



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:06 AM UTC

PDB ID : 4U25 / pdb\_00004u25  
Title : Crystal structure of the E. coli ribosome bound to virginiamycin M1.  
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.  
Deposited on : 2014-07-16  
Resolution : 2.90 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                                                             |

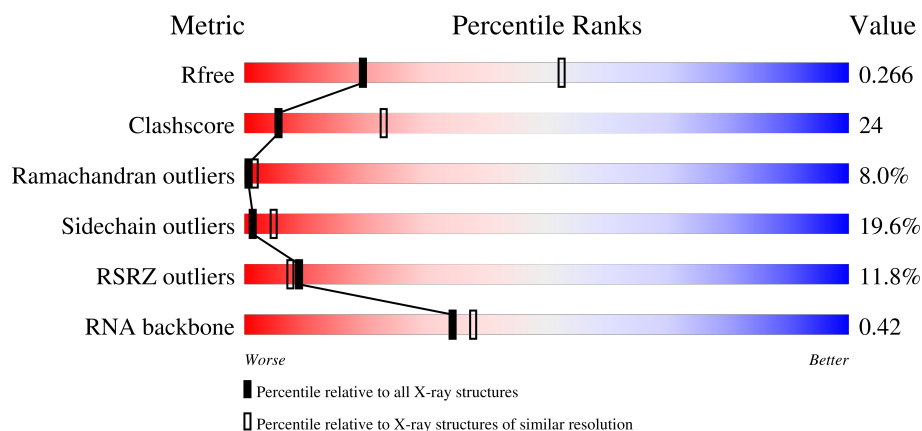
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |
| RNA backbone          | 3983                        | 1120 (3.10-2.70)                                      |

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    | 1539   | <div> <div>3%</div> <div>33% 52% 15%</div> </div>    |
| 1   | CA    | 1539   | <div> <div>6%</div> <div>33% 53% 13%</div> </div>    |
| 2   | AB    | 218    | <div> <div>9%</div> <div>19% 50% 24% 7%</div> </div> |
| 2   | CB    | 218    | <div> <div>21%</div> <div>26% 51% 20% .</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AC    | 206    |                  |
| 3   | CC    | 206    |                  |
| 4   | AD    | 205    |                  |
| 4   | CD    | 205    |                  |
| 5   | AE    | 150    |                  |
| 5   | CE    | 150    |                  |
| 6   | AF    | 100    |                  |
| 6   | CF    | 100    |                  |
| 7   | AG    | 151    |                  |
| 7   | CG    | 151    |                  |
| 8   | AH    | 129    |                  |
| 8   | CH    | 129    |                  |
| 9   | AI    | 127    |                  |
| 9   | CI    | 127    |                  |
| 10  | AJ    | 98     |                  |
| 10  | CJ    | 98     |                  |
| 11  | AK    | 117    |                  |
| 11  | CK    | 117    |                  |
| 12  | AL    | 123    |                  |
| 12  | CL    | 123    |                  |
| 13  | AM    | 114    |                  |
| 13  | CM    | 114    |                  |
| 14  | AN    | 100    |                  |
| 14  | CN    | 100    |                  |
| 15  | AO    | 88     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | CO    | 88     |                  |
| 16  | AP    | 82     |                  |
| 16  | CP    | 82     |                  |
| 17  | AQ    | 80     |                  |
| 17  | CQ    | 80     |                  |
| 18  | AR    | 55     |                  |
| 18  | CR    | 55     |                  |
| 19  | AS    | 79     |                  |
| 19  | CS    | 79     |                  |
| 20  | AT    | 85     |                  |
| 20  | CT    | 85     |                  |
| 21  | AU    | 51     |                  |
| 21  | CU    | 51     |                  |
| 22  | BA    | 2903   |                  |
| 22  | DA    | 2903   |                  |
| 23  | BB    | 119    |                  |
| 23  | DB    | 119    |                  |
| 24  | BC    | 271    |                  |
| 24  | DC    | 271    |                  |
| 25  | BD    | 209    |                  |
| 25  | DD    | 209    |                  |
| 26  | BE    | 201    |                  |
| 26  | DE    | 201    |                  |
| 27  | BF    | 177    |                  |
| 27  | DF    | 177    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BG    | 176    |                  |
| 28  | DG    | 176    |                  |
| 29  | BH    | 149    |                  |
| 29  | DH    | 149    |                  |
| 30  | BI    | 141    |                  |
| 30  | DI    | 141    |                  |
| 31  | BJ    | 142    |                  |
| 31  | DJ    | 142    |                  |
| 32  | BK    | 122    |                  |
| 32  | DK    | 122    |                  |
| 33  | BL    | 143    |                  |
| 33  | DL    | 143    |                  |
| 34  | BM    | 136    |                  |
| 34  | DM    | 136    |                  |
| 35  | BN    | 120    |                  |
| 35  | DN    | 120    |                  |
| 36  | BO    | 116    |                  |
| 36  | DO    | 116    |                  |
| 37  | BP    | 114    |                  |
| 37  | DP    | 114    |                  |
| 38  | BQ    | 117    |                  |
| 38  | DQ    | 117    |                  |
| 39  | BR    | 103    |                  |
| 39  | DR    | 103    |                  |
| 40  | BS    | 110    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | DS    | 110    |                  |
| 41  | BT    | 93     |                  |
| 41  | DT    | 93     |                  |
| 42  | BU    | 102    |                  |
| 42  | DU    | 102    |                  |
| 43  | BV    | 94     |                  |
| 43  | DV    | 94     |                  |
| 44  | BW    | 76     |                  |
| 44  | DW    | 76     |                  |
| 45  | BX    | 77     |                  |
| 45  | DX    | 77     |                  |
| 46  | BY    | 63     |                  |
| 46  | DY    | 63     |                  |
| 47  | BZ    | 58     |                  |
| 47  | DZ    | 58     |                  |
| 48  | B0    | 56     |                  |
| 48  | D0    | 56     |                  |
| 49  | B1    | 50     |                  |
| 49  | D1    | 50     |                  |
| 50  | B2    | 46     |                  |
| 50  | D2    | 46     |                  |
| 51  | B3    | 64     |                  |
| 51  | D3    | 64     |                  |
| 52  | B4    | 38     |                  |
| 52  | D4    | 38     |                  |

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| Mol | Chain | Length | Quality of chain               |
|-----|-------|--------|--------------------------------|
| 53  | B5    | 228    | <p>51%<br/>49% 23% 11% 16%</p> |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | AA    | 1659 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3027 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3062 | -         | -        | -       | X                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288258 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1538     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32995 | 14716 | 6050 | 10691 | 1538 |         |         |       |
| 1   | CA    | 1539     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 33015 | 14725 | 6052 | 10699 | 1539 |         |         |       |

- 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     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |         |       |
| 2   | CB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |         |       |

- 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     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |
| 3   | CC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 4   | CD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |

- 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     |
|     |       |          | 1106  | 687 | 211 | 202 | 6 |         |         |       |
| 5   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1106  | 687 | 211 | 202 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 818   | 515 | 148 | 149 | 6 |         |         |       |
| 6   | CF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 818   | 515 | 148 | 149 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |         |       |
| 7   | CG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |
| 8   | CH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

- 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     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |
| 11  | CK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |
| 12  | CL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |         |       |
| 13  | CM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |
| 14  | CN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |

- 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     |
|     |       |          | 710   | 437 | 143 | 129 | 1 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 710   | 437 | 143 | 129 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |
| 16  | CP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |         |       |
| 17  | CQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18  | AR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |         |         |       |
| 18  | CR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |         |       |
| 19  | CS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |
| 20  | CT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21  | AU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 426   | 265 | 86 | 74 | 1 |         |         |       |
| 21  | CU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 426   | 265 | 86 | 74 | 1 |         |         |       |

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22  | BA    | 2897     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62195 | 27745 | 11446 | 20107 | 2897 |         |         |       |
| 22  | DA    | 2897     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62195 | 27745 | 11446 | 20107 | 2897 |         |         |       |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23  | BB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2549  | 1135 | 466 | 829 | 119 |         |         |       |
| 23  | DB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2529  | 1126 | 464 | 821 | 118 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | BC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |         |       |
| 24  | DC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |
| 25  | DD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |         |       |
| 27  | DF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 28  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |
| 29  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |
| 30  | DI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |
| 31  | DJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |         |       |
| 32  | DK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |
| 33  | DL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |
| 34  | DM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |         |       |
| 35  | DN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36  | BO    | 116      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |         |       |
| 36  | DO    | 116      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 37  | DP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BQ    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |         |       |
| 38  | DQ    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |
| 39  | DR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |
| 40  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |
| 41  | DT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |   |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | DU    | 102      | Total | C   | N   | O   |         |         |       |
|     |       |          | 780   | 492 | 146 | 142 | 0       | 0       | 0     |

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43  | BV    | 94       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 753   | 479 | 137 | 134 | 3       | 0       | 0     |
| 43  | DV    | 94       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 753   | 479 | 137 | 134 | 3       | 0       | 0     |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44  | BW    | 76       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 580   | 359 | 117 | 103 | 1       | 0       | 0     |
| 44  | DW    | 75       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 569   | 353 | 113 | 102 | 1       | 0       | 0     |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 45  | BX    | 77       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 625   | 388 | 129 | 106 | 2       | 0       | 0     |
| 45  | DX    | 77       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 625   | 388 | 129 | 106 | 2       | 0       | 0     |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 46  | BY    | 63       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 509   | 313 | 99 | 95 | 2       | 0       | 0     |
| 46  | DY    | 63       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 509   | 313 | 99 | 95 | 2       | 0       | 0     |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 47  | BZ    | 58       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 449   | 281 | 87 | 79 | 2       | 0       | 0     |
| 47  | DZ    | 58       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 449   | 281 | 87 | 79 | 2       | 0       | 0     |



- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | B0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |
| 48  | D0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49  | B1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |         |       |
| 49  | D1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |
| 50  | D2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 51  | D3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |
| 52  | D4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

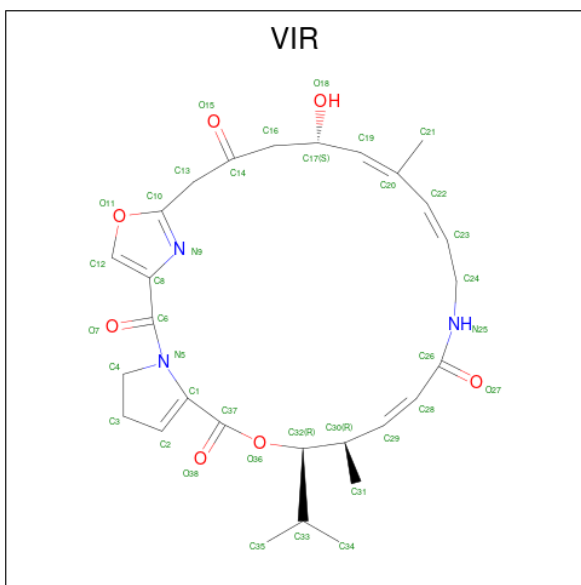
- Molecule 53 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 53  | B5    | 191      | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 1142  | 691 | 221 | 230 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54  | AA    | 71       | Total | Mg  | 0       | 0       |
|     |       |          | 71    | 71  |         |         |
| 54  | AN    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | BA    | 193      | Total | Mg  | 0       | 0       |
|     |       |          | 193   | 193 |         |         |
| 54  | BB    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | BD    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | BQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | CA    | 56       | Total | Mg  | 0       | 0       |
|     |       |          | 56    | 56  |         |         |
| 54  | DA    | 166      | Total | Mg  | 0       | 0       |
|     |       |          | 166   | 166 |         |         |
| 54  | DB    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 54  | DQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | D2    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 55 is VIRGINIAMYCIN M1 (CCD ID: VIR) (formula: C<sub>28</sub>H<sub>35</sub>N<sub>3</sub>O<sub>7</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 55  | BA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 38    | 28 | 3 | 7 |         |         |
| 55  | DA    | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 38    | 28 | 3 | 7 |         |         |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | D4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 57 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | AA    | 192      | Total | O   | 0       | 0       |
|     |       |          | 192   | 192 |         |         |
| 57  | AL    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 57  | AN    | 6        | Total | O   | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 57  | AT    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 57  | AU    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57  | BA    | 620      | Total<br>620 | O<br>620 | 0       | 0       |
| 57  | BB    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 57  | BC    | 7        | Total<br>7   | O<br>7   | 0       | 0       |
| 57  | BD    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 57  | BE    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | BF    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | BJ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | BL    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 57  | BN    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 57  | BQ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | BS    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | BT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | BV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | B2    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | B3    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | B4    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | CA    | 191      | Total<br>191 | O<br>191 | 0       | 0       |
| 57  | CL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | CN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | CT    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | CU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |

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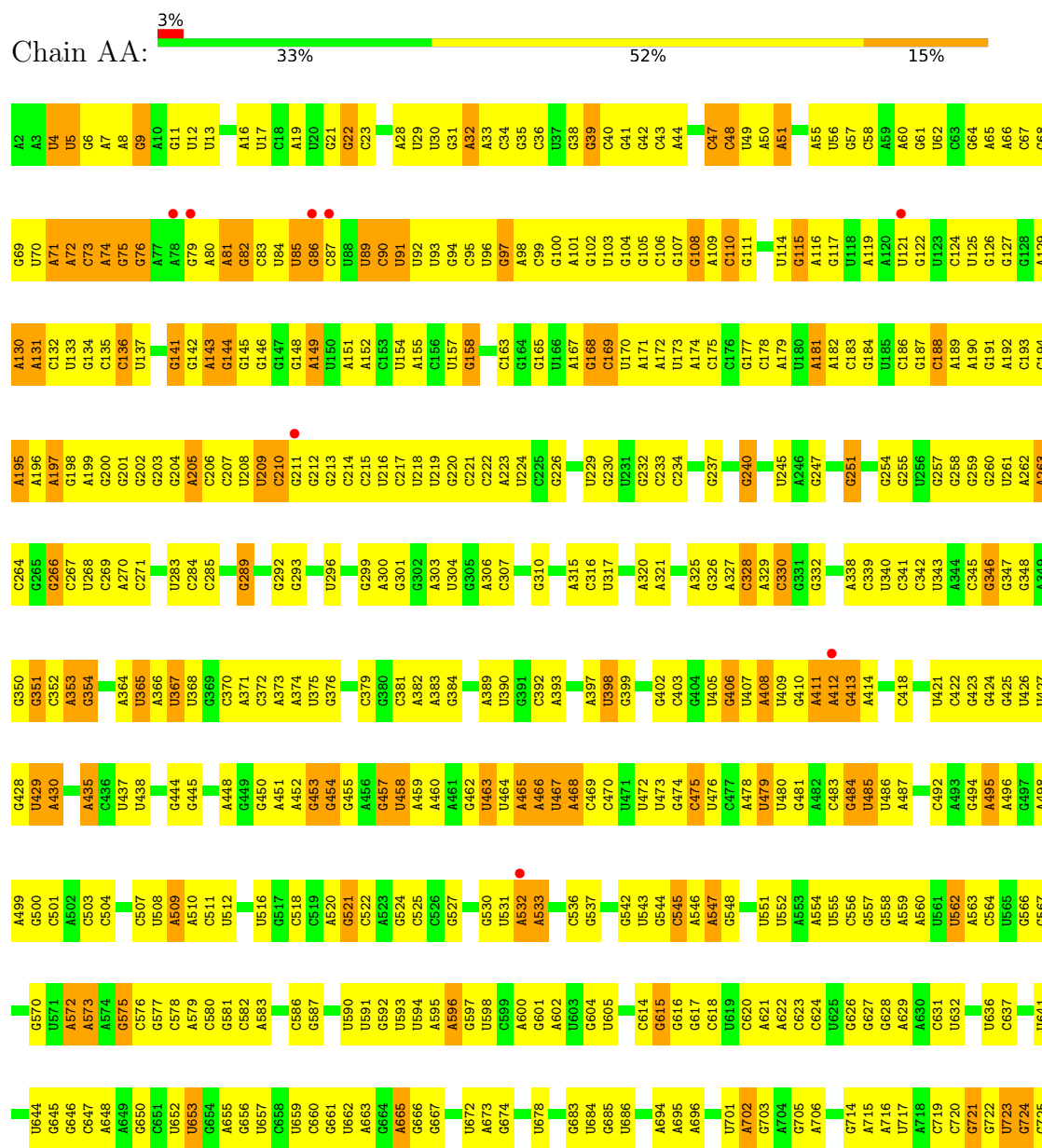
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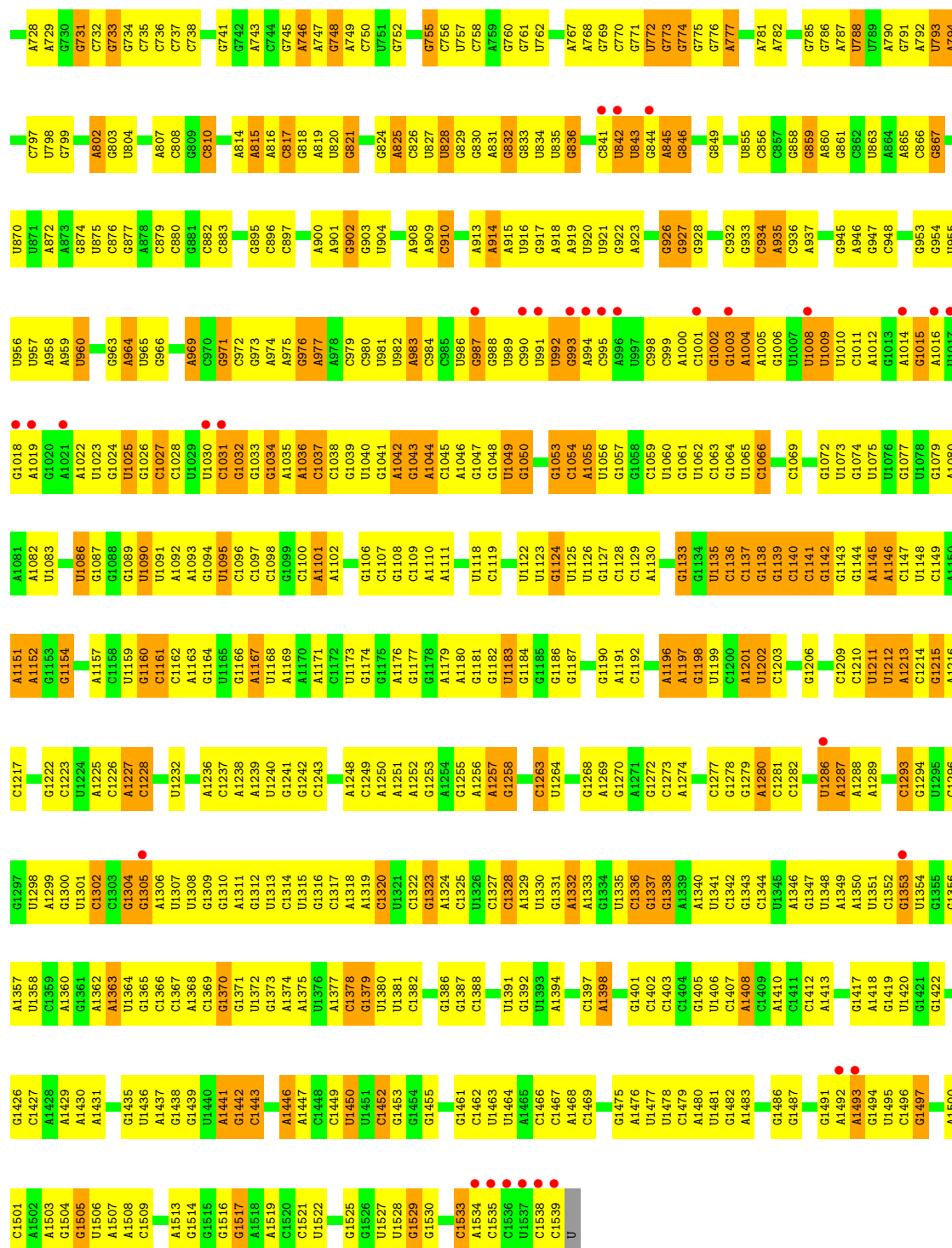
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57  | DA    | 607      | Total<br>607 | O<br>607 | 0       | 0       |
| 57  | DB    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 57  | DC    | 12       | Total<br>12  | O<br>12  | 0       | 0       |
| 57  | DD    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | DE    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 57  | DJ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DL    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | DN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | DT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | D2    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | D3    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | D4    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

### 3 Residue-property plots

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

#### • Molecule 1: 16S rRNA

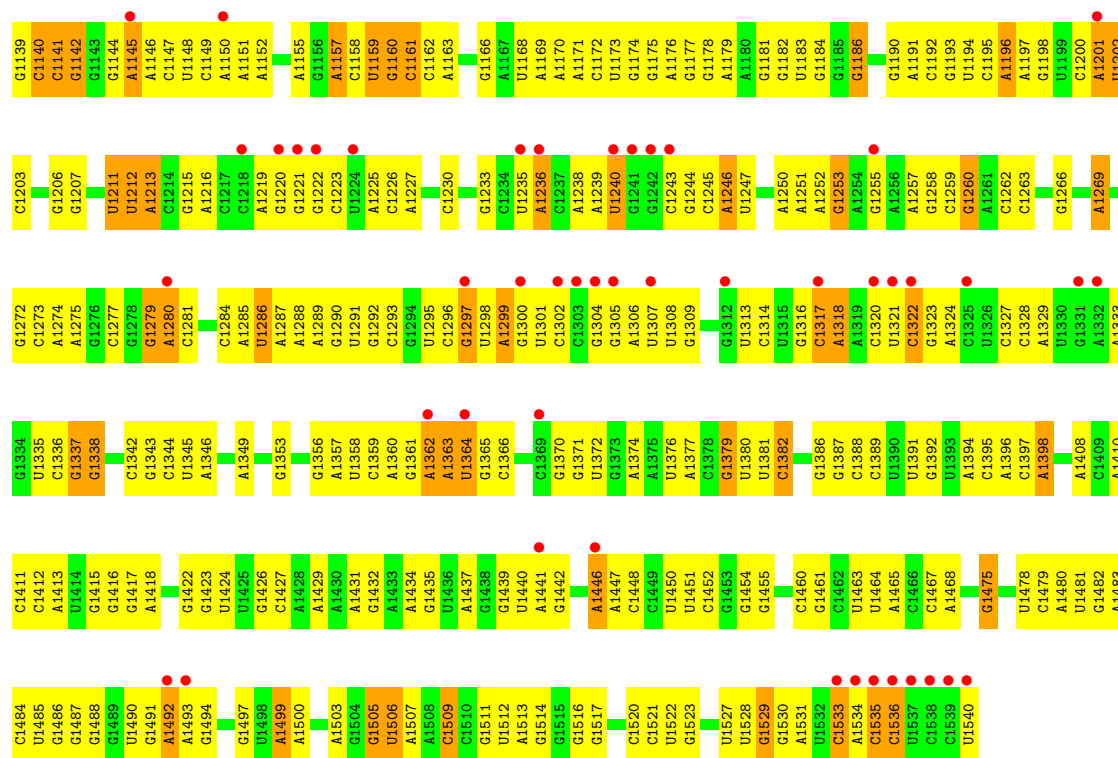




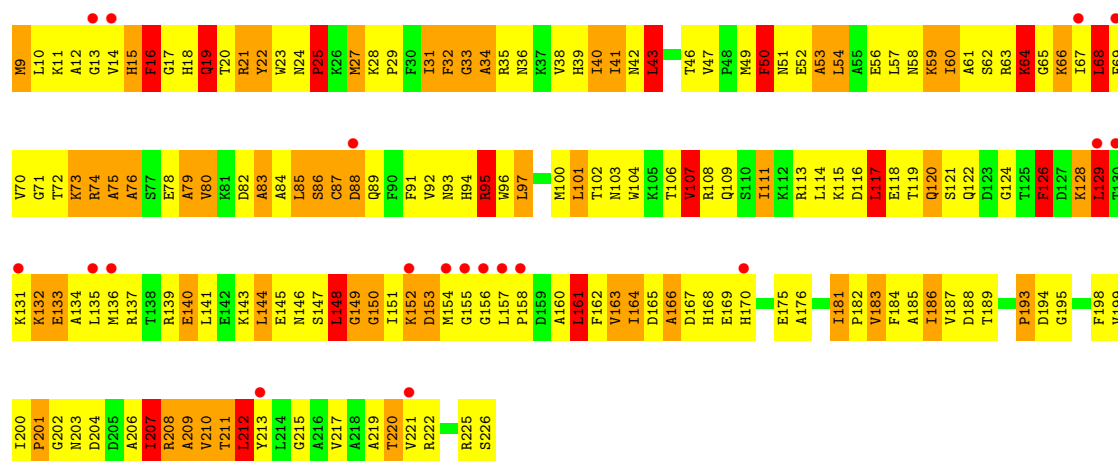
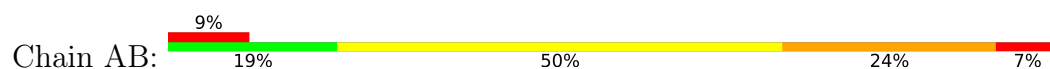
Chain CA:



