



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 02:06 am BST

PDB ID : 4V7V  
Title : Crystal structure of the E. coli ribosome bound to clindamycin.  
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.  
Deposited on : 2010-08-16  
Resolution : 3.29 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.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

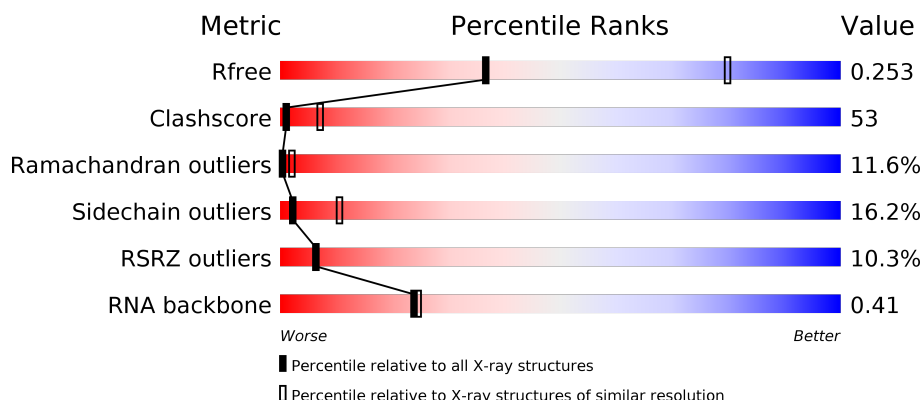
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1177 (3.32-3.24)                                      |
| Clashscore            | 141614                      | 1044 (3.30-3.26)                                      |
| Ramachandran outliers | 138981                      | 1026 (3.30-3.26)                                      |
| Sidechain outliers    | 138945                      | 1025 (3.30-3.26)                                      |
| RSRZ outliers         | 127900                      | 1141 (3.32-3.24)                                      |
| RNA backbone          | 3102                        | 1091 (3.66-2.90)                                      |

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 on 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    | 1533   | <div> <div>19%</div> <div>48%</div> <div>18%</div> <div>14%</div> </div> |
| 2   | AB    | 218    | <div> <div>22%</div> <div>21%</div> <div>54%</div> <div>23%</div> </div> |
| 2   | CB    | 218    | <div> <div>42%</div> <div>25%</div> <div>60%</div> <div>14%</div> </div> |
| 3   | AC    | 206    | <div> <div>5%</div> <div>33%</div> <div>50%</div> <div>14%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | CC    | 206    |                  |
| 4   | AD    | 205    |                  |
| 4   | CD    | 205    |                  |
| 5   | AE    | 150    |                  |
| 5   | CE    | 150    |                  |
| 6   | AF    | 100    |                  |
| 6   | CF    | 100    |                  |
| 7   | AG    | 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    |                  |
| 14  | AN    | 100    |                  |
| 14  | CN    | 100    |                  |
| 15  | AO    | 88     |                  |
| 15  | CO    | 88     |                  |
| 16  | AP    | 82     |                  |
| 17  | AQ    | 80     |                  |

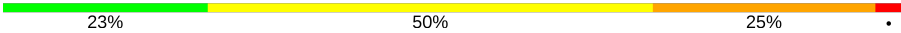
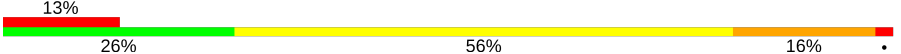
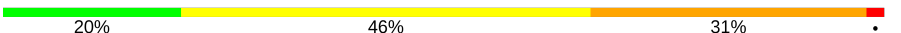
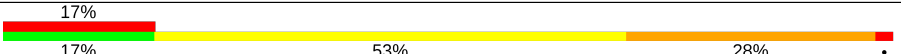

