332 | 0        | 16317    | 1105    | 0            |
| 2   | AB    | 1784  | 0        | 1833     | 175     | 0            |
| 2   | CB    | 1900  | 0        | 1951     | 156     | 0            |
| 3   | AC    | 1612  | 0        | 1677     | 113     | 0            |
| 3   | CC    | 1620  | 0        | 1689     | 125     | 0            |
| 4   | AD    | 1703  | 0        | 1763     | 158     | 0            |
| 4   | CD    | 1703  | 0        | 1763     | 124     | 0            |
| 5   | AE    | 1146  | 0        | 1207     | 78      | 0            |
| 5   | CE    | 1155  | 0        | 1213     | 88      | 0            |
| 6   | AF    | 843   | 0        | 857      | 46      | 0            |
| 6   | CF    | 843   | 0        | 857      | 46      | 0            |
| 7   | AG    | 1257  | 0        | 1296     | 103     | 0            |
| 7   | CG    | 1257  | 0        | 1296     | 81      | 0            |
| 8   | AH    | 1116  | 0        | 1177     | 118     | 0            |
| 8   | CH    | 1116  | 0        | 1177     | 75      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | AI    | 947   | 0        | 979      | 95      | 0            |
| 9   | CI    | 1010  | 0        | 1037     | 90      | 0            |
| 10  | AJ    | 794   | 0        | 840      | 90      | 0            |
| 10  | CJ    | 794   | 0        | 840      | 74      | 0            |
| 11  | AK    | 885   | 0        | 904      | 48      | 0            |
| 11  | CK    | 885   | 0        | 904      | 50      | 0            |
| 12  | AL    | 956   | 0        | 1046     | 89      | 0            |
| 12  | CL    | 970   | 0        | 1057     | 62      | 0            |
| 13  | AM    | 922   | 0        | 979      | 100     | 0            |
| 13  | CM    | 946   | 0        | 1008     | 83      | 0            |
| 14  | AN    | 491   | 0        | 529      | 72      | 0            |
| 14  | CN    | 492   | 0        | 530      | 58      | 0            |
| 15  | AO    | 734   | 0        | 771      | 63      | 0            |
| 15  | CO    | 734   | 0        | 771      | 49      | 0            |
| 16  | AP    | 700   | 0        | 720      | 47      | 0            |
| 16  | CP    | 700   | 0        | 720      | 57      | 0            |
| 17  | AQ    | 823   | 0        | 891      | 58      | 0            |
| 17  | CQ    | 823   | 0        | 889      | 69      | 0            |
| 18  | AR    | 574   | 0        | 642      | 39      | 0            |
| 18  | CR    | 574   | 0        | 644      | 58      | 0            |
| 19  | AS    | 629   | 0        | 652      | 80      | 0            |
| 19  | CS    | 629   | 0        | 652      | 66      | 0            |
| 20  | AT    | 763   | 0        | 861      | 56      | 0            |
| 20  | CT    | 763   | 0        | 861      | 66      | 0            |
| 21  | AU    | 208   | 0        | 221      | 14      | 0            |
| 21  | CU    | 217   | 0        | 234      | 18      | 0            |
| 22  | AV    | 1622  | 0        | 825      | 36      | 0            |
| 22  | CV    | 1643  | 0        | 836      | 50      | 0            |
| 23  | AW    | 1623  | 0        | 820      | 45      | 0            |
| 23  | AY    | 410   | 0        | 207      | 18      | 0            |
| 23  | CW    | 1623  | 0        | 821      | 66      | 0            |
| 23  | CY    | 453   | 0        | 229      | 10      | 0            |
| 24  | AX    | 255   | 0        | 129      | 6       | 0            |
| 24  | CX    | 255   | 0        | 129      | 10      | 0            |
| 25  | B0    | 607   | 0        | 628      | 52      | 0            |
| 25  | D0    | 645   | 0        | 673      | 45      | 0            |
| 26  | B1    | 692   | 0        | 764      | 110     | 0            |
| 26  | D1    | 692   | 0        | 764      | 103     | 0            |
| 27  | B2    | 420   | 0        | 461      | 72      | 0            |
| 27  | D2    | 446   | 0        | 486      | 91      | 0            |
| 28  | B3    | 459   | 0        | 512      | 25      | 0            |
| 28  | D3    | 476   | 0        | 529      | 31      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | B4    | 222   | 0        | 91       | 4       | 0            |
| 29  | D4    | 241   | 0        | 103      | 7       | 0            |
| 30  | B5    | 418   | 0        | 432      | 45      | 0            |
| 30  | D5    | 467   | 0        | 492      | 50      | 0            |
| 31  | B6    | 398   | 0        | 417      | 61      | 0            |
| 31  | D6    | 408   | 0        | 426      | 56      | 0            |
| 32  | B7    | 418   | 0        | 467      | 39      | 0            |
| 32  | D7    | 418   | 0        | 467      | 32      | 0            |
| 33  | B8    | 507   | 0        | 576      | 96      | 0            |
| 33  | D8    | 495   | 0        | 567      | 96      | 0            |
| 34  | B9    | 307   | 0        | 336      | 31      | 0            |
| 34  | D9    | 307   | 0        | 335      | 19      | 0            |
| 35  | BA    | 60821 | 0        | 30654    | 2035    | 0            |
| 35  | DA    | 60821 | 0        | 30655    | 1781    | 0            |
| 36  | BB    | 2576  | 0        | 1305     | 114     | 0            |
| 36  | DB    | 2551  | 0        | 1295     | 89      | 0            |
| 37  | BC    | 1141  | 0        | 865      | 43      | 0            |
| 37  | DC    | 1141  | 0        | 865      | 58      | 0            |
| 38  | BD    | 2126  | 0        | 2208     | 202     | 0            |
| 38  | DD    | 2144  | 0        | 2234     | 194     | 0            |
| 39  | BE    | 1563  | 0        | 1629     | 150     | 0            |
| 39  | DE    | 1563  | 0        | 1629     | 144     | 0            |
| 40  | BF    | 1615  | 0        | 1665     | 172     | 0            |
| 40  | DF    | 1627  | 0        | 1679     | 132     | 0            |
| 41  | BG    | 1449  | 0        | 1503     | 115     | 0            |
| 41  | DG    | 1474  | 0        | 1535     | 119     | 0            |
| 42  | BH    | 1222  | 0        | 1282     | 93      | 0            |
| 42  | DH    | 1270  | 0        | 1339     | 101     | 0            |
| 43  | BI    | 1131  | 0        | 1218     | 100     | 0            |
| 43  | DI    | 1124  | 0        | 1209     | 75      | 0            |
| 44  | BJ    | 651   | 0        | 171      | 9       | 0            |
| 44  | DJ    | 651   | 0        | 163      | 4       | 0            |
| 45  | BK    | 700   | 0        | 166      | 0       | 0            |
| 45  | DK    | 700   | 0        | 179      | 5       | 0            |
| 46  | BN    | 1096  | 0        | 1168     | 108     | 0            |
| 46  | DN    | 1120  | 0        | 1195     | 114     | 0            |
| 47  | BO    | 933   | 0        | 996      | 78      | 0            |
| 47  | DO    | 933   | 0        | 996      | 62      | 0            |
| 48  | BP    | 1099  | 0        | 1176     | 225     | 0            |
| 48  | DP    | 1114  | 0        | 1187     | 208     | 0            |
| 49  | BQ    | 1074  | 0        | 1129     | 117     | 0            |
| 49  | DQ    | 1083  | 0        | 1135     | 118     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 50  | BR    | 949   | 0        | 1008     | 114     | 0            |
| 50  | DR    | 960   | 0        | 1021     | 103     | 0            |
| 51  | BS    | 813   | 0        | 873      | 121     | 0            |
| 51  | DS    | 781   | 0        | 845      | 87      | 0            |
| 52  | BT    | 1100  | 0        | 1164     | 130     | 0            |
| 52  | DT    | 1141  | 0        | 1202     | 130     | 0            |
| 53  | BU    | 964   | 0        | 1022     | 122     | 0            |
| 53  | DU    | 964   | 0        | 1022     | 110     | 0            |
| 54  | BV    | 779   | 0        | 852      | 123     | 0            |
| 54  | DV    | 779   | 0        | 852      | 114     | 0            |
| 55  | BW    | 886   | 0        | 948      | 95      | 0            |
| 55  | DW    | 886   | 0        | 948      | 55      | 0            |
| 56  | BX    | 704   | 0        | 758      | 106     | 0            |
| 56  | DX    | 742   | 0        | 801      | 134     | 0            |
| 57  | BY    | 775   | 0        | 870      | 93      | 0            |
| 57  | DY    | 835   | 0        | 920      | 129     | 0            |
| 58  | BZ    | 1403  | 0        | 1432     | 121     | 0            |
| 58  | DZ    | 1403  | 0        | 1432     | 93      | 0            |
| 59  | AA    | 209   | 0        | 0        | 0       | 0            |
| 59  | AC    | 1     | 0        | 0        | 0       | 0            |
| 59  | AD    | 1     | 0        | 0        | 0       | 0            |
| 59  | AE    | 1     | 0        | 0        | 0       | 0            |
| 59  | AL    | 1     | 0        | 0        | 0       | 0            |
| 59  | AT    | 1     | 0        | 0        | 0       | 0            |
| 59  | AV    | 7     | 0        | 0        | 0       | 0            |
| 59  | AW    | 20    | 0        | 0        | 0       | 0            |
| 59  | AX    | 3     | 0        | 0        | 0       | 0            |
| 59  | B0    | 1     | 0        | 0        | 0       | 0            |
| 59  | B1    | 2     | 0        | 0        | 0       | 0            |
| 59  | B2    | 1     | 0        | 0        | 0       | 0            |
| 59  | B5    | 1     | 0        | 0        | 0       | 0            |
| 59  | B7    | 1     | 0        | 0        | 0       | 0            |
| 59  | B8    | 2     | 0        | 0        | 0       | 0            |
| 59  | BA    | 457   | 0        | 0        | 0       | 0            |
| 59  | BB    | 17    | 0        | 0        | 0       | 0            |
| 59  | BC    | 2     | 0        | 0        | 0       | 0            |
| 59  | BE    | 2     | 0        | 0        | 0       | 0            |
| 59  | BF    | 3     | 0        | 0        | 0       | 0            |
| 59  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 59  | BS    | 1     | 0        | 0        | 0       | 0            |
| 59  | BU    | 5     | 0        | 0        | 0       | 0            |
| 59  | BV    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 59  | BX    | 2      | 0        | 0        | 0       | 0            |
| 59  | CA    | 195    | 0        | 0        | 0       | 0            |
| 59  | CE    | 1      | 0        | 0        | 0       | 0            |
| 59  | CF    | 1      | 0        | 0        | 0       | 0            |
| 59  | CG    | 1      | 0        | 0        | 0       | 0            |
| 59  | CI    | 1      | 0        | 0        | 0       | 0            |
| 59  | CU    | 1      | 0        | 0        | 0       | 0            |
| 59  | CV    | 4      | 0        | 0        | 0       | 0            |
| 59  | CW    | 13     | 0        | 0        | 0       | 0            |
| 59  | CX    | 2      | 0        | 0        | 0       | 0            |
| 59  | D2    | 2      | 0        | 0        | 0       | 0            |
| 59  | D5    | 1      | 0        | 0        | 0       | 0            |
| 59  | DA    | 392    | 0        | 0        | 0       | 0            |
| 59  | DB    | 12     | 0        | 0        | 0       | 0            |
| 59  | DE    | 1      | 0        | 0        | 0       | 0            |
| 59  | DF    | 2      | 0        | 0        | 0       | 0            |
| 59  | DN    | 1      | 0        | 0        | 0       | 0            |
| 59  | DO    | 2      | 0        | 0        | 0       | 0            |
| 59  | DV    | 1      | 0        | 0        | 0       | 0            |
| 60  | AA    | 41     | 0        | 0        | 2       | 0            |
| 60  | CA    | 41     | 0        | 0        | 1       | 0            |
| 61  | AD    | 1      | 0        | 0        | 0       | 0            |
| 61  | AN    | 1      | 0        | 0        | 0       | 0            |
| 61  | B9    | 1      | 0        | 0        | 0       | 0            |
| 61  | CD    | 1      | 0        | 0        | 0       | 0            |
| 61  | CN    | 1      | 0        | 0        | 0       | 0            |
| 61  | D9    | 1      | 0        | 0        | 0       | 0            |
| 62  | AA    | 2      | 0        | 0        | 1       | 0            |
| All | All   | 296449 | 0        | 198495   | 13850   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 13850 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) |
|-------------------|------------------|--------------------------|-------------------|
| 2:AB:142:LEU:CD2  | 2:AB:142:LEU:CG  | 1.77                     | 1.58              |
| 4:AD:122:ARG:HH12 | 4:AD:136:PRO:CD  | 1.22                     | 1.50              |
| 4:AD:122:ARG:NH1  | 4:AD:136:PRO:HD3 | 1.27                     | 1.48              |
| 8:AH:104:ARG:CD   | 8:AH:104:ARG:CG  | 1.95                     | 1.43              |
| 58:DZ:61:LEU:HD12 | 58:DZ:62:PRO:CD  | 1.52                     | 1.35              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AB    | 216/256 (84%) | 148 (68%) | 42 (19%) | 26 (12%) | 0           | 1  |
| 2   | CB    | 232/256 (91%) | 148 (64%) | 59 (25%) | 25 (11%) | 0           | 2  |
| 3   | AC    | 204/239 (85%) | 145 (71%) | 41 (20%) | 18 (9%)  | 0           | 4  |
| 3   | CC    | 205/239 (86%) | 153 (75%) | 37 (18%) | 15 (7%)  | 1           | 6  |
| 4   | AD    | 206/209 (99%) | 148 (72%) | 35 (17%) | 23 (11%) | 0           | 2  |
| 4   | CD    | 206/209 (99%) | 150 (73%) | 41 (20%) | 15 (7%)  | 1           | 6  |
| 5   | AE    | 148/162 (91%) | 113 (76%) | 24 (16%) | 11 (7%)  | 1           | 6  |
| 5   | CE    | 149/162 (92%) | 114 (76%) | 27 (18%) | 8 (5%)   | 1           | 10 |
| 6   | AF    | 99/101 (98%)  | 80 (81%)  | 12 (12%) | 7 (7%)   | 1           | 6  |
| 6   | CF    | 99/101 (98%)  | 84 (85%)  | 12 (12%) | 3 (3%)   | 3           | 20 |
| 7   | AG    | 153/156 (98%) | 103 (67%) | 33 (22%) | 17 (11%) | 0           | 2  |
| 7   | CG    | 153/156 (98%) | 112 (73%) | 30 (20%) | 11 (7%)  | 1           | 6  |
| 8   | AH    | 136/138 (99%) | 98 (72%)  | 25 (18%) | 13 (10%) | 0           | 3  |
| 8   | CH    | 136/138 (99%) | 100 (74%) | 26 (19%) | 10 (7%)  | 1           | 6  |
| 9   | AI    | 119/128 (93%) | 80 (67%)  | 20 (17%) | 19 (16%) | 0           | 1  |
| 9   | CI    | 125/128 (98%) | 87 (70%)  | 23 (18%) | 15 (12%) | 0           | 1  |
| 10  | AJ    | 96/105 (91%)  | 61 (64%)  | 23 (24%) | 12 (12%) | 0           | 1  |
| 10  | CJ    | 96/105 (91%)  | 66 (69%)  | 20 (21%) | 10 (10%) | 0           | 2  |
| 11  | AK    | 117/129 (91%) | 89 (76%)  | 19 (16%) | 9 (8%)   | 1           | 5  |
| 11  | CK    | 117/129 (91%) | 86 (74%)  | 23 (20%) | 8 (7%)   | 1           | 7  |
| 12  | AL    | 120/132 (91%) | 81 (68%)  | 23 (19%) | 16 (13%) | 0           | 1  |
| 12  | CL    | 122/132 (92%) | 86 (70%)  | 21 (17%) | 15 (12%) | 0           | 1  |

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| Mol | Chain | Analysed      | Favoured | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 13  | AM    | 114/126 (90%) | 78 (68%) | 22 (19%) | 14 (12%) | 0           | 1  |
| 13  | CM    | 117/126 (93%) | 88 (75%) | 16 (14%) | 13 (11%) | 0           | 2  |
| 14  | AN    | 58/61 (95%)   | 35 (60%) | 16 (28%) | 7 (12%)  | 0           | 1  |
| 14  | CN    | 58/61 (95%)   | 36 (62%) | 13 (22%) | 9 (16%)  | 0           | 1  |
| 15  | AO    | 86/89 (97%)   | 67 (78%) | 14 (16%) | 5 (6%)   | 1           | 9  |
| 15  | CO    | 86/89 (97%)   | 61 (71%) | 19 (22%) | 6 (7%)   | 1           | 6  |
| 16  | AP    | 81/88 (92%)   | 58 (72%) | 17 (21%) | 6 (7%)   | 1           | 6  |
| 16  | CP    | 81/88 (92%)   | 53 (65%) | 22 (27%) | 6 (7%)   | 1           | 6  |
| 17  | AQ    | 97/105 (92%)  | 81 (84%) | 13 (13%) | 3 (3%)   | 3           | 19 |
| 17  | CQ    | 97/105 (92%)  | 74 (76%) | 13 (13%) | 10 (10%) | 0           | 2  |
| 18  | AR    | 68/88 (77%)   | 55 (81%) | 8 (12%)  | 5 (7%)   | 1           | 6  |
| 18  | CR    | 68/88 (77%)   | 48 (71%) | 12 (18%) | 8 (12%)  | 0           | 1  |
| 19  | AS    | 76/93 (82%)   | 33 (43%) | 30 (40%) | 13 (17%) | 0           | 1  |
| 19  | CS    | 76/93 (82%)   | 46 (60%) | 15 (20%) | 15 (20%) | 0           | 0  |
| 20  | AT    | 97/106 (92%)  | 64 (66%) | 23 (24%) | 10 (10%) | 0           | 2  |
| 20  | CT    | 97/106 (92%)  | 67 (69%) | 18 (19%) | 12 (12%) | 0           | 1  |
| 21  | AU    | 22/27 (82%)   | 15 (68%) | 3 (14%)  | 4 (18%)  | 0           | 0  |
| 21  | CU    | 23/27 (85%)   | 19 (83%) | 1 (4%)   | 3 (13%)  | 0           | 1  |
| 25  | B0    | 74/85 (87%)   | 56 (76%) | 13 (18%) | 5 (7%)   | 1           | 7  |
| 25  | D0    | 80/85 (94%)   | 59 (74%) | 13 (16%) | 8 (10%)  | 0           | 3  |
| 26  | B1    | 86/98 (88%)   | 45 (52%) | 21 (24%) | 20 (23%) | 0           | 0  |
| 26  | D1    | 86/98 (88%)   | 60 (70%) | 12 (14%) | 14 (16%) | 0           | 1  |
| 27  | B2    | 48/72 (67%)   | 14 (29%) | 20 (42%) | 14 (29%) | 0           | 0  |
| 27  | D2    | 51/72 (71%)   | 22 (43%) | 16 (31%) | 13 (26%) | 0           | 0  |
| 28  | B3    | 56/60 (93%)   | 47 (84%) | 7 (12%)  | 2 (4%)   | 2           | 17 |
| 28  | D3    | 58/60 (97%)   | 46 (79%) | 7 (12%)  | 5 (9%)   | 0           | 4  |
| 29  | B4    | 43/71 (61%)   | 10 (23%) | 13 (30%) | 20 (46%) | 0           | 0  |
| 29  | D4    | 47/71 (66%)   | 11 (23%) | 17 (36%) | 19 (40%) | 0           | 0  |
| 30  | B5    | 52/60 (87%)   | 34 (65%) | 9 (17%)  | 9 (17%)  | 0           | 1  |
| 30  | D5    | 58/60 (97%)   | 40 (69%) | 14 (24%) | 4 (7%)   | 1           | 6  |
| 31  | B6    | 44/54 (82%)   | 19 (43%) | 8 (18%)  | 17 (39%) | 0           | 0  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 31  | D6    | 45/54 (83%)   | 19 (42%)  | 14 (31%) | 12 (27%) | 0           | 0   |
| 32  | B7    | 46/49 (94%)   | 36 (78%)  | 6 (13%)  | 4 (9%)   | 0           | 4   |
| 32  | D7    | 46/49 (94%)   | 42 (91%)  | 4 (9%)   | 0        | 100         | 100 |
| 33  | B8    | 61/65 (94%)   | 37 (61%)  | 15 (25%) | 9 (15%)  | 0           | 1   |
| 33  | D8    | 60/65 (92%)   | 35 (58%)  | 13 (22%) | 12 (20%) | 0           | 0   |
| 34  | B9    | 35/37 (95%)   | 28 (80%)  | 5 (14%)  | 2 (6%)   | 1           | 9   |
| 34  | D9    | 35/37 (95%)   | 25 (71%)  | 7 (20%)  | 3 (9%)   | 0           | 4   |
| 37  | BC    | 182/229 (80%) | 82 (45%)  | 54 (30%) | 46 (25%) | 0           | 0   |
| 37  | DC    | 182/229 (80%) | 78 (43%)  | 63 (35%) | 41 (22%) | 0           | 0   |
| 38  | BD    | 271/276 (98%) | 203 (75%) | 45 (17%) | 23 (8%)  | 0           | 4   |
| 38  | DD    | 273/276 (99%) | 212 (78%) | 43 (16%) | 18 (7%)  | 1           | 7   |
| 39  | BE    | 202/206 (98%) | 147 (73%) | 35 (17%) | 20 (10%) | 0           | 3   |
| 39  | DE    | 202/206 (98%) | 137 (68%) | 36 (18%) | 29 (14%) | 0           | 1   |
| 40  | BF    | 204/210 (97%) | 130 (64%) | 39 (19%) | 35 (17%) | 0           | 1   |
| 40  | DF    | 206/210 (98%) | 152 (74%) | 35 (17%) | 19 (9%)  | 0           | 3   |
| 41  | BG    | 176/182 (97%) | 117 (66%) | 42 (24%) | 17 (10%) | 0           | 3   |
| 41  | DG    | 179/182 (98%) | 132 (74%) | 32 (18%) | 15 (8%)  | 0           | 4   |
| 42  | BH    | 157/180 (87%) | 92 (59%)  | 43 (27%) | 22 (14%) | 0           | 1   |
| 42  | DH    | 163/180 (91%) | 104 (64%) | 33 (20%) | 26 (16%) | 0           | 1   |
| 43  | BI    | 143/148 (97%) | 88 (62%)  | 35 (24%) | 20 (14%) | 0           | 1   |
| 43  | DI    | 142/148 (96%) | 91 (64%)  | 30 (21%) | 21 (15%) | 0           | 1   |
| 46  | BN    | 135/140 (96%) | 91 (67%)  | 20 (15%) | 24 (18%) | 0           | 0   |
| 46  | DN    | 138/140 (99%) | 90 (65%)  | 22 (16%) | 26 (19%) | 0           | 0   |
| 47  | BO    | 120/122 (98%) | 89 (74%)  | 21 (18%) | 10 (8%)  | 0           | 4   |
| 47  | DO    | 120/122 (98%) | 106 (88%) | 13 (11%) | 1 (1%)   | 16          | 44  |
| 48  | BP    | 142/150 (95%) | 64 (45%)  | 38 (27%) | 40 (28%) | 0           | 0   |
| 48  | DP    | 144/150 (96%) | 63 (44%)  | 35 (24%) | 46 (32%) | 0           | 0   |
| 49  | BQ    | 133/141 (94%) | 76 (57%)  | 34 (26%) | 23 (17%) | 0           | 1   |
| 49  | DQ    | 134/141 (95%) | 91 (68%)  | 27 (20%) | 16 (12%) | 0           | 1   |
| 50  | BR    | 114/118 (97%) | 83 (73%)  | 19 (17%) | 12 (10%) | 0           | 2   |
| 50  | DR    | 115/118 (98%) | 92 (80%)  | 12 (10%) | 11 (10%) | 0           | 3   |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |   |
|-----|-------|-------------------|------------|------------|------------|-------------|---|
| 51  | BS    | 100/112 (89%)     | 58 (58%)   | 21 (21%)   | 21 (21%)   | 0           | 0 |
| 51  | DS    | 97/112 (87%)      | 59 (61%)   | 22 (23%)   | 16 (16%)   | 0           | 1 |
| 52  | BT    | 130/146 (89%)     | 70 (54%)   | 34 (26%)   | 26 (20%)   | 0           | 0 |
| 52  | DT    | 135/146 (92%)     | 96 (71%)   | 25 (18%)   | 14 (10%)   | 0           | 2 |
| 53  | BU    | 115/118 (98%)     | 86 (75%)   | 17 (15%)   | 12 (10%)   | 0           | 2 |
| 53  | DU    | 115/118 (98%)     | 96 (84%)   | 11 (10%)   | 8 (7%)     | 1           | 6 |
| 54  | BV    | 99/101 (98%)      | 50 (50%)   | 21 (21%)   | 28 (28%)   | 0           | 0 |
| 54  | DV    | 99/101 (98%)      | 62 (63%)   | 22 (22%)   | 15 (15%)   | 0           | 1 |
| 55  | BW    | 109/113 (96%)     | 84 (77%)   | 16 (15%)   | 9 (8%)     | 0           | 4 |
| 55  | DW    | 109/113 (96%)     | 95 (87%)   | 5 (5%)     | 9 (8%)     | 0           | 4 |
| 56  | BX    | 87/96 (91%)       | 46 (53%)   | 25 (29%)   | 16 (18%)   | 0           | 0 |
| 56  | DX    | 92/96 (96%)       | 63 (68%)   | 9 (10%)    | 20 (22%)   | 0           | 0 |
| 57  | BY    | 98/110 (89%)      | 45 (46%)   | 27 (28%)   | 26 (26%)   | 0           | 0 |
| 57  | DY    | 107/110 (97%)     | 53 (50%)   | 26 (24%)   | 28 (26%)   | 0           | 0 |
| 58  | BZ    | 174/206 (84%)     | 113 (65%)  | 43 (25%)   | 18 (10%)   | 0           | 2 |
| 58  | DZ    | 174/206 (84%)     | 120 (69%)  | 33 (19%)   | 21 (12%)   | 0           | 1 |
| All | All   | 11584/12586 (92%) | 7801 (67%) | 2288 (20%) | 1495 (13%) | 0           | 1 |