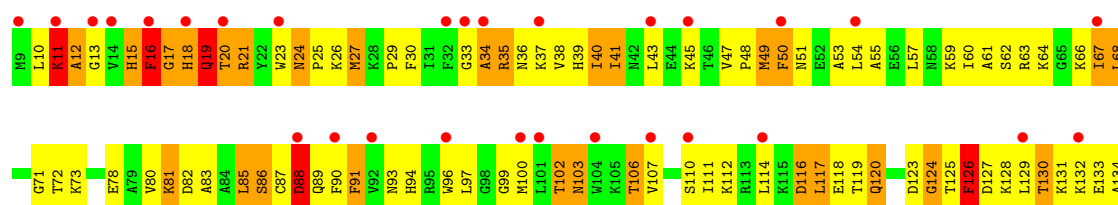


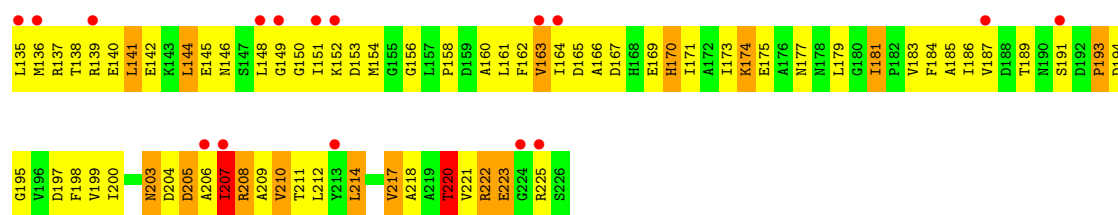


• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

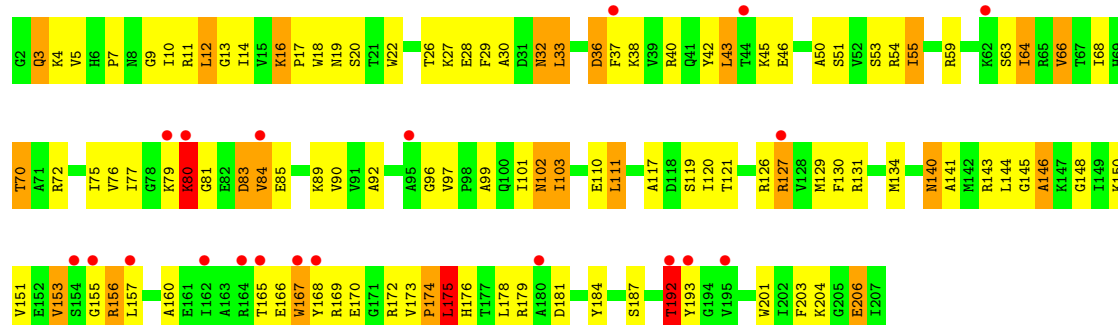




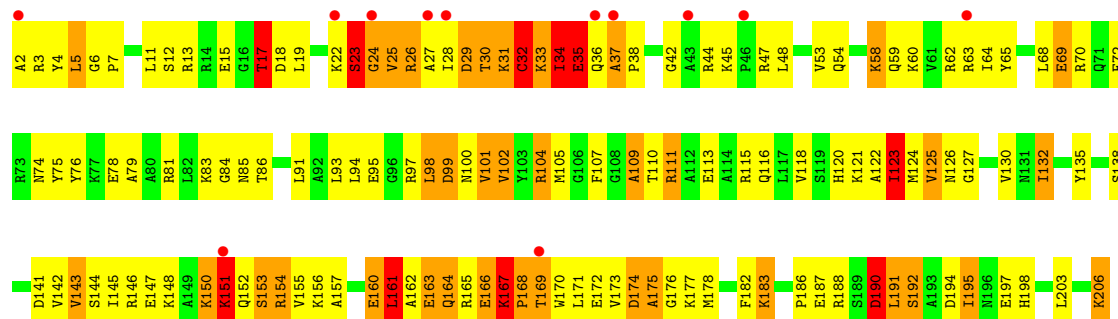
• Molecule 3: 30S ribosomal protein S3



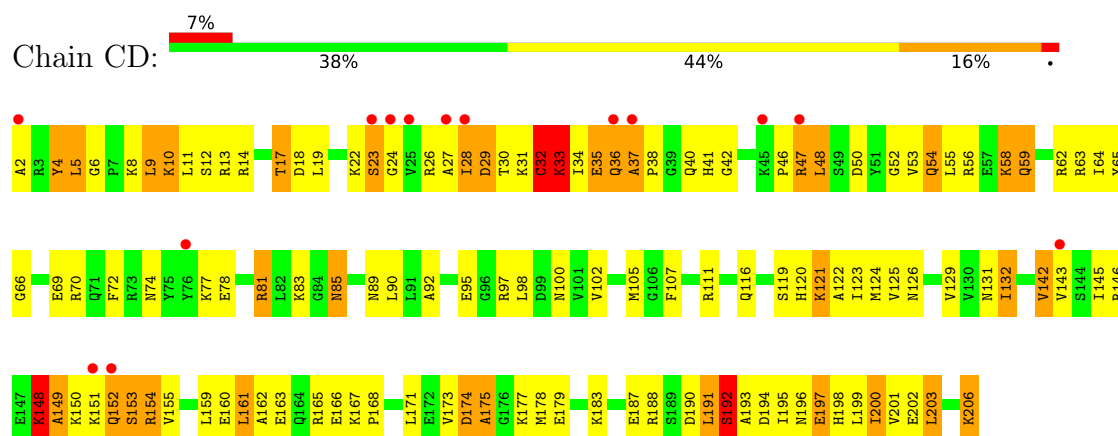
• Molecule 3: 30S ribosomal protein S3



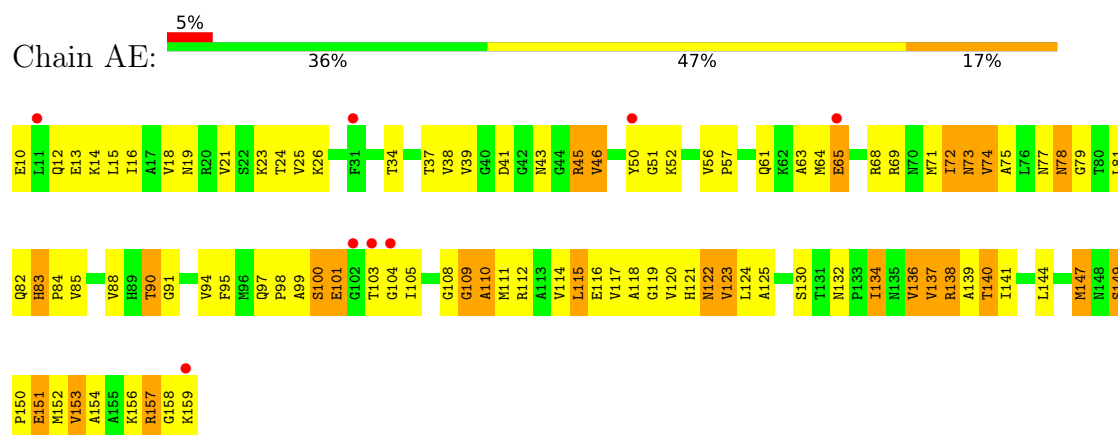
• Molecule 4: 30S ribosomal protein S4



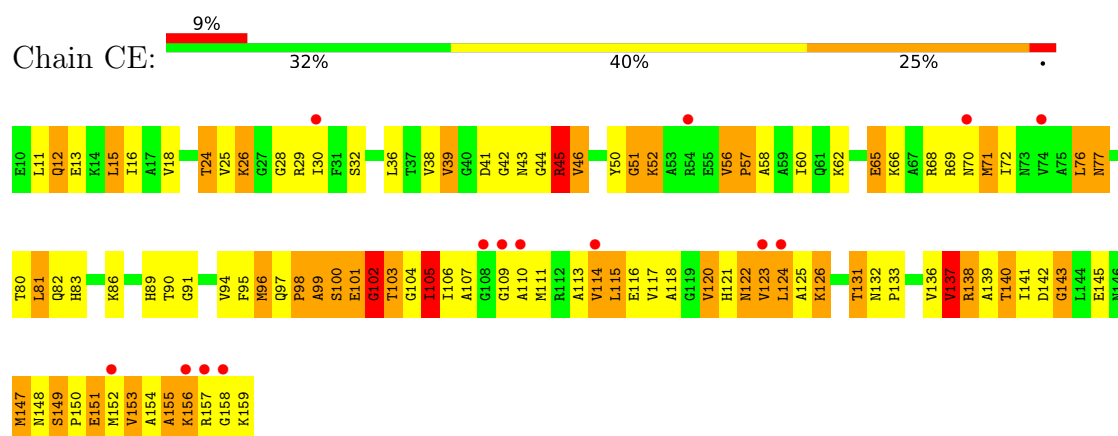
- Molecule 4: 30S ribosomal protein S4



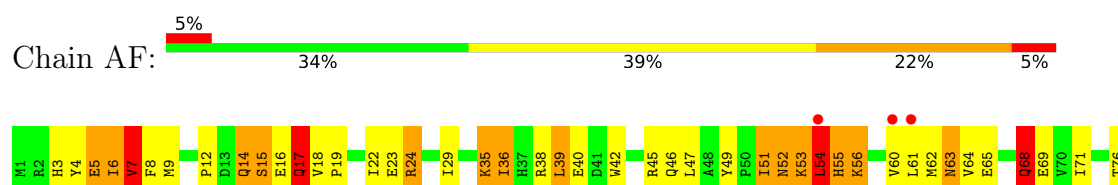
- Molecule 5: 30S ribosomal protein S5

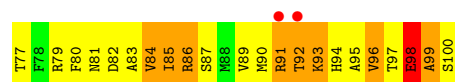


- Molecule 5: 30S ribosomal protein S5

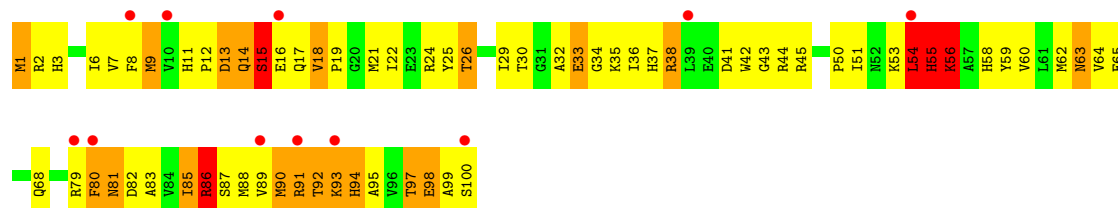


- Molecule 6: 30S ribosomal protein S6

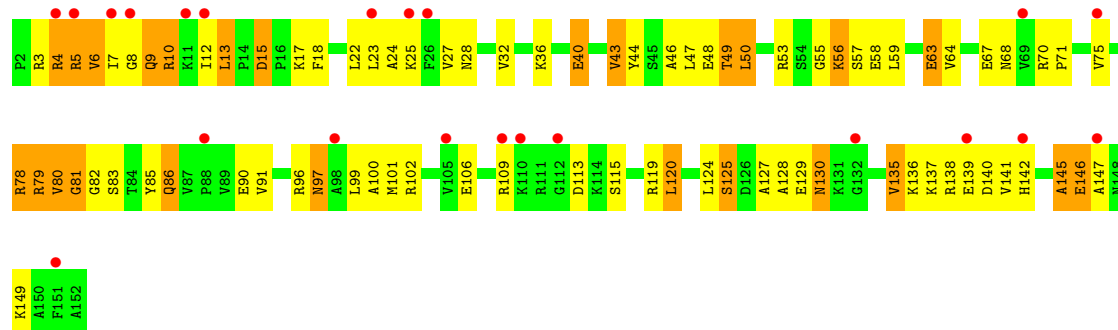




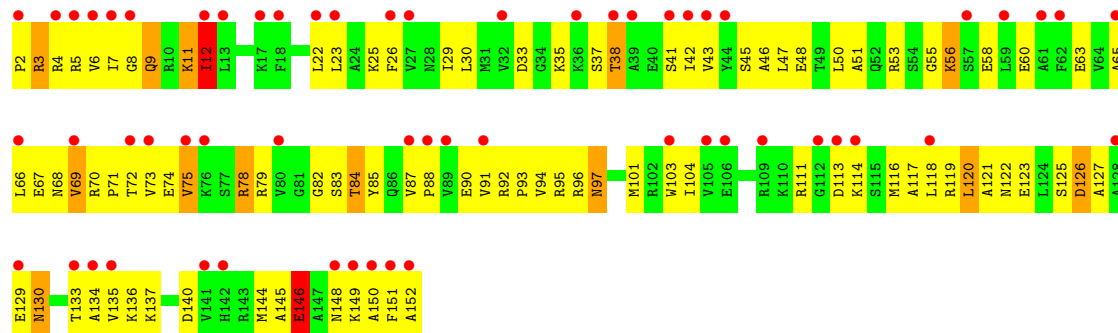
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

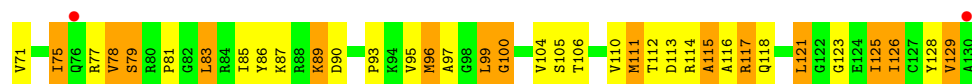


- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

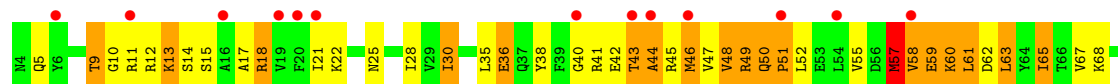




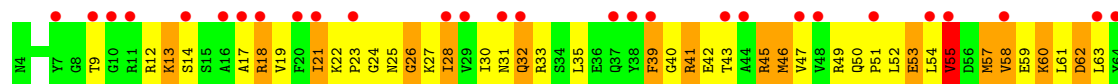
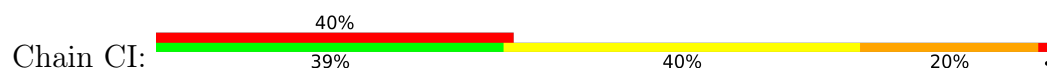
• Molecule 8: 30S ribosomal protein S8



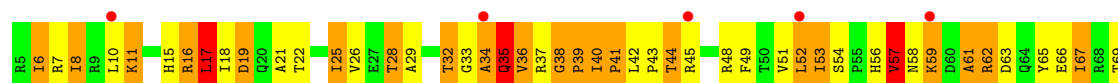
• Molecule 9: 30S ribosomal protein S9



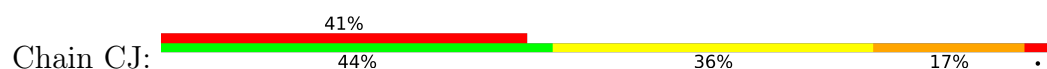
• Molecule 9: 30S ribosomal protein S9

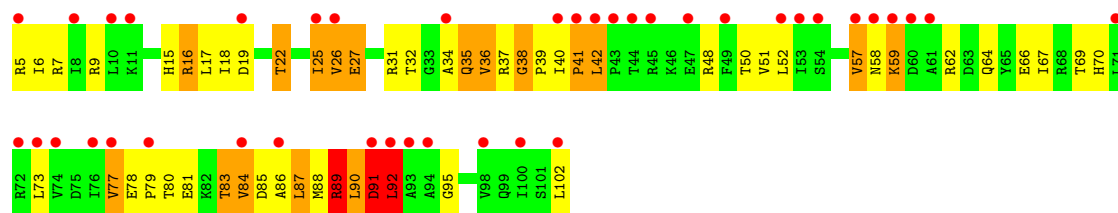


• Molecule 10: 30S ribosomal protein S10

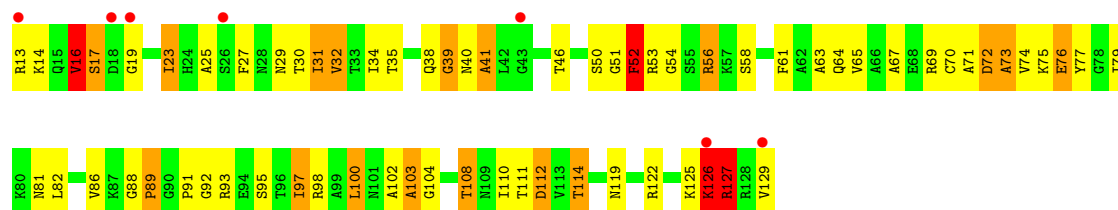
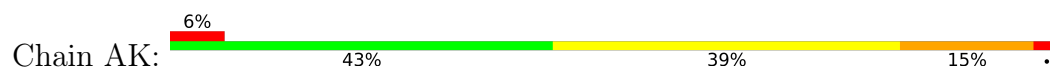


• Molecule 10: 30S ribosomal protein S10

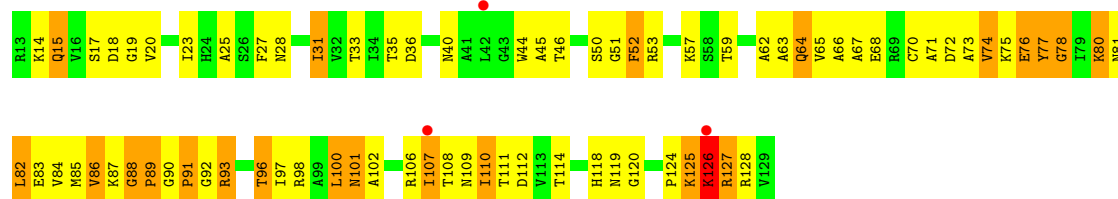




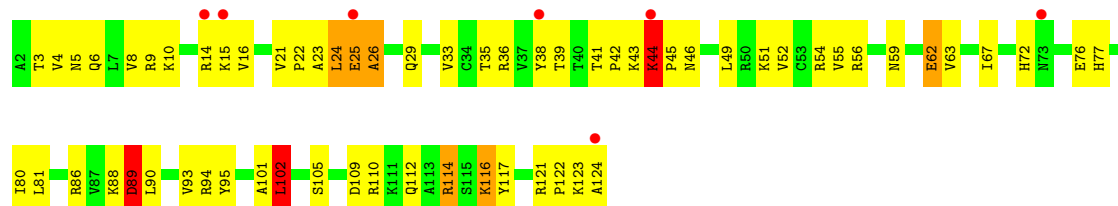
• Molecule 11: 30S ribosomal protein S11



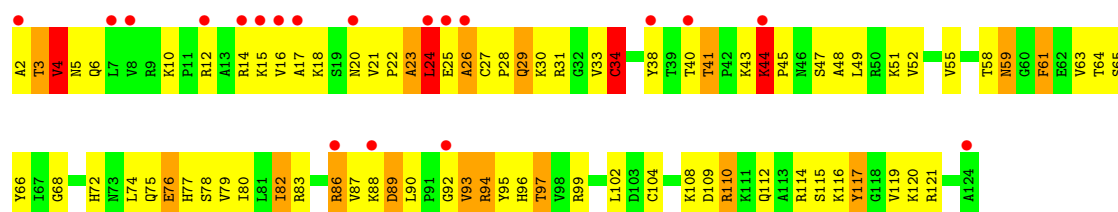
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



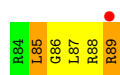
• Molecule 12: 30S ribosomal protein S12



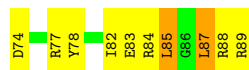
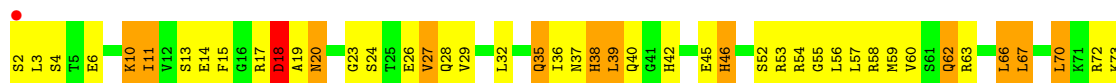
Chain AO:

| Category | Percentage |
|----------|------------|
| Red      | 6%         |
| Green    | 48%        |
| Yellow   | 39%        |
| Orange   | 14%        |

Below the chart, a list of 32 items (S2 to T82) is shown, each with a small colored square indicating its status. The colors correspond to the categories in the chart above: Red (S2, T22, T25, T31, T32, T38, T40, T41, T42, T43, T44, T45, T46, T47, T48, T49, T50, T51, T52, T53, T54, T55, T56, T57, T58, T59, T60, T61, T62, T63, T64, T65, T66, T67, T68, T69, T70, T71, T72, T73, T74, T75, T76, T77, T78, T79, T80, T81, T82).



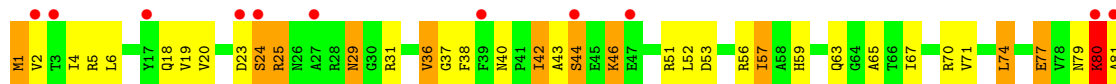
- Molecule 15: 30S ribosomal protein S15



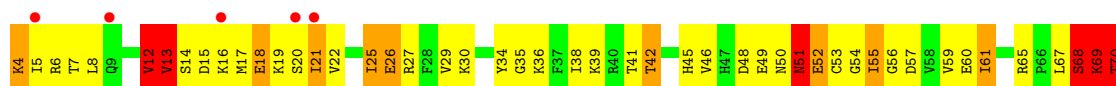
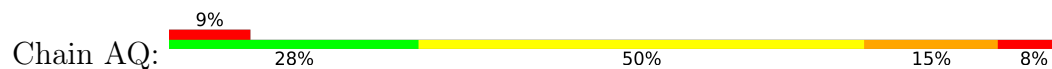
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



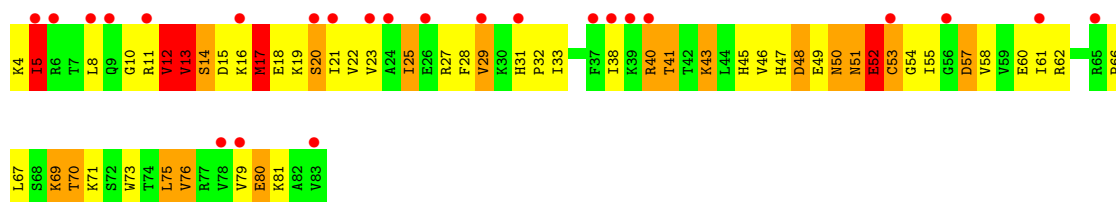
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17







• Molecule 18: 30S ribosomal protein S18



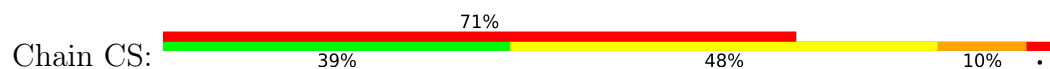
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S19

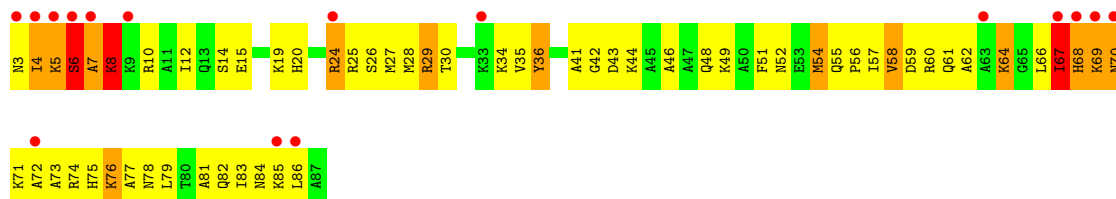


• Molecule 20: 30S ribosomal protein S20

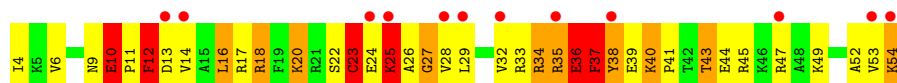




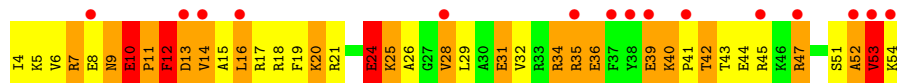
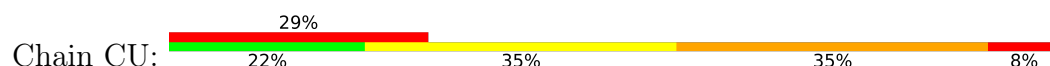
- Molecule 20: 30S ribosomal protein S20



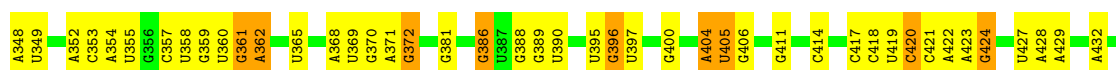
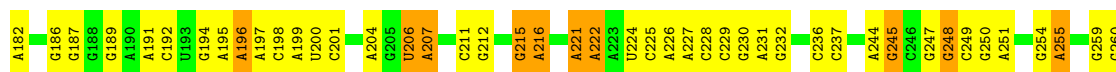
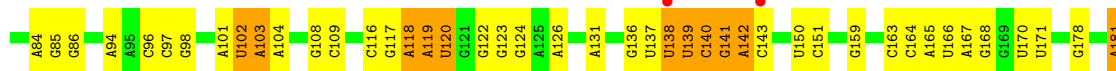
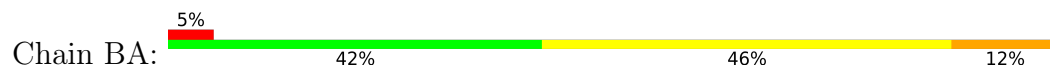
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA