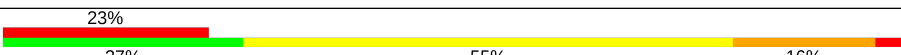
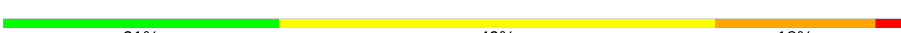
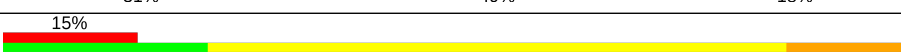

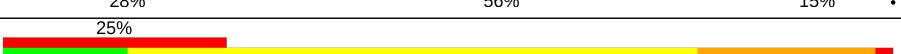

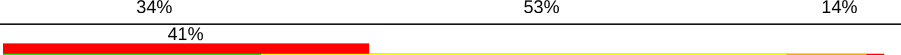


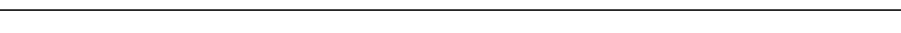

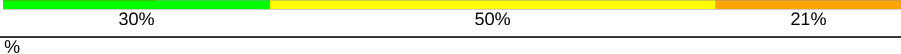
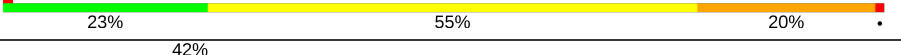


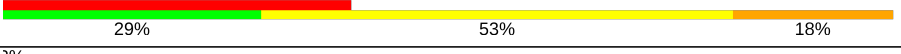
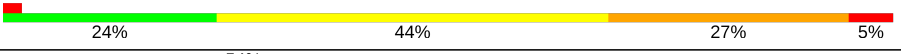
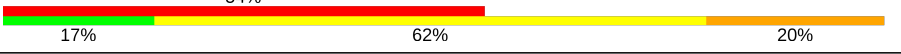
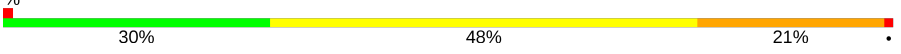
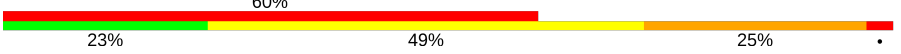
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 17  | CQ    | 80     |                  |
| 18  | AR    | 55     |                  |
| 18  | CR    | 55     |                  |
| 19  | AS    | 79     |                  |
| 19  | CS    | 79     |                  |
| 20  | AT    | 85     |                  |
| 20  | CT    | 85     |                  |
| 21  | AU    | 51     |                  |
| 21  | CU    | 51     |                  |
| 22  | BA    | 2903   |                  |
| 22  | DA    | 2903   |                  |
| 23  | BB    | 118    |                  |
| 24  | BC    | 271    |                  |
| 24  | DC    | 271    |                  |
| 25  | BD    | 209    |                  |
| 25  | DD    | 209    |                  |
| 26  | BE    | 201    |                  |
| 26  | DE    | 201    |                  |
| 27  | BF    | 177    |                  |
| 28  | BG    | 176    |                  |
| 28  | DG    | 176    |                  |
| 29  | BH    | 149    |                  |
| 29  | DH    | 149    |                  |
| 30  | BI    | 141    |                  |
| 30  | DI    | 141    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 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    |  |
| 40  | DS    | 110    |  |
| 41  | BT    | 93     |  |
| 41  | DT    | 93     |  |
| 42  | BU    | 102    |  |
| 42  | DU    | 102    |  |
| 43  | BV    | 94     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 43  | DV    | 94     |                  |
| 44  | BW    | 79     |                  |
| 44  | DW    | 79     |                  |
| 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     |                  |
| 53  | CA    | 1530   |                  |
| 54  | CG    | 150    |                  |
| 55  | CM    | 113    |                  |
| 56  | CP    | 80     |                  |
| 57  | DB    | 117    |                  |
| 58  | DF    | 178    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 59  | MG   | CA    | 1624 | -         | -        | -       | X                |
| 59  | MG   | CA    | 1628 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3003 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3005 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3007 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3010 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3019 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3025 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3027 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3056 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3059 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3061 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3062 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3073 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3075 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3107 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3108 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3124 | -         | -        | -       | X                |
| 59  | MG   | DA    | 3129 | -         | -        | -       | X                |
| 59  | MG   | DE    | 301  | -         | -        | -       | X                |
| 59  | MG   | DJ    | 201  | -         | -        | -       | X                |