5 of 1495 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 22  | LYS  |
| 2   | AB    | 48  | MET  |
| 2   | AB    | 124 | SER  |
| 2   | AB    | 132 | LYS  |
| 2   | AB    | 150 | SER  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | AB    | 189/220 (86%)  | 189 (100%) | 0        | 100         | 100 |
| 2   | CB    | 202/220 (92%)  | 202 (100%) | 0        | 100         | 100 |
| 3   | AC    | 160/188 (85%)  | 159 (99%)  | 1 (1%)   | 78          | 82  |
| 3   | CC    | 161/188 (86%)  | 161 (100%) | 0        | 100         | 100 |
| 4   | AD    | 180/181 (99%)  | 180 (100%) | 0        | 100         | 100 |
| 4   | CD    | 180/181 (99%)  | 180 (100%) | 0        | 100         | 100 |
| 5   | AE    | 115/123 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 5   | CE    | 116/123 (94%)  | 115 (99%)  | 1 (1%)   | 70          | 78  |
| 6   | AF    | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 6   | CF    | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 7   | AG    | 126/127 (99%)  | 126 (100%) | 0        | 100         | 100 |
| 7   | CG    | 126/127 (99%)  | 126 (100%) | 0        | 100         | 100 |
| 8   | AH    | 119/119 (100%) | 119 (100%) | 0        | 100         | 100 |
| 8   | CH    | 119/119 (100%) | 119 (100%) | 0        | 100         | 100 |
| 9   | AI    | 92/99 (93%)    | 92 (100%)  | 0        | 100         | 100 |
| 9   | CI    | 98/99 (99%)    | 98 (100%)  | 0        | 100         | 100 |
| 10  | AJ    | 88/92 (96%)    | 87 (99%)   | 1 (1%)   | 65          | 76  |
| 10  | CJ    | 88/92 (96%)    | 88 (100%)  | 0        | 100         | 100 |
| 11  | AK    | 90/99 (91%)    | 90 (100%)  | 0        | 100         | 100 |
| 11  | CK    | 90/99 (91%)    | 90 (100%)  | 0        | 100         | 100 |
| 12  | AL    | 103/109 (94%)  | 103 (100%) | 0        | 100         | 100 |
| 12  | CL    | 104/109 (95%)  | 104 (100%) | 0        | 100         | 100 |
| 13  | AM    | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 13  | CM    | 95/101 (94%)   | 95 (100%)  | 0        | 100         | 100 |
| 14  | AN    | 49/50 (98%)    | 49 (100%)  | 0        | 100         | 100 |
| 14  | CN    | 49/50 (98%)    | 49 (100%)  | 0        | 100         | 100 |
| 15  | AO    | 79/80 (99%)    | 78 (99%)   | 1 (1%)   | 61          | 75  |
| 15  | CO    | 79/80 (99%)    | 79 (100%)  | 0        | 100         | 100 |
| 16  | AP    | 72/74 (97%)    | 72 (100%)  | 0        | 100         | 100 |
| 16  | CP    | 72/74 (97%)    | 71 (99%)   | 1 (1%)   | 59          | 74  |
| 17  | AQ    | 94/97 (97%)    | 94 (100%)  | 0        | 100         | 100 |
| 17  | CQ    | 94/97 (97%)    | 94 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 18  | AR    | 61/77 (79%)    | 61 (100%)  | 0        | 100         | 100 |
| 18  | CR    | 61/77 (79%)    | 61 (100%)  | 0        | 100         | 100 |
| 19  | AS    | 69/80 (86%)    | 69 (100%)  | 0        | 100         | 100 |
| 19  | CS    | 69/80 (86%)    | 69 (100%)  | 0        | 100         | 100 |
| 20  | AT    | 76/82 (93%)    | 75 (99%)   | 1 (1%)   | 61          | 75  |
| 20  | CT    | 76/82 (93%)    | 76 (100%)  | 0        | 100         | 100 |
| 21  | AU    | 19/22 (86%)    | 19 (100%)  | 0        | 100         | 100 |
| 21  | CU    | 20/22 (91%)    | 20 (100%)  | 0        | 100         | 100 |
| 25  | B0    | 61/67 (91%)    | 61 (100%)  | 0        | 100         | 100 |
| 25  | D0    | 64/67 (96%)    | 64 (100%)  | 0        | 100         | 100 |
| 26  | B1    | 73/83 (88%)    | 73 (100%)  | 0        | 100         | 100 |
| 26  | D1    | 73/83 (88%)    | 73 (100%)  | 0        | 100         | 100 |
| 27  | B2    | 46/67 (69%)    | 46 (100%)  | 0        | 100         | 100 |
| 27  | D2    | 49/67 (73%)    | 49 (100%)  | 0        | 100         | 100 |
| 28  | B3    | 50/52 (96%)    | 50 (100%)  | 0        | 100         | 100 |
| 28  | D3    | 52/52 (100%)   | 51 (98%)   | 1 (2%)   | 50          | 69  |
| 30  | B5    | 46/52 (88%)    | 46 (100%)  | 0        | 100         | 100 |
| 30  | D5    | 52/52 (100%)   | 52 (100%)  | 0        | 100         | 100 |
| 31  | B6    | 45/52 (86%)    | 45 (100%)  | 0        | 100         | 100 |
| 31  | D6    | 46/52 (88%)    | 46 (100%)  | 0        | 100         | 100 |
| 32  | B7    | 41/42 (98%)    | 41 (100%)  | 0        | 100         | 100 |
| 32  | D7    | 41/42 (98%)    | 41 (100%)  | 0        | 100         | 100 |
| 33  | B8    | 53/55 (96%)    | 53 (100%)  | 0        | 100         | 100 |
| 33  | D8    | 52/55 (94%)    | 52 (100%)  | 0        | 100         | 100 |
| 34  | B9    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 34  | D9    | 34/34 (100%)   | 34 (100%)  | 0        | 100         | 100 |
| 37  | BC    | 61/181 (34%)   | 61 (100%)  | 0        | 100         | 100 |
| 37  | DC    | 61/181 (34%)   | 61 (100%)  | 0        | 100         | 100 |
| 38  | BD    | 215/218 (99%)  | 215 (100%) | 0        | 100         | 100 |
| 38  | DD    | 217/218 (100%) | 217 (100%) | 0        | 100         | 100 |
| 39  | BE    | 165/166 (99%)  | 165 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 39  | DE    | 165/166 (99%)  | 164 (99%)  | 1 (1%)   | 78          | 82  |
| 40  | BF    | 164/166 (99%)  | 164 (100%) | 0        | 100         | 100 |
| 40  | DF    | 165/166 (99%)  | 164 (99%)  | 1 (1%)   | 78          | 82  |
| 41  | BG    | 152/156 (97%)  | 152 (100%) | 0        | 100         | 100 |
| 41  | DG    | 155/156 (99%)  | 155 (100%) | 0        | 100         | 100 |
| 42  | BH    | 132/148 (89%)  | 132 (100%) | 0        | 100         | 100 |
| 42  | DH    | 138/148 (93%)  | 138 (100%) | 0        | 100         | 100 |
| 43  | BI    | 122/124 (98%)  | 121 (99%)  | 1 (1%)   | 73          | 79  |
| 43  | DI    | 121/124 (98%)  | 121 (100%) | 0        | 100         | 100 |
| 46  | BN    | 116/119 (98%)  | 115 (99%)  | 1 (1%)   | 70          | 78  |
| 46  | DN    | 119/119 (100%) | 119 (100%) | 0        | 100         | 100 |
| 47  | BO    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 47  | DO    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 48  | BP    | 111/116 (96%)  | 111 (100%) | 0        | 100         | 100 |
| 48  | DP    | 112/116 (97%)  | 112 (100%) | 0        | 100         | 100 |
| 49  | BQ    | 106/111 (96%)  | 106 (100%) | 0        | 100         | 100 |
| 49  | DQ    | 107/111 (96%)  | 107 (100%) | 0        | 100         | 100 |
| 50  | BR    | 99/101 (98%)   | 99 (100%)  | 0        | 100         | 100 |
| 50  | DR    | 100/101 (99%)  | 100 (100%) | 0        | 100         | 100 |
| 51  | BS    | 81/88 (92%)    | 81 (100%)  | 0        | 100         | 100 |
| 51  | DS    | 78/88 (89%)    | 78 (100%)  | 0        | 100         | 100 |
| 52  | BT    | 116/127 (91%)  | 116 (100%) | 0        | 100         | 100 |
| 52  | DT    | 120/127 (94%)  | 120 (100%) | 0        | 100         | 100 |
| 53  | BU    | 93/94 (99%)    | 93 (100%)  | 0        | 100         | 100 |
| 53  | DU    | 93/94 (99%)    | 93 (100%)  | 0        | 100         | 100 |
| 54  | BV    | 82/82 (100%)   | 82 (100%)  | 0        | 100         | 100 |
| 54  | DV    | 82/82 (100%)   | 82 (100%)  | 0        | 100         | 100 |
| 55  | BW    | 91/92 (99%)    | 91 (100%)  | 0        | 100         | 100 |
| 55  | DW    | 91/92 (99%)    | 91 (100%)  | 0        | 100         | 100 |
| 56  | BX    | 72/78 (92%)    | 71 (99%)   | 1 (1%)   | 59          | 74  |
| 56  | DX    | 76/78 (97%)    | 76 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 57  | BY    | 84/91 (92%)      | 84 (100%)   | 0        | 100         | 100 |
| 57  | DY    | 90/91 (99%)      | 90 (100%)   | 0        | 100         | 100 |
| 58  | BZ    | 155/179 (87%)    | 155 (100%)  | 0        | 100         | 100 |
| 58  | DZ    | 155/179 (87%)    | 155 (100%)  | 0        | 100         | 100 |
| All | All   | 9527/10302 (92%) | 9515 (100%) | 12 (0%)  | 88          | 91  |

5 of 12 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CE    | 18  | ARG  |
| 16  | CP    | 53  | VAL  |
| 40  | DF    | 161 | GLU  |
| 28  | D3    | 30  | ARG  |
| 20  | AT    | 55  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | DG    | 108 | ASN  |
| 43  | DI    | 54  | GLN  |
| 52  | DT    | 79  | HIS  |
| 39  | BE    | 55  | ASN  |
| 39  | BE    | 48  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1503/1520 (98%) | 539 (35%)         | 67 (4%)         |
| 1   | CA    | 1503/1520 (98%) | 451 (30%)         | 39 (2%)         |
| 22  | AV    | 75/77 (97%)     | 27 (36%)          | 1 (1%)          |
| 22  | CV    | 76/77 (98%)     | 30 (39%)          | 0               |
| 23  | AW    | 75/76 (98%)     | 63 (84%)          | 8 (10%)         |
| 23  | AY    | 18/76 (23%)     | 8 (44%)           | 0               |
| 23  | CW    | 75/76 (98%)     | 50 (66%)          | 4 (5%)          |
| 23  | CY    | 20/76 (26%)     | 6 (30%)           | 0               |
| 24  | AX    | 11/24 (45%)     | 4 (36%)           | 1 (9%)          |
| 24  | CX    | 11/24 (45%)     | 4 (36%)           | 1 (9%)          |
| 35  | BA    | 2823/2839 (99%) | 989 (35%)         | 91 (3%)         |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 35  | DA    | 2823/2839 (99%) | 884 (31%)         | 74 (2%)         |
| 36  | BB    | 119/122 (97%)   | 39 (32%)          | 2 (1%)          |
| 36  | DB    | 118/122 (96%)   | 37 (31%)          | 5 (4%)          |
| All | All   | 9250/9468 (97%) | 3131 (33%)        | 293 (3%)        |

5 of 3131 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 9   | G    |
| 1   | AA    | 10  | A    |
| 1   | AA    | 14  | U    |
| 1   | AA    | 22  | G    |
| 1   | AA    | 31  | G    |

5 of 293 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 35  | DA    | 574  | C    |
| 35  | DA    | 2859 | G    |
| 35  | DA    | 859  | G    |
| 35  | DA    | 1740 | G    |
| 35  | BA    | 405  | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1384 ligands modelled in this entry, 1382 are monoatomic - leaving 2 for Mogul analysis.

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 60  | EDS  | CA    | 1787 | -    | 41,43,43     | 3.00 | 9 (21%)     | 39,61,61    | 2.00 | 16 (41%)    |
| 60  | EDS  | AA    | 1805 | -    | 41,43,43     | 3.05 | 12 (29%)    | 39,61,61    | 1.63 | 9 (23%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 60  | EDS  | CA    | 1787 | -    | -       | 4/23/79/79 | 0/3/3/3 |
| 60  | EDS  | AA    | 1805 | -    | -       | 6/23/79/79 | 0/3/3/3 |

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

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 60  | AA    | 1805 | EDS  | CBJ-CBI | 14.81 | 1.53        | 1.32     |
| 60  | CA    | 1787 | EDS  | CBJ-CBI | 14.33 | 1.52        | 1.32     |
| 60  | CA    | 1787 | EDS  | CAX-NAM | 5.72  | 1.52        | 1.45     |
| 60  | AA    | 1805 | EDS  | CBE-NAK | 5.69  | 1.46        | 1.34     |
| 60  | AA    | 1805 | EDS  | CAX-NAM | 5.54  | 1.52        | 1.45     |

The worst 5 of 25 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 60  | AA    | 1805 | EDS  | CAT-CAS-CAQ | 4.69  | 118.62      | 109.11   |
| 60  | CA    | 1787 | EDS  | CBA-OAC-CAW | 3.74  | 117.30      | 111.53   |
| 60  | CA    | 1787 | EDS  | CAV-CAR-NAK | -3.57 | 105.32      | 110.78   |
| 60  | CA    | 1787 | EDS  | OAJ-CBO-CBN | 3.56  | 124.58      | 111.50   |
| 60  | CA    | 1787 | EDS  | CAT-CAS-CAQ | 3.37  | 115.94      | 109.11   |

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 60  | AA    | 1805 | EDS  | CBO-CBN-NAO-CBL |
| 60  | CA    | 1787 | EDS  | OAG-CBB-OAB-CAT |
| 60  | AA    | 1805 | EDS  | CBI-CBL-NAO-CBN |
| 60  | AA    | 1805 | EDS  | CAY-CAX-NAM-CBH |

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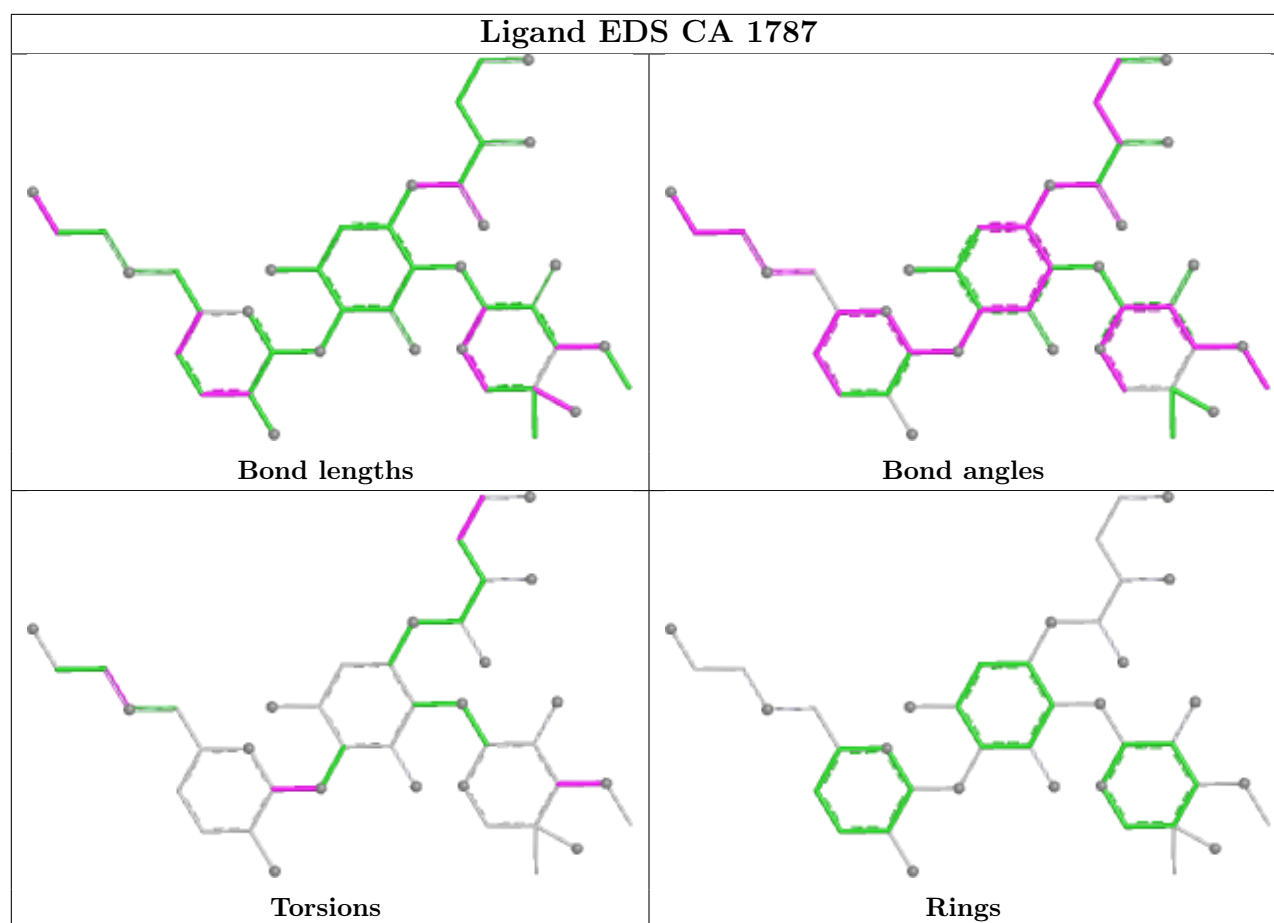
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 60  | CA    | 1787 | EDS  | CAY-CAX-NAM-CBH |