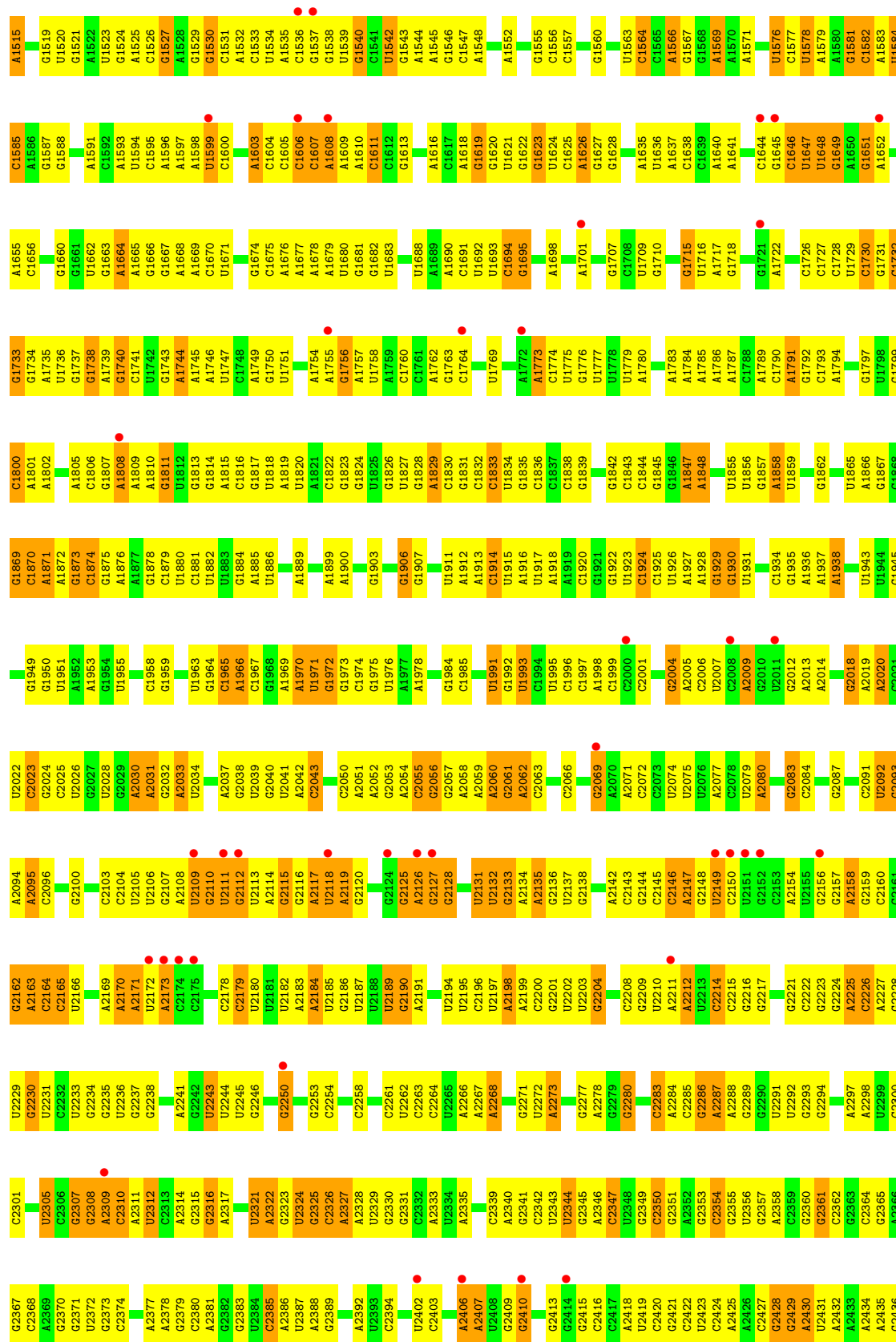


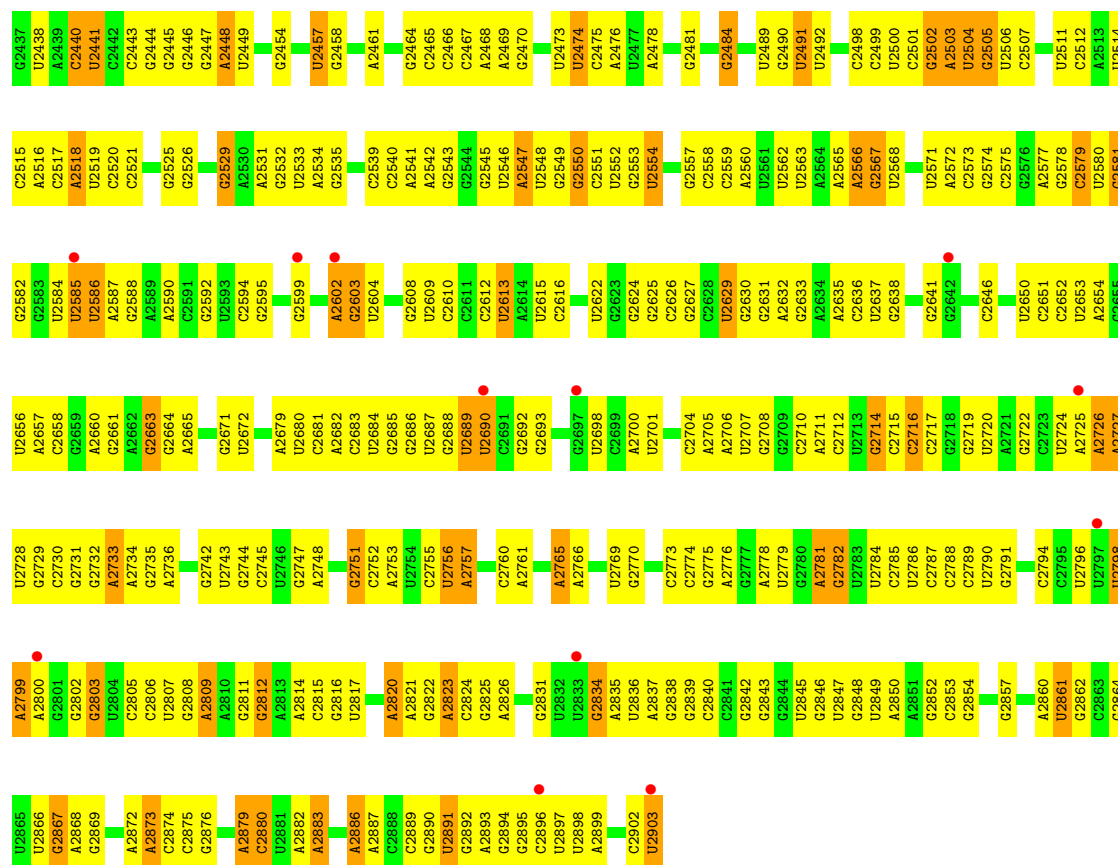
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| C1417 | G1343 | A1265 | C1178 | A1111 | G1051 | C968  | C    | C    | C    | U811 | C731 | G636 | U569 | C435 |
| G1418 | U1344 | G1266 | G1179 | G1112 | C1052 | A972  | C    | C    | C812 | C732 | A637 | A637 | U569 | C436 |
| A1419 | C1345 | U1267 | U1180 | U1113 | C1053 | A973  | G    | G    | U813 | G733 | G538 | G538 | U571 | U441 |
| A1420 | C1351 | A1268 | U1181 | C1114 | A1054 | A974  | C    | C    | C814 | A734 | A644 | A644 | U572 | A442 |
| G1421 | U1352 | A1269 | G1182 | G1115 | G1055 | A975  | C893 | C893 | C815 | A735 | C645 | C645 | U573 | A443 |
| G1423 | U1352 | C1270 | U1183 | G1116 | G1056 | G976  | C894 | C894 | C816 | A736 | U646 | U646 | A574 | C444 |
|       | A1353 | G1271 | U1184 | C1121 | A1057 | G977  | U895 | U895 | C817 | A737 | G647 | G647 | A575 | C445 |
| G1426 | A1354 | A1272 | G1185 | G1122 | U1058 | G977  | A896 | A896 | C818 | A738 | G648 | G648 | U576 | G446 |
| A1427 | G1355 | U1273 | G1186 | C1121 | U1059 | G978  | A897 | A897 | C819 | A739 | G649 | G649 | U577 | C447 |
| C1428 | C1356 | A1274 | U1187 | G1123 | U1060 | A979  | C898 | C898 | A820 | C740 | G651 | G651 | U578 | U448 |
| G1429 | C1357 | A1275 | U1188 | C1124 | U1061 | A980  | C899 | C899 | A821 | C741 | U652 | U652 | U579 | A449 |
| A1430 | G1358 | A1276 | G1189 | G1125 | G1062 | C981  | A900 | A900 | U653 | U744 | U653 | U653 | A513 | C450 |
| G1430 | A1359 | G1277 | G1190 | G1126 | G1063 | C982  | A901 | A901 | U654 | U745 | U654 | U654 | A514 | U451 |
| A1431 | G1360 | G1277 | G1191 | A1127 | C1064 | A983  | A902 | A902 | U655 | U746 | A655 | A655 | A515 | G452 |
| G1432 | G1361 | G1280 | C1196 | G1128 | U1065 | C984  | A903 | A903 | U656 | U747 | G656 | G656 | C517 | A453 |
| A1433 | C1362 | G1187 | G1197 | G1131 | U1066 | C985  | A904 | A904 | U657 | U748 | G657 | G657 | C518 | A454 |
| G1434 | G1363 | A1198 | U1198 | U1132 | A1067 | C986  | C908 | C908 | U658 | U749 | U658 | U658 | C519 | C455 |
| G1435 | G1364 | G1364 | U1199 | A1133 | G1068 | G989  | C909 | C909 | U659 | A753 | A661 | A661 | C520 | C456 |
| G1436 | A1365 | A1285 | U1203 | A1134 | A1069 | C990  | A910 | A910 | U660 | U754 | G662 | G662 | C521 | A457 |
| A1439 | A1366 | A1286 | U1204 | A1135 | A1070 | C991  | A911 | A911 | U661 | U755 | A663 | A663 | C522 | U464 |
| U1440 | A1367 | A1287 | G1206 | C1135 | C1071 | C992  | A912 | A912 | U662 | U756 | A664 | A664 | C523 | A466 |
| G1441 | G1368 | G1288 | G1207 | G1136 | C1072 | A996  | C913 | C913 | U663 | A757 | A665 | A665 | C524 | U467 |
| U1442 | C1371 | C1293 | C1208 | G1137 | A1073 | G997  | U913 | U913 | U664 | C601 | A666 | A666 | C525 | A468 |
| U1443 | U1372 | U1294 | U1209 | G1138 | G1074 | C998  | C914 | C914 | U665 | C602 | A667 | A667 | C526 | C461 |
| G1444 | A1373 | C1295 | U1210 | C1140 | C1075 | U999  | C915 | C915 | U666 | C603 | A668 | A668 | C527 | U469 |
| G1445 | G1374 | G1223 | G1224 | U1141 | C1076 | A1000 | C916 | C916 | U667 | C604 | A669 | A669 | C528 | A477 |
| G1446 | U1375 | U1224 | U1224 | A1142 | U1078 | A1001 | C917 | C917 | U668 | C605 | A670 | A670 | C529 | A478 |
| C1447 | C1376 | G1225 | A1143 | A1143 | C1079 | C1007 | U918 | U918 | U669 | C606 | A671 | A671 | C530 | A479 |
| G1448 | C1377 | A1226 | G1226 | G1150 | A1080 | C1008 | U919 | U919 | U670 | C607 | A672 | A672 | C531 | A480 |
| G1449 | A1378 | G1227 | C1227 | C1145 | U1081 | A1009 | C921 | C921 | U671 | C608 | A673 | A673 | C532 | G481 |
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| U1458 | C1386 | G1311 | A1237 | C1152 | G1087 | U1015 | U933 | U933 | U677 | C614 | A679 | A679 | C538 | G489 |
| U1459 | A1387 | C1315 | G1238 | C1153 | A1088 | G1016 | U934 | U934 | U678 | C615 | A680 | A680 | C539 | C490 |
| U1460 | C1394 | U1316 | U1240 | G1154 | A1089 | A1020 | C935 | C935 | U679 | C616 | A681 | A681 | C540 | G491 |
| C1461 | A1395 | G1317 | A1241 | A1156 | G1091 | G1022 | C936 | C936 | U680 | C617 | A682 | A682 | C541 | A492 |
| U1467 | U1400 | G1324 | U1242 | G1157 | G1093 | U1023 | A941 | A941 | U681 | C618 | A683 | A683 | C542 | G493 |
| U1468 | G1401 | U1325 | C1243 | C1158 | U1094 | G1024 | A942 | A942 | U682 | C619 | A684 | A684 | C543 | G494 |
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| A1470 | A1403 | A1327 | G1245 | G1160 | U1096 | G1026 | C946 | C946 | U684 | C621 | A686 | A686 | C545 | C496 |
| U1474 | C1404 | A1328 | A1246 | C1161 | U1097 | A1027 | C947 | C947 | U685 | C622 | A687 | A687 | C546 | A497 |
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| A1477 | G1407 | G1334 | C1251 | A1168 | U1101 | A1032 | C957 | C957 | U688 | C625 | A690 | A690 | C549 | G500 |
| G1478 | U1408 | G1335 | G1252 | A1169 | C1102 | U1033 | U958 | U958 | U689 | C626 | A691 | A691 | C550 |      |
| U1482 | U1409 | C1336 | C1253 | C1170 | C1103 | G1041 | A959 | A959 | U690 | C627 | A692 | A692 | C551 |      |
| U1485 | G1410 | A1337 | A1254 | G1171 | C1104 | A960  | A960 | A960 | U691 | C628 | A693 | A693 | C552 |      |
| U1486 | U1411 | G1337 | U1255 | C1172 | U1105 | C961  | C961 | C961 | U692 | C629 | A694 | A694 | C553 |      |
| U1487 | U1412 | G1338 | U1256 | U1173 | G1106 | G962  | G880 | G880 | U693 | C630 | A695 | A695 | C554 |      |
| C1488 | A1413 | G1339 | G1256 | U1174 | G1107 | A1046 | G881 | G881 | U694 | C631 | A696 | A696 | C555 |      |
|       | U1414 | U1340 | U1263 | A1175 | U1108 | G1047 | C964 | C964 | U695 | C632 | A697 | A697 | C556 |      |
|       | U1415 | G1341 | U1264 | U1176 | C1109 | U1047 | C965 | C965 | U696 | C633 | A698 | A698 | C557 |      |
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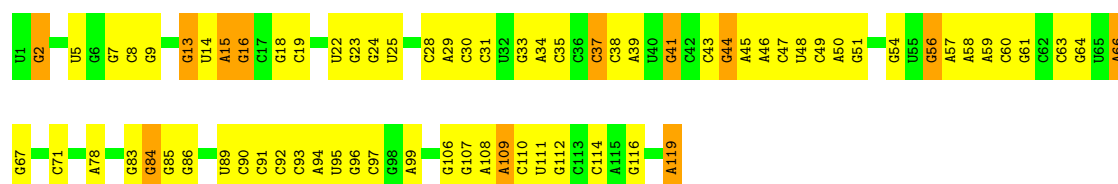
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|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|
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| G1444 | G1380 | U1258 | G1110 | C1049 | A975  | U906 | U842 | G778 | U703 | G636 | U571 |
| G1445 | G1381 | G1259 | A1111 | A1050 | G976  | G907 | U843 | G779 | G704 | A637 | A572 |
| G1446 | G1382 | A1196 | G1112 | G1051 | G977  | U908 | G943 | G780 | U705 | G638 | U573 |
| C1447 | A1383 | G1261 | G1115 | C1052 | G978  | A910 | A844 | G781 | G707 | U639 | A574 |
| C1448 | A1384 | A1262 | G1116 | C1053 | A979  | A911 | A845 | A782 | G708 | U640 | A575 |
| G1449 | U1263 | U1199 | G1117 | A1054 | A980  | C912 | U846 | A783 | U712 | C645 | U576 |
| G1450 | U1264 | C1200 | G1118 | G1055 | A981  | U913 | U847 | G784 | G712 | U646 | G577 |
| G1451 | A1265 | U1203 | G1119 | G1056 | C982  | G914 | C948 | G785 | U716 | U647 | G578 |
| A1452 | U1267 | A1204 | U1110 | A1057 | A983  | C915 | A849 | G786 | A717 | G648 | G579 |
| G1453 | U1268 | U1205 | G1121 | U1058 | A984  | G916 | U850 | C787 | C717 | U649 | U580 |
| C1454 | A1269 | A1206 | G1122 | G1059 | C985  | G917 | C951 | U788 | U720 | C650 | C581 |
| G1455 | U1270 | C1207 | U1060 | U1061 | A986  | A920 | G956 | A789 | U721 | G651 | A582 |
| A1456 | G1270 | G1208 | U1062 | A987  | G989  | C921 | G957 | U790 | A721 | A654 | G583 |
| A1393 | G1271 | U1209 | G1063 | A990  | A990  | C922 | G958 | C791 | U724 | A655 | C584 |
| A1394 | A1272 | A1126 | G1064 | A991  | G993  | G923 | G959 | A792 | U725 | G656 | G585 |
| A1395 | U1273 | A1127 | U1065 | C994  | G994  | U931 | U860 | A793 | G726 | U657 | A586 |
| U1396 | A1274 | G1128 | U1066 | C995  | C995  | U932 | A861 | A794 | G727 | U658 | C587 |
| U1397 | A1275 | G1129 | U1067 | C996  | C996  | U933 | C862 | C795 | A727 | U659 | U588 |
| C1398 | A1276 | U1131 | A1068 | A996  | A996  | A933 | A863 | C796 | G728 | C660 | U589 |
| G1463 | G1277 | U1132 | G1069 | A997  | C997  | U934 | G864 | G797 | G729 | A661 | A590 |
| G1464 | G1278 | A1133 | A1070 | C998  | C998  | U935 | C865 | G798 | A730 | U662 | U591 |
| U1466 | G1279 | G1134 | G1071 | G1002 | G1002 | C937 | A866 | G799 | C731 | G663 | A592 |
| G1469 | U1280 | C1135 | G1072 | G1003 | G1003 | C938 | C867 | G801 | C732 | G664 | U593 |
| A1403 | G1341 | G1136 | A1073 | G1004 | G1004 | G939 | U868 | A802 | A734 | U665 | U594 |
| A1404 | G1281 | U1218 | G1074 | C1006 | C1006 | G940 | G869 | A803 | A735 | A666 | C595 |
| U1405 | U1282 | U1219 | C1007 | C1007 | C1007 | A941 | U870 | A804 | C740 | U667 | A599 |
| U1406 | A1285 | G1220 | C1008 | C1008 | C1008 | A942 | U871 | G805 | C741 | A668 | G600 |
| G1407 | A1286 | G1221 | A1009 | A1009 | A1009 | G943 | G875 | C906 | U741 | C669 | C601 |
| G1408 | A1287 | U1222 | A1010 | A1010 | A1010 | C944 | C876 | U907 | A742 | A670 | A602 |
| U1409 | G1288 | U1223 | U1078 | G1011 | G1011 | C945 | C877 | G808 | A743 | C671 | A603 |
| G1410 | U1289 | U1224 | C1079 | C1012 | C1012 | C946 | A877 | U910 | U747 | C672 | G604 |
| U1411 | C1290 | G1225 | U1081 | U1012 | U1012 | C947 | G878 | U911 | G748 | C673 | G605 |
| U1412 | A1226 | U1226 | U1082 | C1013 | C1013 | C948 | G879 | C812 | A749 | C674 | U606 |
| G1482 | G1288 | A1230 | U1083 | U1019 | U1019 | G949 | G880 | U913 | A750 | A675 | U607 |
| G1483 | U1293 | U1231 | A1084 | A1020 | A1020 | G950 | C881 | C914 | A751 | A676 | A608 |
| U1484 | U1294 | G1232 | A1085 | A1021 | A1021 | C951 | G882 | C915 | A752 | A677 | A609 |
| G1417 | C1295 | C1233 | A1086 | C1022 | C1022 | G952 | G883 | C916 | U753 | C678 | C610 |
| G1418 | C1296 | G1236 | A1087 | G1025 | G1025 | G953 | U884 | C917 | U754 | C679 | A613 |
| U1487 | C1297 | A1237 | A1088 | U1026 | U1026 | G954 | C885 | G918 | G757 | C680 | A614 |
| C1488 | C1298 | G1238 | A1089 | A1027 | A1027 | U955 | A    | A819 | C758 | C681 | U615 |
| C1489 | G1299 | G1239 | A1090 | A1028 | A1028 | U956 | U    | A820 | U759 | U682 | A616 |
| A1490 | G1300 | U1240 | A1091 | A1029 | A1029 | G957 | C    | A821 | G760 | G683 | G617 |
| G1423 | A1301 | U1241 | C1092 | U1093 | U1093 | U958 | C    | G822 | A761 | U686 | G618 |
| G1424 | G1302 | U1242 | A1095 | A1032 | A1032 | U959 | C    | A825 | U764 | C687 | G619 |
| A1427 | G1303 | A1243 | A1096 | U1033 | U1033 | A960 | A826 | U826 | A765 | A621 | G622 |
| C1428 | A1304 | U1244 | U1097 | G1034 | G1034 | G962 | C    | U827 | C766 | G690 | A626 |
| G1430 | C1305 | U1245 | U1098 | U1035 | U1035 | U963 | U894 | U828 | U766 | A693 | A627 |
| A1431 | C1306 | A1246 | U1099 | G1036 | G1036 | C964 | U895 | A829 | G768 | U694 | G628 |
| G1432 | A1307 | A1247 | U1181 | U1037 | U1037 | C965 | U896 | G830 | U769 | G695 | G629 |
| A1433 | G1308 | G1248 | U1182 | U1038 | U1038 | U966 | C997 | G833 | G770 | G696 | G630 |
| A1434 | G1309 | U1249 | U1183 | G1039 | G1039 | G967 | A900 | C834 | C771 | U697 | A631 |
| G1435 | C1310 | G1250 | U1184 | C1100 | C1100 | U968 | C901 | C835 | C772 | G698 | A632 |
| G1436 | U1371 | U1251 | U1185 | U1101 | U1101 | C969 | C902 | G836 | G775 | A699 | A633 |
| G1437 | U1372 | C1252 | G1186 | C1102 | C1102 | U970 | C903 | G837 | G776 | G701 | G634 |
| A1438 | U1313 | G1253 | G1187 | C1103 | C1103 | G971 | C904 | A972 |      |      |      |
| A1439 | C1314 | A1254 | G1188 | G1104 | G1104 | A972 | C905 | A972 |      |      |      |
| U1509 | U1375 | U1255 | A1189 | C1105 | C1105 | A973 | G906 | A973 |      |      |      |
| G1501 | C1376 | G1256 | A1190 | U1108 | U1108 |      | G907 |      |      |      |      |
| A1504 | U1377 |       | G1190 |       |       |      | G908 |      |      |      |      |
| G1500 | A1378 |       |       |       |       |      | G909 |      |      |      |      |
| G1501 |       |       |       |       |       |      | G910 |      |      |      |      |
| A1504 |       |       |       |       |       |      | G911 |      |      |      |      |
| A1509 |       |       |       |       |       |      | G912 |      |      |      |      |
| G1510 |       |       |       |       |       |      | G913 |      |      |      |      |
| G1511 |       |       |       |       |       |      | G914 |      |      |      |      |
| G1512 |       |       |       |       |       |      | G915 |      |      |      |      |
| U1513 |       |       |       |       |       |      | G916 |      |      |      |      |
| G1514 |       |       |       |       |       |      | G917 |      |      |      |      |





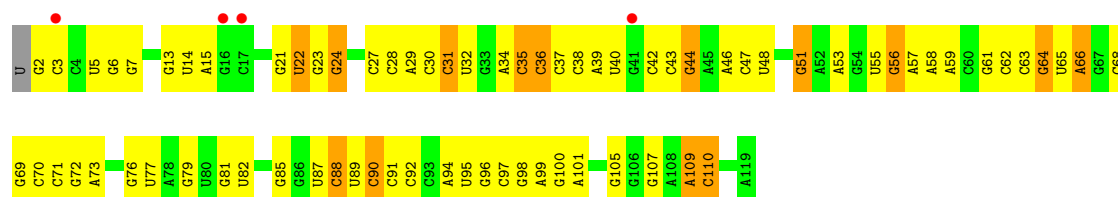
### • Molecule 23: 5S rRNA

Chain BB: 39% 50% 10%



### • Molecule 23: 5S rRNA

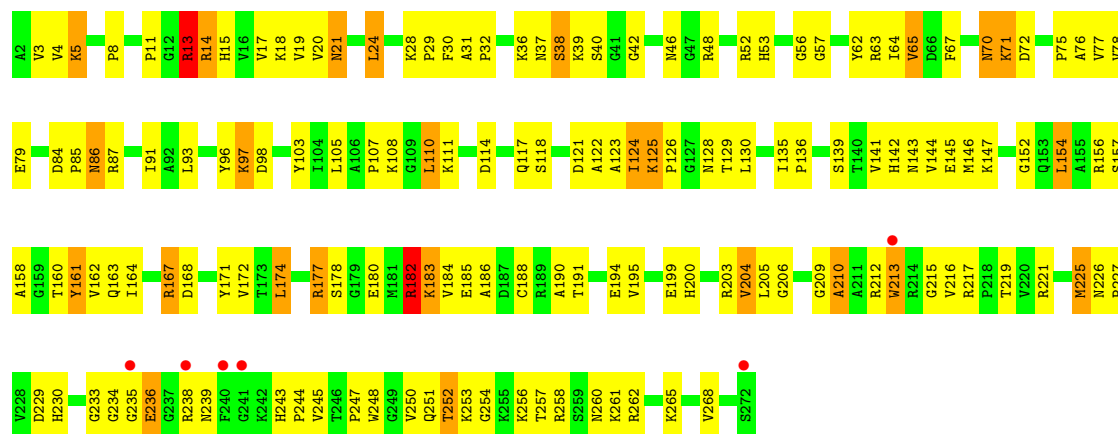
Chain DB: 37% 50% 12%



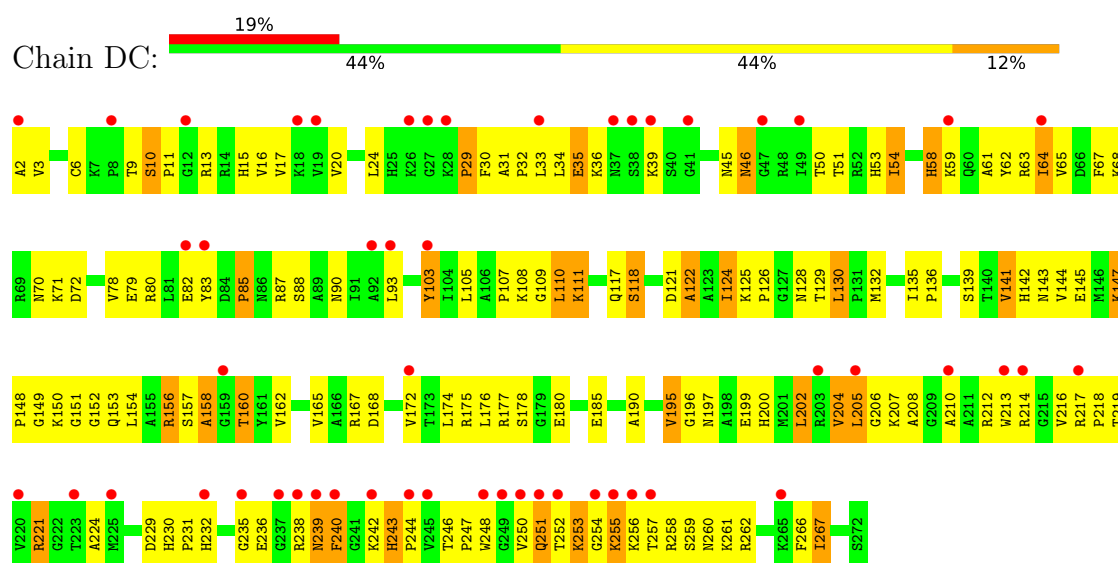
### • Molecule 24: 50S ribosomal protein L2

Chain BC: 44% 46% 9%

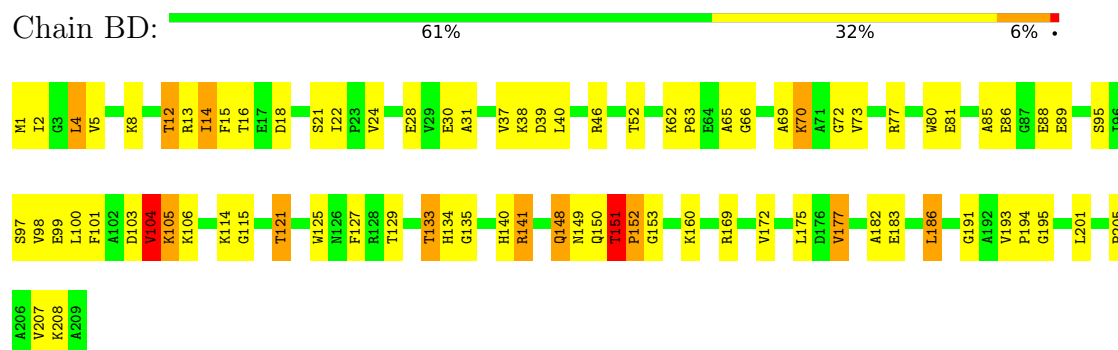




• Molecule 24: 50S ribosomal protein L2

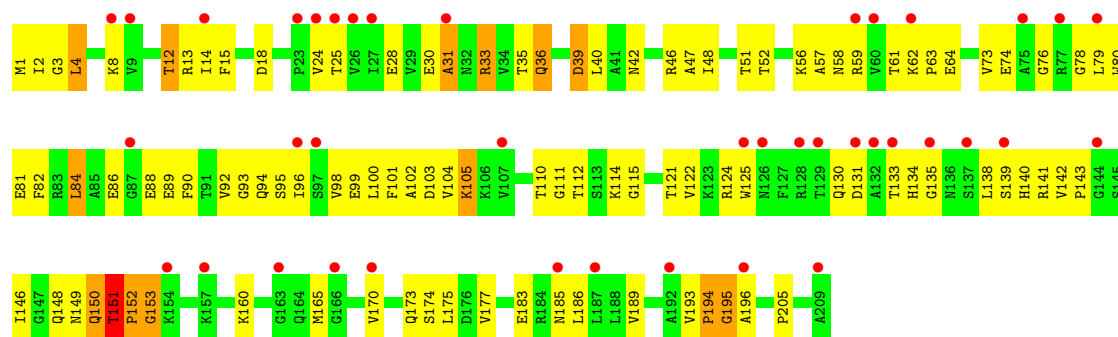


• Molecule 25: 50S ribosomal protein L3



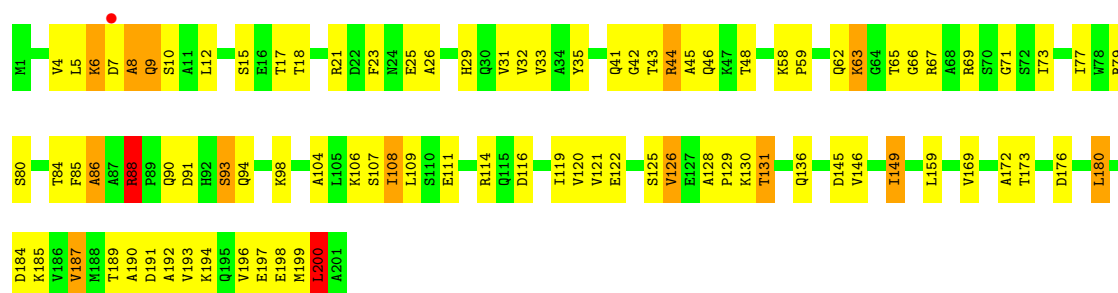
• Molecule 25: 50S ribosomal protein L3





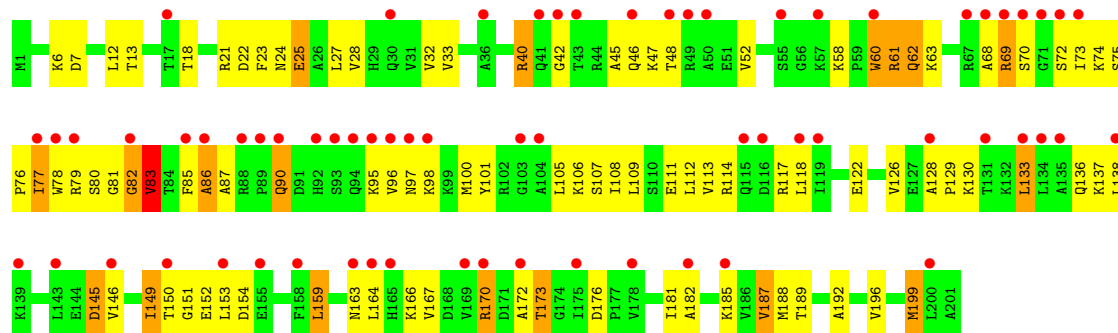
• Molecule 26: 50S ribosomal protein L4

Chain BE: 55% 38% 6% .



• Molecule 26: 50S ribosomal protein L4

Chain DE: 33% 52% 39% 9% .



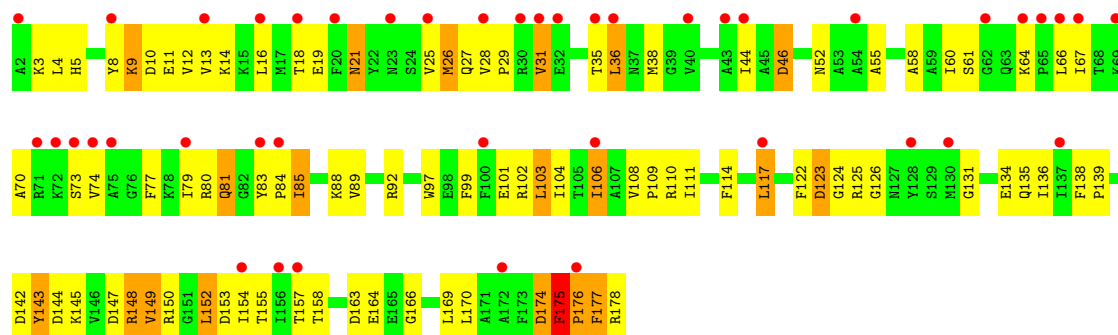
• Molecule 27: 50S ribosomal protein L5

Chain BF: 2% 39% 44% 16% .