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 284501 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    | 1533     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32895 | 14671 | 6036 | 10655 | 1533 |         |         |       |

- 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 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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 |         |         |       |

- 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 |         |         |       |
| 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 |         |         |       |

- 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    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 480 | 159 | 127 | 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     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 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 |         |         |       |

- 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  | S | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |   |         |         |       |
| 18  | CR    | 55       | Total | C   | N  | O  | S | 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    | 2854     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61274 | 27334 | 11279 | 19807 | 2854 |         |         |       |

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| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22  | DA    | 2841     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 60995 | 27210 | 11229 | 19715 | 2841 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23  | BB    | 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 |         |         |       |
| 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 |         |         |       |

- 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     |
|     |       |          | 1111  | 699 | 197 | 214 | 1 |         |         |       |
| 29  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1111  | 699 | 197 | 214 | 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 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 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   | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |         |       |
| 38  | DQ    | 117      | Total | C   | N   | O   | 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   | 0       | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |         |         |       |
| 42  | DU    | 102      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |         |         |       |

- 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 | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |
| 43  | DV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BW    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 596   | 367 | 120 | 108 | 1 |         |         |       |
| 44  | DW    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 596   | 367 | 120 | 108 | 1 |         |         |       |

- 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 | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |
| 45  | DX    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |

- 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 | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |
| 46  | DY    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |

- 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 | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |
| 47  | DZ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |

- 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 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 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 RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 53  | CA    | 1530     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32831 | 14642 | 6024 | 10635 | 1530 |         |         |       |

- Molecule 54 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | CG    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1175  | 730 | 226 | 215 | 4 |         |         |       |

- Molecule 55 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | CM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 541 | 177 | 156 | 3 |         |         |       |

- Molecule 56 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | CP    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 639   | 400 | 126 | 112 | 1 |         |         |       |

- Molecule 57 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 57  | DB    | 117      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2507  | 1116 | 459 | 815 | 117 |         |         |       |

- Molecule 58 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 58  | DF    | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 905 | 251 | 258 | 6 |         |         |       |

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

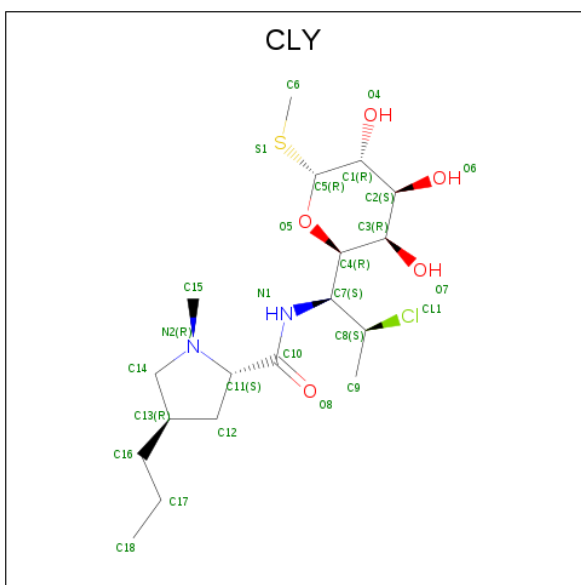
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 59  | BB    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 59  | DE    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | BA    | 134      | Total | Mg  | 0       | 0       |
|     |       |          | 134   | 134 |         |         |
| 59  | CA    | 42       | Total | Mg  | 0       | 0       |
|     |       |          | 42    | 42  |         |         |
| 59  | DJ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | BL    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 59  | DA    | 132      | Total | Mg  | 0       | 0       |
|     |       |          | 132   | 132 |         |         |
| 59  | AA    | 42       | Total | Mg  | 0       | 0       |
|     |       |          | 42    | 42  |         |         |
| 59  | AN    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59  | DC    | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 59  | DB    | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 60 is CLINDAMYCIN (three-letter code: CLY) (formula:  $C_{18}H_{33}ClN_2O_5S$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|---------|
| 60  | BA    | 1        | Total | C  | Cl | N | O | S | 0       | 0       |
|     |       |          | 27    | 18 | 1  | 2 | 5 | 1 |         |         |