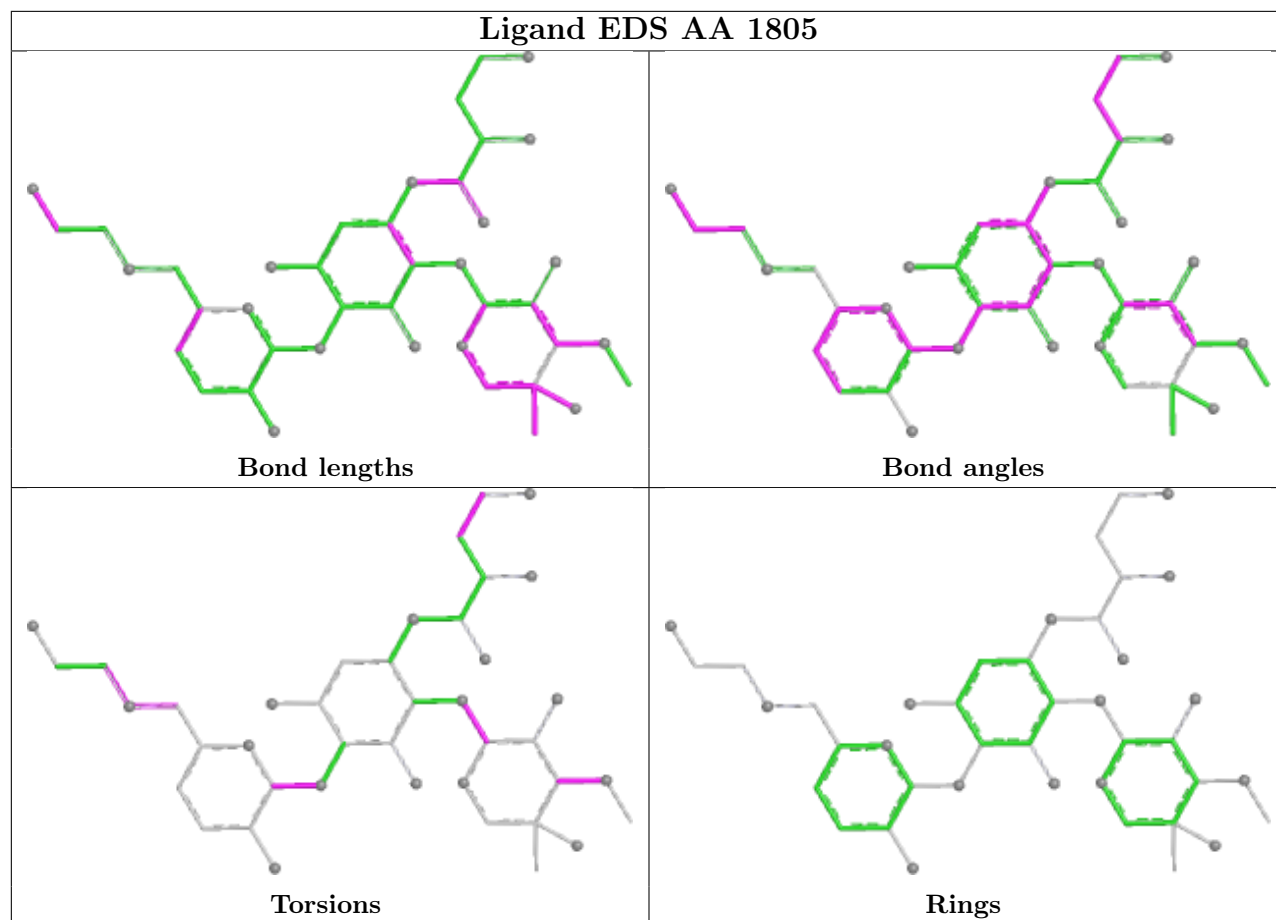
There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60  | CA    | 1787 | EDS  | 1       | 0            |
| 60  | AA    | 1805 | EDS  | 2       | 0            |

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | AA    | 1504/1520 (98%) | -0.12  | 46 (3%) 51 34  | 45, 87, 160, 209      | 0     |
| 1   | CA    | 1504/1520 (98%) | -0.27  | 13 (0%) 81 65  | 41, 84, 187, 269      | 0     |
| 2   | AB    | 218/256 (85%)   | 1.01   | 33 (15%) 5 5   | 101, 144, 193, 209    | 0     |
| 2   | CB    | 234/256 (91%)   | 0.73   | 13 (5%) 30 20  | 92, 134, 190, 208     | 0     |
| 3   | AC    | 206/239 (86%)   | 0.96   | 21 (10%) 12 10 | 89, 116, 150, 163     | 0     |
| 3   | CC    | 207/239 (86%)   | 0.96   | 22 (10%) 11 10 | 77, 109, 151, 174     | 0     |
| 4   | AD    | 208/209 (99%)   | 0.41   | 3 (1%) 73 55   | 65, 80, 100, 111      | 0     |
| 4   | CD    | 208/209 (99%)   | 1.18   | 34 (16%) 4 4   | 73, 93, 118, 130      | 0     |
| 5   | AE    | 150/162 (92%)   | 0.88   | 19 (12%) 8 7   | 70, 91, 117, 132      | 0     |
| 5   | CE    | 151/162 (93%)   | 0.75   | 18 (11%) 9 8   | 63, 83, 110, 144      | 0     |
| 6   | AF    | 101/101 (100%)  | 0.24   | 2 (1%) 65 46   | 69, 87, 102, 133      | 0     |
| 6   | CF    | 101/101 (100%)  | 0.81   | 13 (12%) 7 6   | 68, 89, 110, 129      | 0     |
| 7   | AG    | 155/156 (99%)   | 0.74   | 19 (12%) 8 7   | 90, 114, 148, 163     | 0     |
| 7   | CG    | 155/156 (99%)   | 1.19   | 21 (13%) 7 6   | 90, 109, 144, 150     | 0     |
| 8   | AH    | 138/138 (100%)  | 0.44   | 7 (5%) 33 23   | 69, 95, 112, 129      | 0     |
| 8   | CH    | 138/138 (100%)  | 0.17   | 6 (4%) 40 26   | 70, 87, 103, 110      | 0     |
| 9   | AI    | 121/128 (94%)   | 0.64   | 9 (7%) 20 16   | 90, 141, 171, 181     | 0     |
| 9   | CI    | 127/128 (99%)   | 1.16   | 22 (17%) 4 4   | 77, 134, 175, 186     | 0     |
| 10  | AJ    | 98/105 (93%)    | 1.28   | 20 (20%) 3 2   | 87, 150, 182, 186     | 0     |
| 10  | CJ    | 98/105 (93%)    | 0.97   | 12 (12%) 8 7   | 75, 151, 194, 200     | 0     |
| 11  | AK    | 119/129 (92%)   | 1.12   | 23 (19%) 3 3   | 72, 89, 120, 186      | 0     |
| 11  | CK    | 119/129 (92%)   | 0.85   | 13 (10%) 10 9  | 54, 90, 135, 188      | 0     |
| 12  | AL    | 122/132 (92%)   | 0.86   | 19 (15%) 5 4   | 56, 70, 94, 129       | 0     |
| 12  | CL    | 124/132 (93%)   | 0.86   | 20 (16%) 4 4   | 49, 64, 106, 170      | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 13  | AM    | 116/126 (92%) | 0.65   | 13 (11%) 10 9 | 84, 121, 142, 155     | 0     |
| 13  | CM    | 119/126 (94%) | 1.21   | 26 (21%) 2 2  | 68, 110, 127, 143     | 0     |
| 14  | AN    | 60/61 (98%)   | 0.79   | 6 (10%) 12 10 | 92, 111, 123, 129     | 0     |
| 14  | CN    | 60/61 (98%)   | 0.56   | 4 (6%) 24 17  | 75, 96, 112, 123      | 0     |
| 15  | AO    | 88/89 (98%)   | 0.11   | 0 100 100     | 68, 89, 116, 119      | 0     |
| 15  | CO    | 88/89 (98%)   | 0.34   | 6 (6%) 23 17  | 64, 86, 110, 123      | 0     |
| 16  | AP    | 83/88 (94%)   | 0.09   | 0 100 100     | 65, 77, 100, 140      | 0     |
| 16  | CP    | 83/88 (94%)   | 0.31   | 2 (2%) 59 40  | 75, 88, 119, 176      | 0     |
| 17  | AQ    | 99/105 (94%)  | 0.10   | 1 (1%) 79 63  | 65, 81, 105, 117      | 0     |
| 17  | CQ    | 99/105 (94%)  | 0.64   | 6 (6%) 27 19  | 76, 88, 106, 117      | 0     |
| 18  | AR    | 70/88 (79%)   | 0.64   | 4 (5%) 29 20  | 70, 90, 121, 132      | 0     |
| 18  | CR    | 70/88 (79%)   | 0.48   | 3 (4%) 40 26  | 67, 86, 131, 149      | 0     |
| 19  | AS    | 78/93 (83%)   | 0.76   | 8 (10%) 12 10 | 106, 141, 172, 180    | 0     |
| 19  | CS    | 78/93 (83%)   | 0.94   | 8 (10%) 12 10 | 85, 113, 165, 167     | 0     |
| 20  | AT    | 99/106 (93%)  | 0.22   | 1 (1%) 79 63  | 71, 89, 135, 151      | 0     |
| 20  | CT    | 99/106 (93%)  | 0.31   | 3 (3%) 52 35  | 78, 104, 140, 145     | 0     |
| 21  | AU    | 24/27 (88%)   | 0.33   | 0 100 100     | 90, 114, 134, 139     | 0     |
| 21  | CU    | 25/27 (92%)   | 0.37   | 1 (4%) 42 28  | 86, 96, 126, 130      | 0     |
| 22  | AV    | 76/77 (98%)   | 0.14   | 4 (5%) 32 22  | 56, 97, 125, 154      | 0     |
| 22  | CV    | 77/77 (100%)  | -0.25  | 2 (2%) 57 38  | 43, 88, 118, 155      | 0     |
| 23  | AW    | 76/76 (100%)  | 1.69   | 26 (34%) 1 1  | 51, 193, 217, 221     | 0     |
| 23  | AY    | 19/76 (25%)   | 1.17   | 4 (21%) 2 2   | 75, 101, 161, 166     | 0     |
| 23  | CW    | 76/76 (100%)  | 0.87   | 9 (11%) 9 8   | 48, 194, 225, 230     | 0     |
| 23  | CY    | 21/76 (27%)   | 0.75   | 3 (14%) 6 5   | 63, 99, 162, 202      | 0     |
| 24  | AX    | 12/24 (50%)   | 0.91   | 3 (25%) 2 1   | 64, 74, 143, 145      | 0     |
| 24  | CX    | 12/24 (50%)   | 0.32   | 3 (25%) 2 1   | 53, 60, 121, 127      | 0     |
| 25  | B0    | 76/85 (89%)   | 0.14   | 3 (3%) 43 29  | 49, 69, 93, 149       | 0     |
| 25  | D0    | 82/85 (96%)   | 0.43   | 11 (13%) 7 6  | 42, 57, 88, 102       | 0     |
| 26  | B1    | 88/98 (89%)   | 1.49   | 23 (26%) 1 1  | 46, 65, 124, 140      | 0     |
| 26  | D1    | 88/98 (89%)   | 1.42   | 23 (26%) 1 1  | 38, 60, 110, 120      | 0     |
| 27  | B2    | 50/72 (69%)   | 3.41   | 36 (72%) 0 0  | 92, 120, 151, 164     | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 27  | D2    | 53/72 (73%)     | 1.98   | 23 (43%) 0 0   | 54, 69, 107, 120      | 0     |
| 28  | B3    | 58/60 (96%)     | 0.39   | 3 (5%) 33 22   | 60, 74, 106, 109      | 0     |
| 28  | D3    | 60/60 (100%)    | 0.06   | 0 100 100      | 43, 57, 101, 113      | 0     |
| 29  | B4    | 45/71 (63%)     | 1.66   | 15 (33%) 1 1   | 91, 152, 167, 176     | 0     |
| 29  | D4    | 49/71 (69%)     | 1.21   | 11 (22%) 2 2   | 81, 130, 153, 160     | 0     |
| 30  | B5    | 54/60 (90%)     | 1.02   | 7 (12%) 7 6    | 38, 65, 120, 134      | 0     |
| 30  | D5    | 60/60 (100%)    | 1.00   | 11 (18%) 3 3   | 28, 64, 147, 159      | 0     |
| 31  | B6    | 46/54 (85%)     | 1.31   | 10 (21%) 2 2   | 68, 89, 104, 117      | 0     |
| 31  | D6    | 47/54 (87%)     | 1.21   | 8 (17%) 4 4    | 67, 82, 116, 132      | 0     |
| 32  | B7    | 48/49 (97%)     | 0.61   | 5 (10%) 11 10  | 38, 49, 78, 83        | 0     |
| 32  | D7    | 48/49 (97%)     | 0.01   | 3 (6%) 26 18   | 29, 34, 68, 88        | 0     |
| 33  | B8    | 63/65 (96%)     | 1.59   | 22 (34%) 1 1   | 49, 70, 86, 122       | 0     |
| 33  | D8    | 62/65 (95%)     | 0.91   | 11 (17%) 4 3   | 41, 53, 71, 82        | 0     |
| 34  | B9    | 37/37 (100%)    | 0.31   | 1 (2%) 56 37   | 77, 92, 106, 114      | 0     |
| 34  | D9    | 37/37 (100%)    | 0.70   | 5 (13%) 7 6    | 59, 77, 98, 101       | 0     |
| 35  | BA    | 2824/2839 (99%) | -0.07  | 133 (4%) 36 25 | 36, 63, 194, 265      | 0     |
| 35  | DA    | 2824/2839 (99%) | -0.29  | 92 (3%) 49 33  | 27, 50, 193, 262      | 0     |
| 36  | BB    | 120/122 (98%)   | -0.12  | 4 (3%) 49 33   | 76, 99, 132, 148      | 0     |
| 36  | DB    | 119/122 (97%)   | -0.27  | 7 (5%) 28 19   | 53, 78, 113, 159      | 0     |
| 37  | BC    | 190/229 (82%)   | 1.23   | 31 (16%) 4 4   | 161, 211, 232, 239    | 0     |
| 37  | DC    | 190/229 (82%)   | 0.87   | 18 (9%) 14 11  | 166, 210, 231, 235    | 0     |
| 38  | BD    | 273/276 (98%)   | 0.62   | 25 (9%) 14 11  | 34, 55, 77, 89        | 0     |
| 38  | DD    | 275/276 (99%)   | 0.22   | 14 (5%) 33 23  | 28, 47, 73, 112       | 0     |
| 39  | BE    | 204/206 (99%)   | 0.35   | 7 (3%) 48 32   | 41, 68, 120, 139      | 0     |
| 39  | DE    | 204/206 (99%)   | 0.32   | 10 (4%) 35 24  | 27, 55, 101, 125      | 0     |
| 40  | BF    | 206/210 (98%)   | 0.93   | 34 (16%) 4 4   | 34, 76, 149, 186      | 0     |
| 40  | DF    | 208/210 (99%)   | 0.22   | 17 (8%) 17 14  | 29, 56, 138, 190      | 0     |
| 41  | BG    | 178/182 (97%)   | 0.59   | 13 (7%) 21 16  | 84, 108, 143, 182     | 0     |
| 41  | DG    | 181/182 (99%)   | 0.24   | 5 (2%) 55 36   | 67, 91, 134, 186      | 0     |
| 42  | BH    | 159/180 (88%)   | 1.45   | 41 (25%) 1 1   | 117, 156, 198, 206    | 0     |
| 42  | DH    | 165/180 (91%)   | 0.56   | 15 (9%) 15 12  | 57, 80, 107, 168      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 43  | BI    | 145/148 (97%)  | 0.51   | 9 (6%) 26 19   | 61, 99, 133, 152      | 0     |
| 43  | DI    | 144/148 (97%)  | 1.24   | 31 (21%) 2 2   | 55, 140, 180, 195     | 0     |
| 44  | BJ    | 0/173          | -      | -              | -                     | -     |
| 44  | DJ    | 0/173          | -      | -              | -                     | -     |
| 45  | BK    | 0/147          | -      | -              | -                     | -     |
| 45  | DK    | 0/147          | -      | -              | -                     | -     |
| 46  | BN    | 137/140 (97%)  | 0.67   | 14 (10%) 12 10 | 50, 81, 126, 143      | 0     |
| 46  | DN    | 140/140 (100%) | 0.66   | 14 (10%) 12 10 | 42, 60, 102, 120      | 0     |
| 47  | BO    | 122/122 (100%) | 0.69   | 9 (7%) 20 16   | 46, 66, 87, 98        | 0     |
| 47  | DO    | 122/122 (100%) | 0.13   | 2 (1%) 70 52   | 38, 53, 77, 90        | 0     |
| 48  | BP    | 144/150 (96%)  | 1.41   | 41 (28%) 1 1   | 44, 90, 126, 143      | 0     |
| 48  | DP    | 146/150 (97%)  | 0.91   | 21 (14%) 6 5   | 32, 69, 100, 190      | 0     |
| 49  | BQ    | 135/141 (95%)  | 1.13   | 23 (17%) 4 4   | 54, 85, 119, 154      | 0     |
| 49  | DQ    | 136/141 (96%)  | 1.19   | 30 (22%) 2 2   | 45, 66, 106, 139      | 0     |
| 50  | BR    | 116/118 (98%)  | 0.48   | 10 (8%) 16 13  | 46, 64, 103, 117      | 0     |
| 50  | DR    | 117/118 (99%)  | -0.12  | 1 (0%) 81 65   | 37, 53, 73, 90        | 0     |
| 51  | BS    | 102/112 (91%)  | 0.99   | 16 (15%) 5 4   | 71, 102, 120, 127     | 0     |
| 51  | DS    | 99/112 (88%)   | 0.64   | 11 (11%) 10 9  | 62, 82, 104, 107      | 0     |
| 52  | BT    | 132/146 (90%)  | 0.75   | 17 (12%) 7 6   | 54, 77, 131, 169      | 0     |
| 52  | DT    | 137/146 (93%)  | 0.67   | 17 (12%) 8 7   | 48, 68, 157, 221      | 0     |
| 53  | BU    | 117/118 (99%)  | 0.45   | 4 (3%) 48 32   | 44, 72, 113, 127      | 0     |
| 53  | DU    | 117/118 (99%)  | 0.43   | 6 (5%) 33 23   | 33, 53, 80, 106       | 0     |
| 54  | BV    | 101/101 (100%) | 1.48   | 27 (26%) 1 1   | 48, 110, 134, 183     | 0     |
| 54  | DV    | 101/101 (100%) | 1.02   | 14 (13%) 6 5   | 37, 81, 121, 153      | 0     |
| 55  | BW    | 111/113 (98%)  | 1.19   | 24 (21%) 2 2   | 47, 61, 106, 123      | 0     |
| 55  | DW    | 111/113 (98%)  | 0.33   | 7 (6%) 26 18   | 37, 46, 80, 135       | 0     |
| 56  | BX    | 89/96 (92%)    | 1.82   | 37 (41%) 0 1   | 61, 82, 138, 159      | 0     |
| 56  | DX    | 94/96 (97%)    | 0.86   | 14 (14%) 5 5   | 40, 55, 97, 140       | 0     |
| 57  | BY    | 100/110 (90%)  | 1.84   | 40 (40%) 1 1   | 63, 105, 143, 160     | 0     |
| 57  | DY    | 109/110 (99%)  | 1.18   | 26 (23%) 2 1   | 49, 76, 174, 200      | 0     |
| 58  | BZ    | 176/206 (85%)  | 1.51   | 53 (30%) 1 1   | 92, 153, 201, 217     | 0     |
| 58  | DZ    | 176/206 (85%)  | 1.21   | 39 (22%) 2 2   | 68, 128, 208, 216     | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| All | All   | 21060/22694 (92%) | 0.37   | 1828 (8%) 16 13 | 27, 80, 183, 269      | 0     |