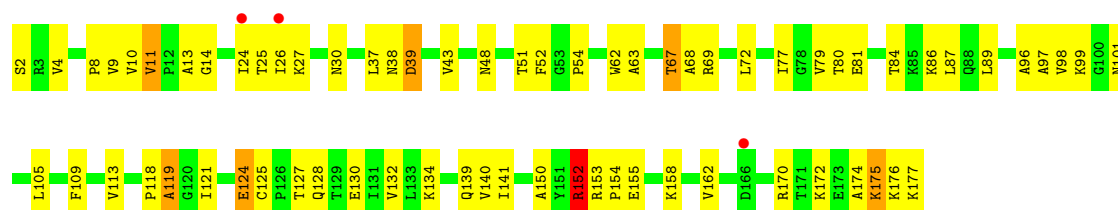




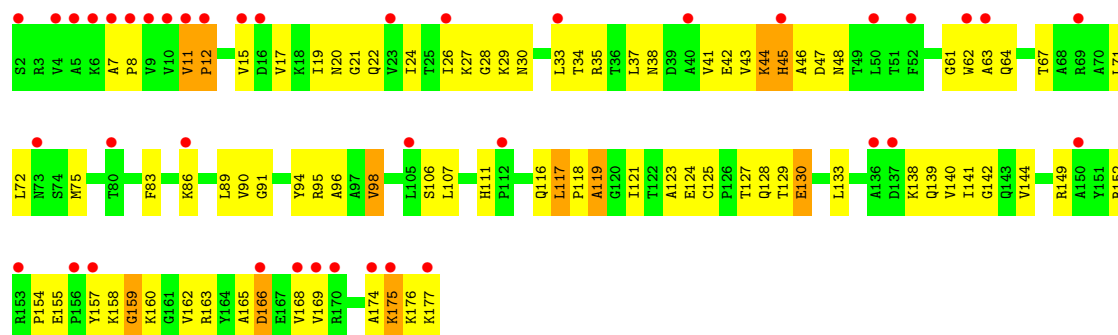
- Molecule 27: 50S ribosomal protein L5



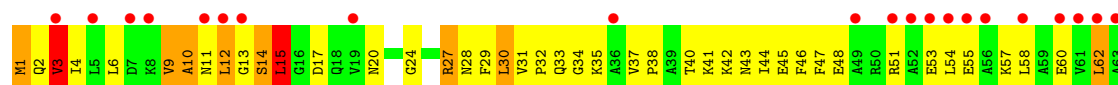
- Molecule 28: 50S ribosomal protein L6

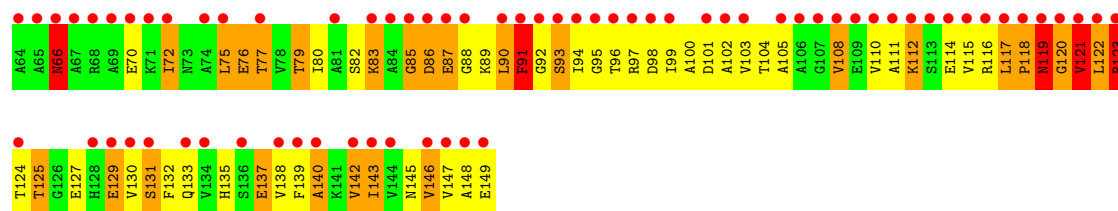


- Molecule 28: 50S ribosomal protein L6

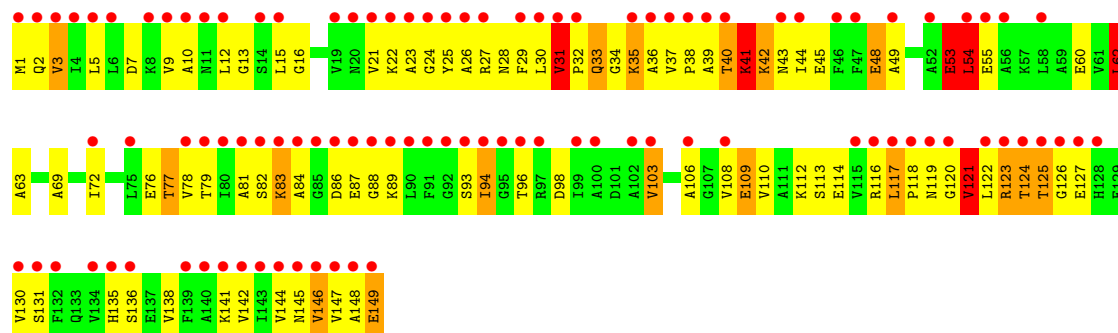
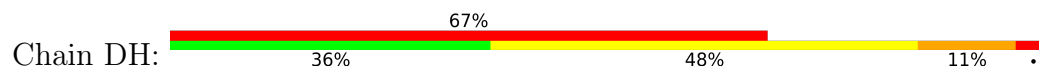


- Molecule 29: 50S ribosomal protein L9

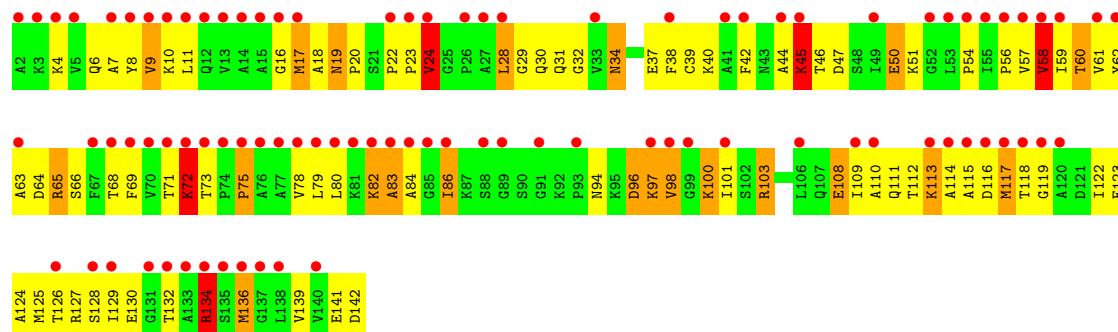




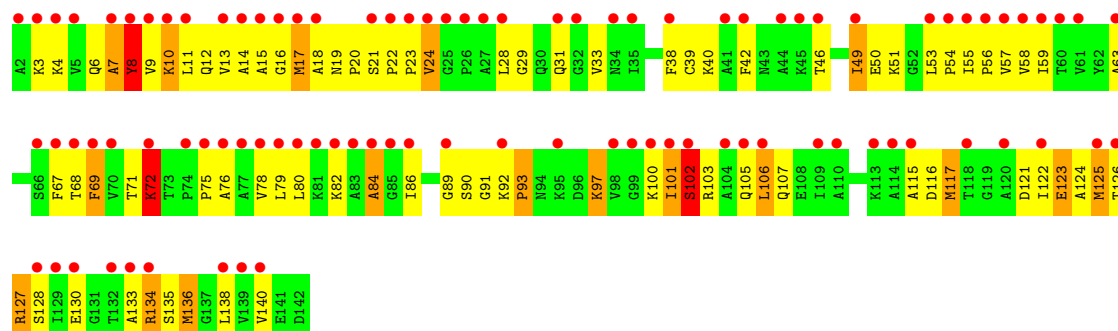
• Molecule 29: 50S ribosomal protein L9



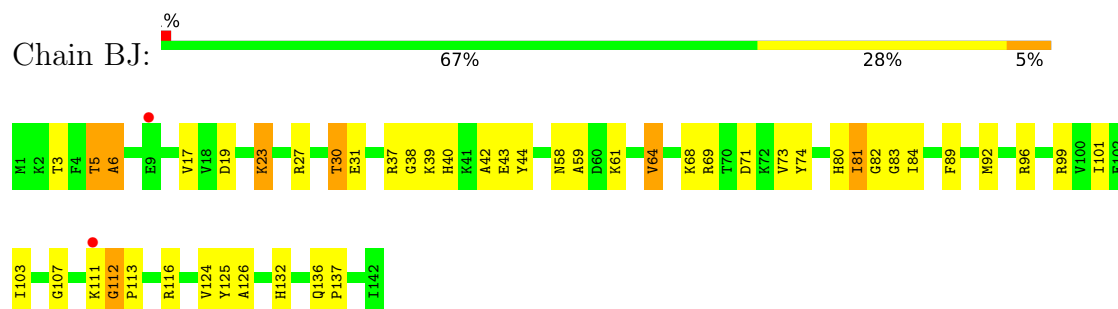
• Molecule 30: 50S ribosomal protein L11



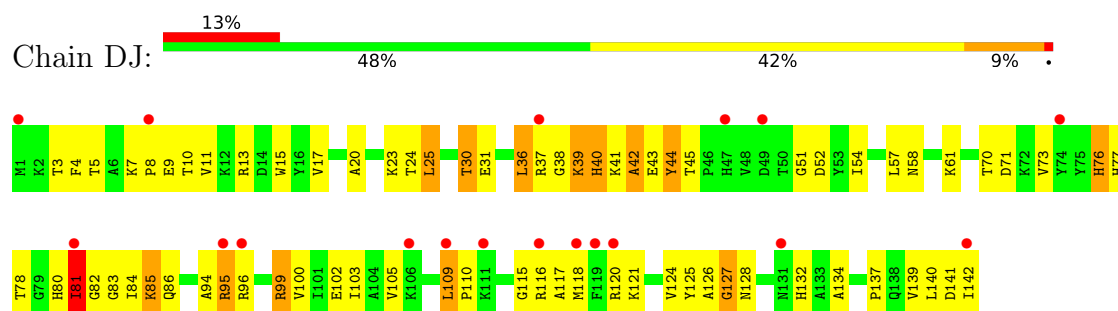
• Molecule 30: 50S ribosomal protein L11



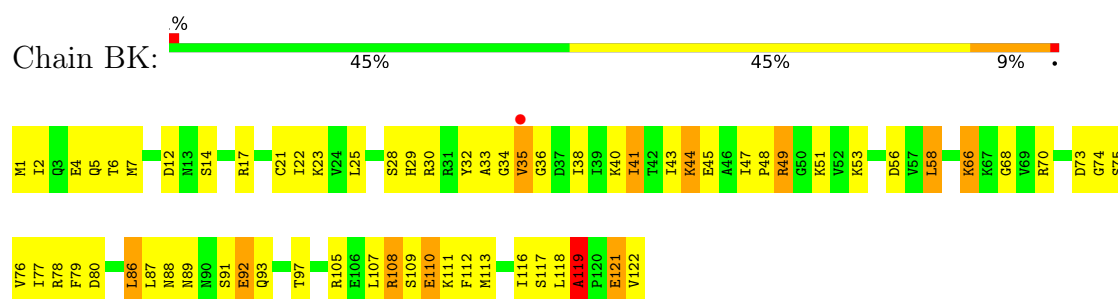
- Molecule 31: 50S ribosomal protein L13



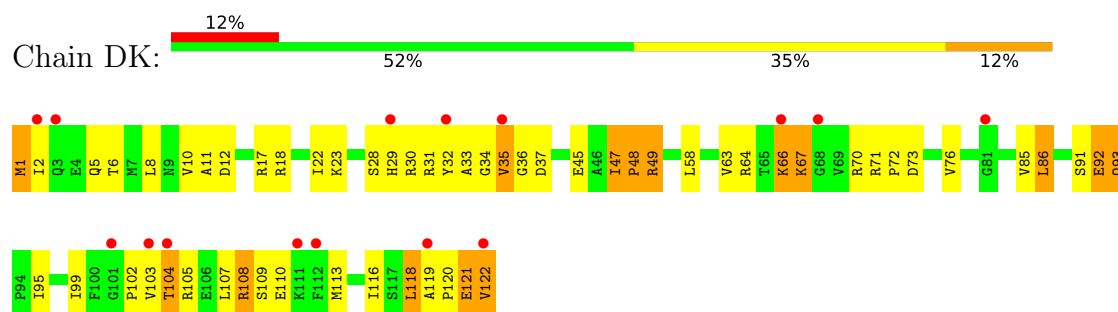
- Molecule 31: 50S ribosomal protein L13



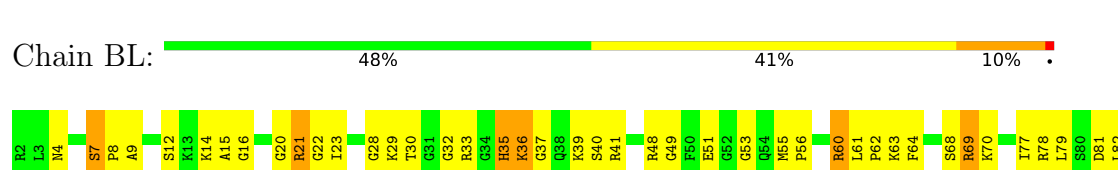
- Molecule 32: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L14

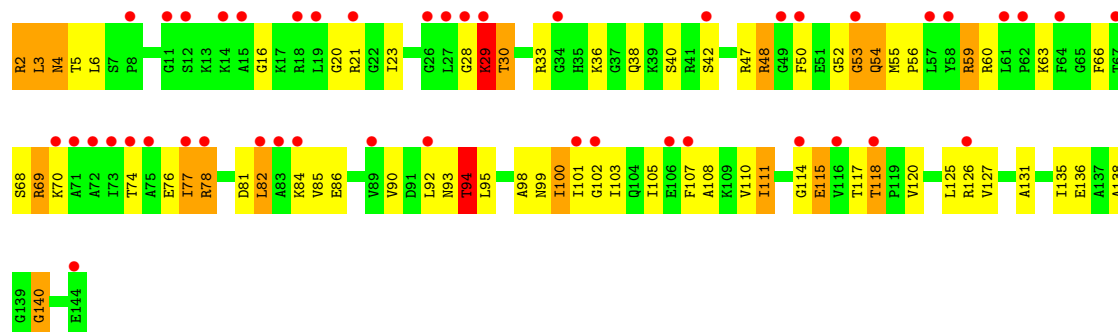


- Molecule 33: 50S ribosomal protein L15

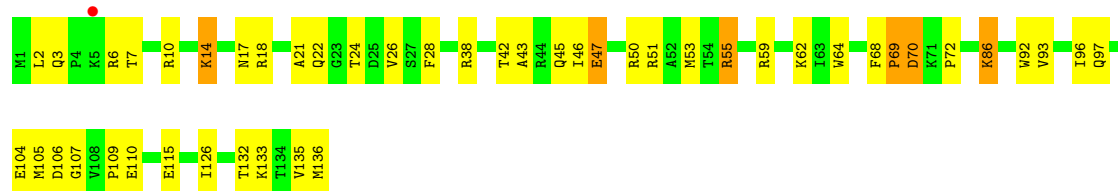




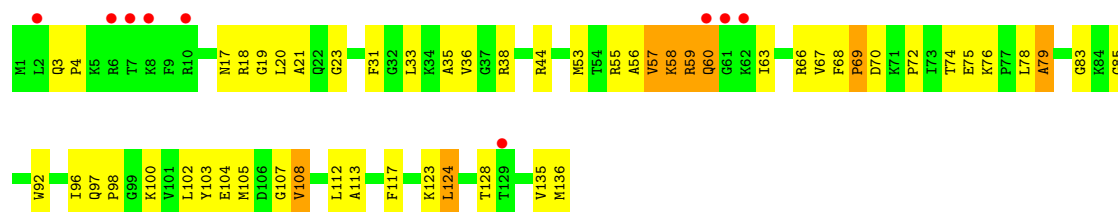
• Molecule 33: 50S ribosomal protein L15



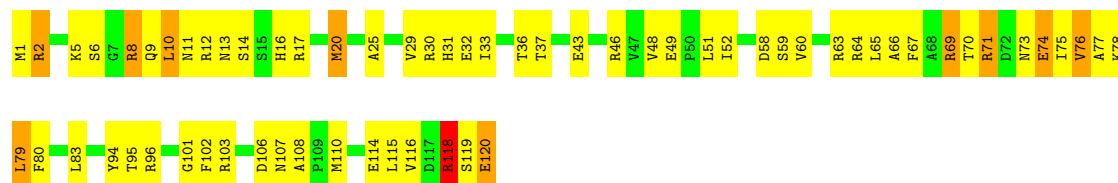
• Molecule 34: 50S ribosomal protein L16



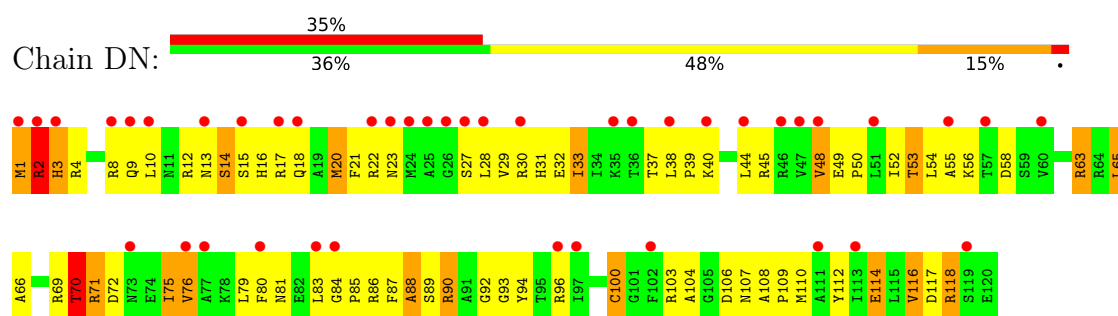
• Molecule 34: 50S ribosomal protein L16



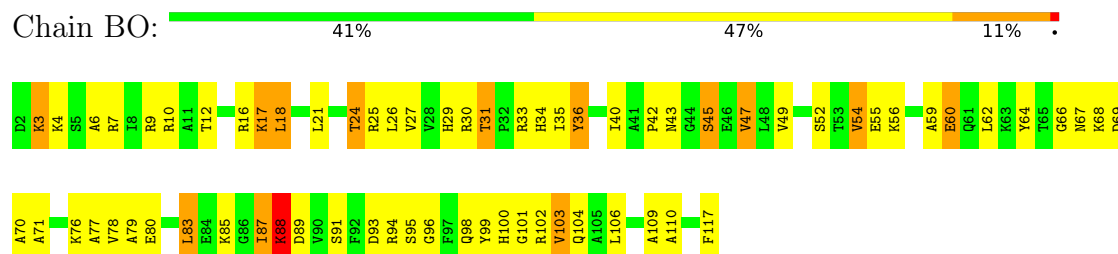
• Molecule 35: 50S ribosomal protein L17



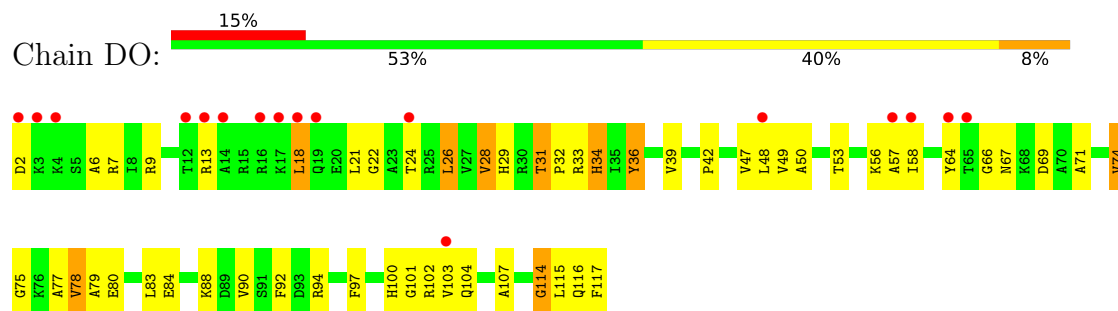
• Molecule 35: 50S ribosomal protein L17



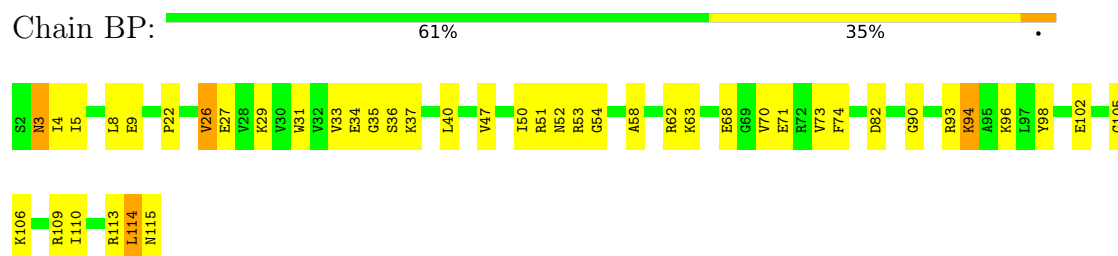
- Molecule 36: 50S ribosomal protein L18



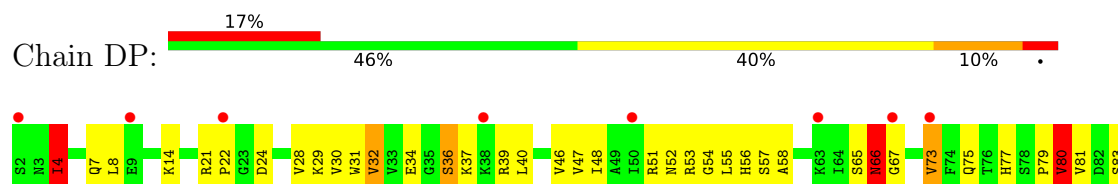
- Molecule 36: 50S ribosomal protein L18

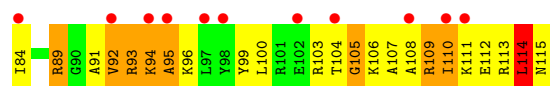


- Molecule 37: 50S ribosomal protein L19



- Molecule 37: 50S ribosomal protein L19

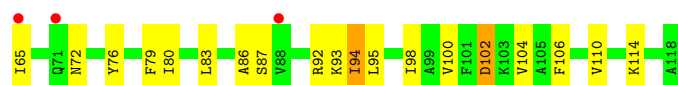
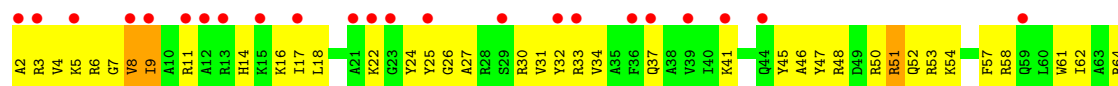




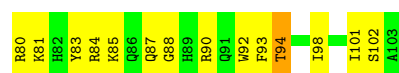
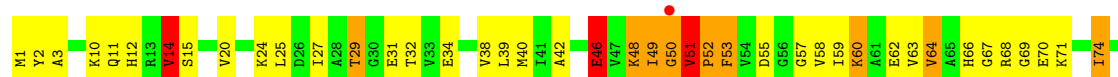
- Molecule 38: 50S ribosomal protein L20



- Molecule 38: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L21



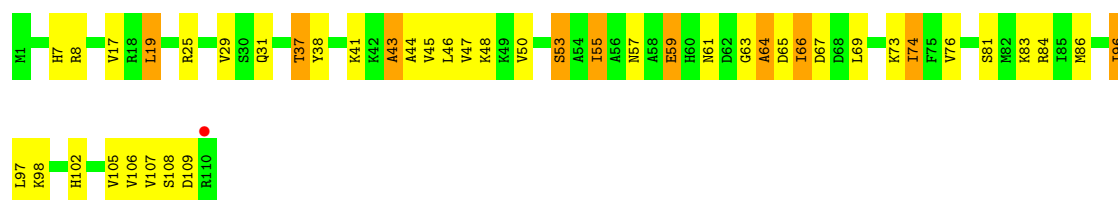
- Molecule 39: 50S ribosomal protein L21



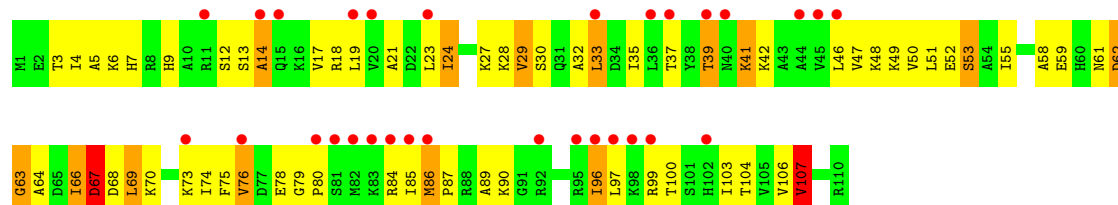
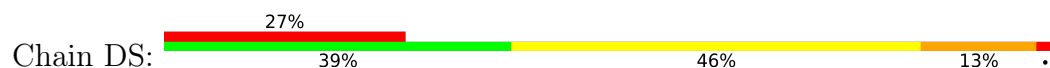
- Molecule 40: 50S ribosomal protein L22



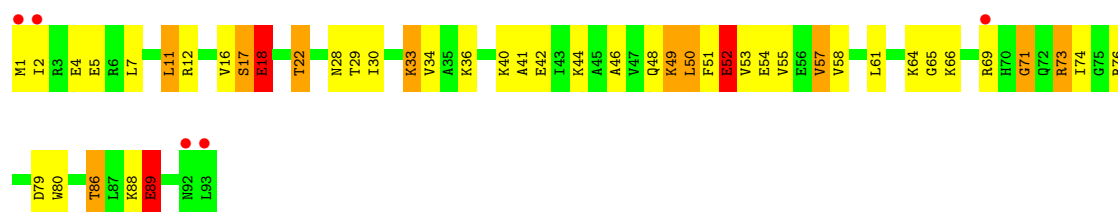




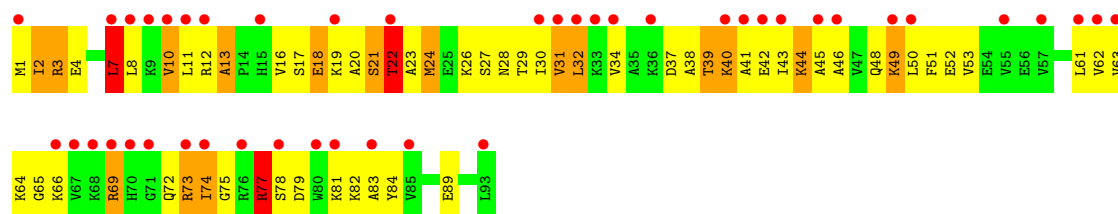
• Molecule 40: 50S ribosomal protein L22



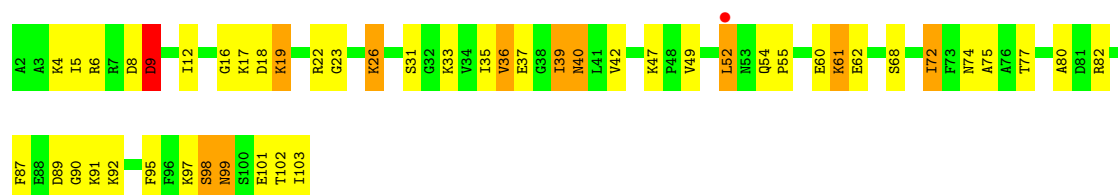
• Molecule 41: 50S ribosomal protein L23



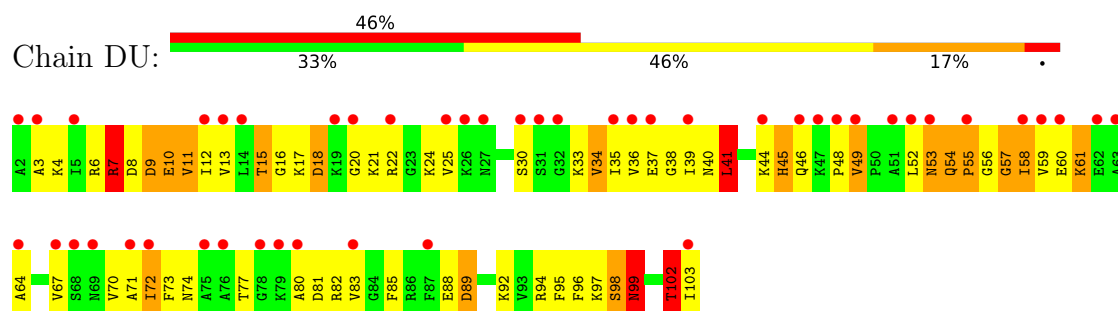
• Molecule 41: 50S ribosomal protein L23



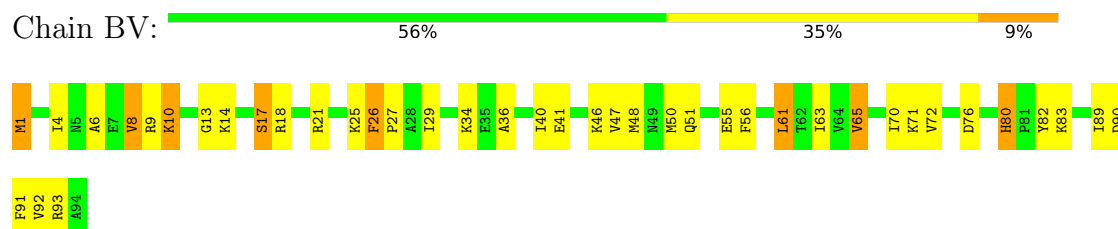
• Molecule 42: 50S ribosomal protein L24



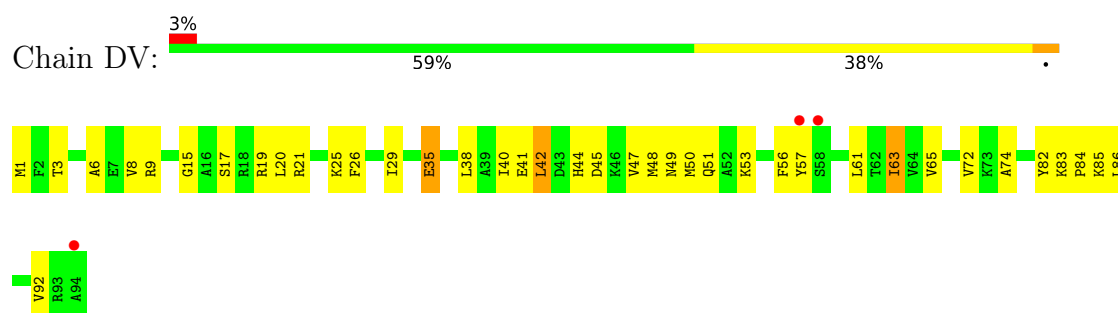
- Molecule 42: 50S ribosomal protein L24



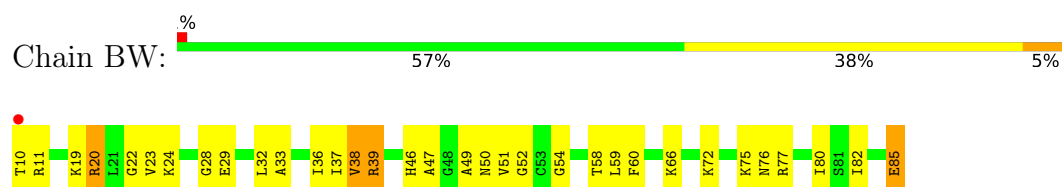
- Molecule 43: 50S ribosomal protein L25



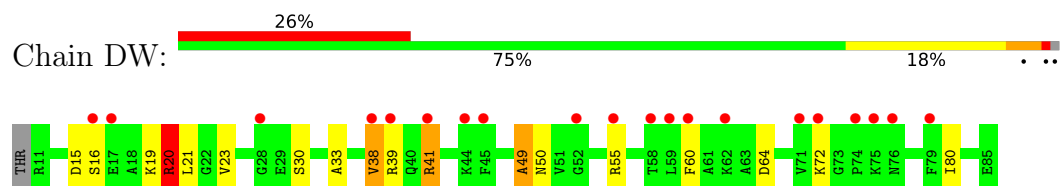
- Molecule 43: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L27



- Molecule 44: 50S ribosomal protein L27

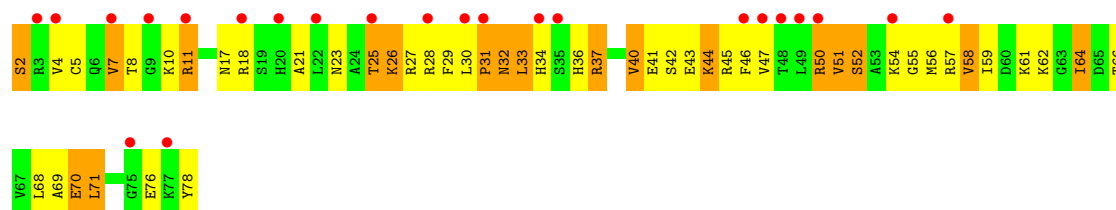


- Molecule 45: 50S ribosomal protein L28





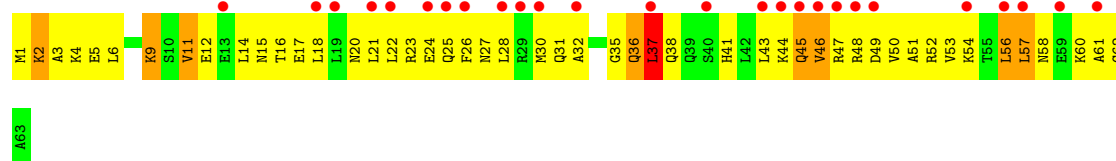
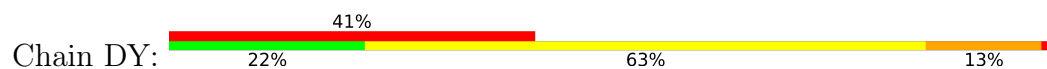
- Molecule 45: 50S ribosomal protein L28