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 61  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 61  | D4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 62 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 62  | AA    | 197      | Total | O   | 0       | 0       |
|     |       |          | 197   | 197 |         |         |
| 62  | AE    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62  | AL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | AN    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 62  | AT    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | AU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | BA    | 601      | Total<br>601 | O<br>601 | 0       | 0       |
| 62  | BB    | 20       | Total<br>20  | O<br>20  | 0       | 0       |
| 62  | BC    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 62  | BD    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 62  | BE    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | BL    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | BN    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | BQ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | BR    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | BT    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | B2    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | B3    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | B4    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | CA    | 193      | Total<br>193 | O<br>193 | 0       | 0       |
| 62  | CE    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 62  | CI    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | CL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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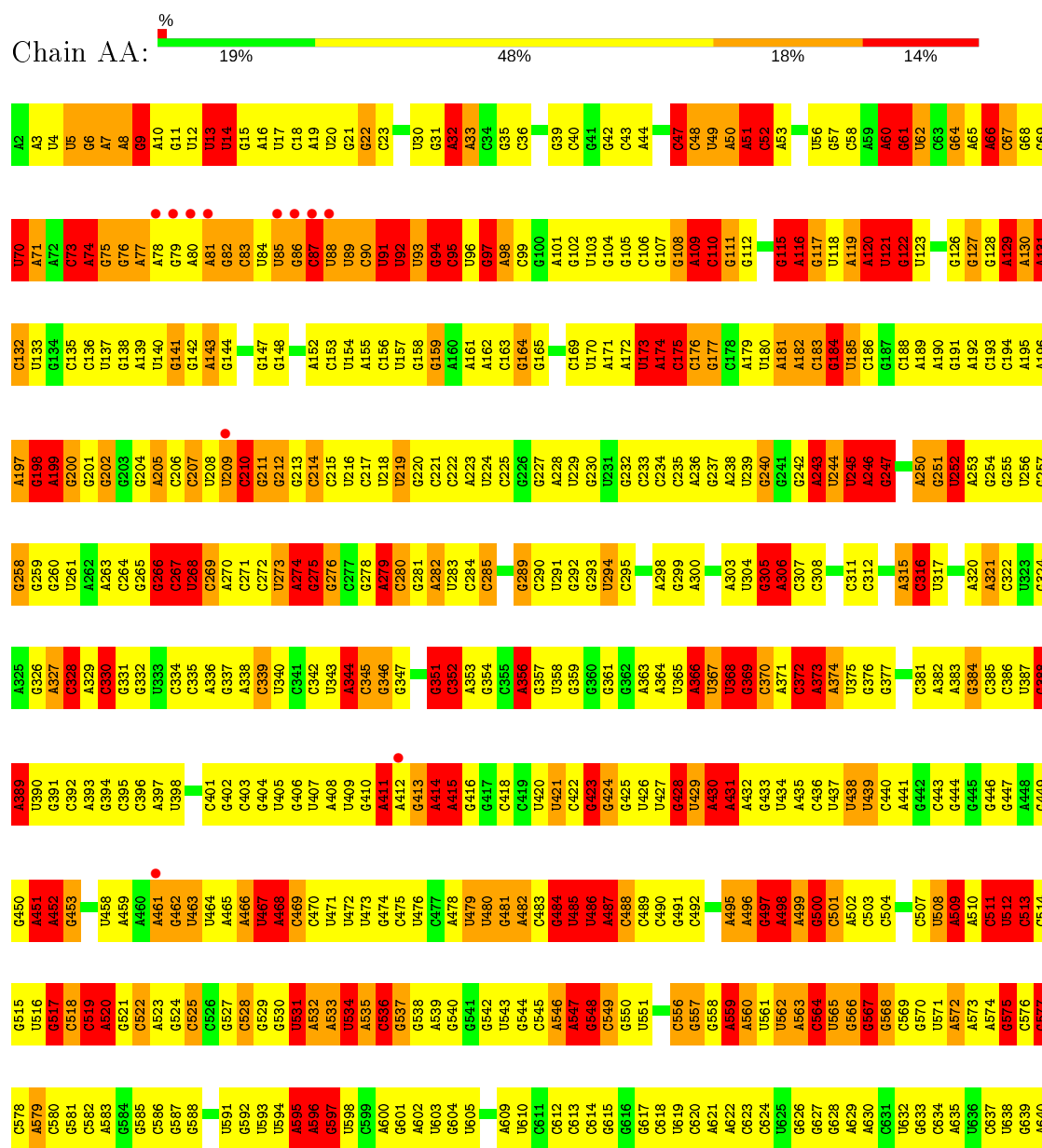
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62  | CN    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | CT    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | CU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | DA    | 599      | Total<br>599 | O<br>599 | 0       | 0       |
| 62  | DB    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 62  | DC    | 9        | Total<br>9   | O<br>9   | 0       | 0       |
| 62  | DD    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | DE    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | DJ    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 62  | DL    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 62  | DN    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | DT    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 62  | DU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | DV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | D2    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 62  | D3    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 62  | D4    | 4        | Total<br>4   | O<br>4   | 0       | 0       |