The worst 5 of 1828 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30  | B5    | 2   | ALA  | 15.9 |
| 7   | CG    | 84  | ASN  | 12.6 |
| 30  | D5    | 1   | MET  | 12.1 |
| 7   | CG    | 85  | TYR  | 11.5 |
| 11  | AK    | 128 | ALA  | 10.6 |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 59  | MG   | AW    | 104  | 1/1   | -0.70 | 0.49 | 171,171,171,171            | 0     |
| 59  | MG   | BA    | 3397 | 1/1   | -0.37 | 0.27 | 190,190,190,190            | 0     |
| 59  | MG   | AW    | 105  | 1/1   | -0.31 | 0.39 | 170,170,170,170            | 0     |
| 59  | MG   | CW    | 110  | 1/1   | -0.13 | 0.14 | 197,197,197,197            | 0     |
| 59  | MG   | CW    | 112  | 1/1   | -0.10 | 0.14 | 191,191,191,191            | 0     |
| 59  | MG   | AA    | 1804 | 1/1   | 0.02  | 0.23 | 80,80,80,80                | 0     |
| 59  | MG   | BA    | 3323 | 1/1   | 0.10  | 0.27 | 159,159,159,159            | 0     |
| 59  | MG   | CW    | 104  | 1/1   | 0.10  | 0.23 | 174,174,174,174            | 0     |
| 59  | MG   | AW    | 118  | 1/1   | 0.13  | 0.14 | 188,188,188,188            | 0     |
| 59  | MG   | AW    | 115  | 1/1   | 0.21  | 0.29 | 193,193,193,193            | 0     |
| 59  | MG   | BC    | 302  | 1/1   | 0.22  | 0.17 | 171,171,171,171            | 0     |
| 59  | MG   | AW    | 114  | 1/1   | 0.22  | 0.25 | 193,193,193,193            | 0     |
| 59  | MG   | BA    | 3453 | 1/1   | 0.28  | 0.72 | 172,172,172,172            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AW    | 110  | 1/1   | 0.28 | 0.17 | 134,134,134,134             | 0     |
| 59  | MG   | CW    | 103  | 1/1   | 0.28 | 0.25 | 178,178,178,178             | 0     |
| 59  | MG   | BA    | 3326 | 1/1   | 0.29 | 0.19 | 130,130,130,130             | 0     |
| 59  | MG   | AA    | 1713 | 1/1   | 0.30 | 0.16 | 137,137,137,137             | 0     |
| 59  | MG   | CW    | 102  | 1/1   | 0.30 | 0.15 | 165,165,165,165             | 0     |
| 59  | MG   | BA    | 3285 | 1/1   | 0.31 | 0.28 | 103,103,103,103             | 0     |
| 59  | MG   | BA    | 3322 | 1/1   | 0.31 | 0.25 | 130,130,130,130             | 0     |
| 59  | MG   | AW    | 111  | 1/1   | 0.31 | 0.33 | 139,139,139,139             | 0     |
| 59  | MG   | AA    | 1756 | 1/1   | 0.31 | 0.31 | 107,107,107,107             | 0     |
| 59  | MG   | CW    | 101  | 1/1   | 0.33 | 0.12 | 101,101,101,101             | 0     |
| 59  | MG   | BA    | 3293 | 1/1   | 0.35 | 0.25 | 108,108,108,108             | 0     |
| 59  | MG   | AA    | 1777 | 1/1   | 0.36 | 0.25 | 81,81,81,81                 | 0     |
| 59  | MG   | AW    | 117  | 1/1   | 0.38 | 0.28 | 125,125,125,125             | 0     |
| 59  | MG   | AW    | 101  | 1/1   | 0.39 | 0.23 | 154,154,154,154             | 0     |
| 59  | MG   | AW    | 119  | 1/1   | 0.39 | 0.19 | 194,194,194,194             | 0     |
| 59  | MG   | DA    | 3386 | 1/1   | 0.40 | 0.14 | 181,181,181,181             | 0     |
| 59  | MG   | DA    | 3328 | 1/1   | 0.41 | 0.21 | 155,155,155,155             | 0     |
| 59  | MG   | CW    | 107  | 1/1   | 0.41 | 0.13 | 145,145,145,145             | 0     |
| 59  | MG   | CA    | 1725 | 1/1   | 0.42 | 0.28 | 80,80,80,80                 | 0     |
| 59  | MG   | CA    | 1620 | 1/1   | 0.43 | 0.15 | 105,105,105,105             | 0     |
| 59  | MG   | AA    | 1719 | 1/1   | 0.44 | 0.27 | 112,112,112,112             | 0     |
| 59  | MG   | BC    | 301  | 1/1   | 0.44 | 0.35 | 166,166,166,166             | 0     |
| 59  | MG   | CW    | 109  | 1/1   | 0.45 | 0.12 | 125,125,125,125             | 0     |
| 59  | MG   | BA    | 3410 | 1/1   | 0.47 | 0.16 | 206,206,206,206             | 0     |
| 59  | MG   | DA    | 3230 | 1/1   | 0.48 | 0.12 | 98,98,98,98                 | 0     |
| 59  | MG   | AA    | 1789 | 1/1   | 0.48 | 0.25 | 126,126,126,126             | 0     |
| 59  | MG   | BA    | 3320 | 1/1   | 0.48 | 0.16 | 173,173,173,173             | 0     |
| 59  | MG   | BA    | 3427 | 1/1   | 0.49 | 0.26 | 84,84,84,84                 | 0     |
| 59  | MG   | BB    | 204  | 1/1   | 0.50 | 0.23 | 98,98,98,98                 | 0     |
| 59  | MG   | CW    | 108  | 1/1   | 0.50 | 0.27 | 130,130,130,130             | 0     |
| 59  | MG   | CA    | 1742 | 1/1   | 0.50 | 0.31 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3351 | 1/1   | 0.50 | 0.15 | 116,116,116,116             | 0     |
| 59  | MG   | BA    | 3317 | 1/1   | 0.52 | 0.20 | 99,99,99,99                 | 0     |
| 59  | MG   | BA    | 3431 | 1/1   | 0.54 | 0.15 | 94,94,94,94                 | 0     |
| 59  | MG   | DB    | 211  | 1/1   | 0.54 | 0.22 | 106,106,106,106             | 0     |
| 59  | MG   | BA    | 3324 | 1/1   | 0.55 | 0.19 | 194,194,194,194             | 0     |
| 59  | MG   | AA    | 1760 | 1/1   | 0.55 | 0.12 | 105,105,105,105             | 0     |
| 59  | MG   | AA    | 1748 | 1/1   | 0.55 | 0.31 | 98,98,98,98                 | 0     |
| 59  | MG   | AV    | 103  | 1/1   | 0.56 | 0.18 | 93,93,93,93                 | 0     |
| 59  | MG   | BA    | 3438 | 1/1   | 0.58 | 0.13 | 104,104,104,104             | 0     |
| 59  | MG   | BB    | 217  | 1/1   | 0.58 | 0.20 | 98,98,98,98                 | 0     |
| 59  | MG   | CW    | 105  | 1/1   | 0.58 | 0.18 | 107,107,107,107             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3301 | 1/1   | 0.58 | 0.28 | 115,115,115,115             | 0     |
| 59  | MG   | AA    | 1746 | 1/1   | 0.59 | 0.17 | 87,87,87,87                 | 0     |
| 59  | MG   | AA    | 1647 | 1/1   | 0.59 | 0.13 | 95,95,95,95                 | 0     |
| 59  | MG   | AA    | 1707 | 1/1   | 0.59 | 0.18 | 87,87,87,87                 | 0     |
| 59  | MG   | AA    | 1790 | 1/1   | 0.59 | 0.20 | 120,120,120,120             | 0     |
| 59  | MG   | BA    | 3434 | 1/1   | 0.59 | 0.35 | 90,90,90,90                 | 0     |
| 59  | MG   | BA    | 3327 | 1/1   | 0.59 | 0.11 | 109,109,109,109             | 0     |
| 59  | MG   | BA    | 3003 | 1/1   | 0.59 | 0.22 | 84,84,84,84                 | 0     |
| 59  | MG   | AA    | 1724 | 1/1   | 0.60 | 0.12 | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1675 | 1/1   | 0.60 | 0.23 | 85,85,85,85                 | 0     |
| 59  | MG   | BA    | 3342 | 1/1   | 0.60 | 0.28 | 64,64,64,64                 | 0     |
| 59  | MG   | AA    | 1801 | 1/1   | 0.60 | 0.18 | 69,69,69,69                 | 0     |
| 59  | MG   | AW    | 109  | 1/1   | 0.61 | 0.20 | 154,154,154,154             | 0     |
| 59  | MG   | AA    | 1611 | 1/1   | 0.62 | 0.37 | 87,87,87,87                 | 0     |
| 59  | MG   | DA    | 3007 | 1/1   | 0.62 | 0.24 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3216 | 1/1   | 0.63 | 0.17 | 88,88,88,88                 | 0     |
| 59  | MG   | DB    | 206  | 1/1   | 0.63 | 0.08 | 91,91,91,91                 | 0     |
| 59  | MG   | AA    | 1657 | 1/1   | 0.63 | 0.20 | 92,92,92,92                 | 0     |
| 59  | MG   | BA    | 3187 | 1/1   | 0.64 | 0.21 | 93,93,93,93                 | 0     |
| 59  | MG   | AW    | 112  | 1/1   | 0.64 | 0.20 | 112,112,112,112             | 0     |
| 59  | MG   | CA    | 1791 | 1/1   | 0.64 | 0.11 | 78,78,78,78                 | 0     |
| 59  | MG   | DA    | 3244 | 1/1   | 0.64 | 0.08 | 147,147,147,147             | 0     |
| 59  | MG   | DV    | 201  | 1/1   | 0.64 | 0.15 | 100,100,100,100             | 0     |
| 59  | MG   | BS    | 201  | 1/1   | 0.65 | 0.16 | 97,97,97,97                 | 0     |
| 59  | MG   | CA    | 1641 | 1/1   | 0.65 | 0.32 | 71,71,71,71                 | 0     |
| 59  | MG   | CW    | 106  | 1/1   | 0.65 | 0.14 | 133,133,133,133             | 0     |
| 59  | MG   | CA    | 1642 | 1/1   | 0.65 | 0.16 | 83,83,83,83                 | 0     |
| 59  | MG   | CA    | 1648 | 1/1   | 0.66 | 0.09 | 96,96,96,96                 | 0     |
| 59  | MG   | CA    | 1652 | 1/1   | 0.66 | 0.17 | 85,85,85,85                 | 0     |
| 59  | MG   | AW    | 107  | 1/1   | 0.66 | 0.23 | 115,115,115,115             | 0     |
| 59  | MG   | BA    | 3234 | 1/1   | 0.66 | 0.32 | 83,83,83,83                 | 0     |
| 59  | MG   | BA    | 3325 | 1/1   | 0.66 | 0.21 | 164,164,164,164             | 0     |
| 59  | MG   | BA    | 3344 | 1/1   | 0.66 | 0.27 | 81,81,81,81                 | 0     |
| 59  | MG   | BA    | 3276 | 1/1   | 0.67 | 0.13 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3387 | 1/1   | 0.67 | 0.26 | 102,102,102,102             | 0     |
| 59  | MG   | AW    | 103  | 1/1   | 0.67 | 0.27 | 105,105,105,105             | 0     |
| 59  | MG   | DA    | 3315 | 1/1   | 0.67 | 0.12 | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1656 | 1/1   | 0.67 | 0.21 | 74,74,74,74                 | 0     |
| 59  | MG   | CA    | 1739 | 1/1   | 0.68 | 0.16 | 131,131,131,131             | 0     |
| 59  | MG   | BB    | 207  | 1/1   | 0.68 | 0.17 | 115,115,115,115             | 0     |
| 59  | MG   | CA    | 1686 | 1/1   | 0.68 | 0.18 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3346 | 1/1   | 0.68 | 0.10 | 128,128,128,128             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3264 | 1/1   | 0.69 | 0.31 | 64,64,64,64                 | 0     |
| 59  | MG   | AW    | 106  | 1/1   | 0.69 | 0.19 | 149,149,149,149             | 0     |
| 59  | MG   | CA    | 1638 | 1/1   | 0.69 | 0.26 | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1686 | 1/1   | 0.69 | 0.09 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3222 | 1/1   | 0.69 | 0.32 | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3171 | 1/1   | 0.69 | 0.08 | 76,76,76,76                 | 0     |
| 59  | MG   | BB    | 206  | 1/1   | 0.69 | 0.24 | 94,94,94,94                 | 0     |
| 59  | MG   | CA    | 1793 | 1/1   | 0.69 | 0.24 | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3254 | 1/1   | 0.70 | 0.22 | 89,89,89,89                 | 0     |
| 59  | MG   | CA    | 1700 | 1/1   | 0.70 | 0.13 | 87,87,87,87                 | 0     |
| 59  | MG   | DA    | 3320 | 1/1   | 0.70 | 0.31 | 67,67,67,67                 | 0     |
| 59  | MG   | DB    | 207  | 1/1   | 0.70 | 0.23 | 73,73,73,73                 | 0     |
| 59  | MG   | AA    | 1656 | 1/1   | 0.70 | 0.26 | 102,102,102,102             | 0     |
| 59  | MG   | DA    | 3357 | 1/1   | 0.70 | 0.16 | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1783 | 1/1   | 0.71 | 0.28 | 74,74,74,74                 | 0     |
| 59  | MG   | CA    | 1672 | 1/1   | 0.71 | 0.16 | 94,94,94,94                 | 0     |
| 59  | MG   | AA    | 1737 | 1/1   | 0.71 | 0.19 | 78,78,78,78                 | 0     |
| 59  | MG   | CA    | 1690 | 1/1   | 0.71 | 0.28 | 84,84,84,84                 | 0     |
| 59  | MG   | BA    | 3168 | 1/1   | 0.71 | 0.23 | 89,89,89,89                 | 0     |
| 59  | MG   | CA    | 1650 | 1/1   | 0.71 | 0.25 | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3328 | 1/1   | 0.71 | 0.26 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3366 | 1/1   | 0.72 | 0.11 | 89,89,89,89                 | 0     |
| 59  | MG   | CA    | 1688 | 1/1   | 0.72 | 0.17 | 81,81,81,81                 | 0     |
| 59  | MG   | CA    | 1637 | 1/1   | 0.72 | 0.36 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3319 | 1/1   | 0.72 | 0.36 | 81,81,81,81                 | 0     |
| 59  | MG   | BA    | 3385 | 1/1   | 0.72 | 0.08 | 84,84,84,84                 | 0     |
| 59  | MG   | AA    | 1634 | 1/1   | 0.72 | 0.14 | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1700 | 1/1   | 0.72 | 0.13 | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3319 | 1/1   | 0.72 | 0.16 | 133,133,133,133             | 0     |
| 59  | MG   | AA    | 1706 | 1/1   | 0.72 | 0.09 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3298 | 1/1   | 0.72 | 0.25 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3357 | 1/1   | 0.72 | 0.09 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3008 | 1/1   | 0.72 | 0.19 | 76,76,76,76                 | 0     |
| 59  | MG   | CA    | 1605 | 1/1   | 0.72 | 0.14 | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1674 | 1/1   | 0.73 | 0.28 | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1645 | 1/1   | 0.73 | 0.18 | 79,79,79,79                 | 0     |
| 59  | MG   | DA    | 3337 | 1/1   | 0.73 | 0.19 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3405 | 1/1   | 0.73 | 0.28 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3321 | 1/1   | 0.73 | 0.07 | 175,175,175,175             | 0     |
| 59  | MG   | AA    | 1701 | 1/1   | 0.73 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | AW    | 102  | 1/1   | 0.73 | 0.18 | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3116 | 1/1   | 0.73 | 0.24 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3303 | 1/1   | 0.73 | 0.27 | 73,73,73,73                 | 0     |
| 59  | MG   | AA    | 1802 | 1/1   | 0.73 | 0.18 | 85,85,85,85                 | 0     |
| 59  | MG   | AA    | 1714 | 1/1   | 0.74 | 0.12 | 88,88,88,88                 | 0     |
| 59  | MG   | BA    | 3230 | 1/1   | 0.74 | 0.16 | 89,89,89,89                 | 0     |
| 59  | MG   | BA    | 3367 | 1/1   | 0.74 | 0.18 | 85,85,85,85                 | 0     |
| 59  | MG   | BB    | 208  | 1/1   | 0.74 | 0.11 | 83,83,83,83                 | 0     |
| 59  | MG   | CA    | 1619 | 1/1   | 0.74 | 0.29 | 66,66,66,66                 | 0     |
| 59  | MG   | CA    | 1792 | 1/1   | 0.74 | 0.23 | 76,76,76,76                 | 0     |
| 59  | MG   | BA    | 3257 | 1/1   | 0.74 | 0.35 | 77,77,77,77                 | 0     |
| 59  | MG   | BF    | 302  | 1/1   | 0.75 | 0.19 | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1776 | 1/1   | 0.75 | 0.30 | 72,72,72,72                 | 0     |
| 59  | MG   | CA    | 1710 | 1/1   | 0.75 | 0.08 | 120,120,120,120             | 0     |
| 59  | MG   | BA    | 3299 | 1/1   | 0.75 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3372 | 1/1   | 0.75 | 0.15 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3160 | 1/1   | 0.75 | 0.16 | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3278 | 1/1   | 0.75 | 0.19 | 86,86,86,86                 | 0     |
| 59  | MG   | BB    | 209  | 1/1   | 0.75 | 0.11 | 109,109,109,109             | 0     |
| 59  | MG   | BA    | 3350 | 1/1   | 0.75 | 0.07 | 91,91,91,91                 | 0     |
| 59  | MG   | AA    | 1617 | 1/1   | 0.75 | 0.33 | 81,81,81,81                 | 0     |
| 59  | MG   | AA    | 1672 | 1/1   | 0.75 | 0.31 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3233 | 1/1   | 0.76 | 0.10 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1695 | 1/1   | 0.76 | 0.28 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3376 | 1/1   | 0.76 | 0.24 | 81,81,81,81                 | 0     |
| 59  | MG   | CA    | 1640 | 1/1   | 0.76 | 0.23 | 91,91,91,91                 | 0     |
| 59  | MG   | AA    | 1772 | 1/1   | 0.76 | 0.13 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3399 | 1/1   | 0.77 | 0.10 | 89,89,89,89                 | 0     |
| 59  | MG   | BA    | 3200 | 1/1   | 0.77 | 0.20 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3203 | 1/1   | 0.77 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1644 | 1/1   | 0.77 | 0.20 | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3202 | 1/1   | 0.77 | 0.36 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1677 | 1/1   | 0.77 | 0.18 | 72,72,72,72                 | 0     |
| 59  | MG   | CA    | 1796 | 1/1   | 0.77 | 0.19 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3219 | 1/1   | 0.77 | 0.09 | 181,181,181,181             | 0     |
| 59  | MG   | BA    | 3093 | 1/1   | 0.77 | 0.17 | 75,75,75,75                 | 0     |
| 59  | MG   | CA    | 1601 | 1/1   | 0.77 | 0.30 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3332 | 1/1   | 0.77 | 0.20 | 68,68,68,68                 | 0     |
| 59  | MG   | AA    | 1763 | 1/1   | 0.77 | 0.11 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3142 | 1/1   | 0.77 | 0.16 | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1765 | 1/1   | 0.77 | 0.18 | 84,84,84,84                 | 0     |
| 59  | MG   | DA    | 3374 | 1/1   | 0.77 | 0.22 | 65,65,65,65                 | 0     |
| 59  | MG   | DA    | 3383 | 1/1   | 0.77 | 0.10 | 92,92,92,92                 | 0     |
| 59  | MG   | DA    | 3384 | 1/1   | 0.77 | 0.07 | 188,188,188,188             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1626 | 1/1   | 0.77 | 0.29 | 94,94,94,94                 | 0     |
| 59  | MG   | AA    | 1792 | 1/1   | 0.77 | 0.08 | 99,99,99,99                 | 0     |
| 59  | MG   | B8    | 101  | 1/1   | 0.77 | 0.26 | 79,79,79,79                 | 0     |
| 59  | MG   | CA    | 1721 | 1/1   | 0.77 | 0.22 | 81,81,81,81                 | 0     |
| 59  | MG   | BA    | 3398 | 1/1   | 0.77 | 0.16 | 104,104,104,104             | 0     |
| 59  | MG   | CA    | 1737 | 1/1   | 0.77 | 0.21 | 82,82,82,82                 | 0     |
| 59  | MG   | BA    | 3164 | 1/1   | 0.78 | 0.16 | 78,78,78,78                 | 0     |
| 59  | MG   | AA    | 1742 | 1/1   | 0.78 | 0.13 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3338 | 1/1   | 0.78 | 0.13 | 89,89,89,89                 | 0     |
| 59  | MG   | DA    | 3311 | 1/1   | 0.78 | 0.17 | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3408 | 1/1   | 0.78 | 0.12 | 93,93,93,93                 | 0     |
| 59  | MG   | BA    | 3304 | 1/1   | 0.78 | 0.07 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3313 | 1/1   | 0.78 | 0.22 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3327 | 1/1   | 0.78 | 0.26 | 89,89,89,89                 | 0     |
| 59  | MG   | BA    | 3025 | 1/1   | 0.78 | 0.11 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1692 | 1/1   | 0.78 | 0.16 | 96,96,96,96                 | 0     |
| 59  | MG   | BA    | 3255 | 1/1   | 0.78 | 0.28 | 85,85,85,85                 | 0     |
| 59  | MG   | CA    | 1697 | 1/1   | 0.78 | 0.23 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3041 | 1/1   | 0.78 | 0.25 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3353 | 1/1   | 0.78 | 0.17 | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3080 | 1/1   | 0.78 | 0.13 | 43,43,43,43                 | 0     |
| 59  | MG   | AW    | 108  | 1/1   | 0.78 | 0.13 | 154,154,154,154             | 0     |
| 59  | MG   | AA    | 1697 | 1/1   | 0.78 | 0.20 | 76,76,76,76                 | 0     |
| 59  | MG   | AA    | 1655 | 1/1   | 0.78 | 0.34 | 73,73,73,73                 | 0     |
| 59  | MG   | DA    | 3014 | 1/1   | 0.78 | 0.13 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3160 | 1/1   | 0.78 | 0.21 | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3161 | 1/1   | 0.78 | 0.35 | 35,35,35,35                 | 0     |
| 59  | MG   | DB    | 212  | 1/1   | 0.78 | 0.22 | 99,99,99,99                 | 0     |
| 59  | MG   | DA    | 3213 | 1/1   | 0.78 | 0.10 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3192 | 1/1   | 0.79 | 0.14 | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3304 | 1/1   | 0.79 | 0.08 | 70,70,70,70                 | 0     |
| 59  | MG   | CA    | 1667 | 1/1   | 0.79 | 0.13 | 62,62,62,62                 | 0     |
| 59  | MG   | CA    | 1722 | 1/1   | 0.79 | 0.07 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3365 | 1/1   | 0.79 | 0.21 | 54,54,54,54                 | 0     |
| 59  | MG   | CA    | 1729 | 1/1   | 0.79 | 0.20 | 77,77,77,77                 | 0     |
| 59  | MG   | CA    | 1678 | 1/1   | 0.79 | 0.26 | 78,78,78,78                 | 0     |
| 59  | MG   | CA    | 1682 | 1/1   | 0.79 | 0.22 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3331 | 1/1   | 0.79 | 0.13 | 99,99,99,99                 | 0     |
| 59  | MG   | BA    | 3232 | 1/1   | 0.79 | 0.16 | 74,74,74,74                 | 0     |
| 59  | MG   | CA    | 1767 | 1/1   | 0.79 | 0.23 | 67,67,67,67                 | 0     |
| 59  | MG   | CA    | 1775 | 1/1   | 0.79 | 0.18 | 76,76,76,76                 | 0     |
| 59  | MG   | BU    | 203  | 1/1   | 0.79 | 0.17 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AE    | 201  | 1/1   | 0.79 | 0.27 | 86,86,86,86                 | 0     |
| 59  | MG   | DA    | 3118 | 1/1   | 0.79 | 0.32 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1623 | 1/1   | 0.79 | 0.24 | 79,79,79,79                 | 0     |
| 59  | MG   | DA    | 3168 | 1/1   | 0.79 | 0.38 | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3182 | 1/1   | 0.79 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | CA    | 1794 | 1/1   | 0.79 | 0.28 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3133 | 1/1   | 0.79 | 0.38 | 94,94,94,94                 | 0     |
| 59  | MG   | AA    | 1679 | 1/1   | 0.79 | 0.24 | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3232 | 1/1   | 0.79 | 0.09 | 93,93,93,93                 | 0     |
| 59  | MG   | AA    | 1619 | 1/1   | 0.79 | 0.20 | 83,83,83,83                 | 0     |
| 59  | MG   | BA    | 3014 | 1/1   | 0.80 | 0.25 | 55,55,55,55                 | 0     |
| 59  | MG   | AW    | 113  | 1/1   | 0.80 | 0.20 | 96,96,96,96                 | 0     |
| 59  | MG   | CA    | 1723 | 1/1   | 0.80 | 0.08 | 132,132,132,132             | 0     |
| 59  | MG   | CA    | 1655 | 1/1   | 0.80 | 0.30 | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1615 | 1/1   | 0.80 | 0.20 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3228 | 1/1   | 0.80 | 0.16 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3185 | 1/1   | 0.80 | 0.18 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3330 | 1/1   | 0.80 | 0.21 | 55,55,55,55                 | 0     |
| 59  | MG   | CA    | 1625 | 1/1   | 0.80 | 0.25 | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1759 | 1/1   | 0.80 | 0.25 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1681 | 1/1   | 0.80 | 0.28 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3354 | 1/1   | 0.80 | 0.25 | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3081 | 1/1   | 0.80 | 0.34 | 39,39,39,39                 | 0     |
| 59  | MG   | AA    | 1635 | 1/1   | 0.80 | 0.26 | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1633 | 1/1   | 0.80 | 0.28 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3375 | 1/1   | 0.80 | 0.14 | 84,84,84,84                 | 0     |
| 59  | MG   | BB    | 214  | 1/1   | 0.80 | 0.12 | 84,84,84,84                 | 0     |
| 59  | MG   | AA    | 1671 | 1/1   | 0.80 | 0.19 | 85,85,85,85                 | 0     |
| 59  | MG   | BA    | 3373 | 1/1   | 0.80 | 0.18 | 73,73,73,73                 | 0     |
| 59  | MG   | CA    | 1693 | 1/1   | 0.80 | 0.07 | 87,87,87,87                 | 0     |
| 59  | MG   | AA    | 1780 | 1/1   | 0.80 | 0.16 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3162 | 1/1   | 0.80 | 0.23 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3108 | 1/1   | 0.80 | 0.19 | 69,69,69,69                 | 0     |
| 59  | MG   | BB    | 203  | 1/1   | 0.80 | 0.18 | 99,99,99,99                 | 0     |
| 59  | MG   | DA    | 3282 | 1/1   | 0.80 | 0.39 | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1654 | 1/1   | 0.81 | 0.09 | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3019 | 1/1   | 0.81 | 0.20 | 68,68,68,68                 | 0     |
| 59  | MG   | AA    | 1762 | 1/1   | 0.81 | 0.10 | 100,100,100,100             | 0     |
| 59  | MG   | AA    | 1741 | 1/1   | 0.81 | 0.09 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1715 | 1/1   | 0.81 | 0.09 | 104,104,104,104             | 0     |
| 59  | MG   | BA    | 3253 | 1/1   | 0.81 | 0.21 | 97,97,97,97                 | 0     |
| 59  | MG   | BA    | 3043 | 1/1   | 0.81 | 0.24 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1648 | 1/1   | 0.81 | 0.14 | 81,81,81,81                 | 0     |
| 59  | MG   | CA    | 1668 | 1/1   | 0.81 | 0.27 | 75,75,75,75                 | 0     |
| 59  | MG   | CA    | 1728 | 1/1   | 0.81 | 0.15 | 73,73,73,73                 | 0     |
| 59  | MG   | CA    | 1669 | 1/1   | 0.81 | 0.38 | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3081 | 1/1   | 0.81 | 0.24 | 37,37,37,37                 | 0     |
| 59  | MG   | CA    | 1673 | 1/1   | 0.81 | 0.25 | 92,92,92,92                 | 0     |
| 59  | MG   | CA    | 1674 | 1/1   | 0.81 | 0.35 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1744 | 1/1   | 0.81 | 0.07 | 94,94,94,94                 | 0     |
| 59  | MG   | AA    | 1794 | 1/1   | 0.81 | 0.14 | 103,103,103,103             | 0     |
| 59  | MG   | CA    | 1627 | 1/1   | 0.81 | 0.24 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1770 | 1/1   | 0.81 | 0.22 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3227 | 1/1   | 0.81 | 0.14 | 78,78,78,78                 | 0     |
| 59  | MG   | CA    | 1778 | 1/1   | 0.81 | 0.23 | 77,77,77,77                 | 0     |
| 59  | MG   | DA    | 3206 | 1/1   | 0.81 | 0.27 | 82,82,82,82                 | 0     |
| 59  | MG   | BA    | 3281 | 1/1   | 0.81 | 0.34 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3007 | 1/1   | 0.81 | 0.16 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3413 | 1/1   | 0.81 | 0.29 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3420 | 1/1   | 0.81 | 0.12 | 77,77,77,77                 | 0     |
| 59  | MG   | DN    | 201  | 1/1   | 0.81 | 0.27 | 98,98,98,98                 | 0     |
| 59  | MG   | BA    | 3286 | 1/1   | 0.81 | 0.18 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1609 | 1/1   | 0.82 | 0.22 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1675 | 1/1   | 0.82 | 0.17 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3059 | 1/1   | 0.82 | 0.11 | 65,65,65,65                 | 0     |
| 59  | MG   | BB    | 216  | 1/1   | 0.82 | 0.24 | 92,92,92,92                 | 0     |
| 59  | MG   | AA    | 1803 | 1/1   | 0.82 | 0.13 | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3456 | 1/1   | 0.82 | 0.13 | 73,73,73,73                 | 0     |
| 59  | MG   | AA    | 1726 | 1/1   | 0.82 | 0.14 | 72,72,72,72                 | 0     |
| 59  | MG   | CE    | 201  | 1/1   | 0.82 | 0.24 | 84,84,84,84                 | 0     |
| 59  | MG   | CG    | 201  | 1/1   | 0.82 | 0.10 | 72,72,72,72                 | 0     |
| 59  | MG   | CU    | 101  | 1/1   | 0.82 | 0.17 | 84,84,84,84                 | 0     |
| 59  | MG   | CA    | 1735 | 1/1   | 0.82 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3186 | 1/1   | 0.82 | 0.33 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1608 | 1/1   | 0.82 | 0.26 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3382 | 1/1   | 0.82 | 0.27 | 80,80,80,80                 | 0     |
| 59  | MG   | CA    | 1741 | 1/1   | 0.82 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3234 | 1/1   | 0.82 | 0.37 | 72,72,72,72                 | 0     |
| 59  | MG   | AA    | 1747 | 1/1   | 0.82 | 0.09 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3252 | 1/1   | 0.82 | 0.11 | 68,68,68,68                 | 0     |
| 59  | MG   | AA    | 1601 | 1/1   | 0.82 | 0.23 | 73,73,73,73                 | 0     |
| 59  | MG   | CA    | 1750 | 1/1   | 0.82 | 0.20 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3285 | 1/1   | 0.82 | 0.27 | 44,44,44,44                 | 0     |
| 59  | MG   | CA    | 1671 | 1/1   | 0.82 | 0.11 | 106,106,106,106             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3269 | 1/1   | 0.82 | 0.14 | 166,166,166,166             | 0     |
| 59  | MG   | DO    | 202  | 1/1   | 0.82 | 0.18 | 86,86,86,86                 | 0     |
| 59  | MG   | CA    | 1608 | 1/1   | 0.82 | 0.17 | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1743 | 1/1   | 0.83 | 0.14 | 80,80,80,80                 | 0     |
| 59  | MG   | AA    | 1750 | 1/1   | 0.83 | 0.30 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3169 | 1/1   | 0.83 | 0.33 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3297 | 1/1   | 0.83 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | BB    | 211  | 1/1   | 0.83 | 0.12 | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3419 | 1/1   | 0.83 | 0.27 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1732 | 1/1   | 0.83 | 0.18 | 85,85,85,85                 | 0     |
| 59  | MG   | BB    | 215  | 1/1   | 0.83 | 0.21 | 76,76,76,76                 | 0     |
| 59  | MG   | AA    | 1644 | 1/1   | 0.83 | 0.15 | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1788 | 1/1   | 0.83 | 0.08 | 94,94,94,94                 | 0     |
| 59  | MG   | AA    | 1766 | 1/1   | 0.83 | 0.06 | 54,54,54,54                 | 0     |
| 59  | MG   | AA    | 1808 | 1/1   | 0.83 | 0.11 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3151 | 1/1   | 0.83 | 0.20 | 78,78,78,78                 | 0     |
| 59  | MG   | BQ    | 201  | 1/1   | 0.83 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3157 | 1/1   | 0.83 | 0.18 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3348 | 1/1   | 0.83 | 0.24 | 72,72,72,72                 | 0     |
| 59  | MG   | CA    | 1761 | 1/1   | 0.83 | 0.08 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3084 | 1/1   | 0.83 | 0.20 | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3367 | 1/1   | 0.83 | 0.15 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3091 | 1/1   | 0.83 | 0.20 | 37,37,37,37                 | 0     |
| 59  | MG   | CA    | 1689 | 1/1   | 0.83 | 0.10 | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1759 | 1/1   | 0.83 | 0.10 | 93,93,93,93                 | 0     |
| 59  | MG   | DA    | 3380 | 1/1   | 0.83 | 0.25 | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3163 | 1/1   | 0.83 | 0.20 | 79,79,79,79                 | 0     |
| 59  | MG   | CA    | 1649 | 1/1   | 0.83 | 0.12 | 76,76,76,76                 | 0     |
| 59  | MG   | DA    | 3170 | 1/1   | 0.83 | 0.12 | 87,87,87,87                 | 0     |
| 59  | MG   | AA    | 1791 | 1/1   | 0.83 | 0.22 | 91,91,91,91                 | 0     |
| 59  | MG   | AA    | 1650 | 1/1   | 0.83 | 0.23 | 80,80,80,80                 | 0     |
| 59  | MG   | BB    | 205  | 1/1   | 0.83 | 0.19 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3163 | 1/1   | 0.83 | 0.20 | 81,81,81,81                 | 0     |
| 59  | MG   | CA    | 1707 | 1/1   | 0.83 | 0.26 | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1709 | 1/1   | 0.83 | 0.28 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1662 | 1/1   | 0.83 | 0.12 | 60,60,60,60                 | 0     |
| 59  | MG   | CA    | 1663 | 1/1   | 0.83 | 0.28 | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1664 | 1/1   | 0.83 | 0.31 | 75,75,75,75                 | 0     |
| 59  | MG   | DA    | 3321 | 1/1   | 0.84 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3326 | 1/1   | 0.84 | 0.07 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3198 | 1/1   | 0.84 | 0.13 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3450 | 1/1   | 0.84 | 0.07 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3167 | 1/1   | 0.84 | 0.13 | 76,76,76,76                 | 0     |
| 59  | MG   | CA    | 1666 | 1/1   | 0.84 | 0.22 | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1633 | 1/1   | 0.84 | 0.22 | 64,64,64,64                 | 0     |
| 59  | MG   | AA    | 1629 | 1/1   | 0.84 | 0.25 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3344 | 1/1   | 0.84 | 0.20 | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3192 | 1/1   | 0.84 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3212 | 1/1   | 0.84 | 0.24 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3092 | 1/1   | 0.84 | 0.21 | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3352 | 1/1   | 0.84 | 0.29 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3180 | 1/1   | 0.84 | 0.14 | 79,79,79,79                 | 0     |
| 59  | MG   | DA    | 3373 | 1/1   | 0.84 | 0.29 | 75,75,75,75                 | 0     |
| 59  | MG   | CA    | 1765 | 1/1   | 0.84 | 0.30 | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3412 | 1/1   | 0.84 | 0.08 | 64,64,64,64                 | 0     |
| 59  | MG   | CA    | 1720 | 1/1   | 0.84 | 0.12 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3246 | 1/1   | 0.84 | 0.21 | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1676 | 1/1   | 0.84 | 0.13 | 88,88,88,88                 | 0     |
| 59  | MG   | AL    | 201  | 1/1   | 0.84 | 0.18 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3271 | 1/1   | 0.84 | 0.16 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1610 | 1/1   | 0.84 | 0.12 | 76,76,76,76                 | 0     |
| 59  | MG   | BA    | 3166 | 1/1   | 0.84 | 0.12 | 105,105,105,105             | 0     |
| 59  | MG   | BA    | 3306 | 1/1   | 0.84 | 0.34 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3167 | 1/1   | 0.84 | 0.21 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3314 | 1/1   | 0.84 | 0.39 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3101 | 1/1   | 0.84 | 0.27 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3105 | 1/1   | 0.84 | 0.20 | 40,40,40,40                 | 0     |
| 59  | MG   | CA    | 1733 | 1/1   | 0.84 | 0.14 | 81,81,81,81                 | 0     |
| 59  | MG   | AA    | 1658 | 1/1   | 0.85 | 0.22 | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1692 | 1/1   | 0.85 | 0.26 | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1738 | 1/1   | 0.85 | 0.23 | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1676 | 1/1   | 0.85 | 0.24 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1757 | 1/1   | 0.85 | 0.28 | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1696 | 1/1   | 0.85 | 0.10 | 81,81,81,81                 | 0     |
| 59  | MG   | BA    | 3271 | 1/1   | 0.85 | 0.24 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3001 | 1/1   | 0.85 | 0.35 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3317 | 1/1   | 0.85 | 0.25 | 52,52,52,52                 | 0     |
| 59  | MG   | CA    | 1683 | 1/1   | 0.85 | 0.11 | 74,74,74,74                 | 0     |
| 59  | MG   | CA    | 1743 | 1/1   | 0.85 | 0.13 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3273 | 1/1   | 0.85 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1660 | 1/1   | 0.85 | 0.33 | 84,84,84,84                 | 0     |
| 59  | MG   | BA    | 3213 | 1/1   | 0.85 | 0.12 | 72,72,72,72                 | 0     |
| 59  | MG   | DA    | 3089 | 1/1   | 0.85 | 0.25 | 46,46,46,46                 | 0     |
| 59  | MG   | B8    | 102  | 1/1   | 0.85 | 0.24 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1614 | 1/1   | 0.85 | 0.10 | 85,85,85,85                 | 0     |
| 59  | MG   | BA    | 3335 | 1/1   | 0.85 | 0.15 | 81,81,81,81                 | 0     |
| 59  | MG   | DA    | 3116 | 1/1   | 0.85 | 0.23 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3220 | 1/1   | 0.85 | 0.09 | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3119 | 1/1   | 0.85 | 0.20 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3149 | 1/1   | 0.85 | 0.27 | 40,40,40,40                 | 0     |
| 59  | MG   | AA    | 1745 | 1/1   | 0.85 | 0.27 | 77,77,77,77                 | 0     |
| 59  | MG   | CA    | 1777 | 1/1   | 0.85 | 0.28 | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3011 | 1/1   | 0.85 | 0.37 | 65,65,65,65                 | 0     |
| 59  | MG   | CA    | 1785 | 1/1   | 0.85 | 0.22 | 46,46,46,46                 | 0     |
| 59  | MG   | CA    | 1706 | 1/1   | 0.85 | 0.11 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3176 | 1/1   | 0.85 | 0.20 | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1721 | 1/1   | 0.85 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3193 | 1/1   | 0.85 | 0.25 | 50,50,50,50                 | 0     |
| 59  | MG   | CA    | 1602 | 1/1   | 0.85 | 0.09 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3302 | 1/1   | 0.85 | 0.26 | 75,75,75,75                 | 0     |
| 59  | MG   | CA    | 1718 | 1/1   | 0.85 | 0.10 | 81,81,81,81                 | 0     |
| 59  | MG   | DA    | 3216 | 1/1   | 0.85 | 0.18 | 26,26,26,26                 | 0     |
| 59  | MG   | DB    | 202  | 1/1   | 0.85 | 0.21 | 83,83,83,83                 | 0     |
| 59  | MG   | DA    | 3224 | 1/1   | 0.85 | 0.12 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3184 | 1/1   | 0.85 | 0.21 | 59,59,59,59                 | 0     |
| 59  | MG   | AA    | 1683 | 1/1   | 0.85 | 0.23 | 74,74,74,74                 | 0     |
| 59  | MG   | AA    | 1793 | 1/1   | 0.85 | 0.16 | 85,85,85,85                 | 0     |
| 59  | MG   | BB    | 201  | 1/1   | 0.85 | 0.06 | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3245 | 1/1   | 0.85 | 0.14 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3246 | 1/1   | 0.85 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3207 | 1/1   | 0.86 | 0.37 | 83,83,83,83                 | 0     |
| 59  | MG   | BA    | 3237 | 1/1   | 0.86 | 0.26 | 37,37,37,37                 | 0     |
| 59  | MG   | AA    | 1754 | 1/1   | 0.86 | 0.13 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3311 | 1/1   | 0.86 | 0.20 | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1664 | 1/1   | 0.86 | 0.17 | 89,89,89,89                 | 0     |
| 59  | MG   | CA    | 1634 | 1/1   | 0.86 | 0.18 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3364 | 1/1   | 0.86 | 0.30 | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1604 | 1/1   | 0.86 | 0.27 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3044 | 1/1   | 0.86 | 0.25 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3248 | 1/1   | 0.86 | 0.24 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3051 | 1/1   | 0.86 | 0.16 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3057 | 1/1   | 0.86 | 0.26 | 52,52,52,52                 | 0     |
| 59  | MG   | B2    | 101  | 1/1   | 0.86 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1646 | 1/1   | 0.86 | 0.12 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3384 | 1/1   | 0.86 | 0.24 | 63,63,63,63                 | 0     |
| 59  | MG   | AV    | 102  | 1/1   | 0.86 | 0.28 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3299 | 1/1   | 0.86 | 0.22 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3386 | 1/1   | 0.86 | 0.05 | 83,83,83,83                 | 0     |
| 59  | MG   | AA    | 1631 | 1/1   | 0.86 | 0.28 | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3086 | 1/1   | 0.86 | 0.28 | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1779 | 1/1   | 0.86 | 0.32 | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1727 | 1/1   | 0.86 | 0.10 | 99,99,99,99                 | 0     |