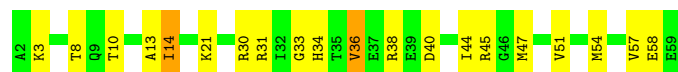
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

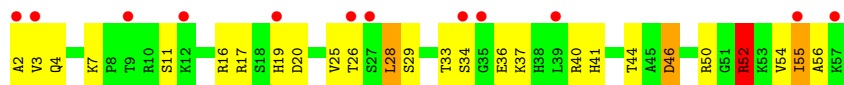


- Molecule 48: 50S ribosomal protein L32





- Molecule 48: 50S ribosomal protein L32



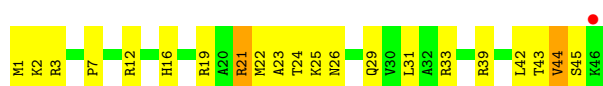
- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33



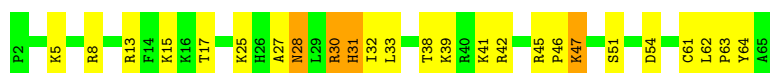
- Molecule 50: 50S ribosomal protein L34



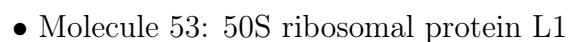
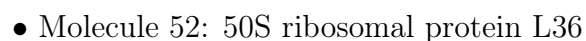
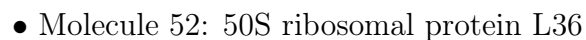
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.64Å 434.61Å 625.01Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 69.41 – 2.90<br>69.41 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.0 (69.41-2.90)<br>90.0 (69.41-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.15                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.39 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8.1_1168)                          | Depositor        |
| R, $R_{free}$                                                           | 0.223 , 0.265<br>0.226 , 0.266                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4560 reflections (0.40%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 47.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.436                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 48.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 288258                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: MG, ZN, VIR

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    | 0.27         | 0/36944     | 0.47        | 0/57632       |
| 1   | CA    | 0.23         | 0/36966     | 0.41        | 0/57666       |
| 2   | AB    | 0.45         | 0/1736      | 0.90        | 5/2338 (0.2%) |
| 2   | CB    | 0.43         | 0/1736      | 0.83        | 4/2338 (0.2%) |
| 3   | AC    | 0.44         | 0/1652      | 0.86        | 5/2225 (0.2%) |
| 3   | CC    | 0.42         | 0/1652      | 0.79        | 0/2225        |
| 4   | AD    | 0.44         | 0/1665      | 0.93        | 7/2227 (0.3%) |
| 4   | CD    | 0.49         | 0/1665      | 0.89        | 2/2227 (0.1%) |
| 5   | AE    | 0.51         | 0/1119      | 0.93        | 3/1504 (0.2%) |
| 5   | CE    | 0.52         | 0/1119      | 0.95        | 4/1504 (0.3%) |
| 6   | AF    | 0.52         | 0/836       | 0.91        | 1/1128 (0.1%) |
| 6   | CF    | 0.43         | 0/836       | 0.87        | 3/1128 (0.3%) |
| 7   | AG    | 0.44         | 0/1196      | 0.86        | 1/1602 (0.1%) |
| 7   | CG    | 0.45         | 0/1196      | 0.83        | 0/1602        |
| 8   | AH    | 0.51         | 0/989       | 0.91        | 3/1326 (0.2%) |
| 8   | CH    | 0.39         | 0/989       | 0.79        | 1/1326 (0.1%) |
| 9   | AI    | 0.41         | 0/1034      | 0.84        | 1/1375 (0.1%) |
| 9   | CI    | 0.39         | 0/1034      | 0.81        | 0/1375        |
| 10  | AJ    | 0.50         | 0/797       | 0.84        | 1/1077 (0.1%) |
| 10  | CJ    | 0.49         | 0/797       | 0.83        | 1/1077 (0.1%) |
| 11  | AK    | 0.47         | 0/893       | 0.84        | 1/1205 (0.1%) |
| 11  | CK    | 0.46         | 0/893       | 0.97        | 5/1205 (0.4%) |
| 12  | AL    | 0.51         | 0/969       | 0.93        | 1/1300 (0.1%) |
| 12  | CL    | 0.48         | 0/969       | 0.92        | 2/1300 (0.2%) |
| 13  | AM    | 0.45         | 0/893       | 0.92        | 2/1193 (0.2%) |
| 13  | CM    | 0.45         | 0/893       | 0.86        | 0/1193        |
| 14  | AN    | 0.46         | 0/785       | 0.90        | 3/1043 (0.3%) |
| 14  | CN    | 0.38         | 0/785       | 0.83        | 2/1043 (0.2%) |
| 15  | AO    | 0.43         | 0/718       | 0.81        | 1/959 (0.1%)  |
| 15  | CO    | 0.39         | 0/718       | 0.78        | 0/959         |
| 16  | AP    | 0.54         | 0/659       | 0.89        | 0/884         |
| 16  | CP    | 0.43         | 0/659       | 0.83        | 2/884 (0.2%)  |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 17  | AQ    | 0.46         | 0/658   | 0.85        | 0/881           |
| 17  | CQ    | 0.45         | 0/658   | 0.84        | 0/881           |
| 18  | AR    | 0.42         | 0/463   | 0.80        | 0/621           |
| 18  | CR    | 0.47         | 0/463   | 0.81        | 0/621           |
| 19  | AS    | 0.47         | 0/653   | 0.93        | 2/877 (0.2%)    |
| 19  | CS    | 0.49         | 0/653   | 0.87        | 2/877 (0.2%)    |
| 20  | AT    | 0.48         | 0/671   | 0.90        | 1/888 (0.1%)    |
| 20  | CT    | 0.41         | 0/671   | 0.87        | 1/888 (0.1%)    |
| 21  | AU    | 0.54         | 0/431   | 0.90        | 0/570           |
| 21  | CU    | 0.53         | 0/431   | 0.87        | 0/570           |
| 22  | BA    | 0.44         | 0/69659 | 0.62        | 1/108672 (0.0%) |
| 22  | DA    | 0.22         | 0/69659 | 0.40        | 0/108672        |
| 23  | BB    | 0.40         | 0/2850  | 0.60        | 0/4444          |
| 23  | DB    | 0.17         | 0/2828  | 0.32        | 0/4410          |
| 24  | BC    | 0.63         | 0/2122  | 1.02        | 10/2852 (0.4%)  |
| 24  | DC    | 0.43         | 0/2122  | 0.86        | 4/2852 (0.1%)   |
| 25  | BD    | 0.75         | 0/1586  | 1.09        | 6/2134 (0.3%)   |
| 25  | DD    | 0.42         | 0/1586  | 0.84        | 3/2134 (0.1%)   |
| 26  | BE    | 0.67         | 0/1571  | 0.99        | 5/2113 (0.2%)   |
| 26  | DE    | 0.45         | 0/1571  | 0.84        | 1/2113 (0.0%)   |
| 27  | BF    | 0.54         | 0/1435  | 0.94        | 2/1926 (0.1%)   |
| 27  | DF    | 0.40         | 0/1435  | 0.78        | 2/1926 (0.1%)   |
| 28  | BG    | 0.52         | 0/1343  | 0.92        | 0/1816          |
| 28  | DG    | 0.42         | 0/1343  | 0.80        | 2/1816 (0.1%)   |
| 29  | BH    | 0.49         | 0/1121  | 0.99        | 5/1515 (0.3%)   |
| 29  | DH    | 0.47         | 0/1121  | 0.92        | 5/1515 (0.3%)   |
| 30  | BI    | 0.55         | 0/1046  | 0.89        | 1/1410 (0.1%)   |
| 30  | DI    | 0.55         | 0/1046  | 0.90        | 2/1410 (0.1%)   |
| 31  | BJ    | 0.79         | 0/1152  | 1.05        | 6/1551 (0.4%)   |
| 31  | DJ    | 0.44         | 0/1152  | 0.85        | 3/1551 (0.2%)   |
| 32  | BK    | 0.70         | 0/948   | 1.06        | 3/1268 (0.2%)   |
| 32  | DK    | 0.45         | 0/948   | 0.85        | 3/1268 (0.2%)   |
| 33  | BL    | 0.72         | 0/1054  | 1.07        | 4/1403 (0.3%)   |
| 33  | DL    | 0.44         | 0/1054  | 0.90        | 0/1403          |
| 34  | BM    | 0.73         | 0/1093  | 1.02        | 4/1460 (0.3%)   |
| 34  | DM    | 0.40         | 0/1093  | 0.76        | 0/1460          |
| 35  | BN    | 0.76         | 0/974   | 1.05        | 0/1301          |
| 35  | DN    | 0.45         | 0/974   | 0.84        | 0/1301          |
| 36  | BO    | 0.61         | 0/902   | 0.95        | 0/1209          |
| 36  | DO    | 0.38         | 0/902   | 0.78        | 0/1209          |
| 37  | BP    | 0.66         | 0/929   | 0.90        | 1/1242 (0.1%)   |
| 37  | DP    | 0.41         | 0/929   | 0.80        | 1/1242 (0.1%)   |
| 38  | BQ    | 0.86         | 0/960   | 1.10        | 3/1278 (0.2%)   |



| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | DQ    | 0.43         | 0/960           | 0.84        | 1/1278 (0.1%)     |
| 39  | BR    | 0.79         | 0/829           | 1.11        | 4/1107 (0.4%)     |
| 39  | DR    | 0.41         | 0/829           | 0.88        | 4/1107 (0.4%)     |
| 40  | BS    | 0.91         | 0/864           | 1.06        | 2/1156 (0.2%)     |
| 40  | DS    | 0.45         | 0/864           | 0.80        | 0/1156            |
| 41  | BT    | 0.59         | 0/745           | 0.90        | 0/994             |
| 41  | DT    | 0.42         | 0/745           | 0.76        | 0/994             |
| 42  | BU    | 0.56         | 0/788           | 0.91        | 1/1051 (0.1%)     |
| 42  | DU    | 0.51         | 0/788           | 0.86        | 0/1051            |
| 43  | BV    | 0.66         | 0/766           | 1.01        | 4/1025 (0.4%)     |
| 43  | DV    | 0.36         | 0/766           | 0.73        | 0/1025            |
| 44  | BW    | 0.71         | 0/587           | 1.01        | 0/776             |
| 44  | DW    | 0.35         | 0/576           | 0.76        | 0/762             |
| 45  | BX    | 0.58         | 0/635           | 0.89        | 0/848             |
| 45  | DX    | 0.44         | 0/635           | 0.87        | 2/848 (0.2%)      |
| 46  | BY    | 0.56         | 0/510           | 0.92        | 2/677 (0.3%)      |
| 46  | DY    | 0.38         | 0/510           | 0.82        | 0/677             |
| 47  | BZ    | 0.84         | 0/453           | 1.02        | 0/605             |
| 47  | DZ    | 0.43         | 0/453           | 0.83        | 1/605 (0.2%)      |
| 48  | B0    | 0.74         | 1/450 (0.2%)    | 1.03        | 2/599 (0.3%)      |
| 48  | D0    | 0.46         | 0/450           | 0.77        | 0/599             |
| 49  | B1    | 0.53         | 0/417           | 0.81        | 0/554             |
| 49  | D1    | 0.45         | 0/417           | 0.72        | 0/554             |
| 50  | B2    | 0.74         | 0/380           | 1.04        | 0/498             |
| 50  | D2    | 0.45         | 0/380           | 0.92        | 0/498             |
| 51  | B3    | 0.71         | 0/513           | 0.98        | 1/676 (0.1%)      |
| 51  | D3    | 0.43         | 0/513           | 0.78        | 0/676             |
| 52  | B4    | 0.73         | 0/303           | 1.08        | 3/397 (0.8%)      |
| 52  | D4    | 0.38         | 0/303           | 0.83        | 2/397 (0.5%)      |
| 53  | B5    | 0.54         | 0/1145          | 1.05        | 9/1556 (0.6%)     |
| All | All   | 0.39         | 1/310626 (0.0%) | 0.63        | 182/464366 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | CE    | 0                   | 1                   |
| 6   | CF    | 0                   | 1                   |
| 11  | AK    | 0                   | 1                   |
| 12  | CL    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 21  | AU    | 0                   | 1                   |
| 21  | CU    | 0                   | 1                   |
| 25  | BD    | 0                   | 1                   |
| All | All   | 0                   | 7                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 48  | B0    | 21  | ALA  | CA-CB | -5.56 | 1.44        | 1.53     |

The worst 5 of 182 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 25  | BD    | 151 | THR  | CA-C-N | 12.13 | 135.00      | 119.84   |
| 25  | BD    | 151 | THR  | C-N-CA | 12.13 | 135.00      | 119.84   |
| 53  | B5    | 181 | PHE  | CA-C-N | 10.33 | 131.02      | 120.38   |
| 53  | B5    | 181 | PHE  | C-N-CA | 10.33 | 131.02      | 120.38   |
| 20  | AT    | 8   | LYS  | N-CA-C | -9.73 | 100.66      | 111.07   |

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 11  | AK    | 126 | LYS  | Peptide |
| 21  | AU    | 39  | GLU  | Peptide |
| 25  | BD    | 151 | THR  | Peptide |
| 5   | CE    | 102 | GLY  | Peptide |
| 6   | CF    | 54  | LEU  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32995 | 0        | 16607    | 1127    | 4            |
| 1   | CA    | 33015 | 0        | 16617    | 1086    | 0            |
| 2   | AB    | 1705  | 0        | 1732     | 198     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | CB    | 1705  | 0        | 1732     | 144     | 0            |
| 3   | AC    | 1625  | 0        | 1696     | 89      | 0            |
| 3   | CC    | 1625  | 0        | 1696     | 76      | 0            |
| 4   | AD    | 1643  | 0        | 1707     | 164     | 0            |
| 4   | CD    | 1643  | 0        | 1707     | 131     | 0            |
| 5   | AE    | 1106  | 0        | 1148     | 81      | 0            |
| 5   | CE    | 1106  | 0        | 1148     | 125     | 0            |
| 6   | AF    | 818   | 0        | 808      | 71      | 0            |
| 6   | CF    | 818   | 0        | 808      | 67      | 0            |
| 7   | AG    | 1182  | 0        | 1238     | 59      | 0            |
| 7   | CG    | 1182  | 0        | 1238     | 67      | 0            |
| 8   | AH    | 979   | 0        | 1031     | 74      | 0            |
| 8   | CH    | 979   | 0        | 1031     | 50      | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 86      | 0            |
| 9   | CI    | 1022  | 0        | 1070     | 65      | 0            |
| 10  | AJ    | 787   | 0        | 828      | 80      | 0            |
| 10  | CJ    | 787   | 0        | 828      | 50      | 0            |
| 11  | AK    | 877   | 0        | 887      | 70      | 0            |
| 11  | CK    | 877   | 0        | 887      | 70      | 0            |
| 12  | AL    | 955   | 0        | 1016     | 69      | 0            |
| 12  | CL    | 955   | 0        | 1016     | 78      | 0            |
| 13  | AM    | 884   | 0        | 941      | 72      | 0            |
| 13  | CM    | 884   | 0        | 941      | 49      | 0            |
| 14  | AN    | 774   | 0        | 824      | 73      | 0            |
| 14  | CN    | 774   | 0        | 824      | 51      | 0            |
| 15  | AO    | 710   | 0        | 728      | 34      | 0            |
| 15  | CO    | 710   | 0        | 728      | 44      | 0            |
| 16  | AP    | 649   | 0        | 666      | 67      | 0            |
| 16  | CP    | 649   | 0        | 666      | 29      | 0            |
| 17  | AQ    | 649   | 0        | 691      | 74      | 0            |
| 17  | CQ    | 649   | 0        | 691      | 56      | 0            |
| 18  | AR    | 456   | 0        | 478      | 22      | 0            |
| 18  | CR    | 456   | 0        | 478      | 36      | 0            |
| 19  | AS    | 638   | 0        | 665      | 59      | 0            |
| 19  | CS    | 638   | 0        | 665      | 36      | 0            |
| 20  | AT    | 665   | 0        | 714      | 63      | 0            |
| 20  | CT    | 665   | 0        | 714      | 49      | 0            |
| 21  | AU    | 426   | 0        | 449      | 60      | 0            |
| 21  | CU    | 426   | 0        | 449      | 55      | 0            |
| 22  | BA    | 62195 | 0        | 31280    | 1629    | 0            |
| 22  | DA    | 62195 | 0        | 31280    | 2239    | 0            |
| 23  | BB    | 2549  | 0        | 1291     | 54      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 23  | DB    | 2529  | 0        | 1281     | 62      | 0            |
| 24  | BC    | 2083  | 0        | 2154     | 130     | 0            |
| 24  | DC    | 2083  | 0        | 2154     | 132     | 0            |
| 25  | BD    | 1565  | 0        | 1616     | 71      | 0            |
| 25  | DD    | 1565  | 0        | 1616     | 83      | 0            |
| 26  | BE    | 1552  | 0        | 1619     | 70      | 0            |
| 26  | DE    | 1552  | 0        | 1619     | 80      | 0            |
| 27  | BF    | 1411  | 0        | 1444     | 101     | 0            |
| 27  | DF    | 1411  | 0        | 1444     | 64      | 0            |
| 28  | BG    | 1323  | 0        | 1371     | 53      | 0            |
| 28  | DG    | 1323  | 0        | 1371     | 56      | 0            |
| 29  | BH    | 1110  | 0        | 1147     | 161     | 0            |
| 29  | DH    | 1110  | 0        | 1148     | 125     | 4            |
| 30  | BI    | 1032  | 0        | 1085     | 75      | 0            |
| 30  | DI    | 1032  | 0        | 1085     | 69      | 0            |
| 31  | BJ    | 1129  | 0        | 1162     | 37      | 0            |
| 31  | DJ    | 1129  | 0        | 1162     | 54      | 0            |
| 32  | BK    | 939   | 0        | 1012     | 55      | 0            |
| 32  | DK    | 939   | 0        | 1012     | 52      | 0            |
| 33  | BL    | 1045  | 0        | 1117     | 66      | 0            |
| 33  | DL    | 1045  | 0        | 1117     | 70      | 0            |
| 34  | BM    | 1074  | 0        | 1157     | 32      | 0            |
| 34  | DM    | 1074  | 0        | 1157     | 33      | 0            |
| 35  | BN    | 961   | 0        | 1000     | 57      | 0            |
| 35  | DN    | 961   | 0        | 1000     | 75      | 0            |
| 36  | BO    | 892   | 0        | 923      | 57      | 0            |
| 36  | DO    | 892   | 0        | 923      | 45      | 0            |
| 37  | BP    | 917   | 0        | 962      | 32      | 0            |
| 37  | DP    | 917   | 0        | 962      | 47      | 0            |
| 38  | BQ    | 947   | 0        | 1019     | 55      | 0            |
| 38  | DQ    | 947   | 0        | 1019     | 53      | 0            |
| 39  | BR    | 816   | 0        | 839      | 75      | 0            |
| 39  | DR    | 816   | 0        | 839      | 48      | 0            |
| 40  | BS    | 857   | 0        | 922      | 37      | 0            |
| 40  | DS    | 857   | 0        | 922      | 53      | 0            |
| 41  | BT    | 739   | 0        | 807      | 42      | 0            |
| 41  | DT    | 739   | 0        | 807      | 65      | 0            |
| 42  | BU    | 780   | 0        | 831      | 30      | 0            |
| 42  | DU    | 780   | 0        | 831      | 72      | 0            |
| 43  | BV    | 753   | 0        | 780      | 29      | 0            |
| 43  | DV    | 753   | 0        | 780      | 28      | 0            |
| 44  | BW    | 580   | 0        | 594      | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | DW    | 569   | 0        | 581      | 17      | 0            |
| 45  | BX    | 625   | 0        | 652      | 26      | 0            |
| 45  | DX    | 625   | 0        | 652      | 48      | 0            |
| 46  | BY    | 509   | 0        | 543      | 33      | 0            |
| 46  | DY    | 509   | 0        | 543      | 49      | 0            |
| 47  | BZ    | 449   | 0        | 488      | 12      | 0            |
| 47  | DZ    | 449   | 0        | 488      | 17      | 0            |
| 48  | B0    | 444   | 0        | 458      | 24      | 0            |
| 48  | D0    | 444   | 0        | 458      | 20      | 0            |
| 49  | B1    | 410   | 0        | 440      | 27      | 0            |
| 49  | D1    | 410   | 0        | 440      | 18      | 0            |
| 50  | B2    | 377   | 0        | 418      | 20      | 0            |
| 50  | D2    | 377   | 0        | 418      | 24      | 0            |
| 51  | B3    | 504   | 0        | 572      | 27      | 0            |
| 51  | D3    | 504   | 0        | 572      | 21      | 0            |
| 52  | B4    | 302   | 0        | 340      | 15      | 0            |
| 52  | D4    | 302   | 0        | 342      | 15      | 0            |
| 53  | B5    | 1142  | 0        | 865      | 50      | 0            |
| 54  | AA    | 71    | 0        | 0        | 0       | 0            |
| 54  | AN    | 1     | 0        | 0        | 0       | 0            |
| 54  | BA    | 193   | 0        | 0        | 0       | 0            |
| 54  | BB    | 4     | 0        | 0        | 0       | 0            |
| 54  | BD    | 1     | 0        | 0        | 0       | 0            |
| 54  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 54  | CA    | 56    | 0        | 0        | 0       | 0            |
| 54  | D2    | 1     | 0        | 0        | 0       | 0            |
| 54  | DA    | 166   | 0        | 0        | 0       | 0            |
| 54  | DB    | 3     | 0        | 0        | 0       | 0            |
| 54  | DQ    | 1     | 0        | 0        | 0       | 0            |
| 55  | BA    | 38    | 0        | 35       | 5       | 0            |
| 55  | DA    | 38    | 0        | 35       | 15      | 0            |
| 56  | B4    | 1     | 0        | 0        | 0       | 0            |
| 56  | D4    | 1     | 0        | 0        | 0       | 0            |
| 57  | AA    | 192   | 0        | 0        | 25      | 0            |
| 57  | AL    | 2     | 0        | 0        | 0       | 0            |
| 57  | AN    | 6     | 0        | 0        | 1       | 0            |
| 57  | AT    | 2     | 0        | 0        | 0       | 0            |
| 57  | AU    | 1     | 0        | 0        | 0       | 0            |
| 57  | B2    | 1     | 0        | 0        | 0       | 0            |
| 57  | B3    | 2     | 0        | 0        | 0       | 0            |
| 57  | B4    | 2     | 0        | 0        | 0       | 0            |
| 57  | BA    | 620   | 0        | 0        | 65      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | BB    | 13     | 0        | 0        | 0       | 0            |
| 57  | BC    | 7      | 0        | 0        | 1       | 0            |
| 57  | BD    | 3      | 0        | 0        | 2       | 0            |
| 57  | BE    | 4      | 0        | 0        | 0       | 0            |
| 57  | BF    | 1      | 0        | 0        | 1       | 0            |
| 57  | BJ    | 1      | 0        | 0        | 0       | 0            |
| 57  | BL    | 5      | 0        | 0        | 0       | 0            |
| 57  | BN    | 3      | 0        | 0        | 0       | 0            |
| 57  | BQ    | 1      | 0        | 0        | 0       | 0            |
| 57  | BS    | 1      | 0        | 0        | 0       | 0            |
| 57  | BT    | 1      | 0        | 0        | 0       | 0            |
| 57  | BV    | 1      | 0        | 0        | 0       | 0            |
| 57  | CA    | 191    | 0        | 0        | 26      | 0            |
| 57  | CL    | 1      | 0        | 0        | 0       | 0            |
| 57  | CN    | 2      | 0        | 0        | 0       | 0            |
| 57  | CT    | 2      | 0        | 0        | 0       | 0            |
| 57  | CU    | 2      | 0        | 0        | 1       | 0            |
| 57  | D2    | 1      | 0        | 0        | 0       | 0            |
| 57  | D3    | 2      | 0        | 0        | 0       | 0            |
| 57  | D4    | 1      | 0        | 0        | 0       | 0            |
| 57  | DA    | 607    | 0        | 0        | 105     | 0            |
| 57  | DB    | 13     | 0        | 0        | 0       | 0            |
| 57  | DC    | 12     | 0        | 0        | 2       | 0            |
| 57  | DD    | 4      | 0        | 0        | 2       | 0            |
| 57  | DE    | 6      | 0        | 0        | 2       | 0            |
| 57  | DJ    | 1      | 0        | 0        | 0       | 0            |
| 57  | DL    | 4      | 0        | 0        | 1       | 0            |
| 57  | DN    | 2      | 0        | 0        | 0       | 0            |
| 57  | DT    | 1      | 0        | 0        | 0       | 0            |
| 57  | DU    | 1      | 0        | 0        | 0       | 0            |
| 57  | DV    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 288258 | 0        | 192859   | 11151   | 4            |

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 24.