| 59  | MG   | CW    | 113  | 1/1   | 0.86 | 0.10 | 123,123,123,123             | 0     |
| 59  | MG   | BA    | 3402 | 1/1   | 0.86 | 0.10 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3003 | 1/1   | 0.86 | 0.14 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3221 | 1/1   | 0.86 | 0.23 | 87,87,87,87                 | 0     |
| 59  | MG   | CA    | 1730 | 1/1   | 0.86 | 0.06 | 93,93,93,93                 | 0     |
| 59  | MG   | AA    | 1740 | 1/1   | 0.86 | 0.16 | 114,114,114,114             | 0     |
| 59  | MG   | DA    | 3049 | 1/1   | 0.86 | 0.36 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3172 | 1/1   | 0.86 | 0.07 | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1694 | 1/1   | 0.86 | 0.08 | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1749 | 1/1   | 0.86 | 0.12 | 105,105,105,105             | 0     |
| 59  | MG   | BA    | 3341 | 1/1   | 0.86 | 0.22 | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1670 | 1/1   | 0.86 | 0.29 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3231 | 1/1   | 0.86 | 0.23 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3358 | 1/1   | 0.86 | 0.11 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3422 | 1/1   | 0.86 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3182 | 1/1   | 0.86 | 0.09 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1606 | 1/1   | 0.86 | 0.25 | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3120 | 1/1   | 0.86 | 0.33 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3124 | 1/1   | 0.86 | 0.14 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3138 | 1/1   | 0.86 | 0.41 | 34,34,34,34                 | 0     |
| 59  | MG   | DA    | 3143 | 1/1   | 0.86 | 0.06 | 67,67,67,67                 | 0     |
| 59  | MG   | CA    | 1751 | 1/1   | 0.86 | 0.07 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3428 | 1/1   | 0.86 | 0.25 | 71,71,71,71                 | 0     |
| 59  | MG   | AA    | 1652 | 1/1   | 0.86 | 0.16 | 92,92,92,92                 | 0     |
| 59  | MG   | BA    | 3433 | 1/1   | 0.86 | 0.23 | 94,94,94,94                 | 0     |
| 59  | MG   | BA    | 3022 | 1/1   | 0.86 | 0.20 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3435 | 1/1   | 0.86 | 0.09 | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3436 | 1/1   | 0.86 | 0.14 | 65,65,65,65                 | 0     |
| 59  | MG   | DB    | 209  | 1/1   | 0.86 | 0.24 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3187 | 1/1   | 0.86 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1685 | 1/1   | 0.86 | 0.13 | 56,56,56,56                 | 0     |
| 59  | MG   | CA    | 1621 | 1/1   | 0.86 | 0.14 | 67,67,67,67                 | 0     |
| 59  | MG   | CA    | 1783 | 1/1   | 0.86 | 0.21 | 64,64,64,64                 | 0     |
| 59  | MG   | CA    | 1623 | 1/1   | 0.86 | 0.23 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3266 | 1/1   | 0.87 | 0.24 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3145 | 1/1   | 0.87 | 0.20 | 62,62,62,62                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1727 | 1/1   | 0.87 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | CA    | 1747 | 1/1   | 0.87 | 0.15 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3362 | 1/1   | 0.87 | 0.08 | 83,83,83,83                 | 0     |
| 59  | MG   | DA    | 3275 | 1/1   | 0.87 | 0.15 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3278 | 1/1   | 0.87 | 0.23 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3280 | 1/1   | 0.87 | 0.11 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3363 | 1/1   | 0.87 | 0.26 | 43,43,43,43                 | 0     |
| 59  | MG   | CA    | 1753 | 1/1   | 0.87 | 0.16 | 82,82,82,82                 | 0     |
| 59  | MG   | AA    | 1630 | 1/1   | 0.87 | 0.07 | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1680 | 1/1   | 0.87 | 0.16 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1625 | 1/1   | 0.87 | 0.15 | 66,66,66,66                 | 0     |
| 59  | MG   | CA    | 1653 | 1/1   | 0.87 | 0.24 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3094 | 1/1   | 0.87 | 0.21 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3099 | 1/1   | 0.87 | 0.27 | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3280 | 1/1   | 0.87 | 0.12 | 107,107,107,107             | 0     |
| 59  | MG   | AA    | 1718 | 1/1   | 0.87 | 0.25 | 89,89,89,89                 | 0     |
| 59  | MG   | DA    | 3110 | 1/1   | 0.87 | 0.15 | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3113 | 1/1   | 0.87 | 0.12 | 23,23,23,23                 | 0     |
| 59  | MG   | CA    | 1657 | 1/1   | 0.87 | 0.07 | 88,88,88,88                 | 0     |
| 59  | MG   | CA    | 1659 | 1/1   | 0.87 | 0.27 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3437 | 1/1   | 0.87 | 0.12 | 126,126,126,126             | 0     |
| 59  | MG   | CA    | 1714 | 1/1   | 0.87 | 0.15 | 67,67,67,67                 | 0     |
| 59  | MG   | CA    | 1788 | 1/1   | 0.87 | 0.08 | 124,124,124,124             | 0     |
| 59  | MG   | BA    | 3087 | 1/1   | 0.87 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1716 | 1/1   | 0.87 | 0.22 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3383 | 1/1   | 0.87 | 0.10 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3152 | 1/1   | 0.87 | 0.20 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3194 | 1/1   | 0.87 | 0.24 | 54,54,54,54                 | 0     |
| 59  | MG   | AA    | 1685 | 1/1   | 0.87 | 0.18 | 104,104,104,104             | 0     |
| 59  | MG   | AA    | 1627 | 1/1   | 0.87 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | CF    | 201  | 1/1   | 0.87 | 0.27 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3392 | 1/1   | 0.87 | 0.80 | 83,83,83,83                 | 0     |
| 59  | MG   | AW    | 120  | 1/1   | 0.87 | 0.22 | 104,104,104,104             | 0     |
| 59  | MG   | CV    | 102  | 1/1   | 0.87 | 0.20 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3188 | 1/1   | 0.87 | 0.23 | 30,30,30,30                 | 0     |
| 59  | MG   | CV    | 104  | 1/1   | 0.87 | 0.24 | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1705 | 1/1   | 0.87 | 0.17 | 83,83,83,83                 | 0     |
| 59  | MG   | BA    | 3252 | 1/1   | 0.87 | 0.34 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3127 | 1/1   | 0.87 | 0.14 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3132 | 1/1   | 0.87 | 0.07 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3305 | 1/1   | 0.87 | 0.34 | 77,77,77,77                 | 0     |
| 59  | MG   | AV    | 104  | 1/1   | 0.87 | 0.20 | 102,102,102,102             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1734 | 1/1   | 0.87 | 0.29 | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1615 | 1/1   | 0.87 | 0.32 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3312 | 1/1   | 0.87 | 0.07 | 65,65,65,65                 | 0     |
| 59  | MG   | DA    | 3233 | 1/1   | 0.87 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | DF    | 301  | 1/1   | 0.87 | 0.11 | 66,66,66,66                 | 0     |
| 59  | MG   | CA    | 1639 | 1/1   | 0.87 | 0.25 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3235 | 1/1   | 0.87 | 0.41 | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3415 | 1/1   | 0.87 | 0.29 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3270 | 1/1   | 0.88 | 0.11 | 73,73,73,73                 | 0     |
| 59  | MG   | CA    | 1795 | 1/1   | 0.88 | 0.09 | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3124 | 1/1   | 0.88 | 0.22 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3198 | 1/1   | 0.88 | 0.23 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3202 | 1/1   | 0.88 | 0.08 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3340 | 1/1   | 0.88 | 0.19 | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3126 | 1/1   | 0.88 | 0.20 | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1784 | 1/1   | 0.88 | 0.18 | 70,70,70,70                 | 0     |
| 59  | MG   | CI    | 201  | 1/1   | 0.88 | 0.24 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3012 | 1/1   | 0.88 | 0.22 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3221 | 1/1   | 0.88 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1670 | 1/1   | 0.88 | 0.25 | 68,68,68,68                 | 0     |
| 59  | MG   | CV    | 103  | 1/1   | 0.88 | 0.09 | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3231 | 1/1   | 0.88 | 0.10 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3203 | 1/1   | 0.88 | 0.25 | 58,58,58,58                 | 0     |
| 59  | MG   | AT    | 201  | 1/1   | 0.88 | 0.07 | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3444 | 1/1   | 0.88 | 0.16 | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1717 | 1/1   | 0.88 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1612 | 1/1   | 0.88 | 0.27 | 50,50,50,50                 | 0     |
| 59  | MG   | CA    | 1719 | 1/1   | 0.88 | 0.13 | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3291 | 1/1   | 0.88 | 0.21 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3149 | 1/1   | 0.88 | 0.31 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3253 | 1/1   | 0.88 | 0.12 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3024 | 1/1   | 0.88 | 0.08 | 82,82,82,82                 | 0     |
| 59  | MG   | AA    | 1643 | 1/1   | 0.88 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | DA    | 3274 | 1/1   | 0.88 | 0.18 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3030 | 1/1   | 0.88 | 0.16 | 52,52,52,52                 | 0     |
| 59  | MG   | CW    | 111  | 1/1   | 0.88 | 0.35 | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1698 | 1/1   | 0.88 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | AV    | 105  | 1/1   | 0.88 | 0.32 | 62,62,62,62                 | 0     |
| 59  | MG   | D2    | 102  | 1/1   | 0.88 | 0.08 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3290 | 1/1   | 0.88 | 0.09 | 68,68,68,68                 | 0     |
| 59  | MG   | AV    | 106  | 1/1   | 0.88 | 0.18 | 96,96,96,96                 | 0     |
| 59  | MG   | BA    | 3368 | 1/1   | 0.88 | 0.14 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1658 | 1/1   | 0.88 | 0.35 | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1673 | 1/1   | 0.88 | 0.08 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3012 | 1/1   | 0.88 | 0.22 | 45,45,45,45                 | 0     |
| 59  | MG   | BB    | 210  | 1/1   | 0.88 | 0.20 | 93,93,93,93                 | 0     |
| 59  | MG   | DA    | 3039 | 1/1   | 0.88 | 0.45 | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1646 | 1/1   | 0.88 | 0.32 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3050 | 1/1   | 0.88 | 0.13 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3322 | 1/1   | 0.88 | 0.17 | 56,56,56,56                 | 0     |
| 59  | MG   | AA    | 1703 | 1/1   | 0.88 | 0.25 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3063 | 1/1   | 0.88 | 0.23 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3085 | 1/1   | 0.88 | 0.20 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3077 | 1/1   | 0.88 | 0.22 | 52,52,52,52                 | 0     |
| 59  | MG   | AX    | 102  | 1/1   | 0.88 | 0.13 | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3244 | 1/1   | 0.88 | 0.34 | 85,85,85,85                 | 0     |
| 59  | MG   | DA    | 3336 | 1/1   | 0.88 | 0.24 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3095 | 1/1   | 0.88 | 0.28 | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3396 | 1/1   | 0.88 | 0.27 | 63,63,63,63                 | 0     |
| 59  | MG   | B1    | 101  | 1/1   | 0.88 | 0.08 | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1663 | 1/1   | 0.88 | 0.29 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3108 | 1/1   | 0.88 | 0.20 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3178 | 1/1   | 0.88 | 0.12 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3400 | 1/1   | 0.88 | 0.12 | 59,59,59,59                 | 0     |
| 59  | MG   | AA    | 1736 | 1/1   | 0.88 | 0.23 | 56,56,56,56                 | 0     |
| 59  | MG   | CA    | 1760 | 1/1   | 0.88 | 0.07 | 92,92,92,92                 | 0     |
| 59  | MG   | BA    | 3404 | 1/1   | 0.88 | 0.19 | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1688 | 1/1   | 0.88 | 0.24 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3002 | 1/1   | 0.88 | 0.17 | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3134 | 1/1   | 0.88 | 0.33 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3096 | 1/1   | 0.88 | 0.15 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3411 | 1/1   | 0.88 | 0.11 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3146 | 1/1   | 0.88 | 0.19 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3264 | 1/1   | 0.88 | 0.25 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3150 | 1/1   | 0.88 | 0.12 | 54,54,54,54                 | 0     |
| 59  | MG   | DB    | 204  | 1/1   | 0.88 | 0.21 | 77,77,77,77                 | 0     |
| 59  | MG   | AA    | 1651 | 1/1   | 0.88 | 0.19 | 78,78,78,78                 | 0     |
| 59  | MG   | CA    | 1687 | 1/1   | 0.88 | 0.20 | 56,56,56,56                 | 0     |
| 59  | MG   | AA    | 1708 | 1/1   | 0.88 | 0.22 | 61,61,61,61                 | 0     |
| 59  | MG   | DB    | 210  | 1/1   | 0.88 | 0.09 | 88,88,88,88                 | 0     |
| 59  | MG   | BA    | 3418 | 1/1   | 0.88 | 0.28 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1790 | 1/1   | 0.88 | 0.21 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3330 | 1/1   | 0.88 | 0.10 | 104,104,104,104             | 0     |
| 59  | MG   | BA    | 3333 | 1/1   | 0.88 | 0.22 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3186 | 1/1   | 0.88 | 0.50 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3334 | 1/1   | 0.88 | 0.27 | 54,54,54,54                 | 0     |
| 59  | MG   | CA    | 1691 | 1/1   | 0.89 | 0.21 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3394 | 1/1   | 0.89 | 0.08 | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1723 | 1/1   | 0.89 | 0.06 | 64,64,64,64                 | 0     |
| 59  | MG   | CA    | 1772 | 1/1   | 0.89 | 0.31 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1628 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3224 | 1/1   | 0.89 | 0.12 | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3331 | 1/1   | 0.89 | 0.10 | 88,88,88,88                 | 0     |
| 59  | MG   | CA    | 1782 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1701 | 1/1   | 0.89 | 0.15 | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1703 | 1/1   | 0.89 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1702 | 1/1   | 0.89 | 0.10 | 93,93,93,93                 | 0     |
| 59  | MG   | BA    | 3177 | 1/1   | 0.89 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3229 | 1/1   | 0.89 | 0.21 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3140 | 1/1   | 0.89 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | AV    | 101  | 1/1   | 0.89 | 0.17 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3313 | 1/1   | 0.89 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3294 | 1/1   | 0.89 | 0.16 | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1678 | 1/1   | 0.89 | 0.10 | 82,82,82,82                 | 0     |
| 59  | MG   | AA    | 1800 | 1/1   | 0.89 | 0.22 | 74,74,74,74                 | 0     |
| 59  | MG   | AA    | 1666 | 1/1   | 0.89 | 0.25 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3347 | 1/1   | 0.89 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3153 | 1/1   | 0.89 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | BU    | 202  | 1/1   | 0.89 | 0.33 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3238 | 1/1   | 0.89 | 0.26 | 42,42,42,42                 | 0     |
| 59  | MG   | CV    | 101  | 1/1   | 0.89 | 0.21 | 31,31,31,31                 | 0     |
| 59  | MG   | BU    | 205  | 1/1   | 0.89 | 0.31 | 57,57,57,57                 | 0     |
| 59  | MG   | CA    | 1665 | 1/1   | 0.89 | 0.20 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3155 | 1/1   | 0.89 | 0.08 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3156 | 1/1   | 0.89 | 0.23 | 78,78,78,78                 | 0     |
| 59  | MG   | AA    | 1785 | 1/1   | 0.89 | 0.25 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3307 | 1/1   | 0.89 | 0.35 | 39,39,39,39                 | 0     |
| 59  | MG   | DA    | 3181 | 1/1   | 0.89 | 0.06 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3036 | 1/1   | 0.89 | 0.25 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3040 | 1/1   | 0.89 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3095 | 1/1   | 0.89 | 0.28 | 30,30,30,30                 | 0     |
| 59  | MG   | CA    | 1614 | 1/1   | 0.89 | 0.07 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1641 | 1/1   | 0.89 | 0.07 | 78,78,78,78                 | 0     |
| 59  | MG   | CA    | 1617 | 1/1   | 0.89 | 0.15 | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3197 | 1/1   | 0.89 | 0.24 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3256 | 1/1   | 0.89 | 0.34 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3204 | 1/1   | 0.89 | 0.13 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3259 | 1/1   | 0.89 | 0.14 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3439 | 1/1   | 0.89 | 0.11 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3102 | 1/1   | 0.89 | 0.23 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3211 | 1/1   | 0.89 | 0.17 | 55,55,55,55                 | 0     |
| 59  | MG   | AA    | 1775 | 1/1   | 0.89 | 0.07 | 75,75,75,75                 | 0     |
| 59  | MG   | AA    | 1681 | 1/1   | 0.89 | 0.09 | 76,76,76,76                 | 0     |
| 59  | MG   | CA    | 1752 | 1/1   | 0.89 | 0.24 | 41,41,41,41                 | 0     |
| 59  | MG   | DB    | 205  | 1/1   | 0.89 | 0.13 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3218 | 1/1   | 0.89 | 0.07 | 77,77,77,77                 | 0     |
| 59  | MG   | CA    | 1756 | 1/1   | 0.89 | 0.18 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3048 | 1/1   | 0.89 | 0.22 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3019 | 1/1   | 0.89 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3032 | 1/1   | 0.89 | 0.26 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3389 | 1/1   | 0.89 | 0.29 | 74,74,74,74                 | 0     |
| 59  | MG   | DA    | 3045 | 1/1   | 0.89 | 0.23 | 38,38,38,38                 | 0     |
| 59  | MG   | AD    | 301  | 1/1   | 0.89 | 0.24 | 69,69,69,69                 | 0     |
| 59  | MG   | CA    | 1762 | 1/1   | 0.89 | 0.19 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3063 | 1/1   | 0.89 | 0.25 | 19,19,19,19                 | 0     |
| 59  | MG   | AA    | 1626 | 1/1   | 0.90 | 0.21 | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1781 | 1/1   | 0.90 | 0.23 | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3109 | 1/1   | 0.90 | 0.18 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3113 | 1/1   | 0.90 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3360 | 1/1   | 0.90 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1807 | 1/1   | 0.90 | 0.30 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3123 | 1/1   | 0.90 | 0.12 | 34,34,34,34                 | 0     |
| 59  | MG   | AA    | 1782 | 1/1   | 0.90 | 0.09 | 116,116,116,116             | 0     |
| 59  | MG   | BA    | 3020 | 1/1   | 0.90 | 0.13 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1636 | 1/1   | 0.90 | 0.28 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1717 | 1/1   | 0.90 | 0.14 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3173 | 1/1   | 0.90 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3293 | 1/1   | 0.90 | 0.21 | 16,16,16,16                 | 0     |
| 59  | MG   | BA    | 3372 | 1/1   | 0.90 | 0.07 | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3272 | 1/1   | 0.90 | 0.25 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3223 | 1/1   | 0.90 | 0.13 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3441 | 1/1   | 0.90 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3144 | 1/1   | 0.90 | 0.08 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3381 | 1/1   | 0.90 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3316 | 1/1   | 0.90 | 0.13 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3382 | 1/1   | 0.90 | 0.20 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3079 | 1/1   | 0.90 | 0.22 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3137 | 1/1   | 0.90 | 0.16 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3153 | 1/1   | 0.90 | 0.10 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3155 | 1/1   | 0.90 | 0.12 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3158 | 1/1   | 0.90 | 0.29 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1795 | 1/1   | 0.90 | 0.22 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3162 | 1/1   | 0.90 | 0.15 | 53,53,53,53                 | 0     |
| 59  | MG   | BB    | 202  | 1/1   | 0.90 | 0.13 | 98,98,98,98                 | 0     |
| 59  | MG   | BA    | 3028 | 1/1   | 0.90 | 0.17 | 23,23,23,23                 | 0     |
| 59  | MG   | CA    | 1636 | 1/1   | 0.90 | 0.18 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3029 | 1/1   | 0.90 | 0.26 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3329 | 1/1   | 0.90 | 0.12 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3183 | 1/1   | 0.90 | 0.14 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3347 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 59  | MG   | CX    | 101  | 1/1   | 0.90 | 0.32 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3287 | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1752 | 1/1   | 0.90 | 0.22 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3292 | 1/1   | 0.90 | 0.20 | 48,48,48,48                 | 0     |
| 59  | MG   | CA    | 1643 | 1/1   | 0.90 | 0.22 | 100,100,100,100             | 0     |
| 59  | MG   | BA    | 3090 | 1/1   | 0.90 | 0.09 | 73,73,73,73                 | 0     |
| 59  | MG   | BA    | 3337 | 1/1   | 0.90 | 0.20 | 80,80,80,80                 | 0     |
| 59  | MG   | CA    | 1647 | 1/1   | 0.90 | 0.25 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3018 | 1/1   | 0.90 | 0.15 | 73,73,73,73                 | 0     |
| 59  | MG   | DA    | 3379 | 1/1   | 0.90 | 0.11 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3001 | 1/1   | 0.90 | 0.28 | 56,56,56,56                 | 0     |
| 59  | MG   | CA    | 1704 | 1/1   | 0.90 | 0.22 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3154 | 1/1   | 0.90 | 0.21 | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1710 | 1/1   | 0.90 | 0.07 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3385 | 1/1   | 0.90 | 0.11 | 226,226,226,226             | 0     |
| 59  | MG   | CA    | 1708 | 1/1   | 0.90 | 0.15 | 55,55,55,55                 | 0     |
| 59  | MG   | CA    | 1780 | 1/1   | 0.90 | 0.09 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3053 | 1/1   | 0.90 | 0.24 | 29,29,29,29                 | 0     |
| 59  | MG   | DB    | 203  | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3227 | 1/1   | 0.90 | 0.11 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3229 | 1/1   | 0.90 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3300 | 1/1   | 0.90 | 0.17 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3064 | 1/1   | 0.90 | 0.35 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3071 | 1/1   | 0.90 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | AW    | 116  | 1/1   | 0.90 | 0.22 | 76,76,76,76                 | 0     |
| 59  | MG   | CA    | 1711 | 1/1   | 0.90 | 0.25 | 72,72,72,72                 | 0     |
| 59  | MG   | BA    | 3197 | 1/1   | 0.90 | 0.42 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3238 | 1/1   | 0.90 | 0.32 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3241 | 1/1   | 0.90 | 0.23 | 33,33,33,33                 | 0     |
| 59  | MG   | AA    | 1712 | 1/1   | 0.90 | 0.09 | 67,67,67,67                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3101 | 1/1   | 0.90 | 0.18 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3250 | 1/1   | 0.91 | 0.14 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3251 | 1/1   | 0.91 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1618 | 1/1   | 0.91 | 0.17 | 65,65,65,65                 | 0     |
| 59  | MG   | CA    | 1726 | 1/1   | 0.91 | 0.07 | 64,64,64,64                 | 0     |
| 59  | MG   | DA    | 3254 | 1/1   | 0.91 | 0.30 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3260 | 1/1   | 0.91 | 0.27 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3391 | 1/1   | 0.91 | 0.17 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3448 | 1/1   | 0.91 | 0.22 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3208 | 1/1   | 0.91 | 0.07 | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3393 | 1/1   | 0.91 | 0.26 | 34,34,34,34                 | 0     |
| 59  | MG   | CA    | 1731 | 1/1   | 0.91 | 0.28 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3454 | 1/1   | 0.91 | 0.28 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1624 | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |
| 59  | MG   | DA    | 3123 | 1/1   | 0.91 | 0.24 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1687 | 1/1   | 0.91 | 0.10 | 84,84,84,84                 | 0     |
| 59  | MG   | DA    | 3127 | 1/1   | 0.91 | 0.20 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3296 | 1/1   | 0.91 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3457 | 1/1   | 0.91 | 0.32 | 82,82,82,82                 | 0     |
| 59  | MG   | BA    | 3013 | 1/1   | 0.91 | 0.12 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3301 | 1/1   | 0.91 | 0.12 | 136,136,136,136             | 0     |
| 59  | MG   | DA    | 3140 | 1/1   | 0.91 | 0.26 | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3307 | 1/1   | 0.91 | 0.37 | 64,64,64,64                 | 0     |
| 59  | MG   | CA    | 1630 | 1/1   | 0.91 | 0.04 | 120,120,120,120             | 0     |
| 59  | MG   | BA    | 3147 | 1/1   | 0.91 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3217 | 1/1   | 0.91 | 0.25 | 72,72,72,72                 | 0     |
| 59  | MG   | CA    | 1635 | 1/1   | 0.91 | 0.20 | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1764 | 1/1   | 0.91 | 0.09 | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3260 | 1/1   | 0.91 | 0.15 | 59,59,59,59                 | 0     |
| 59  | MG   | CA    | 1748 | 1/1   | 0.91 | 0.19 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3308 | 1/1   | 0.91 | 0.08 | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1798 | 1/1   | 0.91 | 0.13 | 75,75,75,75                 | 0     |
| 59  | MG   | BA    | 3107 | 1/1   | 0.91 | 0.19 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3161 | 1/1   | 0.91 | 0.22 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3179 | 1/1   | 0.91 | 0.07 | 66,66,66,66                 | 0     |
| 59  | MG   | D2    | 101  | 1/1   | 0.91 | 0.11 | 59,59,59,59                 | 0     |
| 59  | MG   | AA    | 1613 | 1/1   | 0.91 | 0.14 | 89,89,89,89                 | 0     |
| 59  | MG   | B0    | 101  | 1/1   | 0.91 | 0.15 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3333 | 1/1   | 0.91 | 0.09 | 57,57,57,57                 | 0     |
| 59  | MG   | AA    | 1711 | 1/1   | 0.91 | 0.10 | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3004 | 1/1   | 0.91 | 0.21 | 89,89,89,89                 | 0     |
| 59  | MG   | DA    | 3342 | 1/1   | 0.91 | 0.14 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3343 | 1/1   | 0.91 | 0.24 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3006 | 1/1   | 0.91 | 0.19 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3185 | 1/1   | 0.91 | 0.23 | 31,31,31,31                 | 0     |
| 59  | MG   | CA    | 1699 | 1/1   | 0.91 | 0.06 | 66,66,66,66                 | 0     |
| 59  | MG   | AA    | 1767 | 1/1   | 0.91 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3356 | 1/1   | 0.91 | 0.28 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3414 | 1/1   | 0.91 | 0.21 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3158 | 1/1   | 0.91 | 0.09 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3361 | 1/1   | 0.91 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3362 | 1/1   | 0.91 | 0.13 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3363 | 1/1   | 0.91 | 0.23 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3118 | 1/1   | 0.91 | 0.20 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3368 | 1/1   | 0.91 | 0.35 | 50,50,50,50                 | 0     |
| 59  | MG   | CA    | 1771 | 1/1   | 0.91 | 0.08 | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1620 | 1/1   | 0.91 | 0.23 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3035 | 1/1   | 0.91 | 0.39 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3036 | 1/1   | 0.91 | 0.16 | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3191 | 1/1   | 0.91 | 0.23 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3284 | 1/1   | 0.91 | 0.10 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3210 | 1/1   | 0.91 | 0.17 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3047 | 1/1   | 0.91 | 0.19 | 16,16,16,16                 | 0     |
| 59  | MG   | BA    | 3425 | 1/1   | 0.91 | 0.09 | 67,67,67,67                 | 0     |
| 59  | MG   | CA    | 1779 | 1/1   | 0.91 | 0.21 | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1667 | 1/1   | 0.91 | 0.20 | 64,64,64,64                 | 0     |
| 59  | MG   | AV    | 107  | 1/1   | 0.91 | 0.21 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3226 | 1/1   | 0.91 | 0.11 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3429 | 1/1   | 0.91 | 0.25 | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1640 | 1/1   | 0.91 | 0.31 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3074 | 1/1   | 0.91 | 0.12 | 40,40,40,40                 | 0     |
| 59  | MG   | CA    | 1661 | 1/1   | 0.91 | 0.25 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3083 | 1/1   | 0.91 | 0.25 | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3379 | 1/1   | 0.91 | 0.09 | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3236 | 1/1   | 0.91 | 0.25 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3165 | 1/1   | 0.91 | 0.33 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3199 | 1/1   | 0.91 | 0.18 | 60,60,60,60                 | 0     |
| 59  | MG   | BA    | 3088 | 1/1   | 0.91 | 0.12 | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1730 | 1/1   | 0.91 | 0.23 | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3098 | 1/1   | 0.91 | 0.24 | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1603 | 1/1   | 0.91 | 0.11 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3068 | 1/1   | 0.92 | 0.17 | 36,36,36,36                 | 0     |
| 59  | MG   | AA    | 1770 | 1/1   | 0.92 | 0.29 | 74,74,74,74                 | 0     |
| 59  | MG   | DA    | 3117 | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3255 | 1/1   | 0.92 | 0.18 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3259 | 1/1   | 0.92 | 0.28 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3268 | 1/1   | 0.92 | 0.15 | 48,48,48,48                 | 0     |
| 59  | MG   | CA    | 1616 | 1/1   | 0.92 | 0.26 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3265 | 1/1   | 0.92 | 0.12 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3270 | 1/1   | 0.92 | 0.14 | 45,45,45,45                 | 0     |
| 59  | MG   | CA    | 1736 | 1/1   | 0.92 | 0.25 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3129 | 1/1   | 0.92 | 0.32 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1738 | 1/1   | 0.92 | 0.13 | 95,95,95,95                 | 0     |
| 59  | MG   | BA    | 3015 | 1/1   | 0.92 | 0.12 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3133 | 1/1   | 0.92 | 0.26 | 22,22,22,22                 | 0     |
| 59  | MG   | AA    | 1649 | 1/1   | 0.92 | 0.18 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3136 | 1/1   | 0.92 | 0.24 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3175 | 1/1   | 0.92 | 0.19 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3139 | 1/1   | 0.92 | 0.36 | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3446 | 1/1   | 0.92 | 0.28 | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1810 | 1/1   | 0.92 | 0.07 | 88,88,88,88                 | 0     |
| 59  | MG   | DA    | 3298 | 1/1   | 0.92 | 0.07 | 50,50,50,50                 | 0     |
| 59  | MG   | AX    | 101  | 1/1   | 0.92 | 0.24 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3277 | 1/1   | 0.92 | 0.16 | 56,56,56,56                 | 0     |
| 59  | MG   | AC    | 301  | 1/1   | 0.92 | 0.17 | 66,66,66,66                 | 0     |
| 59  | MG   | CX    | 102  | 1/1   | 0.92 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3143 | 1/1   | 0.92 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1632 | 1/1   | 0.92 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3144 | 1/1   | 0.92 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | AA    | 1704 | 1/1   | 0.92 | 0.21 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1757 | 1/1   | 0.92 | 0.44 | 60,60,60,60                 | 0     |
| 59  | MG   | CA    | 1758 | 1/1   | 0.92 | 0.16 | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1610 | 1/1   | 0.92 | 0.13 | 95,95,95,95                 | 0     |
| 59  | MG   | BA    | 3148 | 1/1   | 0.92 | 0.35 | 24,24,24,24                 | 0     |
| 59  | MG   | DA    | 3164 | 1/1   | 0.92 | 0.07 | 57,57,57,57                 | 0     |
| 59  | MG   | AA    | 1729 | 1/1   | 0.92 | 0.12 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3288 | 1/1   | 0.92 | 0.21 | 78,78,78,78                 | 0     |
| 59  | MG   | DA    | 3017 | 1/1   | 0.92 | 0.21 | 29,29,29,29                 | 0     |
| 59  | MG   | B5    | 101  | 1/1   | 0.92 | 0.15 | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1624 | 1/1   | 0.92 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3184 | 1/1   | 0.92 | 0.06 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3027 | 1/1   | 0.92 | 0.18 | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1734 | 1/1   | 0.92 | 0.18 | 75,75,75,75                 | 0     |
| 59  | MG   | CA    | 1702 | 1/1   | 0.92 | 0.18 | 75,75,75,75                 | 0     |
| 59  | MG   | DA    | 3338 | 1/1   | 0.92 | 0.32 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3340 | 1/1   | 0.92 | 0.08 | 84,84,84,84                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3343 | 1/1   | 0.92 | 0.09 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3190 | 1/1   | 0.92 | 0.38 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3098 | 1/1   | 0.92 | 0.22 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3040 | 1/1   | 0.92 | 0.16 | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3194 | 1/1   | 0.92 | 0.10 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3195 | 1/1   | 0.92 | 0.16 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3409 | 1/1   | 0.92 | 0.24 | 61,61,61,61                 | 0     |
| 59  | MG   | BB    | 212  | 1/1   | 0.92 | 0.20 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3199 | 1/1   | 0.92 | 0.08 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3200 | 1/1   | 0.92 | 0.22 | 45,45,45,45                 | 0     |
| 59  | MG   | BB    | 213  | 1/1   | 0.92 | 0.23 | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1797 | 1/1   | 0.92 | 0.08 | 73,73,73,73                 | 0     |
| 59  | MG   | DA    | 3366 | 1/1   | 0.92 | 0.33 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3243 | 1/1   | 0.92 | 0.17 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3055 | 1/1   | 0.92 | 0.20 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3208 | 1/1   | 0.92 | 0.22 | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1605 | 1/1   | 0.92 | 0.31 | 37,37,37,37                 | 0     |
| 59  | MG   | AA    | 1653 | 1/1   | 0.92 | 0.24 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3212 | 1/1   | 0.92 | 0.14 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3070 | 1/1   | 0.92 | 0.30 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3004 | 1/1   | 0.92 | 0.32 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3381 | 1/1   | 0.92 | 0.07 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3220 | 1/1   | 0.92 | 0.19 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3249 | 1/1   | 0.92 | 0.14 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3077 | 1/1   | 0.92 | 0.27 | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3080 | 1/1   | 0.92 | 0.20 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1669 | 1/1   | 0.92 | 0.14 | 57,57,57,57                 | 0     |
| 59  | MG   | BF    | 303  | 1/1   | 0.92 | 0.17 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3111 | 1/1   | 0.92 | 0.07 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3052 | 1/1   | 0.92 | 0.22 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3056 | 1/1   | 0.92 | 0.17 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3423 | 1/1   | 0.92 | 0.14 | 61,61,61,61                 | 0     |
| 59  | MG   | AA    | 1751 | 1/1   | 0.92 | 0.27 | 52,52,52,52                 | 0     |
| 59  | MG   | BX    | 102  | 1/1   | 0.92 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1693 | 1/1   | 0.92 | 0.15 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3258 | 1/1   | 0.92 | 0.43 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3243 | 1/1   | 0.92 | 0.26 | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1768 | 1/1   | 0.92 | 0.17 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3103 | 1/1   | 0.92 | 0.42 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3215 | 1/1   | 0.92 | 0.22 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3371 | 1/1   | 0.92 | 0.27 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3261 | 1/1   | 0.92 | 0.14 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3377 | 1/1   | 0.93 | 0.07 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3279 | 1/1   | 0.93 | 0.17 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3256 | 1/1   | 0.93 | 0.18 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3380 | 1/1   | 0.93 | 0.13 | 60,60,60,60                 | 0     |
| 59  | MG   | CA    | 1618 | 1/1   | 0.93 | 0.21 | 65,65,65,65                 | 0     |
| 59  | MG   | BA    | 3070 | 1/1   | 0.93 | 0.15 | 21,21,21,21                 | 0     |
| 59  | MG   | CA    | 1677 | 1/1   | 0.93 | 0.19 | 68,68,68,68                 | 0     |
| 59  | MG   | CA    | 1740 | 1/1   | 0.93 | 0.14 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3190 | 1/1   | 0.93 | 0.18 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3130 | 1/1   | 0.93 | 0.16 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3282 | 1/1   | 0.93 | 0.22 | 76,76,76,76                 | 0     |
| 59  | MG   | CA    | 1622 | 1/1   | 0.93 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3073 | 1/1   | 0.93 | 0.18 | 37,37,37,37                 | 0     |
| 59  | MG   | CA    | 1745 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3115 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3076 | 1/1   | 0.93 | 0.13 | 65,65,65,65                 | 0     |
| 59  | MG   | DA    | 3291 | 1/1   | 0.93 | 0.10 | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1695 | 1/1   | 0.93 | 0.16 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3332 | 1/1   | 0.93 | 0.09 | 75,75,75,75                 | 0     |
| 59  | MG   | DA    | 3002 | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | B1    | 102  | 1/1   | 0.93 | 0.06 | 67,67,67,67                 | 0     |
| 59  | MG   | AA    | 1690 | 1/1   | 0.93 | 0.07 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3005 | 1/1   | 0.93 | 0.35 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3302 | 1/1   | 0.93 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1761 | 1/1   | 0.93 | 0.31 | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1809 | 1/1   | 0.93 | 0.27 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3157 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3251 | 1/1   | 0.93 | 0.15 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3010 | 1/1   | 0.93 | 0.13 | 40,40,40,40                 | 0     |
| 59  | MG   | DA    | 3011 | 1/1   | 0.93 | 0.22 | 27,27,27,27                 | 0     |
| 59  | MG   | CA    | 1694 | 1/1   | 0.93 | 0.08 | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3013 | 1/1   | 0.93 | 0.20 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3295 | 1/1   | 0.93 | 0.24 | 51,51,51,51                 | 0     |
| 59  | MG   | CA    | 1696 | 1/1   | 0.93 | 0.24 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3296 | 1/1   | 0.93 | 0.36 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3017 | 1/1   | 0.93 | 0.07 | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3020 | 1/1   | 0.93 | 0.20 | 29,29,29,29                 | 0     |
| 59  | MG   | CA    | 1766 | 1/1   | 0.93 | 0.13 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3046 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 59  | MG   | DA    | 3034 | 1/1   | 0.93 | 0.15 | 36,36,36,36                 | 0     |
| 59  | MG   | CA    | 1768 | 1/1   | 0.93 | 0.29 | 58,58,58,58                 | 0     |
| 59  | MG   | CA    | 1769 | 1/1   | 0.93 | 0.28 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3335 | 1/1   | 0.93 | 0.23 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1722 | 1/1   | 0.93 | 0.09 | 75,75,75,75                 | 0     |
| 59  | MG   | DA    | 3189 | 1/1   | 0.93 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3345 | 1/1   | 0.93 | 0.09 | 74,74,74,74                 | 0     |
| 59  | MG   | DA    | 3042 | 1/1   | 0.93 | 0.23 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3135 | 1/1   | 0.93 | 0.09 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3046 | 1/1   | 0.93 | 0.20 | 35,35,35,35                 | 0     |
| 59  | MG   | AA    | 1659 | 1/1   | 0.93 | 0.18 | 74,74,74,74                 | 0     |
| 59  | MG   | BA    | 3170 | 1/1   | 0.93 | 0.15 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3139 | 1/1   | 0.93 | 0.17 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3350 | 1/1   | 0.93 | 0.20 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3021 | 1/1   | 0.93 | 0.06 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3355 | 1/1   | 0.93 | 0.19 | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3141 | 1/1   | 0.93 | 0.21 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3061 | 1/1   | 0.93 | 0.20 | 21,21,21,21                 | 0     |
| 59  | MG   | CA    | 1781 | 1/1   | 0.93 | 0.12 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3354 | 1/1   | 0.93 | 0.21 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3069 | 1/1   | 0.93 | 0.12 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3356 | 1/1   | 0.93 | 0.11 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3365 | 1/1   | 0.93 | 0.07 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3416 | 1/1   | 0.93 | 0.17 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3174 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1744 | 1/1   | 0.93 | 0.18 | 70,70,70,70                 | 0     |
| 59  | MG   | AA    | 1602 | 1/1   | 0.93 | 0.18 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3421 | 1/1   | 0.93 | 0.25 | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3218 | 1/1   | 0.93 | 0.30 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3097 | 1/1   | 0.93 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3058 | 1/1   | 0.93 | 0.08 | 47,47,47,47                 | 0     |
| 59  | MG   | CA    | 1660 | 1/1   | 0.93 | 0.11 | 65,65,65,65                 | 0     |
| 59  | MG   | DA    | 3086 | 1/1   | 0.93 | 0.20 | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3088 | 1/1   | 0.93 | 0.27 | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3099 | 1/1   | 0.93 | 0.14 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3315 | 1/1   | 0.93 | 0.09 | 64,64,64,64                 | 0     |
| 59  | MG   | CA    | 1724 | 1/1   | 0.93 | 0.07 | 120,120,120,120             | 0     |
| 59  | MG   | AA    | 1725 | 1/1   | 0.93 | 0.28 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3061 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3430 | 1/1   | 0.93 | 0.09 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3369 | 1/1   | 0.93 | 0.24 | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1637 | 1/1   | 0.93 | 0.22 | 71,71,71,71                 | 0     |
| 59  | MG   | BA    | 3152 | 1/1   | 0.93 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3242 | 1/1   | 0.93 | 0.17 | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3010 | 1/1   | 0.93 | 0.08 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3109 | 1/1   | 0.93 | 0.14 | 17,17,17,17                 | 0     |
| 59  | MG   | CA    | 1613 | 1/1   | 0.93 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3111 | 1/1   | 0.93 | 0.33 | 28,28,28,28                 | 0     |
| 59  | MG   | DA    | 3249 | 1/1   | 0.93 | 0.07 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3112 | 1/1   | 0.93 | 0.17 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3069 | 1/1   | 0.93 | 0.22 | 29,29,29,29                 | 0     |
| 59  | MG   | DO    | 201  | 1/1   | 0.93 | 0.22 | 64,64,64,64                 | 0     |
| 59  | MG   | DA    | 3114 | 1/1   | 0.93 | 0.07 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3115 | 1/1   | 0.93 | 0.25 | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1720 | 1/1   | 0.94 | 0.18 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3008 | 1/1   | 0.94 | 0.22 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3042 | 1/1   | 0.94 | 0.31 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3349 | 1/1   | 0.94 | 0.30 | 73,73,73,73                 | 0     |
| 59  | MG   | AA    | 1632 | 1/1   | 0.94 | 0.14 | 77,77,77,77                 | 0     |
| 59  | MG   | BV    | 201  | 1/1   | 0.94 | 0.23 | 33,33,33,33                 | 0     |
| 59  | MG   | BX    | 101  | 1/1   | 0.94 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3121 | 1/1   | 0.94 | 0.13 | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3258 | 1/1   | 0.94 | 0.22 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1709 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 59  | MG   | AA    | 1609 | 1/1   | 0.94 | 0.13 | 80,80,80,80                 | 0     |
| 59  | MG   | DA    | 3126 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3094 | 1/1   | 0.94 | 0.12 | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3269 | 1/1   | 0.94 | 0.19 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3129 | 1/1   | 0.94 | 0.13 | 34,34,34,34                 | 0     |
| 59  | MG   | CA    | 1603 | 1/1   | 0.94 | 0.24 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3273 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3131 | 1/1   | 0.94 | 0.26 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3132 | 1/1   | 0.94 | 0.16 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3277 | 1/1   | 0.94 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3239 | 1/1   | 0.94 | 0.29 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3279 | 1/1   | 0.94 | 0.31 | 52,52,52,52                 | 0     |
| 59  | MG   | AA    | 1691 | 1/1   | 0.94 | 0.26 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3281 | 1/1   | 0.94 | 0.24 | 38,38,38,38                 | 0     |
| 59  | MG   | CA    | 1607 | 1/1   | 0.94 | 0.15 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3188 | 1/1   | 0.94 | 0.19 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3286 | 1/1   | 0.94 | 0.17 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3049 | 1/1   | 0.94 | 0.18 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3050 | 1/1   | 0.94 | 0.12 | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3141 | 1/1   | 0.94 | 0.08 | 40,40,40,40                 | 0     |
| 59  | MG   | CA    | 1611 | 1/1   | 0.94 | 0.25 | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1754 | 1/1   | 0.94 | 0.20 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3145 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1755 | 1/1   | 0.94 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3147 | 1/1   | 0.94 | 0.15 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3248 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | DA    | 3303 | 1/1   | 0.94 | 0.07 | 48,48,48,48                 | 0     |
| 59  | MG   | AA    | 1771 | 1/1   | 0.94 | 0.16 | 48,48,48,48                 | 0     |
| 59  | MG   | AX    | 103  | 1/1   | 0.94 | 0.16 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3432 | 1/1   | 0.94 | 0.08 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3195 | 1/1   | 0.94 | 0.27 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3156 | 1/1   | 0.94 | 0.28 | 67,67,67,67                 | 0     |
| 59  | MG   | BA    | 3055 | 1/1   | 0.94 | 0.15 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3310 | 1/1   | 0.94 | 0.30 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3031 | 1/1   | 0.94 | 0.19 | 32,32,32,32                 | 0     |
| 59  | MG   | AA    | 1638 | 1/1   | 0.94 | 0.17 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3370 | 1/1   | 0.94 | 0.07 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3105 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3324 | 1/1   | 0.94 | 0.21 | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1773 | 1/1   | 0.94 | 0.24 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3165 | 1/1   | 0.94 | 0.13 | 34,34,34,34                 | 0     |
| 59  | MG   | DA    | 3166 | 1/1   | 0.94 | 0.12 | 63,63,63,63                 | 0     |
| 59  | MG   | BA    | 3201 | 1/1   | 0.94 | 0.28 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3442 | 1/1   | 0.94 | 0.08 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3169 | 1/1   | 0.94 | 0.17 | 37,37,37,37                 | 0     |
| 59  | MG   | AA    | 1774 | 1/1   | 0.94 | 0.17 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3174 | 1/1   | 0.94 | 0.18 | 37,37,37,37                 | 0     |
| 59  | MG   | CA    | 1698 | 1/1   | 0.94 | 0.07 | 74,74,74,74                 | 0     |
| 59  | MG   | AA    | 1758 | 1/1   | 0.94 | 0.22 | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1682 | 1/1   | 0.94 | 0.14 | 117,117,117,117             | 0     |
| 59  | MG   | DA    | 3339 | 1/1   | 0.94 | 0.24 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3048 | 1/1   | 0.94 | 0.26 | 14,14,14,14                 | 0     |
| 59  | MG   | BA    | 3206 | 1/1   | 0.94 | 0.14 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3451 | 1/1   | 0.94 | 0.19 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3263 | 1/1   | 0.94 | 0.26 | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3345 | 1/1   | 0.94 | 0.34 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3207 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3057 | 1/1   | 0.94 | 0.20 | 28,28,28,28                 | 0     |
| 59  | MG   | CA    | 1705 | 1/1   | 0.94 | 0.30 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3062 | 1/1   | 0.94 | 0.19 | 30,30,30,30                 | 0     |
| 59  | MG   | CA    | 1784 | 1/1   | 0.94 | 0.12 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3065 | 1/1   | 0.94 | 0.23 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3066 | 1/1   | 0.94 | 0.25 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3210 | 1/1   | 0.94 | 0.05 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3360 | 1/1   | 0.94 | 0.06 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3114 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1789 | 1/1   | 0.94 | 0.15 | 89,89,89,89                 | 0     |
| 59  | MG   | AA    | 1796 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3364 | 1/1   | 0.94 | 0.17 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3066 | 1/1   | 0.94 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3079 | 1/1   | 0.94 | 0.16 | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1616 | 1/1   | 0.94 | 0.10 | 63,63,63,63                 | 0     |
| 59  | MG   | CA    | 1712 | 1/1   | 0.94 | 0.10 | 86,86,86,86                 | 0     |
| 59  | MG   | DA    | 3209 | 1/1   | 0.94 | 0.06 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3027 | 1/1   | 0.94 | 0.11 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3274 | 1/1   | 0.94 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1716 | 1/1   | 0.94 | 0.08 | 99,99,99,99                 | 0     |
| 59  | MG   | DA    | 3378 | 1/1   | 0.94 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | CA    | 1645 | 1/1   | 0.94 | 0.23 | 50,50,50,50                 | 0     |
| 59  | MG   | AA    | 1606 | 1/1   | 0.94 | 0.14 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1642 | 1/1   | 0.94 | 0.10 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3090 | 1/1   | 0.94 | 0.17 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3035 | 1/1   | 0.94 | 0.21 | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3223 | 1/1   | 0.94 | 0.19 | 19,19,19,19                 | 0     |
| 59  | MG   | DA    | 3092 | 1/1   | 0.94 | 0.15 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3130 | 1/1   | 0.94 | 0.14 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3336 | 1/1   | 0.94 | 0.25 | 73,73,73,73                 | 0     |
| 59  | MG   | CA    | 1651 | 1/1   | 0.94 | 0.16 | 60,60,60,60                 | 0     |
| 59  | MG   | AA    | 1661 | 1/1   | 0.94 | 0.27 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3403 | 1/1   | 0.94 | 0.18 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3102 | 1/1   | 0.94 | 0.22 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3037 | 1/1   | 0.94 | 0.18 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3339 | 1/1   | 0.94 | 0.07 | 58,58,58,58                 | 0     |
| 59  | MG   | DA    | 3106 | 1/1   | 0.94 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3107 | 1/1   | 0.94 | 0.11 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3225 | 1/1   | 0.94 | 0.16 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3134 | 1/1   | 0.94 | 0.17 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3039 | 1/1   | 0.94 | 0.09 | 45,45,45,45                 | 0     |
| 59  | MG   | BE    | 301  | 1/1   | 0.94 | 0.18 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3082 | 1/1   | 0.94 | 0.15 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3247 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3083 | 1/1   | 0.94 | 0.16 | 28,28,28,28                 | 0     |
| 60  | EDS  | CA    | 1787 | 41/41 | 0.94 | 0.09 | 39,46,57,70                 | 0     |
| 59  | MG   | BA    | 3100 | 1/1   | 0.95 | 0.10 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3100 | 1/1   | 0.95 | 0.20 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3355 | 1/1   | 0.95 | 0.06 | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3295 | 1/1   | 0.95 | 0.16 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1684 | 1/1   | 0.95 | 0.33 | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1739 | 1/1   | 0.95 | 0.19 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3358 | 1/1   | 0.95 | 0.08 | 73,73,73,73                 | 0     |
| 59  | MG   | DA    | 3191 | 1/1   | 0.95 | 0.08 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3300 | 1/1   | 0.95 | 0.15 | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3015 | 1/1   | 0.95 | 0.14 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3359 | 1/1   | 0.95 | 0.16 | 78,78,78,78                 | 0     |
| 59  | MG   | AA    | 1621 | 1/1   | 0.95 | 0.11 | 58,58,58,58                 | 0     |
| 59  | MG   | AA    | 1778 | 1/1   | 0.95 | 0.20 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3306 | 1/1   | 0.95 | 0.06 | 39,39,39,39                 | 0     |
| 59  | MG   | DA    | 3196 | 1/1   | 0.95 | 0.18 | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1731 | 1/1   | 0.95 | 0.15 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3022 | 1/1   | 0.95 | 0.23 | 17,17,17,17                 | 0     |
| 59  | MG   | DA    | 3314 | 1/1   | 0.95 | 0.06 | 64,64,64,64                 | 0     |
| 59  | MG   | DA    | 3023 | 1/1   | 0.95 | 0.37 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3025 | 1/1   | 0.95 | 0.20 | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3026 | 1/1   | 0.95 | 0.25 | 28,28,28,28                 | 0     |
| 59  | MG   | AA    | 1806 | 1/1   | 0.95 | 0.28 | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3204 | 1/1   | 0.95 | 0.20 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3029 | 1/1   | 0.95 | 0.18 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3110 | 1/1   | 0.95 | 0.21 | 35,35,35,35                 | 0     |
| 59  | MG   | CA    | 1679 | 1/1   | 0.95 | 0.06 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3325 | 1/1   | 0.95 | 0.07 | 56,56,56,56                 | 0     |
| 59  | MG   | CA    | 1629 | 1/1   | 0.95 | 0.20 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3060 | 1/1   | 0.95 | 0.19 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3417 | 1/1   | 0.95 | 0.22 | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3122 | 1/1   | 0.95 | 0.17 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3112 | 1/1   | 0.95 | 0.32 | 42,42,42,42                 | 0     |
| 59  | MG   | AA    | 1769 | 1/1   | 0.95 | 0.12 | 71,71,71,71                 | 0     |
| 59  | MG   | DA    | 3125 | 1/1   | 0.95 | 0.15 | 43,43,43,43                 | 0     |
| 59  | MG   | DA    | 3219 | 1/1   | 0.95 | 0.17 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3041 | 1/1   | 0.95 | 0.17 | 24,24,24,24                 | 0     |
| 59  | MG   | AA    | 1733 | 1/1   | 0.95 | 0.11 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3222 | 1/1   | 0.95 | 0.25 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3128 | 1/1   | 0.95 | 0.13 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3289 | 1/1   | 0.95 | 0.17 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3290 | 1/1   | 0.95 | 0.30 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3214 | 1/1   | 0.95 | 0.21 | 59,59,59,59                 | 0     |
| 59  | MG   | BA    | 3089 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3005 | 1/1   | 0.95 | 0.10 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3065 | 1/1   | 0.95 | 0.15 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3051 | 1/1   | 0.95 | 0.24 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3349 | 1/1   | 0.95 | 0.44 | 39,39,39,39                 | 1     |
| 59  | MG   | DA    | 3137 | 1/1   | 0.95 | 0.36 | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3353 | 1/1   | 0.95 | 0.14 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3181 | 1/1   | 0.95 | 0.19 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3054 | 1/1   | 0.95 | 0.16 | 18,18,18,18                 | 0     |
| 59  | MG   | DA    | 3237 | 1/1   | 0.95 | 0.16 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3120 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3121 | 1/1   | 0.95 | 0.14 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3359 | 1/1   | 0.95 | 0.06 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3142 | 1/1   | 0.95 | 0.24 | 30,30,30,30                 | 0     |
| 59  | MG   | CA    | 1749 | 1/1   | 0.95 | 0.11 | 60,60,60,60                 | 0     |
| 59  | MG   | DA    | 3062 | 1/1   | 0.95 | 0.28 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3122 | 1/1   | 0.95 | 0.14 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3023 | 1/1   | 0.95 | 0.18 | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1699 | 1/1   | 0.95 | 0.05 | 105,105,105,105             | 0     |
| 59  | MG   | DA    | 3148 | 1/1   | 0.95 | 0.23 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3125 | 1/1   | 0.95 | 0.06 | 65,65,65,65                 | 0     |
| 59  | MG   | AA    | 1715 | 1/1   | 0.95 | 0.17 | 52,52,52,52                 | 0     |
| 59  | MG   | DA    | 3369 | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | DA    | 3371 | 1/1   | 0.95 | 0.28 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3151 | 1/1   | 0.95 | 0.26 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3265 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3390 | 1/1   | 0.95 | 0.16 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3226 | 1/1   | 0.95 | 0.09 | 57,57,57,57                 | 0     |
| 59  | MG   | DA    | 3376 | 1/1   | 0.95 | 0.17 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3075 | 1/1   | 0.95 | 0.07 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3440 | 1/1   | 0.95 | 0.25 | 54,54,54,54                 | 0     |
| 59  | MG   | CA    | 1654 | 1/1   | 0.95 | 0.24 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3159 | 1/1   | 0.95 | 0.05 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3261 | 1/1   | 0.95 | 0.28 | 50,50,50,50                 | 0     |
| 59  | MG   | CA    | 1604 | 1/1   | 0.95 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3009 | 1/1   | 0.95 | 0.05 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3268 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3128 | 1/1   | 0.95 | 0.29 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3348 | 1/1   | 0.95 | 0.09 | 63,63,63,63                 | 0     |
| 59  | MG   | DA    | 3390 | 1/1   | 0.95 | 0.21 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3391 | 1/1   | 0.95 | 0.07 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3392 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3071 | 1/1   | 0.95 | 0.24 | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3272 | 1/1   | 0.95 | 0.17 | 57,57,57,57                 | 0     |
| 59  | MG   | BA    | 3449 | 1/1   | 0.95 | 0.23 | 46,46,46,46                 | 0     |
| 59  | MG   | AA    | 1728 | 1/1   | 0.95 | 0.15 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3131 | 1/1   | 0.95 | 0.25 | 55,55,55,55                 | 0     |
| 59  | MG   | DA    | 3276 | 1/1   | 0.95 | 0.22 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3452 | 1/1   | 0.95 | 0.18 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1755 | 1/1   | 0.95 | 0.17 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3173 | 1/1   | 0.95 | 0.11 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3275 | 1/1   | 0.95 | 0.16 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3179 | 1/1   | 0.95 | 0.21 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3455 | 1/1   | 0.95 | 0.08 | 59,59,59,59                 | 0     |
| 59  | MG   | DA    | 3284 | 1/1   | 0.95 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3097 | 1/1   | 0.95 | 0.29 | 19,19,19,19                 | 0     |
| 59  | MG   | DA    | 3009 | 1/1   | 0.95 | 0.12 | 29,29,29,29                 | 0     |
| 60  | EDS  | AA    | 1805 | 41/41 | 0.95 | 0.09 | 47,55,60,66                 | 0     |
| 59  | MG   | DA    | 3289 | 1/1   | 0.95 | 0.21 | 50,50,50,50                 | 0     |
| 59  | MG   | DA    | 3176 | 1/1   | 0.96 | 0.11 | 70,70,70,70                 | 0     |
| 59  | MG   | BA    | 3038 | 1/1   | 0.96 | 0.31 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3180 | 1/1   | 0.96 | 0.05 | 26,26,26,26                 | 0     |
| 59  | MG   | AA    | 1787 | 1/1   | 0.96 | 0.08 | 84,84,84,84                 | 0     |
| 59  | MG   | BA    | 3084 | 1/1   | 0.96 | 0.09 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3395 | 1/1   | 0.96 | 0.08 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3058 | 1/1   | 0.96 | 0.12 | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3257 | 1/1   | 0.96 | 0.14 | 21,21,21,21                 | 0     |
| 59  | MG   | DA    | 3059 | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 59  | MG   | B7    | 101  | 1/1   | 0.96 | 0.07 | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3361 | 1/1   | 0.96 | 0.14 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3211 | 1/1   | 0.96 | 0.11 | 44,44,44,44                 | 0     |
| 59  | MG   | AA    | 1689 | 1/1   | 0.96 | 0.15 | 53,53,53,53                 | 0     |
| 59  | MG   | AA    | 1639 | 1/1   | 0.96 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3266 | 1/1   | 0.96 | 0.22 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3267 | 1/1   | 0.96 | 0.26 | 53,53,53,53                 | 0     |
| 59  | MG   | CA    | 1786 | 1/1   | 0.96 | 0.32 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3241 | 1/1   | 0.96 | 0.28 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3242 | 1/1   | 0.96 | 0.19 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1662 | 1/1   | 0.96 | 0.39 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3136 | 1/1   | 0.96 | 0.17 | 51,51,51,51                 | 0     |
| 59  | MG   | AA    | 1799 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 59  | MG   | CA    | 1746 | 1/1   | 0.96 | 0.05 | 79,79,79,79                 | 0     |
| 59  | MG   | DA    | 3135 | 1/1   | 0.96 | 0.11 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3443 | 1/1   | 0.96 | 0.18 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3138 | 1/1   | 0.96 | 0.05 | 34,34,34,34                 | 0     |
| 59  | MG   | CA    | 1631 | 1/1   | 0.96 | 0.20 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3082 | 1/1   | 0.96 | 0.23 | 32,32,32,32                 | 0     |
| 59  | MG   | DA    | 3205 | 1/1   | 0.96 | 0.27 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3445 | 1/1   | 0.96 | 0.20 | 36,36,36,36                 | 0     |
| 59  | MG   | BU    | 201  | 1/1   | 0.96 | 0.07 | 74,74,74,74                 | 0     |
| 59  | MG   | DA    | 3021 | 1/1   | 0.96 | 0.22 | 25,25,25,25                 | 0     |
| 59  | MG   | AA    | 1732 | 1/1   | 0.96 | 0.29 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3370 | 1/1   | 0.96 | 0.26 | 37,37,37,37                 | 0     |
| 59  | MG   | CA    | 1713 | 1/1   | 0.96 | 0.04 | 61,61,61,61                 | 0     |
| 59  | MG   | DA    | 3024 | 1/1   | 0.96 | 0.18 | 19,19,19,19                 | 0     |
| 59  | MG   | AA    | 1607 | 1/1   | 0.96 | 0.21 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3250 | 1/1   | 0.96 | 0.25 | 30,30,30,30                 | 0     |
| 59  | MG   | DA    | 3214 | 1/1   | 0.96 | 0.38 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3215 | 1/1   | 0.96 | 0.31 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3016 | 1/1   | 0.96 | 0.23 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3032 | 1/1   | 0.96 | 0.33 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3033 | 1/1   | 0.96 | 0.13 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3096 | 1/1   | 0.96 | 0.13 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3034 | 1/1   | 0.96 | 0.20 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3053 | 1/1   | 0.96 | 0.11 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3154 | 1/1   | 0.96 | 0.09 | 54,54,54,54                 | 0     |
| 59  | MG   | BA    | 3146 | 1/1   | 0.96 | 0.11 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3054 | 1/1   | 0.96 | 0.16 | 16,16,16,16                 | 0     |
| 59  | MG   | DA    | 3305 | 1/1   | 0.96 | 0.05 | 62,62,62,62                 | 0     |
| 59  | MG   | DA    | 3388 | 1/1   | 0.96 | 0.14 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3037 | 1/1   | 0.96 | 0.28 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3038 | 1/1   | 0.96 | 0.05 | 41,41,41,41                 | 0     |
| 59  | MG   | DA    | 3159 | 1/1   | 0.96 | 0.28 | 41,41,41,41                 | 0     |
| 59  | MG   | CA    | 1764 | 1/1   | 0.96 | 0.23 | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1668 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3006 | 1/1   | 0.96 | 0.26 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1735 | 1/1   | 0.96 | 0.32 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3044 | 1/1   | 0.96 | 0.22 | 23,23,23,23                 | 0     |
| 59  | MG   | BA    | 3388 | 1/1   | 0.96 | 0.19 | 59,59,59,59                 | 0     |
| 59  | MG   | DB    | 208  | 1/1   | 0.96 | 0.30 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3424 | 1/1   | 0.96 | 0.14 | 52,52,52,52                 | 0     |
| 59  | MG   | BA    | 3103 | 1/1   | 0.96 | 0.18 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3262 | 1/1   | 0.96 | 0.22 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3323 | 1/1   | 0.96 | 0.17 | 43,43,43,43                 | 0     |
| 59  | MG   | DE    | 301  | 1/1   | 0.96 | 0.14 | 25,25,25,25                 | 0     |
| 59  | MG   | CA    | 1612 | 1/1   | 0.96 | 0.26 | 37,37,37,37                 | 0     |
| 59  | MG   | DF    | 302  | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3104 | 1/1   | 0.96 | 0.34 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3245 | 1/1   | 0.96 | 0.09 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3171 | 1/1   | 0.96 | 0.16 | 46,46,46,46                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1776 | 1/1   | 0.96 | 0.17 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3052 | 1/1   | 0.96 | 0.22 | 20,20,20,20                 | 0     |
| 59  | MG   | DA    | 3175 | 1/1   | 0.96 | 0.15 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3087 | 1/1   | 0.97 | 0.13 | 17,17,17,17                 | 0     |
| 59  | MG   | BA    | 3047 | 1/1   | 0.97 | 0.18 | 37,37,37,37                 | 0     |
| 59  | MG   | BU    | 204  | 1/1   | 0.97 | 0.06 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3297 | 1/1   | 0.97 | 0.03 | 66,66,66,66                 | 0     |
| 59  | MG   | BA    | 3401 | 1/1   | 0.97 | 0.16 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3150 | 1/1   | 0.97 | 0.30 | 37,37,37,37                 | 0     |
| 59  | MG   | DA    | 3093 | 1/1   | 0.97 | 0.05 | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3056 | 1/1   | 0.97 | 0.06 | 32,32,32,32                 | 0     |
| 59  | MG   | BA    | 3091 | 1/1   | 0.97 | 0.10 | 38,38,38,38                 | 0     |
| 59  | MG   | D5    | 101  | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3308 | 1/1   | 0.97 | 0.19 | 47,47,47,47                 | 0     |
| 59  | MG   | DA    | 3309 | 1/1   | 0.97 | 0.06 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3028 | 1/1   | 0.97 | 0.32 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3312 | 1/1   | 0.97 | 0.12 | 46,46,46,46                 | 0     |
| 59  | MG   | BA    | 3447 | 1/1   | 0.97 | 0.07 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3316 | 1/1   | 0.97 | 0.23 | 59,59,59,59                 | 0     |
| 59  | MG   | CA    | 1773 | 1/1   | 0.97 | 0.21 | 44,44,44,44                 | 0     |
| 59  | MG   | DA    | 3262 | 1/1   | 0.97 | 0.21 | 51,51,51,51                 | 0     |
| 59  | MG   | DA    | 3263 | 1/1   | 0.97 | 0.27 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3318 | 1/1   | 0.97 | 0.21 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3033 | 1/1   | 0.97 | 0.06 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3377 | 1/1   | 0.97 | 0.23 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3177 | 1/1   | 0.97 | 0.32 | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3240 | 1/1   | 0.97 | 0.11 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3078 | 1/1   | 0.97 | 0.33 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3104 | 1/1   | 0.97 | 0.07 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3067 | 1/1   | 0.97 | 0.20 | 26,26,26,26                 | 0     |
| 59  | MG   | CA    | 1628 | 1/1   | 0.97 | 0.07 | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3225 | 1/1   | 0.97 | 0.10 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3387 | 1/1   | 0.97 | 0.05 | 42,42,42,42                 | 0     |
| 59  | MG   | BA    | 3189 | 1/1   | 0.97 | 0.16 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3329 | 1/1   | 0.97 | 0.06 | 94,94,94,94                 | 0     |
| 59  | MG   | DA    | 3072 | 1/1   | 0.97 | 0.33 | 22,22,22,22                 | 0     |
| 59  | MG   | DA    | 3389 | 1/1   | 0.97 | 0.12 | 24,24,24,24                 | 0     |
| 59  | MG   | DA    | 3073 | 1/1   | 0.97 | 0.20 | 38,38,38,38                 | 0     |
| 59  | MG   | BA    | 3085 | 1/1   | 0.97 | 0.11 | 30,30,30,30                 | 0     |
| 59  | MG   | AA    | 1622 | 1/1   | 0.97 | 0.06 | 61,61,61,61                 | 0     |
| 59  | MG   | DB    | 201  | 1/1   | 0.97 | 0.08 | 65,65,65,65                 | 0     |
| 59  | MG   | DA    | 3076 | 1/1   | 0.97 | 0.11 | 29,29,29,29                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3018 | 1/1   | 0.97 | 0.21 | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3078 | 1/1   | 0.97 | 0.20 | 33,33,33,33                 | 0     |
| 59  | MG   | DA    | 3236 | 1/1   | 0.97 | 0.38 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3205 | 1/1   | 0.97 | 0.12 | 48,48,48,48                 | 0     |
| 59  | MG   | BF    | 301  | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3341 | 1/1   | 0.97 | 0.20 | 45,45,45,45                 | 0     |
| 59  | MG   | DA    | 3239 | 1/1   | 0.97 | 0.10 | 35,35,35,35                 | 0     |
| 59  | MG   | DA    | 3240 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 59  | MG   | DA    | 3288 | 1/1   | 0.97 | 0.15 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3045 | 1/1   | 0.97 | 0.30 | 38,38,38,38                 | 0     |
| 59  | MG   | DA    | 3346 | 1/1   | 0.97 | 0.19 | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3374 | 1/1   | 0.97 | 0.12 | 49,49,49,49                 | 0     |
| 59  | MG   | AA    | 1786 | 1/1   | 0.97 | 0.15 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3196 | 1/1   | 0.97 | 0.19 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3294 | 1/1   | 0.97 | 0.37 | 34,34,34,34                 | 0     |
| 59  | MG   | DA    | 3352 | 1/1   | 0.97 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3378 | 1/1   | 0.97 | 0.12 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3201 | 1/1   | 0.97 | 0.04 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3209 | 1/1   | 0.97 | 0.10 | 45,45,45,45                 | 0     |
| 59  | MG   | BA    | 3074 | 1/1   | 0.98 | 0.07 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3119 | 1/1   | 0.98 | 0.04 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3067 | 1/1   | 0.98 | 0.28 | 36,36,36,36                 | 0     |
| 59  | MG   | DA    | 3178 | 1/1   | 0.98 | 0.15 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3235 | 1/1   | 0.98 | 0.23 | 29,29,29,29                 | 0     |
| 59  | MG   | CA    | 1763 | 1/1   | 0.98 | 0.07 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3406 | 1/1   | 0.98 | 0.04 | 72,72,72,72                 | 0     |
| 59  | MG   | DA    | 3068 | 1/1   | 0.98 | 0.22 | 16,16,16,16                 | 0     |
| 59  | MG   | DA    | 3183 | 1/1   | 0.98 | 0.18 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3351 | 1/1   | 0.98 | 0.05 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3426 | 1/1   | 0.98 | 0.08 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3016 | 1/1   | 0.98 | 0.19 | 18,18,18,18                 | 0     |
| 59  | MG   | DA    | 3043 | 1/1   | 0.98 | 0.10 | 26,26,26,26                 | 0     |
| 59  | MG   | DA    | 3283 | 1/1   | 0.98 | 0.16 | 33,33,33,33                 | 0     |
| 59  | MG   | BA    | 3407 | 1/1   | 0.98 | 0.08 | 54,54,54,54                 | 0     |
| 59  | MG   | AA    | 1665 | 1/1   | 0.98 | 0.09 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3031 | 1/1   | 0.98 | 0.12 | 25,25,25,25                 | 0     |
| 59  | MG   | DA    | 3287 | 1/1   | 0.98 | 0.08 | 30,30,30,30                 | 0     |
| 59  | MG   | CA    | 1680 | 1/1   | 0.98 | 0.06 | 84,84,84,84                 | 0     |
| 59  | MG   | BA    | 3064 | 1/1   | 0.98 | 0.07 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3375 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1753 | 1/1   | 0.98 | 0.25 | 22,22,22,22                 | 0     |
| 59  | MG   | CA    | 1684 | 1/1   | 0.98 | 0.08 | 79,79,79,79                 | 0     |