The worst 5 of 11151 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) |
|------------------|------------------|--------------------------|-------------------|
| 22:BA:1153:C:OP2 | 57:BA:3360:HOH:O | 1.56                     | 1.23              |
| 22:BA:621:A:OP2  | 57:BA:3293:HOH:O | 1.57                     | 1.23              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BH:117:LEU:O    | 29:BH:121:VAL:HG23 | 1.34                     | 1.22              |
| 29:BH:123:ARG:HH22 | 1:CA:367:U:P       | 1.69                     | 1.15              |
| 29:BH:117:LEU:O    | 29:BH:121:VAL:CG2  | 1.95                     | 1.14              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                   | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|--------------------------|--------------------------|-------------------|
| 1:AA:368:U:OP1 | 29:DH:93:SER:OG[4_455]   | 1.70                     | 0.50              |
| 1:AA:367:U:O5' | 29:DH:123:ARG:NH2[4_455] | 2.02                     | 0.18              |
| 1:AA:368:U:O4  | 29:DH:83:LYS:CE[4_455]   | 2.03                     | 0.17              |
| 1:AA:368:U:O4  | 29:DH:83:LYS:CB[4_455]   | 2.13                     | 0.07              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 2   | AB    | 216/218 (99%) | 126 (58%) | 40 (18%) | 50 (23%) | 0           | 0 |
| 2   | CB    | 216/218 (99%) | 133 (62%) | 52 (24%) | 31 (14%) | 0           | 0 |
| 3   | AC    | 204/206 (99%) | 149 (73%) | 38 (19%) | 17 (8%)  | 0           | 1 |
| 3   | CC    | 204/206 (99%) | 153 (75%) | 40 (20%) | 11 (5%)  | 1           | 5 |
| 4   | AD    | 203/205 (99%) | 139 (68%) | 33 (16%) | 31 (15%) | 0           | 0 |
| 4   | CD    | 203/205 (99%) | 150 (74%) | 31 (15%) | 22 (11%) | 0           | 1 |
| 5   | AE    | 148/150 (99%) | 104 (70%) | 31 (21%) | 13 (9%)  | 0           | 1 |
| 5   | CE    | 148/150 (99%) | 98 (66%)  | 28 (19%) | 22 (15%) | 0           | 0 |
| 6   | AF    | 98/100 (98%)  | 66 (67%)  | 19 (19%) | 13 (13%) | 0           | 0 |
| 6   | CF    | 98/100 (98%)  | 66 (67%)  | 16 (16%) | 16 (16%) | 0           | 0 |
| 7   | AG    | 149/151 (99%) | 111 (74%) | 28 (19%) | 10 (7%)  | 1           | 3 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 7   | CG    | 149/151 (99%) | 121 (81%) | 20 (13%) | 8 (5%)   | 1           | 5   |
| 8   | AH    | 127/129 (98%) | 91 (72%)  | 21 (16%) | 15 (12%) | 0           | 1   |
| 8   | CH    | 127/129 (98%) | 95 (75%)  | 24 (19%) | 8 (6%)   | 1           | 3   |
| 9   | AI    | 125/127 (98%) | 91 (73%)  | 21 (17%) | 13 (10%) | 0           | 1   |
| 9   | CI    | 125/127 (98%) | 86 (69%)  | 28 (22%) | 11 (9%)  | 0           | 1   |
| 10  | AJ    | 96/98 (98%)   | 60 (62%)  | 15 (16%) | 21 (22%) | 0           | 0   |
| 10  | CJ    | 96/98 (98%)   | 71 (74%)  | 13 (14%) | 12 (12%) | 0           | 0   |
| 11  | AK    | 115/117 (98%) | 84 (73%)  | 19 (16%) | 12 (10%) | 0           | 1   |
| 11  | CK    | 115/117 (98%) | 81 (70%)  | 24 (21%) | 10 (9%)  | 0           | 1   |
| 12  | AL    | 121/123 (98%) | 92 (76%)  | 22 (18%) | 7 (6%)   | 1           | 4   |
| 12  | CL    | 121/123 (98%) | 94 (78%)  | 12 (10%) | 15 (12%) | 0           | 0   |
| 13  | AM    | 112/114 (98%) | 81 (72%)  | 20 (18%) | 11 (10%) | 0           | 1   |
| 13  | CM    | 112/114 (98%) | 86 (77%)  | 17 (15%) | 9 (8%)   | 1           | 2   |
| 14  | AN    | 92/100 (92%)  | 62 (67%)  | 18 (20%) | 12 (13%) | 0           | 0   |
| 14  | CN    | 92/100 (92%)  | 59 (64%)  | 18 (20%) | 15 (16%) | 0           | 0   |
| 15  | AO    | 86/88 (98%)   | 65 (76%)  | 16 (19%) | 5 (6%)   | 1           | 4   |
| 15  | CO    | 86/88 (98%)   | 70 (81%)  | 12 (14%) | 4 (5%)   | 2           | 7   |
| 16  | AP    | 80/82 (98%)   | 53 (66%)  | 15 (19%) | 12 (15%) | 0           | 0   |
| 16  | CP    | 80/82 (98%)   | 59 (74%)  | 16 (20%) | 5 (6%)   | 1           | 3   |
| 17  | AQ    | 78/80 (98%)   | 54 (69%)  | 15 (19%) | 9 (12%)  | 0           | 1   |
| 17  | CQ    | 78/80 (98%)   | 56 (72%)  | 11 (14%) | 11 (14%) | 0           | 0   |
| 18  | AR    | 53/55 (96%)   | 43 (81%)  | 10 (19%) | 0        | 100         | 100 |
| 18  | CR    | 53/55 (96%)   | 34 (64%)  | 13 (24%) | 6 (11%)  | 0           | 1   |
| 19  | AS    | 77/79 (98%)   | 54 (70%)  | 12 (16%) | 11 (14%) | 0           | 0   |
| 19  | CS    | 77/79 (98%)   | 60 (78%)  | 12 (16%) | 5 (6%)   | 1           | 3   |
| 20  | AT    | 83/85 (98%)   | 60 (72%)  | 15 (18%) | 8 (10%)  | 0           | 1   |
| 20  | CT    | 83/85 (98%)   | 64 (77%)  | 12 (14%) | 7 (8%)   | 0           | 1   |
| 21  | AU    | 49/51 (96%)   | 27 (55%)  | 9 (18%)  | 13 (26%) | 0           | 0   |
| 21  | CU    | 49/51 (96%)   | 26 (53%)  | 12 (24%) | 11 (22%) | 0           | 0   |
| 24  | BC    | 269/271 (99%) | 211 (78%) | 47 (18%) | 11 (4%)  | 2           | 9   |
| 24  | DC    | 269/271 (99%) | 204 (76%) | 50 (19%) | 15 (6%)  | 1           | 4   |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 25  | BD    | 207/209 (99%) | 180 (87%) | 20 (10%) | 7 (3%)   | 3           | 12 |
| 25  | DD    | 207/209 (99%) | 168 (81%) | 29 (14%) | 10 (5%)  | 2           | 7  |
| 26  | BE    | 199/201 (99%) | 167 (84%) | 26 (13%) | 6 (3%)   | 3           | 14 |
| 26  | DE    | 199/201 (99%) | 160 (80%) | 28 (14%) | 11 (6%)  | 1           | 4  |
| 27  | BF    | 175/177 (99%) | 144 (82%) | 24 (14%) | 7 (4%)   | 2           | 9  |
| 27  | DF    | 175/177 (99%) | 137 (78%) | 24 (14%) | 14 (8%)  | 1           | 2  |
| 28  | BG    | 174/176 (99%) | 149 (86%) | 20 (12%) | 5 (3%)   | 3           | 15 |
| 28  | DG    | 174/176 (99%) | 136 (78%) | 29 (17%) | 9 (5%)   | 1           | 5  |
| 29  | BH    | 147/149 (99%) | 89 (60%)  | 37 (25%) | 21 (14%) | 0           | 0  |
| 29  | DH    | 147/149 (99%) | 100 (68%) | 32 (22%) | 15 (10%) | 0           | 1  |
| 30  | BI    | 139/141 (99%) | 85 (61%)  | 36 (26%) | 18 (13%) | 0           | 0  |
| 30  | DI    | 139/141 (99%) | 82 (59%)  | 44 (32%) | 13 (9%)  | 0           | 1  |
| 31  | BJ    | 140/142 (99%) | 129 (92%) | 10 (7%)  | 1 (1%)   | 18          | 48 |
| 31  | DJ    | 140/142 (99%) | 118 (84%) | 17 (12%) | 5 (4%)   | 2           | 11 |
| 32  | BK    | 120/122 (98%) | 99 (82%)  | 15 (12%) | 6 (5%)   | 1           | 6  |
| 32  | DK    | 120/122 (98%) | 100 (83%) | 13 (11%) | 7 (6%)   | 1           | 4  |
| 33  | BL    | 141/143 (99%) | 112 (79%) | 22 (16%) | 7 (5%)   | 1           | 6  |
| 33  | DL    | 141/143 (99%) | 99 (70%)  | 29 (21%) | 13 (9%)  | 0           | 1  |
| 34  | BM    | 134/136 (98%) | 123 (92%) | 9 (7%)   | 2 (2%)   | 8           | 28 |
| 34  | DM    | 134/136 (98%) | 111 (83%) | 15 (11%) | 8 (6%)   | 1           | 4  |
| 35  | BN    | 118/120 (98%) | 104 (88%) | 10 (8%)  | 4 (3%)   | 3           | 12 |
| 35  | DN    | 118/120 (98%) | 94 (80%)  | 16 (14%) | 8 (7%)   | 1           | 2  |
| 36  | BO    | 114/116 (98%) | 87 (76%)  | 21 (18%) | 6 (5%)   | 1           | 5  |
| 36  | DO    | 114/116 (98%) | 85 (75%)  | 22 (19%) | 7 (6%)   | 1           | 4  |
| 37  | BP    | 112/114 (98%) | 99 (88%)  | 9 (8%)   | 4 (4%)   | 2           | 11 |
| 37  | DP    | 112/114 (98%) | 84 (75%)  | 16 (14%) | 12 (11%) | 0           | 1  |
| 38  | BQ    | 115/117 (98%) | 109 (95%) | 4 (4%)   | 2 (2%)   | 7           | 26 |
| 38  | DQ    | 115/117 (98%) | 101 (88%) | 13 (11%) | 1 (1%)   | 14          | 41 |
| 39  | BR    | 101/103 (98%) | 84 (83%)  | 9 (9%)   | 8 (8%)   | 1           | 2  |
| 39  | DR    | 101/103 (98%) | 76 (75%)  | 18 (18%) | 7 (7%)   | 1           | 2  |
| 40  | BS    | 108/110 (98%) | 98 (91%)  | 7 (6%)   | 3 (3%)   | 4           | 15 |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 40  | DS    | 108/110 (98%)     | 88 (82%)   | 12 (11%)   | 8 (7%)   | 1           | 2   |
| 41  | BT    | 91/93 (98%)       | 72 (79%)   | 13 (14%)   | 6 (7%)   | 1           | 3   |
| 41  | DT    | 91/93 (98%)       | 52 (57%)   | 28 (31%)   | 11 (12%) | 0           | 1   |
| 42  | BU    | 100/102 (98%)     | 76 (76%)   | 16 (16%)   | 8 (8%)   | 1           | 2   |
| 42  | DU    | 100/102 (98%)     | 71 (71%)   | 16 (16%)   | 13 (13%) | 0           | 0   |
| 43  | BV    | 92/94 (98%)       | 87 (95%)   | 5 (5%)     | 0        | 100         | 100 |
| 43  | DV    | 92/94 (98%)       | 79 (86%)   | 12 (13%)   | 1 (1%)   | 11          | 36  |
| 44  | BW    | 74/76 (97%)       | 68 (92%)   | 5 (7%)     | 1 (1%)   | 9           | 30  |
| 44  | DW    | 73/76 (96%)       | 63 (86%)   | 8 (11%)    | 2 (3%)   | 4           | 16  |
| 45  | BX    | 75/77 (97%)       | 68 (91%)   | 6 (8%)     | 1 (1%)   | 9           | 32  |
| 45  | DX    | 75/77 (97%)       | 55 (73%)   | 12 (16%)   | 8 (11%)  | 0           | 1   |
| 46  | BY    | 61/63 (97%)       | 47 (77%)   | 7 (12%)    | 7 (12%)  | 0           | 1   |
| 46  | DY    | 61/63 (97%)       | 43 (70%)   | 13 (21%)   | 5 (8%)   | 0           | 2   |
| 47  | BZ    | 56/58 (97%)       | 53 (95%)   | 3 (5%)     | 0        | 100         | 100 |
| 47  | DZ    | 56/58 (97%)       | 47 (84%)   | 6 (11%)    | 3 (5%)   | 1           | 5   |
| 48  | B0    | 54/56 (96%)       | 44 (82%)   | 8 (15%)    | 2 (4%)   | 2           | 11  |
| 48  | D0    | 54/56 (96%)       | 39 (72%)   | 13 (24%)   | 2 (4%)   | 2           | 11  |
| 49  | B1    | 48/50 (96%)       | 39 (81%)   | 5 (10%)    | 4 (8%)   | 0           | 1   |
| 49  | D1    | 48/50 (96%)       | 37 (77%)   | 8 (17%)    | 3 (6%)   | 1           | 3   |
| 50  | B2    | 44/46 (96%)       | 40 (91%)   | 3 (7%)     | 1 (2%)   | 5           | 19  |
| 50  | D2    | 44/46 (96%)       | 33 (75%)   | 8 (18%)    | 3 (7%)   | 1           | 2   |
| 51  | B3    | 62/64 (97%)       | 55 (89%)   | 6 (10%)    | 1 (2%)   | 7           | 27  |
| 51  | D3    | 62/64 (97%)       | 46 (74%)   | 13 (21%)   | 3 (5%)   | 2           | 7   |
| 52  | B4    | 36/38 (95%)       | 33 (92%)   | 3 (8%)     | 0        | 100         | 100 |
| 52  | D4    | 36/38 (95%)       | 33 (92%)   | 2 (6%)     | 1 (3%)   | 4           | 15  |
| 53  | B5    | 183/228 (80%)     | 97 (53%)   | 57 (31%)   | 29 (16%) | 0           | 0   |
| All | All   | 11418/11672 (98%) | 8663 (76%) | 1837 (16%) | 918 (8%) | 1           | 2   |

5 of 918 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 16  | PHE  |
| 2   | AB    | 21  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 22  | TYR  |
| 2   | AB    | 34  | ALA  |
| 2   | AB    | 64  | LYS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | AB    | 180/180 (100%) | 130 (72%) | 50 (28%) | 0           | 1  |
| 2   | CB    | 180/180 (100%) | 135 (75%) | 45 (25%) | 0           | 2  |
| 3   | AC    | 170/170 (100%) | 128 (75%) | 42 (25%) | 1           | 2  |
| 3   | CC    | 170/170 (100%) | 135 (79%) | 35 (21%) | 1           | 4  |
| 4   | AD    | 172/172 (100%) | 138 (80%) | 34 (20%) | 1           | 5  |
| 4   | CD    | 172/172 (100%) | 141 (82%) | 31 (18%) | 2           | 6  |
| 5   | AE    | 113/113 (100%) | 81 (72%)  | 32 (28%) | 0           | 1  |
| 5   | CE    | 113/113 (100%) | 84 (74%)  | 29 (26%) | 0           | 2  |
| 6   | AF    | 87/87 (100%)   | 63 (72%)  | 24 (28%) | 0           | 1  |
| 6   | CF    | 87/87 (100%)   | 61 (70%)  | 26 (30%) | 0           | 1  |
| 7   | AG    | 124/124 (100%) | 89 (72%)  | 35 (28%) | 0           | 1  |
| 7   | CG    | 124/124 (100%) | 91 (73%)  | 33 (27%) | 0           | 1  |
| 8   | AH    | 104/104 (100%) | 82 (79%)  | 22 (21%) | 1           | 4  |
| 8   | CH    | 104/104 (100%) | 79 (76%)  | 25 (24%) | 1           | 2  |
| 9   | AI    | 105/105 (100%) | 76 (72%)  | 29 (28%) | 0           | 1  |
| 9   | CI    | 105/105 (100%) | 79 (75%)  | 26 (25%) | 1           | 2  |
| 10  | AJ    | 86/86 (100%)   | 63 (73%)  | 23 (27%) | 0           | 1  |
| 10  | CJ    | 86/86 (100%)   | 68 (79%)  | 18 (21%) | 1           | 4  |
| 11  | AK    | 90/90 (100%)   | 67 (74%)  | 23 (26%) | 0           | 2  |
| 11  | CK    | 90/90 (100%)   | 64 (71%)  | 26 (29%) | 0           | 1  |
| 12  | AL    | 103/103 (100%) | 90 (87%)  | 13 (13%) | 4           | 14 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12  | CL    | 103/103 (100%) | 82 (80%)  | 21 (20%) | 1           | 4  |
| 13  | AM    | 92/92 (100%)   | 67 (73%)  | 25 (27%) | 0           | 1  |
| 13  | CM    | 92/92 (100%)   | 70 (76%)  | 22 (24%) | 1           | 3  |
| 14  | AN    | 79/83 (95%)    | 65 (82%)  | 14 (18%) | 2           | 6  |
| 14  | CN    | 79/83 (95%)    | 67 (85%)  | 12 (15%) | 3           | 9  |
| 15  | AO    | 75/76 (99%)    | 63 (84%)  | 12 (16%) | 2           | 8  |
| 15  | CO    | 75/76 (99%)    | 58 (77%)  | 17 (23%) | 1           | 3  |
| 16  | AP    | 65/65 (100%)   | 49 (75%)  | 16 (25%) | 1           | 2  |
| 16  | CP    | 65/65 (100%)   | 52 (80%)  | 13 (20%) | 1           | 4  |
| 17  | AQ    | 74/74 (100%)   | 51 (69%)  | 23 (31%) | 0           | 1  |
| 17  | CQ    | 74/74 (100%)   | 49 (66%)  | 25 (34%) | 0           | 0  |
| 18  | AR    | 48/48 (100%)   | 38 (79%)  | 10 (21%) | 1           | 4  |
| 18  | CR    | 48/48 (100%)   | 37 (77%)  | 11 (23%) | 1           | 3  |
| 19  | AS    | 70/70 (100%)   | 55 (79%)  | 15 (21%) | 1           | 4  |
| 19  | CS    | 70/70 (100%)   | 57 (81%)  | 13 (19%) | 1           | 5  |
| 20  | AT    | 65/65 (100%)   | 48 (74%)  | 17 (26%) | 0           | 2  |
| 20  | CT    | 65/65 (100%)   | 47 (72%)  | 18 (28%) | 0           | 1  |
| 21  | AU    | 44/44 (100%)   | 28 (64%)  | 16 (36%) | 0           | 0  |
| 21  | CU    | 44/44 (100%)   | 28 (64%)  | 16 (36%) | 0           | 0  |
| 24  | BC    | 216/216 (100%) | 182 (84%) | 34 (16%) | 2           | 9  |
| 24  | DC    | 216/216 (100%) | 176 (82%) | 40 (18%) | 1           | 5  |
| 25  | BD    | 164/164 (100%) | 147 (90%) | 17 (10%) | 7           | 23 |
| 25  | DD    | 164/164 (100%) | 144 (88%) | 20 (12%) | 5           | 16 |
| 26  | BE    | 165/165 (100%) | 138 (84%) | 27 (16%) | 2           | 8  |
| 26  | DE    | 165/165 (100%) | 139 (84%) | 26 (16%) | 2           | 8  |
| 27  | BF    | 148/148 (100%) | 111 (75%) | 37 (25%) | 0           | 2  |
| 27  | DF    | 148/148 (100%) | 122 (82%) | 26 (18%) | 2           | 6  |
| 28  | BG    | 137/137 (100%) | 124 (90%) | 13 (10%) | 8           | 26 |
| 28  | DG    | 137/137 (100%) | 117 (85%) | 20 (15%) | 3           | 10 |
| 29  | BH    | 114/114 (100%) | 81 (71%)  | 33 (29%) | 0           | 1  |
| 29  | DH    | 114/114 (100%) | 89 (78%)  | 25 (22%) | 1           | 3  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30  | BI    | 109/109 (100%) | 78 (72%)  | 31 (28%) | 0           | 1  |
| 30  | DI    | 109/109 (100%) | 78 (72%)  | 31 (28%) | 0           | 1  |
| 31  | BJ    | 116/116 (100%) | 106 (91%) | 10 (9%)  | 10          | 30 |
| 31  | DJ    | 116/116 (100%) | 97 (84%)  | 19 (16%) | 2           | 8  |
| 32  | BK    | 103/103 (100%) | 92 (89%)  | 11 (11%) | 6           | 22 |
| 32  | DK    | 103/103 (100%) | 94 (91%)  | 9 (9%)   | 9           | 30 |
| 33  | BL    | 102/102 (100%) | 87 (85%)  | 15 (15%) | 3           | 10 |
| 33  | DL    | 102/102 (100%) | 86 (84%)  | 16 (16%) | 2           | 9  |
| 34  | BM    | 109/109 (100%) | 99 (91%)  | 10 (9%)  | 8           | 27 |
| 34  | DM    | 109/109 (100%) | 100 (92%) | 9 (8%)   | 10          | 32 |
| 35  | BN    | 100/100 (100%) | 88 (88%)  | 12 (12%) | 5           | 16 |
| 35  | DN    | 100/100 (100%) | 80 (80%)  | 20 (20%) | 1           | 4  |
| 36  | BO    | 86/86 (100%)   | 68 (79%)  | 18 (21%) | 1           | 4  |
| 36  | DO    | 86/86 (100%)   | 72 (84%)  | 14 (16%) | 2           | 8  |
| 37  | BP    | 99/99 (100%)   | 91 (92%)  | 8 (8%)   | 11          | 33 |
| 37  | DP    | 99/99 (100%)   | 80 (81%)  | 19 (19%) | 1           | 5  |
| 38  | BQ    | 89/89 (100%)   | 79 (89%)  | 10 (11%) | 6           | 19 |
| 38  | DQ    | 89/89 (100%)   | 77 (86%)  | 12 (14%) | 4           | 12 |
| 39  | BR    | 84/84 (100%)   | 69 (82%)  | 15 (18%) | 2           | 6  |
| 39  | DR    | 84/84 (100%)   | 70 (83%)  | 14 (17%) | 2           | 7  |
| 40  | BS    | 93/93 (100%)   | 78 (84%)  | 15 (16%) | 2           | 8  |
| 40  | DS    | 93/93 (100%)   | 75 (81%)  | 18 (19%) | 1           | 5  |
| 41  | BT    | 80/80 (100%)   | 64 (80%)  | 16 (20%) | 1           | 4  |
| 41  | DT    | 80/80 (100%)   | 65 (81%)  | 15 (19%) | 1           | 5  |
| 42  | BU    | 83/83 (100%)   | 69 (83%)  | 14 (17%) | 2           | 7  |
| 42  | DU    | 83/83 (100%)   | 65 (78%)  | 18 (22%) | 1           | 3  |
| 43  | BV    | 78/78 (100%)   | 66 (85%)  | 12 (15%) | 2           | 9  |
| 43  | DV    | 78/78 (100%)   | 65 (83%)  | 13 (17%) | 2           | 7  |
| 44  | BW    | 57/58 (98%)    | 50 (88%)  | 7 (12%)  | 4           | 15 |
| 44  | DW    | 56/58 (97%)    | 51 (91%)  | 5 (9%)   | 9           | 28 |
| 45  | BX    | 67/67 (100%)   | 55 (82%)  | 12 (18%) | 2           | 6  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 45  | DX    | 67/67 (100%)    | 51 (76%)   | 16 (24%)   | 1           | 3  |
| 46  | BY    | 55/55 (100%)    | 47 (86%)   | 8 (14%)    | 3           | 10 |
| 46  | DY    | 55/55 (100%)    | 40 (73%)   | 15 (27%)   | 0           | 1  |
| 47  | BZ    | 48/48 (100%)    | 42 (88%)   | 6 (12%)    | 4           | 15 |
| 47  | DZ    | 48/48 (100%)    | 33 (69%)   | 15 (31%)   | 0           | 1  |
| 48  | B0    | 47/47 (100%)    | 41 (87%)   | 6 (13%)    | 4           | 14 |
| 48  | D0    | 47/47 (100%)    | 42 (89%)   | 5 (11%)    | 6           | 22 |
| 49  | B1    | 45/45 (100%)    | 35 (78%)   | 10 (22%)   | 1           | 3  |
| 49  | D1    | 45/45 (100%)    | 40 (89%)   | 5 (11%)    | 6           | 20 |
| 50  | B2    | 38/38 (100%)    | 34 (90%)   | 4 (10%)    | 6           | 22 |
| 50  | D2    | 38/38 (100%)    | 30 (79%)   | 8 (21%)    | 1           | 4  |
| 51  | B3    | 51/51 (100%)    | 47 (92%)   | 4 (8%)     | 11          | 35 |
| 51  | D3    | 51/51 (100%)    | 44 (86%)   | 7 (14%)    | 3           | 12 |
| 52  | B4    | 34/34 (100%)    | 27 (79%)   | 7 (21%)    | 1           | 4  |
| 52  | D4    | 34/34 (100%)    | 30 (88%)   | 4 (12%)    | 5           | 17 |
| 53  | B5    | 61/180 (34%)    | 45 (74%)   | 16 (26%)   | 0           | 2  |
| All | All   | 9386/9518 (99%) | 7547 (80%) | 1839 (20%) | 1           | 5  |

5 of 1839 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 67  | ILE  |
| 45  | DX    | 46  | PHE  |
| 9   | CI    | 46  | MET  |
| 43  | DV    | 53  | LYS  |
| 33  | DL    | 82  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | CM    | 100 | GLN  |
| 24  | DC    | 90  | ASN  |
| 51  | D3    | 31  | HIS  |
| 15  | CO    | 46  | HIS  |
| 20  | CT    | 52  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1537/1539 (99%) | 322 (20%)         | 13 (0%)         |
| 1   | CA    | 1538/1539 (99%) | 312 (20%)         | 8 (0%)          |
| 22  | BA    | 2895/2903 (99%) | 516 (17%)         | 22 (0%)         |
| 22  | DA    | 2895/2903 (99%) | 635 (21%)         | 23 (0%)         |
| 23  | BB    | 118/119 (99%)   | 18 (15%)          | 0               |
| 23  | DB    | 117/119 (98%)   | 22 (18%)          | 0               |
| All | All   | 9100/9122 (99%) | 1825 (20%)        | 66 (0%)         |

5 of 1825 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 4   | U    |
| 1   | AA    | 5   | U    |
| 1   | AA    | 6   | G    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 13  | U    |

5 of 66 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 2162 | G    |
| 22  | DA    | 2225 | A    |
| 22  | DA    | 2873 | A    |
| 22  | BA    | 1344 | U    |
| 22  | BA    | 1180 | U    |

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 502 ligands modelled in this entry, 500 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$ |
| 55  | VIR  | BA    | 3001 | -    | 38,40,40     | 3.98 | 16 (42%)    | 42,55,55    | 3.57 | 22 (52%)    |
| 55  | VIR  | DA    | 3001 | -    | 38,40,40     | 3.92 | 16 (42%)    | 42,55,55    | 3.22 | 18 (42%)    |

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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 55  | VIR  | BA    | 3001 | -    | -       | 11/48/58/58 | 0/2/3/3 |
| 55  | VIR  | DA    | 3001 | -    | -       | 13/48/58/58 | 0/2/3/3 |

The worst 5 of 32 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | BA    | 3001 | VIR  | C28-C29 | 10.26 | 1.55        | 1.32     |
| 55  | DA    | 3001 | VIR  | C28-C29 | 9.95  | 1.54        | 1.32     |
| 55  | BA    | 3001 | VIR  | C12-C8  | 9.40  | 1.44        | 1.34     |
| 55  | BA    | 3001 | VIR  | C22-C23 | 8.79  | 1.56        | 1.32     |
| 55  | DA    | 3001 | VIR  | C22-C23 | 8.58  | 1.55        | 1.32     |

The worst 5 of 40 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55  | DA    | 3001 | VIR  | C23-C22-C20 | -9.51 | 111.52      | 125.89   |
| 55  | BA    | 3001 | VIR  | C23-C22-C20 | -8.91 | 112.42      | 125.89   |
| 55  | BA    | 3001 | VIR  | C37-C1-N5   | -7.73 | 113.59      | 123.34   |
| 55  | BA    | 3001 | VIR  | C29-C28-C26 | -7.60 | 104.80      | 122.67   |
| 55  | BA    | 3001 | VIR  | O11-C10-C13 | 7.31  | 124.46      | 117.70   |

There are no chirality outliers.

5 of 24 torsion outliers are listed below:



| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 55  | BA    | 3001 | VIR  | C2-C1-C37-O36   |
| 55  | BA    | 3001 | VIR  | C17-C19-C20-C21 |
| 55  | BA    | 3001 | VIR  | C20-C22-C23-C24 |
| 55  | DA    | 3001 | VIR  | C17-C19-C20-C21 |
| 55  | DA    | 3001 | VIR  | C17-C19-C20-C22 |

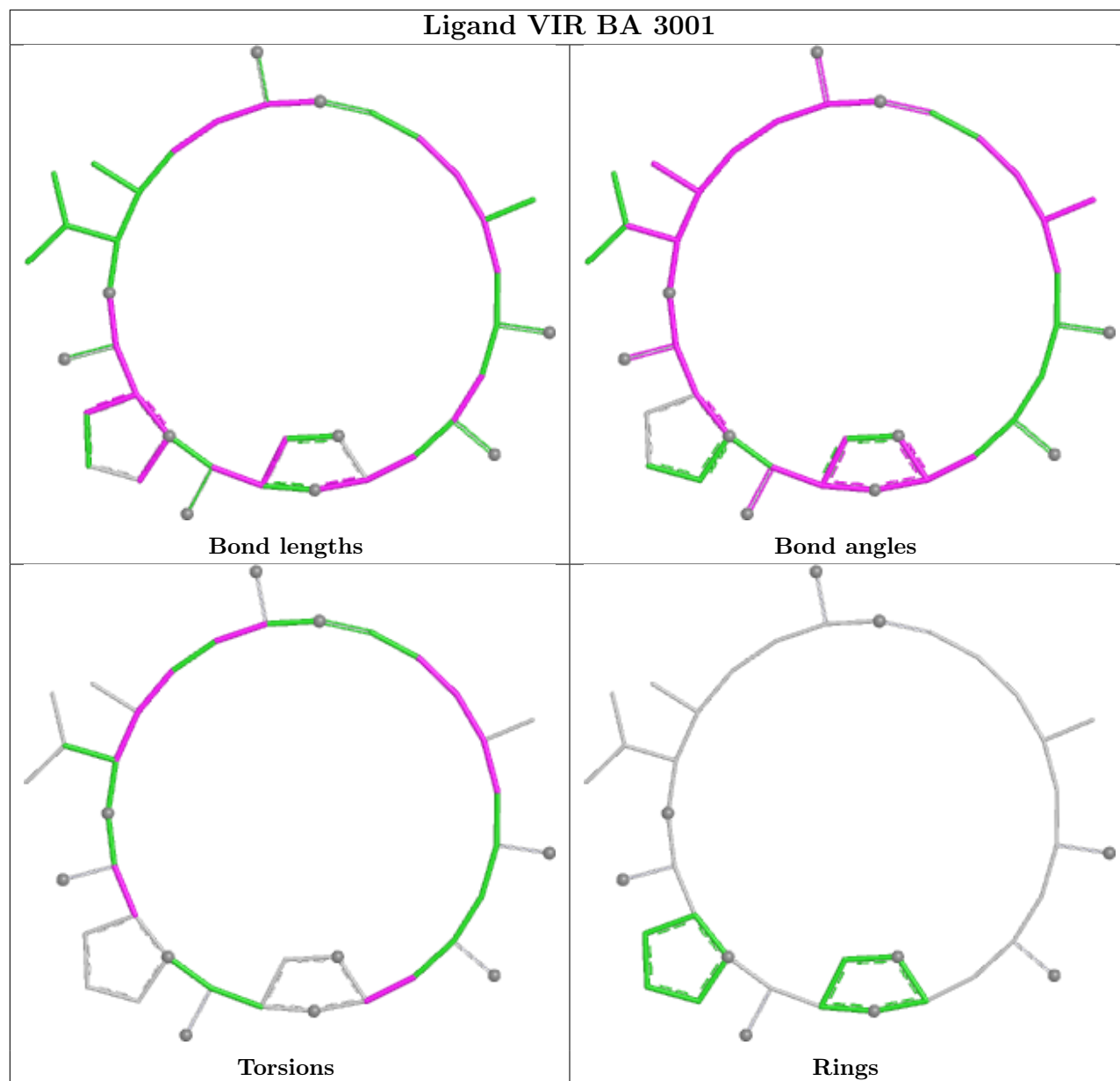
There are no ring outliers.

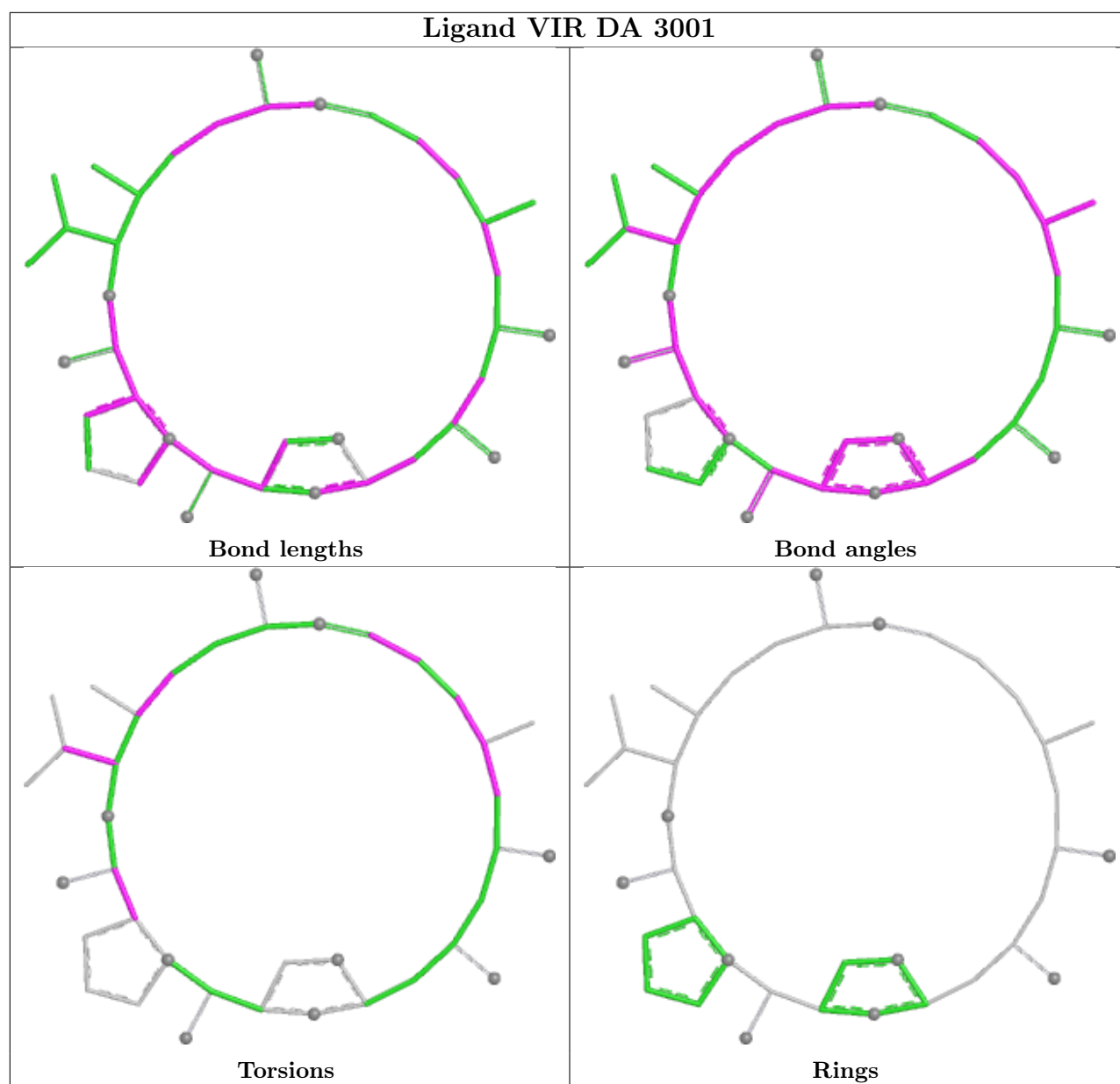
2 monomers are involved in 20 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55  | BA    | 3001 | VIR  | 5       | 0            |
| 55  | DA    | 3001 | VIR  | 15      | 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.

## Ligand VIR BA 3001





## 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    | 1538/1539 (99%)  | 0.05   | 40 (2%) 57 48 | 12, 51, 134, 181      | 0     |
| 1   | CA    | 1539/1539 (100%) | 0.49   | 91 (5%) 28 22 | 25, 70, 145, 177      | 0     |
| 2   | AB    | 218/218 (100%)   | 0.74   | 19 (8%) 16 13 | 38, 75, 100, 123      | 0     |
| 2   | CB    | 218/218 (100%)   | 1.23   | 45 (20%) 2 2  | 61, 87, 107, 126      | 0     |
| 3   | AC    | 206/206 (100%)   | 0.40   | 7 (3%) 48 39  | 35, 57, 78, 93        | 0     |
| 3   | CC    | 206/206 (100%)   | 0.88   | 20 (9%) 13 11 | 51, 80, 95, 105       | 0     |
| 4   | AD    | 205/205 (100%)   | 0.63   | 12 (5%) 28 22 | 33, 56, 78, 104       | 0     |
| 4   | CD    | 205/205 (100%)   | 0.37   | 14 (6%) 23 18 | 17, 38, 63, 87        | 0     |
| 5   | AE    | 150/150 (100%)   | 0.54   | 8 (5%) 32 25  | 32, 48, 79, 101       | 0     |
| 5   | CE    | 150/150 (100%)   | 0.79   | 14 (9%) 14 12 | 30, 56, 82, 103       | 0     |
| 6   | AF    | 100/100 (100%)   | 0.50   | 5 (5%) 34 27  | 34, 57, 73, 87        | 0     |
| 6   | CF    | 100/100 (100%)   | 0.75   | 11 (11%) 10 9 | 45, 74, 94, 105       | 0     |
| 7   | AG    | 151/151 (100%)   | 1.00   | 22 (14%) 6 4  | 54, 77, 96, 102       | 0     |
| 7   | CG    | 151/151 (100%)   | 1.85   | 58 (38%) 1 0  | 82, 101, 110, 115     | 0     |
| 8   | AH    | 129/129 (100%)   | 0.28   | 4 (3%) 51 42  | 31, 49, 66, 75        | 0     |
| 8   | CH    | 129/129 (100%)   | 0.76   | 9 (6%) 22 18  | 50, 65, 81, 92        | 0     |
| 9   | AI    | 127/127 (100%)   | 1.11   | 19 (14%) 5 4  | 44, 74, 96, 110       | 0     |
| 9   | CI    | 127/127 (100%)   | 1.79   | 51 (40%) 0 0  | 73, 94, 111, 122      | 0     |
| 10  | AJ    | 98/98 (100%)     | 1.04   | 14 (14%) 6 5  | 39, 66, 92, 122       | 0     |
| 10  | CJ    | 98/98 (100%)     | 2.00   | 40 (40%) 0 0  | 71, 95, 111, 126      | 0     |
| 11  | AK    | 117/117 (100%)   | 0.70   | 7 (5%) 27 21  | 26, 65, 92, 117       | 0     |
| 11  | CK    | 117/117 (100%)   | 0.52   | 3 (2%) 57 48  | 38, 67, 80, 92        | 0     |
| 12  | AL    | 123/123 (100%)   | 0.33   | 7 (5%) 29 23  | 21, 35, 64, 98        | 0     |
| 12  | CL    | 123/123 (100%)   | 0.89   | 19 (15%) 5 4  | 36, 52, 78, 99        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13  | AM    | 114/114 (100%)  | 0.83   | 12 (10%) 11 10 | 48, 69, 94, 103       | 0     |
| 13  | CM    | 114/114 (100%)  | 2.34   | 68 (59%) 0 0   | 97, 109, 118, 119     | 0     |
| 14  | AN    | 96/100 (96%)    | 1.02   | 15 (15%) 5 4   | 41, 61, 94, 103       | 0     |
| 14  | CN    | 96/100 (96%)    | 1.89   | 39 (40%) 0 0   | 70, 95, 113, 120      | 0     |
| 15  | AO    | 88/88 (100%)    | 0.57   | 5 (5%) 29 23   | 28, 51, 65, 89        | 0     |
| 15  | CO    | 88/88 (100%)    | 0.56   | 1 (1%) 78 71   | 40, 63, 81, 98        | 0     |
| 16  | AP    | 82/82 (100%)    | 0.74   | 8 (9%) 13 11   | 33, 47, 85, 101       | 0     |
| 16  | CP    | 82/82 (100%)    | 1.12   | 11 (13%) 7 5   | 44, 61, 89, 106       | 0     |
| 17  | AQ    | 80/80 (100%)    | 0.71   | 7 (8%) 15 13   | 28, 52, 77, 122       | 0     |
| 17  | CQ    | 80/80 (100%)    | 1.43   | 24 (30%) 1 1   | 44, 76, 98, 103       | 0     |
| 18  | AR    | 55/55 (100%)    | 0.52   | 3 (5%) 30 24   | 39, 52, 79, 108       | 0     |
| 18  | CR    | 55/55 (100%)    | 0.60   | 2 (3%) 46 38   | 39, 55, 79, 111       | 0     |
| 19  | AS    | 79/79 (100%)    | 0.88   | 8 (10%) 12 10  | 54, 69, 89, 101       | 0     |
| 19  | CS    | 79/79 (100%)    | 2.46   | 56 (70%) 0 0   | 90, 110, 119, 125     | 0     |
| 20  | AT    | 85/85 (100%)    | 0.78   | 9 (10%) 11 9   | 35, 48, 71, 101       | 0     |
| 20  | CT    | 85/85 (100%)    | 1.25   | 16 (18%) 3 3   | 55, 74, 92, 99        | 0     |
| 21  | AU    | 51/51 (100%)    | 1.57   | 12 (23%) 2 2   | 46, 75, 97, 106       | 0     |
| 21  | CU    | 51/51 (100%)    | 1.76   | 15 (29%) 1 1   | 45, 72, 97, 105       | 0     |
| 22  | BA    | 2897/2903 (99%) | -0.38  | 139 (4%) 35 28 | 1, 15, 131, 195       | 0     |
| 22  | DA    | 2897/2903 (99%) | 0.86   | 185 (6%) 25 20 | 40, 82, 146, 181      | 0     |
| 23  | BB    | 119/119 (100%)  | -0.57  | 0 100 100      | 3, 25, 52, 85         | 0     |
| 23  | DB    | 118/119 (99%)   | 0.73   | 4 (3%) 48 39   | 67, 112, 133, 144     | 0     |
| 24  | BC    | 271/271 (100%)  | -0.09  | 6 (2%) 62 53   | 5, 21, 36, 54         | 0     |
| 24  | DC    | 271/271 (100%)  | 1.16   | 52 (19%) 3 2   | 43, 62, 77, 90        | 0     |
| 25  | BD    | 209/209 (100%)  | -0.31  | 0 100 100      | 1, 11, 35, 68         | 0     |
| 25  | DD    | 209/209 (100%)  | 1.21   | 40 (19%) 3 2   | 49, 68, 84, 96        | 0     |
| 26  | BE    | 201/201 (100%)  | -0.20  | 1 (0%) 87 83   | 1, 23, 53, 91         | 0     |
| 26  | DE    | 201/201 (100%)  | 1.59   | 66 (32%) 1 1   | 46, 85, 102, 109      | 0     |
| 27  | BF    | 177/177 (100%)  | 0.42   | 4 (2%) 61 52   | 24, 43, 77, 90        | 0     |
| 27  | DF    | 177/177 (100%)  | 1.43   | 43 (24%) 2 1   | 91, 108, 120, 126     | 0     |
| 28  | BG    | 176/176 (100%)  | 0.01   | 3 (1%) 69 61   | 17, 38, 62, 83        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | DG    | 176/176 (100%) | 1.41   | 40 (22%) 2 2  | 72, 94, 106, 116      | 0     |
| 29  | BH    | 149/149 (100%) | 2.48   | 90 (60%) 0 0  | 25, 102, 121, 129     | 0     |
| 29  | DH    | 149/149 (100%) | 2.53   | 100 (67%) 0 0 | 25, 92, 107, 115      | 0     |
| 30  | BI    | 141/141 (100%) | 2.63   | 90 (63%) 0 0  | 90, 112, 122, 133     | 0     |
| 30  | DI    | 141/141 (100%) | 2.61   | 93 (65%) 0 0  | 102, 119, 129, 132    | 0     |
| 31  | BJ    | 142/142 (100%) | -0.35  | 2 (1%) 73 65  | 2, 7, 21, 37          | 0     |
| 31  | DJ    | 142/142 (100%) | 0.89   | 18 (12%) 8 6  | 50, 66, 79, 94        | 0     |
| 32  | BK    | 122/122 (100%) | -0.30  | 1 (0%) 82 77  | 4, 13, 32, 69         | 0     |
| 32  | DK    | 122/122 (100%) | 0.99   | 15 (12%) 8 7  | 47, 64, 83, 97        | 0     |
| 33  | BL    | 143/143 (100%) | -0.06  | 0 100 100     | 1, 18, 44, 73         | 0     |
| 33  | DL    | 143/143 (100%) | 1.69   | 45 (31%) 1 1  | 46, 80, 95, 115       | 0     |
| 34  | BM    | 136/136 (100%) | -0.38  | 1 (0%) 84 79  | 2, 11, 31, 83         | 0     |
| 34  | DM    | 136/136 (100%) | 0.83   | 9 (6%) 24 19  | 42, 69, 82, 101       | 0     |
| 35  | BN    | 120/120 (100%) | -0.39  | 0 100 100     | 3, 8, 19, 53          | 0     |
| 35  | DN    | 120/120 (100%) | 1.77   | 42 (35%) 1 1  | 56, 76, 89, 116       | 0     |
| 36  | BO    | 116/116 (100%) | -0.12  | 0 100 100     | 12, 27, 45, 52        | 0     |
| 36  | DO    | 116/116 (100%) | 1.21   | 17 (14%) 6 4  | 81, 95, 105, 115      | 0     |
| 37  | BP    | 114/114 (100%) | -0.27  | 0 100 100     | 7, 18, 43, 66         | 0     |
| 37  | DP    | 114/114 (100%) | 1.21   | 19 (16%) 4 3  | 58, 70, 85, 93        | 0     |
| 38  | BQ    | 117/117 (100%) | -0.45  | 0 100 100     | 1, 4, 15, 30          | 0     |
| 38  | DQ    | 117/117 (100%) | 1.34   | 26 (22%) 2 2  | 54, 67, 79, 83        | 0     |
| 39  | BR    | 103/103 (100%) | -0.22  | 1 (0%) 79 73  | 1, 13, 33, 67         | 0     |
| 39  | DR    | 103/103 (100%) | 1.30   | 20 (19%) 3 2  | 52, 78, 88, 99        | 0     |
| 40  | BS    | 110/110 (100%) | -0.38  | 1 (0%) 81 75  | 1, 5, 24, 79          | 0     |
| 40  | DS    | 110/110 (100%) | 1.57   | 30 (27%) 1 1  | 57, 75, 89, 101       | 0     |
| 41  | BT    | 93/93 (100%)   | 0.28   | 5 (5%) 31 24  | 8, 26, 75, 104        | 0     |
| 41  | DT    | 93/93 (100%)   | 2.09   | 44 (47%) 0 0  | 68, 87, 103, 119      | 0     |
| 42  | BU    | 102/102 (100%) | -0.08  | 1 (0%) 79 73  | 14, 29, 63, 92        | 0     |
| 42  | DU    | 102/102 (100%) | 2.11   | 47 (46%) 0 0  | 75, 92, 111, 120      | 0     |
| 43  | BV    | 94/94 (100%)   | -0.28  | 0 100 100     | 6, 20, 41, 55         | 0     |
| 43  | DV    | 94/94 (100%)   | 0.83   | 3 (3%) 50 41  | 70, 85, 96, 104       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | BW    | 76/76 (100%)      | -0.10  | 1 (1%) 75 67   | 7, 13, 29, 53         | 0     |
| 44  | DW    | 75/76 (98%)       | 1.60   | 20 (26%) 1 1   | 61, 80, 90, 104       | 0     |
| 45  | BX    | 77/77 (100%)      | 0.02   | 1 (1%) 75 67   | 7, 23, 51, 72         | 0     |
| 45  | DX    | 77/77 (100%)      | 1.60   | 23 (29%) 1 1   | 52, 70, 84, 88        | 0     |
| 46  | BY    | 63/63 (100%)      | 0.40   | 6 (9%) 14 11   | 21, 39, 72, 94        | 0     |
| 46  | DY    | 63/63 (100%)      | 1.92   | 26 (41%) 0 0   | 78, 95, 102, 106      | 0     |
| 47  | BZ    | 58/58 (100%)      | -0.27  | 0 100 100      | 1, 8, 24, 41          | 0     |
| 47  | DZ    | 58/58 (100%)      | 1.14   | 8 (13%) 6 5    | 58, 71, 82, 95        | 0     |
| 48  | B0    | 56/56 (100%)      | -0.37  | 0 100 100      | 1, 12, 36, 69         | 0     |
| 48  | D0    | 56/56 (100%)      | 1.42   | 12 (21%) 2 2   | 58, 79, 92, 102       | 0     |
| 49  | B1    | 50/50 (100%)      | 0.11   | 2 (4%) 42 34   | 18, 29, 48, 76        | 0     |
| 49  | D1    | 50/50 (100%)      | 1.57   | 17 (34%) 1 1   | 70, 86, 94, 105       | 0     |
| 50  | B2    | 46/46 (100%)      | -0.30  | 1 (2%) 62 53   | 4, 9, 15, 86          | 0     |
| 50  | D2    | 46/46 (100%)      | 1.99   | 20 (43%) 0 0   | 55, 69, 80, 102       | 0     |
| 51  | B3    | 64/64 (100%)      | -0.24  | 0 100 100      | 5, 10, 20, 33         | 0     |
| 51  | D3    | 64/64 (100%)      | 2.10   | 31 (48%) 0 0   | 58, 71, 79, 82        | 0     |
| 52  | B4    | 38/38 (100%)      | -0.11  | 0 100 100      | 8, 18, 37, 53         | 0     |
| 52  | D4    | 38/38 (100%)      | 1.73   | 13 (34%) 1 1   | 59, 75, 87, 101       | 0     |
| 53  | B5    | 191/228 (83%)     | 2.34   | 117 (61%) 0 0  | 101, 117, 128, 136    | 0     |
| All | All   | 20734/20794 (99%) | 0.60   | 2451 (11%) 9 7 | 1, 63, 121, 195       | 0     |

The worst 5 of 2451 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | CD    | 25   | VAL  | 10.1 |
| 30  | BI    | 53   | LEU  | 9.6  |
| 22  | BA    | 2184 | A    | 8.8  |
| 22  | BA    | 2185 | U    | 8.5  |
| 22  | BA    | 2140 | G    | 8.4  |