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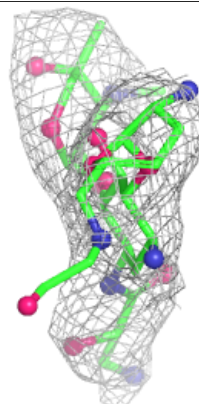
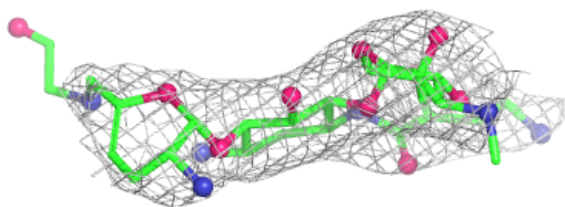
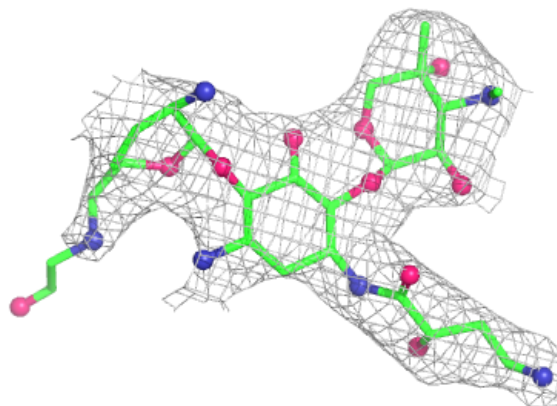
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1774 | 1/1   | 0.98 | 0.26 | 49,49,49,49                 | 0     |
| 59  | MG   | DA    | 3228 | 1/1   | 0.98 | 0.27 | 43,43,43,43                 | 0     |
| 59  | MG   | BA    | 3267 | 1/1   | 0.98 | 0.16 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3072 | 1/1   | 0.98 | 0.08 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3283 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 59  | MG   | DA    | 3334 | 1/1   | 0.98 | 0.11 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3106 | 1/1   | 0.98 | 0.06 | 62,62,62,62                 | 0     |
| 59  | MG   | BA    | 3193 | 1/1   | 0.98 | 0.23 | 37,37,37,37                 | 0     |
| 59  | MG   | BA    | 3026 | 1/1   | 0.98 | 0.19 | 19,19,19,19                 | 0     |
| 59  | MG   | BA    | 3318 | 1/1   | 0.98 | 0.06 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3172 | 1/1   | 0.98 | 0.17 | 48,48,48,48                 | 0     |
| 59  | MG   | DA    | 3060 | 1/1   | 0.98 | 0.30 | 24,24,24,24                 | 0     |
| 59  | MG   | BA    | 3117 | 1/1   | 0.98 | 0.15 | 26,26,26,26                 | 0     |
| 61  | ZN   | AD    | 302  | 1/1   | 0.98 | 0.16 | 64,64,64,64                 | 0     |
| 59  | MG   | DA    | 3217 | 1/1   | 0.99 | 0.05 | 40,40,40,40                 | 0     |
| 59  | MG   | BA    | 3075 | 1/1   | 0.99 | 0.13 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3309 | 1/1   | 0.99 | 0.33 | 31,31,31,31                 | 0     |
| 59  | MG   | DA    | 3292 | 1/1   | 0.99 | 0.08 | 21,21,21,21                 | 0     |
| 59  | MG   | BE    | 302  | 1/1   | 0.99 | 0.07 | 23,23,23,23                 | 0     |
| 59  | MG   | DA    | 3030 | 1/1   | 0.99 | 0.21 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3247 | 1/1   | 0.99 | 0.05 | 34,34,34,34                 | 0     |
| 59  | MG   | DA    | 3310 | 1/1   | 0.99 | 0.30 | 27,27,27,27                 | 0     |
| 61  | ZN   | AN    | 101  | 1/1   | 0.99 | 0.03 | 100,100,100,100             | 0     |
| 61  | ZN   | CD    | 301  | 1/1   | 0.99 | 0.21 | 68,68,68,68                 | 0     |
| 61  | ZN   | B9    | 101  | 1/1   | 1.00 | 0.02 | 91,91,91,91                 | 0     |
| 61  | ZN   | CN    | 101  | 1/1   | 1.00 | 0.02 | 77,77,77,77                 | 0     |
| 61  | ZN   | D9    | 101  | 1/1   | 1.00 | 0.02 | 75,75,75,75                 | 0     |

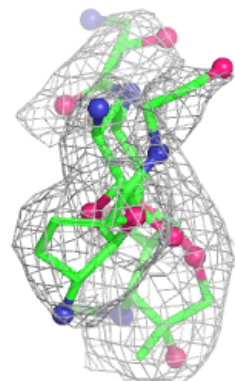
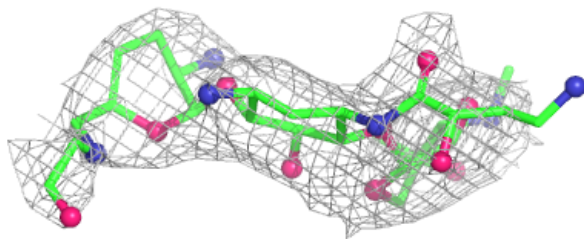
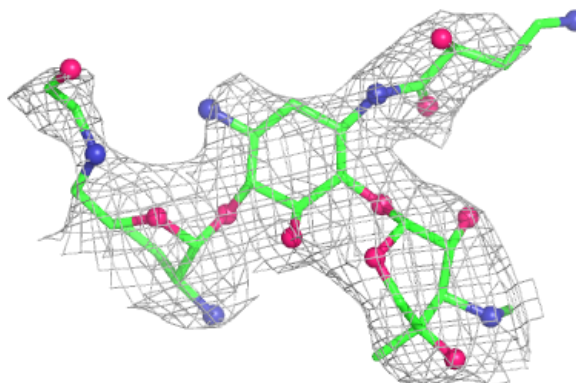
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around EDS CA 1787:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around EDS AA 1805:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.