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

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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54  | MG   | DA    | 3136 | 1/1   | 0.01 | 0.35 | 90,90,90,90                | 0     |
| 54  | MG   | DA    | 3134 | 1/1   | 0.12 | 0.39 | 105,105,105,105            | 0     |
| 54  | MG   | DA    | 3114 | 1/1   | 0.32 | 0.21 | 85,85,85,85                | 0     |
| 54  | MG   | DA    | 3027 | 1/1   | 0.34 | 0.48 | 98,98,98,98                | 0     |
| 54  | MG   | DA    | 3062 | 1/1   | 0.43 | 0.61 | 110,110,110,110            | 0     |
| 54  | MG   | AA    | 1659 | 1/1   | 0.43 | 0.56 | 77,77,77,77                | 0     |
| 54  | MG   | DA    | 3094 | 1/1   | 0.48 | 0.24 | 101,101,101,101            | 0     |
| 54  | MG   | DA    | 3132 | 1/1   | 0.48 | 0.32 | 93,93,93,93                | 0     |
| 54  | MG   | CA    | 1630 | 1/1   | 0.52 | 0.19 | 111,111,111,111            | 0     |
| 54  | MG   | DA    | 3061 | 1/1   | 0.55 | 0.26 | 85,85,85,85                | 0     |
| 54  | MG   | DA    | 3057 | 1/1   | 0.56 | 0.28 | 87,87,87,87                | 0     |
| 54  | MG   | AA    | 1657 | 1/1   | 0.57 | 0.31 | 68,68,68,68                | 0     |
| 54  | MG   | BA    | 3056 | 1/1   | 0.59 | 0.36 | 53,53,53,53                | 0     |
| 54  | MG   | DA    | 3120 | 1/1   | 0.60 | 0.27 | 102,102,102,102            | 0     |
| 54  | MG   | BA    | 3016 | 1/1   | 0.61 | 0.26 | 65,65,65,65                | 0     |
| 54  | MG   | DA    | 3042 | 1/1   | 0.63 | 0.29 | 64,64,64,64                | 0     |
| 54  | MG   | AA    | 1667 | 1/1   | 0.63 | 0.15 | 66,66,66,66                | 0     |
| 54  | MG   | DA    | 3078 | 1/1   | 0.63 | 0.27 | 89,89,89,89                | 0     |
| 54  | MG   | DA    | 3041 | 1/1   | 0.65 | 0.19 | 89,89,89,89                | 0     |
| 54  | MG   | DA    | 3159 | 1/1   | 0.66 | 0.13 | 68,68,68,68                | 0     |
| 54  | MG   | DA    | 3093 | 1/1   | 0.67 | 0.22 | 108,108,108,108            | 0     |
| 54  | MG   | DA    | 3139 | 1/1   | 0.67 | 0.32 | 49,49,49,49                | 0     |
| 54  | MG   | CA    | 1636 | 1/1   | 0.67 | 0.16 | 118,118,118,118            | 0     |
| 54  | MG   | AA    | 1634 | 1/1   | 0.68 | 0.25 | 74,74,74,74                | 0     |
| 54  | MG   | DQ    | 201  | 1/1   | 0.69 | 0.22 | 53,53,53,53                | 0     |
| 54  | MG   | CA    | 1635 | 1/1   | 0.70 | 0.12 | 123,123,123,123            | 0     |
| 54  | MG   | DA    | 3045 | 1/1   | 0.72 | 0.15 | 102,102,102,102            | 0     |
| 54  | MG   | DA    | 3148 | 1/1   | 0.72 | 0.11 | 58,58,58,58                | 0     |
| 54  | MG   | CA    | 1646 | 1/1   | 0.72 | 0.21 | 66,66,66,66                | 0     |
| 54  | MG   | AA    | 1646 | 1/1   | 0.72 | 0.12 | 53,53,53,53                | 0     |
| 54  | MG   | CA    | 1644 | 1/1   | 0.73 | 0.21 | 54,54,54,54                | 0     |
| 54  | MG   | DA    | 3156 | 1/1   | 0.74 | 0.24 | 64,64,64,64                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1611 | 1/1   | 0.75 | 0.13 | 85,85,85,85                 | 0     |
| 54  | MG   | AA    | 1658 | 1/1   | 0.75 | 0.15 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3033 | 1/1   | 0.76 | 0.28 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3036 | 1/1   | 0.76 | 0.16 | 78,78,78,78                 | 0     |
| 54  | MG   | CA    | 1628 | 1/1   | 0.76 | 0.10 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3121 | 1/1   | 0.77 | 0.17 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3059 | 1/1   | 0.77 | 0.19 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3137 | 1/1   | 0.77 | 0.29 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3149 | 1/1   | 0.78 | 0.23 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3125 | 1/1   | 0.78 | 0.24 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3009 | 1/1   | 0.78 | 0.24 | 82,82,82,82                 | 0     |
| 54  | MG   | DA    | 3017 | 1/1   | 0.78 | 0.19 | 90,90,90,90                 | 0     |
| 54  | MG   | DA    | 3100 | 1/1   | 0.79 | 0.20 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3162 | 1/1   | 0.79 | 0.12 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3072 | 1/1   | 0.79 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3005 | 1/1   | 0.80 | 0.17 | 96,96,96,96                 | 0     |
| 54  | MG   | AA    | 1671 | 1/1   | 0.80 | 0.38 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3136 | 1/1   | 0.80 | 0.15 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3113 | 1/1   | 0.80 | 0.11 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1648 | 1/1   | 0.80 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3165 | 1/1   | 0.80 | 0.18 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1633 | 1/1   | 0.80 | 0.26 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3096 | 1/1   | 0.81 | 0.12 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3127 | 1/1   | 0.81 | 0.17 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3074 | 1/1   | 0.81 | 0.09 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3058 | 1/1   | 0.81 | 0.36 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3153 | 1/1   | 0.81 | 0.35 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3014 | 1/1   | 0.82 | 0.13 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3063 | 1/1   | 0.82 | 0.21 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3029 | 1/1   | 0.82 | 0.25 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3145 | 1/1   | 0.82 | 0.16 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3138 | 1/1   | 0.83 | 0.28 | 46,46,46,46                 | 0     |
| 54  | MG   | AA    | 1618 | 1/1   | 0.83 | 0.25 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3164 | 1/1   | 0.83 | 0.16 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3028 | 1/1   | 0.83 | 0.11 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3146 | 1/1   | 0.83 | 0.09 | 62,62,62,62                 | 0     |
| 54  | MG   | DA    | 3050 | 1/1   | 0.84 | 0.15 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3030 | 1/1   | 0.84 | 0.11 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3101 | 1/1   | 0.84 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3161 | 1/1   | 0.84 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 3158 | 1/1   | 0.85 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3077 | 1/1   | 0.85 | 0.22 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3003 | 1/1   | 0.85 | 0.18 | 95,95,95,95                 | 0     |
| 54  | MG   | BA    | 3147 | 1/1   | 0.85 | 0.26 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3152 | 1/1   | 0.85 | 0.20 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3143 | 1/1   | 0.85 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | AA    | 1664 | 1/1   | 0.85 | 0.11 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3048 | 1/1   | 0.86 | 0.13 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3083 | 1/1   | 0.86 | 0.22 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3007 | 1/1   | 0.86 | 0.10 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3085 | 1/1   | 0.86 | 0.14 | 30,30,30,30                 | 0     |
| 54  | MG   | AA    | 1651 | 1/1   | 0.86 | 0.30 | 52,52,52,52                 | 0     |
| 54  | MG   | AA    | 1643 | 1/1   | 0.86 | 0.18 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3020 | 1/1   | 0.86 | 0.13 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3041 | 1/1   | 0.86 | 0.29 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3190 | 1/1   | 0.86 | 0.19 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3193 | 1/1   | 0.86 | 0.07 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1656 | 1/1   | 0.86 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3081 | 1/1   | 0.87 | 0.10 | 83,83,83,83                 | 0     |
| 54  | MG   | BA    | 3159 | 1/1   | 0.87 | 0.11 | 21,21,21,21                 | 0     |
| 54  | MG   | CA    | 1629 | 1/1   | 0.87 | 0.09 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3071 | 1/1   | 0.87 | 0.08 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3099 | 1/1   | 0.87 | 0.10 | 62,62,62,62                 | 0     |
| 54  | MG   | CA    | 1649 | 1/1   | 0.87 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | AA    | 1669 | 1/1   | 0.87 | 0.15 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3133 | 1/1   | 0.87 | 0.21 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3110 | 1/1   | 0.87 | 0.16 | 46,46,46,46                 | 0     |
| 54  | MG   | CA    | 1648 | 1/1   | 0.88 | 0.18 | 25,25,25,25                 | 0     |
| 54  | MG   | AA    | 1662 | 1/1   | 0.88 | 0.14 | 51,51,51,51                 | 0     |
| 54  | MG   | AA    | 1614 | 1/1   | 0.88 | 0.15 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1665 | 1/1   | 0.88 | 0.12 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3189 | 1/1   | 0.88 | 0.23 | 38,38,38,38                 | 0     |
| 54  | MG   | CA    | 1645 | 1/1   | 0.88 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3073 | 1/1   | 0.88 | 0.15 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3104 | 1/1   | 0.88 | 0.10 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1661 | 1/1   | 0.88 | 0.12 | 43,43,43,43                 | 0     |
| 54  | MG   | CA    | 1631 | 1/1   | 0.89 | 0.13 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3099 | 1/1   | 0.89 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3113 | 1/1   | 0.89 | 0.07 | 14,14,14,14                 | 0     |
| 54  | MG   | AA    | 1650 | 1/1   | 0.89 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1660 | 1/1   | 0.89 | 0.17 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3138 | 1/1   | 0.89 | 0.27 | 7,7,7,7                     | 0     |
| 54  | MG   | BA    | 3084 | 1/1   | 0.89 | 0.15 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3137 | 1/1   | 0.89 | 0.12 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1647 | 1/1   | 0.89 | 0.19 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3019 | 1/1   | 0.89 | 0.09 | 84,84,84,84                 | 0     |
| 54  | MG   | AA    | 1652 | 1/1   | 0.89 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3144 | 1/1   | 0.89 | 0.11 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3087 | 1/1   | 0.89 | 0.09 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3187 | 1/1   | 0.90 | 0.16 | 30,30,30,30                 | 0     |
| 54  | MG   | DA    | 3117 | 1/1   | 0.90 | 0.18 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3048 | 1/1   | 0.90 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1638 | 1/1   | 0.90 | 0.08 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1655 | 1/1   | 0.90 | 0.13 | 44,44,44,44                 | 0     |
| 54  | MG   | CA    | 1641 | 1/1   | 0.90 | 0.19 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3129 | 1/1   | 0.90 | 0.10 | 81,81,81,81                 | 0     |
| 54  | MG   | CA    | 1642 | 1/1   | 0.90 | 0.17 | 26,26,26,26                 | 0     |
| 54  | MG   | DA    | 3154 | 1/1   | 0.90 | 0.17 | 42,42,42,42                 | 0     |
| 54  | MG   | CA    | 1643 | 1/1   | 0.90 | 0.17 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1605 | 1/1   | 0.90 | 0.13 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3065 | 1/1   | 0.90 | 0.14 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3160 | 1/1   | 0.90 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3134 | 1/1   | 0.90 | 0.22 | 47,47,47,47                 | 0     |
| 54  | MG   | CA    | 1615 | 1/1   | 0.90 | 0.12 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3163 | 1/1   | 0.90 | 0.30 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3088 | 1/1   | 0.90 | 0.11 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 3140 | 1/1   | 0.90 | 0.22 | 34,34,34,34                 | 0     |
| 54  | MG   | DA    | 3167 | 1/1   | 0.90 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3141 | 1/1   | 0.90 | 0.17 | 40,40,40,40                 | 0     |
| 55  | VIR  | DA    | 3001 | 38/38 | 0.90 | 0.14 | 27,39,47,53                 | 0     |
| 54  | MG   | DA    | 3058 | 1/1   | 0.91 | 0.08 | 75,75,75,75                 | 0     |
| 54  | MG   | BA    | 3061 | 1/1   | 0.91 | 0.28 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3095 | 1/1   | 0.91 | 0.07 | 84,84,84,84                 | 0     |
| 54  | MG   | DA    | 3011 | 1/1   | 0.91 | 0.08 | 57,57,57,57                 | 0     |
| 54  | MG   | AA    | 1631 | 1/1   | 0.91 | 0.10 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3157 | 1/1   | 0.91 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3016 | 1/1   | 0.91 | 0.10 | 75,75,75,75                 | 0     |
| 54  | MG   | AA    | 1602 | 1/1   | 0.91 | 0.23 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1635 | 1/1   | 0.91 | 0.14 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3124 | 1/1   | 0.91 | 0.09 | 18,18,18,18                 | 0     |
| 54  | MG   | DA    | 3026 | 1/1   | 0.91 | 0.09 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3076 | 1/1   | 0.91 | 0.07 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3049 | 1/1   | 0.91 | 0.07 | 108,108,108,108             | 0     |
| 54  | MG   | BA    | 3160 | 1/1   | 0.91 | 0.08 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 3086 | 1/1   | 0.91 | 0.09 | 83,83,83,83                 | 0     |
| 54  | MG   | DA    | 3124 | 1/1   | 0.91 | 0.08 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1654 | 1/1   | 0.91 | 0.21 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1637 | 1/1   | 0.92 | 0.08 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1649 | 1/1   | 0.92 | 0.07 | 26,26,26,26                 | 0     |
| 54  | MG   | DA    | 3151 | 1/1   | 0.92 | 0.09 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3125 | 1/1   | 0.92 | 0.17 | 36,36,36,36                 | 0     |
| 54  | MG   | BA    | 3062 | 1/1   | 0.92 | 0.23 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3173 | 1/1   | 0.92 | 0.10 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3155 | 1/1   | 0.92 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3012 | 1/1   | 0.92 | 0.19 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3098 | 1/1   | 0.92 | 0.08 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3176 | 1/1   | 0.92 | 0.12 | 17,17,17,17                 | 0     |
| 54  | MG   | CA    | 1650 | 1/1   | 0.92 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3070 | 1/1   | 0.92 | 0.12 | 82,82,82,82                 | 0     |
| 54  | MG   | CA    | 1652 | 1/1   | 0.92 | 0.08 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3043 | 1/1   | 0.92 | 0.11 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3055 | 1/1   | 0.92 | 0.09 | 13,13,13,13                 | 0     |
| 54  | MG   | DA    | 3047 | 1/1   | 0.92 | 0.09 | 78,78,78,78                 | 0     |
| 54  | MG   | AA    | 1655 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 54  | MG   | DA    | 3080 | 1/1   | 0.92 | 0.08 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3025 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3147 | 1/1   | 0.92 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3008 | 1/1   | 0.93 | 0.12 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3150 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3112 | 1/1   | 0.93 | 0.11 | 73,73,73,73                 | 0     |
| 54  | MG   | BA    | 3151 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3074 | 1/1   | 0.93 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3116 | 1/1   | 0.93 | 0.10 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3150 | 1/1   | 0.93 | 0.34 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3156 | 1/1   | 0.93 | 0.14 | 21,21,21,21                 | 0     |
| 54  | MG   | CA    | 1614 | 1/1   | 0.93 | 0.06 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3157 | 1/1   | 0.93 | 0.17 | 20,20,20,20                 | 0     |
| 54  | MG   | CA    | 1627 | 1/1   | 0.93 | 0.15 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3084 | 1/1   | 0.93 | 0.07 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3060 | 1/1   | 0.93 | 0.16 | 19,19,19,19                 | 0     |
| 54  | MG   | DA    | 3128 | 1/1   | 0.93 | 0.07 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1663 | 1/1   | 0.93 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3089 | 1/1   | 0.93 | 0.07 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3092 | 1/1   | 0.93 | 0.06 | 79,79,79,79                 | 0     |
| 54  | MG   | AA    | 1666 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1644 | 1/1   | 0.93 | 0.12 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3184 | 1/1   | 0.93 | 0.21 | 11,11,11,11                 | 0     |
| 54  | MG   | BA    | 3026 | 1/1   | 0.93 | 0.17 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3142 | 1/1   | 0.93 | 0.20 | 0,0,0,0                     | 0     |
| 54  | MG   | DA    | 3166 | 1/1   | 0.93 | 0.32 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3037 | 1/1   | 0.93 | 0.13 | 26,26,26,26                 | 0     |
| 54  | MG   | DA    | 3031 | 1/1   | 0.93 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3191 | 1/1   | 0.93 | 0.20 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3003 | 1/1   | 0.94 | 0.06 | 23,23,23,23                 | 0     |
| 54  | MG   | BA    | 3149 | 1/1   | 0.94 | 0.19 | 26,26,26,26                 | 0     |
| 54  | MG   | DA    | 3079 | 1/1   | 0.94 | 0.05 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3015 | 1/1   | 0.94 | 0.07 | 14,14,14,14                 | 0     |
| 54  | MG   | AA    | 1629 | 1/1   | 0.94 | 0.09 | 65,65,65,65                 | 0     |
| 54  | MG   | CA    | 1610 | 1/1   | 0.94 | 0.08 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3034 | 1/1   | 0.94 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1651 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3115 | 1/1   | 0.94 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 3091 | 1/1   | 0.94 | 0.07 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3142 | 1/1   | 0.94 | 0.25 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1654 | 1/1   | 0.94 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1605 | 1/1   | 0.94 | 0.07 | 28,28,28,28                 | 0     |
| 54  | MG   | AA    | 1619 | 1/1   | 0.94 | 0.05 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3046 | 1/1   | 0.94 | 0.07 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3002 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1645 | 1/1   | 0.94 | 0.12 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3161 | 1/1   | 0.94 | 0.07 | 11,11,11,11                 | 0     |
| 54  | MG   | BA    | 3163 | 1/1   | 0.94 | 0.11 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 3055 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3103 | 1/1   | 0.94 | 0.07 | 77,77,77,77                 | 0     |
| 54  | MG   | BA    | 3166 | 1/1   | 0.94 | 0.25 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3106 | 1/1   | 0.94 | 0.14 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3107 | 1/1   | 0.94 | 0.06 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3109 | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3169 | 1/1   | 0.94 | 0.09 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3080 | 1/1   | 0.94 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3174 | 1/1   | 0.94 | 0.06 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3175 | 1/1   | 0.94 | 0.09 | 20,20,20,20                 | 0     |
| 54  | MG   | AA    | 1628 | 1/1   | 0.94 | 0.08 | 53,53,53,53                 | 0     |
| 54  | MG   | CA    | 1639 | 1/1   | 0.94 | 0.07 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3118 | 1/1   | 0.94 | 0.07 | 71,71,71,71                 | 0     |
| 54  | MG   | BA    | 3180 | 1/1   | 0.94 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | BA    | 3181 | 1/1   | 0.94 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | AN    | 201  | 1/1   | 0.94 | 0.14 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3002 | 1/1   | 0.94 | 0.06 | 15,15,15,15                 | 0     |
| 54  | MG   | DB    | 201  | 1/1   | 0.94 | 0.07 | 101,101,101,101             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3146 | 1/1   | 0.94 | 0.09 | 6,6,6,6                     | 0     |
| 54  | MG   | D2    | 101  | 1/1   | 0.94 | 0.10 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3075 | 1/1   | 0.94 | 0.07 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3053 | 1/1   | 0.95 | 0.07 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3178 | 1/1   | 0.95 | 0.07 | 12,12,12,12                 | 0     |
| 54  | MG   | AA    | 1630 | 1/1   | 0.95 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1625 | 1/1   | 0.95 | 0.11 | 19,19,19,19                 | 0     |
| 54  | MG   | DA    | 3126 | 1/1   | 0.95 | 0.08 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3035 | 1/1   | 0.95 | 0.25 | 44,44,44,44                 | 0     |
| 54  | MG   | CA    | 1632 | 1/1   | 0.95 | 0.07 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1609 | 1/1   | 0.95 | 0.07 | 46,46,46,46                 | 0     |
| 54  | MG   | AA    | 1616 | 1/1   | 0.95 | 0.07 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3141 | 1/1   | 0.95 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | DA    | 3040 | 1/1   | 0.95 | 0.10 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3135 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3045 | 1/1   | 0.95 | 0.05 | 20,20,20,20                 | 0     |
| 54  | MG   | BA    | 3167 | 1/1   | 0.95 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | CA    | 1602 | 1/1   | 0.95 | 0.07 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3102 | 1/1   | 0.95 | 0.06 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3170 | 1/1   | 0.95 | 0.07 | 23,23,23,23                 | 0     |
| 54  | MG   | AA    | 1670 | 1/1   | 0.95 | 0.17 | 40,40,40,40                 | 0     |
| 54  | MG   | BA    | 3075 | 1/1   | 0.95 | 0.08 | 19,19,19,19                 | 0     |
| 54  | MG   | DA    | 3082 | 1/1   | 0.95 | 0.07 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3116 | 1/1   | 0.95 | 0.09 | 48,48,48,48                 | 0     |
| 54  | MG   | CA    | 1617 | 1/1   | 0.95 | 0.08 | 36,36,36,36                 | 0     |
| 54  | MG   | CA    | 1618 | 1/1   | 0.95 | 0.07 | 38,38,38,38                 | 0     |
| 54  | MG   | CA    | 1622 | 1/1   | 0.95 | 0.06 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3182 | 1/1   | 0.96 | 0.08 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3122 | 1/1   | 0.96 | 0.08 | 26,26,26,26                 | 0     |
| 54  | MG   | AA    | 1626 | 1/1   | 0.96 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3097 | 1/1   | 0.96 | 0.05 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3081 | 1/1   | 0.96 | 0.05 | 19,19,19,19                 | 0     |
| 54  | MG   | BA    | 3132 | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | AA    | 1612 | 1/1   | 0.96 | 0.07 | 43,43,43,43                 | 0     |
| 54  | MG   | CA    | 1637 | 1/1   | 0.96 | 0.08 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3192 | 1/1   | 0.96 | 0.12 | 17,17,17,17                 | 0     |
| 54  | MG   | BA    | 3017 | 1/1   | 0.96 | 0.14 | 24,24,24,24                 | 0     |
| 54  | MG   | DA    | 3018 | 1/1   | 0.96 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3064 | 1/1   | 0.96 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | CA    | 1601 | 1/1   | 0.96 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | AA    | 1607 | 1/1   | 0.96 | 0.05 | 51,51,51,51                 | 0     |
| 54  | MG   | AA    | 1610 | 1/1   | 0.96 | 0.13 | 69,69,69,69                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | CA    | 1607 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 54  | MG   | CA    | 1608 | 1/1   | 0.96 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1609 | 1/1   | 0.96 | 0.09 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1638 | 1/1   | 0.96 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1639 | 1/1   | 0.96 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3077 | 1/1   | 0.96 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3172 | 1/1   | 0.96 | 0.09 | 26,26,26,26                 | 0     |
| 54  | MG   | BA    | 3103 | 1/1   | 0.96 | 0.14 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3044 | 1/1   | 0.96 | 0.04 | 21,21,21,21                 | 0     |
| 54  | MG   | AA    | 1642 | 1/1   | 0.96 | 0.05 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3038 | 1/1   | 0.96 | 0.05 | 77,77,77,77                 | 0     |
| 54  | MG   | CA    | 1653 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 54  | MG   | CA    | 1619 | 1/1   | 0.96 | 0.07 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 3004 | 1/1   | 0.96 | 0.07 | 27,27,27,27                 | 0     |
| 54  | MG   | BA    | 3120 | 1/1   | 0.96 | 0.17 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3090 | 1/1   | 0.96 | 0.11 | 81,81,81,81                 | 0     |
| 54  | MG   | BA    | 3154 | 1/1   | 0.96 | 0.29 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3155 | 1/1   | 0.96 | 0.12 | 18,18,18,18                 | 0     |
| 55  | VIR  | BA    | 3001 | 38/38 | 0.96 | 0.10 | 3,15,28,31                  | 0     |
| 54  | MG   | DA    | 3004 | 1/1   | 0.96 | 0.06 | 69,69,69,69                 | 0     |
| 54  | MG   | DA    | 3085 | 1/1   | 0.97 | 0.04 | 83,83,83,83                 | 0     |
| 54  | MG   | AA    | 1656 | 1/1   | 0.97 | 0.07 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3188 | 1/1   | 0.97 | 0.06 | 6,6,6,6                     | 0     |
| 54  | MG   | DA    | 3088 | 1/1   | 0.97 | 0.05 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3044 | 1/1   | 0.97 | 0.05 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3106 | 1/1   | 0.97 | 0.09 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3162 | 1/1   | 0.97 | 0.15 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3006 | 1/1   | 0.97 | 0.06 | 99,99,99,99                 | 0     |
| 54  | MG   | AA    | 1623 | 1/1   | 0.97 | 0.06 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3143 | 1/1   | 0.97 | 0.25 | 15,15,15,15                 | 0     |
| 54  | MG   | BA    | 3078 | 1/1   | 0.97 | 0.07 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 3052 | 1/1   | 0.97 | 0.05 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 3054 | 1/1   | 0.97 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | BB    | 201  | 1/1   | 0.97 | 0.05 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 3056 | 1/1   | 0.97 | 0.07 | 61,61,61,61                 | 0     |
| 54  | MG   | BB    | 202  | 1/1   | 0.97 | 0.04 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3168 | 1/1   | 0.97 | 0.07 | 19,19,19,19                 | 0     |
| 54  | MG   | DA    | 3102 | 1/1   | 0.97 | 0.05 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3079 | 1/1   | 0.97 | 0.04 | 41,41,41,41                 | 0     |
| 54  | MG   | CA    | 1604 | 1/1   | 0.97 | 0.05 | 88,88,88,88                 | 0     |
| 54  | MG   | BA    | 3148 | 1/1   | 0.97 | 0.19 | 28,28,28,28                 | 0     |
| 54  | MG   | CA    | 1606 | 1/1   | 0.97 | 0.07 | 68,68,68,68                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3108 | 1/1   | 0.97 | 0.05 | 74,74,74,74                 | 0     |
| 54  | MG   | AA    | 1668 | 1/1   | 0.97 | 0.11 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 3021 | 1/1   | 0.97 | 0.13 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3111 | 1/1   | 0.97 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1653 | 1/1   | 0.97 | 0.13 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3005 | 1/1   | 0.97 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3152 | 1/1   | 0.97 | 0.04 | 14,14,14,14                 | 0     |
| 54  | MG   | DA    | 3115 | 1/1   | 0.97 | 0.07 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3008 | 1/1   | 0.97 | 0.08 | 32,32,32,32                 | 0     |
| 54  | MG   | CA    | 1612 | 1/1   | 0.97 | 0.04 | 43,43,43,43                 | 0     |
| 54  | MG   | AA    | 1601 | 1/1   | 0.97 | 0.06 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3070 | 1/1   | 0.97 | 0.06 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3072 | 1/1   | 0.97 | 0.09 | 13,13,13,13                 | 0     |
| 54  | MG   | BA    | 3158 | 1/1   | 0.97 | 0.05 | 16,16,16,16                 | 0     |
| 54  | MG   | BA    | 3183 | 1/1   | 0.97 | 0.18 | 26,26,26,26                 | 0     |
| 54  | MG   | DB    | 202  | 1/1   | 0.97 | 0.10 | 61,61,61,61                 | 0     |
| 54  | MG   | DB    | 203  | 1/1   | 0.97 | 0.06 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3037 | 1/1   | 0.97 | 0.07 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1621 | 1/1   | 0.97 | 0.05 | 69,69,69,69                 | 0     |
| 54  | MG   | AA    | 1622 | 1/1   | 0.97 | 0.09 | 51,51,51,51                 | 0     |
| 54  | MG   | CA    | 1625 | 1/1   | 0.97 | 0.07 | 22,22,22,22                 | 0     |
| 54  | MG   | CA    | 1634 | 1/1   | 0.98 | 0.04 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3091 | 1/1   | 0.98 | 0.06 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 3024 | 1/1   | 0.98 | 0.03 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3092 | 1/1   | 0.98 | 0.04 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3164 | 1/1   | 0.98 | 0.24 | 15,15,15,15                 | 0     |
| 54  | MG   | BB    | 203  | 1/1   | 0.98 | 0.03 | 11,11,11,11                 | 0     |
| 54  | MG   | BB    | 204  | 1/1   | 0.98 | 0.23 | 6,6,6,6                     | 0     |
| 54  | MG   | CA    | 1640 | 1/1   | 0.98 | 0.10 | 31,31,31,31                 | 0     |
| 54  | MG   | BD    | 301  | 1/1   | 0.98 | 0.04 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3031 | 1/1   | 0.98 | 0.07 | 3,3,3,3                     | 0     |
| 54  | MG   | DA    | 3032 | 1/1   | 0.98 | 0.06 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3139 | 1/1   | 0.98 | 0.19 | 3,3,3,3                     | 0     |
| 54  | MG   | DA    | 3083 | 1/1   | 0.98 | 0.04 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3032 | 1/1   | 0.98 | 0.08 | 6,6,6,6                     | 0     |
| 54  | MG   | DA    | 3035 | 1/1   | 0.98 | 0.05 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3006 | 1/1   | 0.98 | 0.06 | 47,47,47,47                 | 0     |
| 54  | MG   | AA    | 1620 | 1/1   | 0.98 | 0.04 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3171 | 1/1   | 0.98 | 0.08 | 16,16,16,16                 | 0     |
| 54  | MG   | DA    | 3039 | 1/1   | 0.98 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3144 | 1/1   | 0.98 | 0.03 | 12,12,12,12                 | 0     |
| 54  | MG   | BA    | 3145 | 1/1   | 0.98 | 0.24 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3108 | 1/1   | 0.98 | 0.05 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3110 | 1/1   | 0.98 | 0.16 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3111 | 1/1   | 0.98 | 0.03 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3177 | 1/1   | 0.98 | 0.26 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3057 | 1/1   | 0.98 | 0.07 | 6,6,6,6                     | 0     |
| 54  | MG   | CA    | 1616 | 1/1   | 0.98 | 0.06 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3179 | 1/1   | 0.98 | 0.09 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3024 | 1/1   | 0.98 | 0.06 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3059 | 1/1   | 0.98 | 0.05 | 17,17,17,17                 | 0     |
| 54  | MG   | DA    | 3051 | 1/1   | 0.98 | 0.05 | 60,60,60,60                 | 0     |
| 54  | MG   | CA    | 1620 | 1/1   | 0.98 | 0.04 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3053 | 1/1   | 0.98 | 0.03 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3042 | 1/1   | 0.98 | 0.07 | 11,11,11,11                 | 0     |
| 54  | MG   | DA    | 3105 | 1/1   | 0.98 | 0.05 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1615 | 1/1   | 0.98 | 0.04 | 63,63,63,63                 | 0     |
| 54  | MG   | CA    | 1623 | 1/1   | 0.98 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3028 | 1/1   | 0.98 | 0.10 | 16,16,16,16                 | 0     |
| 54  | MG   | CA    | 1626 | 1/1   | 0.98 | 0.05 | 52,52,52,52                 | 0     |
| 54  | MG   | BA    | 3185 | 1/1   | 0.98 | 0.19 | 13,13,13,13                 | 0     |
| 54  | MG   | DA    | 3060 | 1/1   | 0.98 | 0.05 | 41,41,41,41                 | 0     |
| 54  | MG   | BA    | 3063 | 1/1   | 0.98 | 0.06 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3127 | 1/1   | 0.98 | 0.08 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3128 | 1/1   | 0.98 | 0.03 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3086 | 1/1   | 0.98 | 0.05 | 10,10,10,10                 | 0     |
| 54  | MG   | BA    | 3133 | 1/1   | 0.98 | 0.10 | 27,27,27,27                 | 0     |
| 54  | MG   | DA    | 3066 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3069 | 1/1   | 0.98 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | DA    | 3119 | 1/1   | 0.98 | 0.04 | 50,50,50,50                 | 0     |
| 54  | MG   | BA    | 3047 | 1/1   | 0.98 | 0.07 | 4,4,4,4                     | 0     |
| 54  | MG   | AA    | 1621 | 1/1   | 0.99 | 0.12 | 16,16,16,16                 | 0     |
| 54  | MG   | CA    | 1613 | 1/1   | 0.99 | 0.07 | 15,15,15,15                 | 0     |
| 54  | MG   | AA    | 1603 | 1/1   | 0.99 | 0.10 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3089 | 1/1   | 0.99 | 0.13 | 28,28,28,28                 | 0     |
| 54  | MG   | BA    | 3090 | 1/1   | 0.99 | 0.04 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3153 | 1/1   | 0.99 | 0.07 | 6,6,6,6                     | 0     |
| 54  | MG   | AA    | 1632 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 54  | MG   | AA    | 1647 | 1/1   | 0.99 | 0.03 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3093 | 1/1   | 0.99 | 0.05 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3094 | 1/1   | 0.99 | 0.05 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3095 | 1/1   | 0.99 | 0.07 | 30,30,30,30                 | 0     |
| 54  | MG   | BA    | 3096 | 1/1   | 0.99 | 0.03 | 5,5,5,5                     | 0     |
| 54  | MG   | CA    | 1624 | 1/1   | 0.99 | 0.04 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3098 | 1/1   | 0.99 | 0.04 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3007 | 1/1   | 0.99 | 0.04 | 17,17,17,17                 | 0     |
| 54  | MG   | BA    | 3100 | 1/1   | 0.99 | 0.05 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3101 | 1/1   | 0.99 | 0.04 | 5,5,5,5                     | 0     |
| 54  | MG   | AA    | 1633 | 1/1   | 0.99 | 0.06 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3165 | 1/1   | 0.99 | 0.06 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3049 | 1/1   | 0.99 | 0.02 | 11,11,11,11                 | 0     |
| 54  | MG   | BA    | 3104 | 1/1   | 0.99 | 0.04 | 12,12,12,12                 | 0     |
| 54  | MG   | BA    | 3105 | 1/1   | 0.99 | 0.10 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3051 | 1/1   | 0.99 | 0.06 | 4,4,4,4                     | 0     |
| 54  | MG   | DA    | 3122 | 1/1   | 0.99 | 0.05 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3052 | 1/1   | 0.99 | 0.03 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3109 | 1/1   | 0.99 | 0.08 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3009 | 1/1   | 0.99 | 0.06 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3012 | 1/1   | 0.99 | 0.05 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3112 | 1/1   | 0.99 | 0.03 | 7,7,7,7                     | 0     |
| 54  | MG   | BA    | 3013 | 1/1   | 0.99 | 0.08 | 0,0,0,0                     | 0     |
| 54  | MG   | DA    | 3130 | 1/1   | 0.99 | 0.08 | 37,37,37,37                 | 0     |
| 54  | MG   | DA    | 3131 | 1/1   | 0.99 | 0.05 | 69,69,69,69                 | 0     |
| 54  | MG   | BA    | 3114 | 1/1   | 0.99 | 0.07 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3014 | 1/1   | 0.99 | 0.07 | 0,0,0,0                     | 0     |
| 54  | MG   | AA    | 1606 | 1/1   | 0.99 | 0.06 | 35,35,35,35                 | 0     |
| 54  | MG   | BA    | 3117 | 1/1   | 0.99 | 0.07 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3119 | 1/1   | 0.99 | 0.04 | 12,12,12,12                 | 0     |
| 54  | MG   | AA    | 1624 | 1/1   | 0.99 | 0.03 | 32,32,32,32                 | 0     |
| 54  | MG   | BA    | 3121 | 1/1   | 0.99 | 0.03 | 4,4,4,4                     | 0     |
| 54  | MG   | AA    | 1636 | 1/1   | 0.99 | 0.06 | 11,11,11,11                 | 0     |
| 54  | MG   | BA    | 3020 | 1/1   | 0.99 | 0.13 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3021 | 1/1   | 0.99 | 0.05 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3186 | 1/1   | 0.99 | 0.04 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3067 | 1/1   | 0.99 | 0.03 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3068 | 1/1   | 0.99 | 0.03 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3126 | 1/1   | 0.99 | 0.08 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3023 | 1/1   | 0.99 | 0.07 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3068 | 1/1   | 0.99 | 0.11 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3129 | 1/1   | 0.99 | 0.08 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3131 | 1/1   | 0.99 | 0.06 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3069 | 1/1   | 0.99 | 0.04 | 7,7,7,7                     | 0     |
| 54  | MG   | AA    | 1617 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3194 | 1/1   | 0.99 | 0.04 | 28,28,28,28                 | 0     |
| 54  | MG   | BA    | 3071 | 1/1   | 0.99 | 0.04 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3135 | 1/1   | 0.99 | 0.05 | 1,1,1,1                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3025 | 1/1   | 0.99 | 0.04 | 3,3,3,3                     | 0     |
| 54  | MG   | AA    | 1604 | 1/1   | 0.99 | 0.05 | 55,55,55,55                 | 0     |
| 54  | MG   | BA    | 3027 | 1/1   | 0.99 | 0.03 | 3,3,3,3                     | 0     |
| 54  | MG   | DA    | 3010 | 1/1   | 0.99 | 0.05 | 71,71,71,71                 | 0     |
| 54  | MG   | BQ    | 201  | 1/1   | 0.99 | 0.08 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3076 | 1/1   | 0.99 | 0.03 | 12,12,12,12                 | 0     |
| 54  | MG   | DA    | 3013 | 1/1   | 0.99 | 0.06 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3140 | 1/1   | 0.99 | 0.19 | 1,1,1,1                     | 0     |
| 54  | MG   | DA    | 3015 | 1/1   | 0.99 | 0.05 | 46,46,46,46                 | 0     |
| 54  | MG   | CA    | 1603 | 1/1   | 0.99 | 0.07 | 36,36,36,36                 | 0     |
| 54  | MG   | AA    | 1627 | 1/1   | 0.99 | 0.02 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3030 | 1/1   | 0.99 | 0.12 | 14,14,14,14                 | 0     |
| 54  | MG   | AA    | 1640 | 1/1   | 0.99 | 0.05 | 21,21,21,21                 | 0     |
| 54  | MG   | AA    | 1641 | 1/1   | 0.99 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3033 | 1/1   | 0.99 | 0.05 | 6,6,6,6                     | 0     |
| 54  | MG   | DA    | 3022 | 1/1   | 0.99 | 0.10 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3023 | 1/1   | 0.99 | 0.05 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 1613 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 54  | MG   | AA    | 1608 | 1/1   | 0.99 | 0.03 | 18,18,18,18                 | 0     |
| 54  | MG   | BA    | 3040 | 1/1   | 0.99 | 0.03 | 0,0,0,0                     | 0     |
| 56  | ZN   | D4    | 101  | 1/1   | 0.99 | 0.02 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3082 | 1/1   | 1.00 | 0.08 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3034 | 1/1   | 1.00 | 0.14 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3107 | 1/1   | 1.00 | 0.13 | 1,1,1,1                     | 0     |
| 54  | MG   | DA    | 3123 | 1/1   | 1.00 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3010 | 1/1   | 1.00 | 0.03 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3064 | 1/1   | 1.00 | 0.06 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3065 | 1/1   | 1.00 | 0.08 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3087 | 1/1   | 1.00 | 0.07 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3066 | 1/1   | 1.00 | 0.03 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3067 | 1/1   | 1.00 | 0.05 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3036 | 1/1   | 1.00 | 0.03 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3050 | 1/1   | 1.00 | 0.03 | 4,4,4,4                     | 0     |
| 54  | MG   | BA    | 3022 | 1/1   | 1.00 | 0.05 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3038 | 1/1   | 1.00 | 0.08 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3118 | 1/1   | 1.00 | 0.03 | 5,5,5,5                     | 0     |
| 54  | MG   | BA    | 3039 | 1/1   | 1.00 | 0.06 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3073 | 1/1   | 1.00 | 0.06 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3054 | 1/1   | 1.00 | 0.03 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3097 | 1/1   | 1.00 | 0.05 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3123 | 1/1   | 1.00 | 0.09 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3029 | 1/1   | 1.00 | 0.06 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3011 | 1/1   | 1.00 | 0.04 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3018 | 1/1   | 1.00 | 0.04 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3043 | 1/1   | 1.00 | 0.05 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3019 | 1/1   | 1.00 | 0.07 | 15,15,15,15                 | 0     |
| 54  | MG   | AA    | 1611 | 1/1   | 1.00 | 0.03 | 12,12,12,12                 | 0     |
| 54  | MG   | BA    | 3130 | 1/1   | 1.00 | 0.04 | 0,0,0,0                     | 0     |
| 56  | ZN   | B4    | 101  | 1/1   | 1.00 | 0.01 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 3046 | 1/1   | 1.00 | 0.02 | 5,5,5,5                     | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.