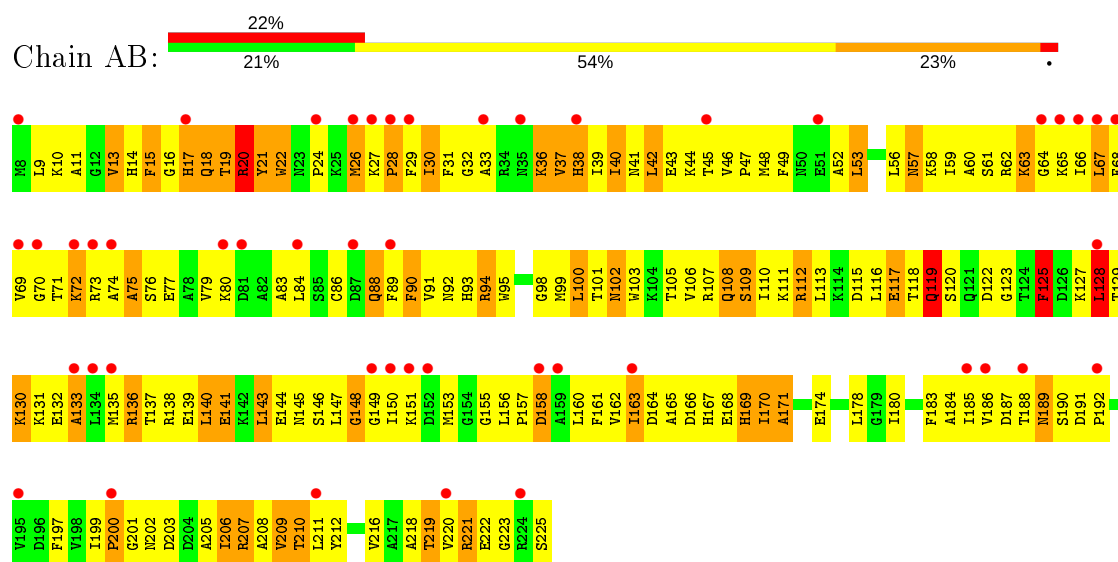
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

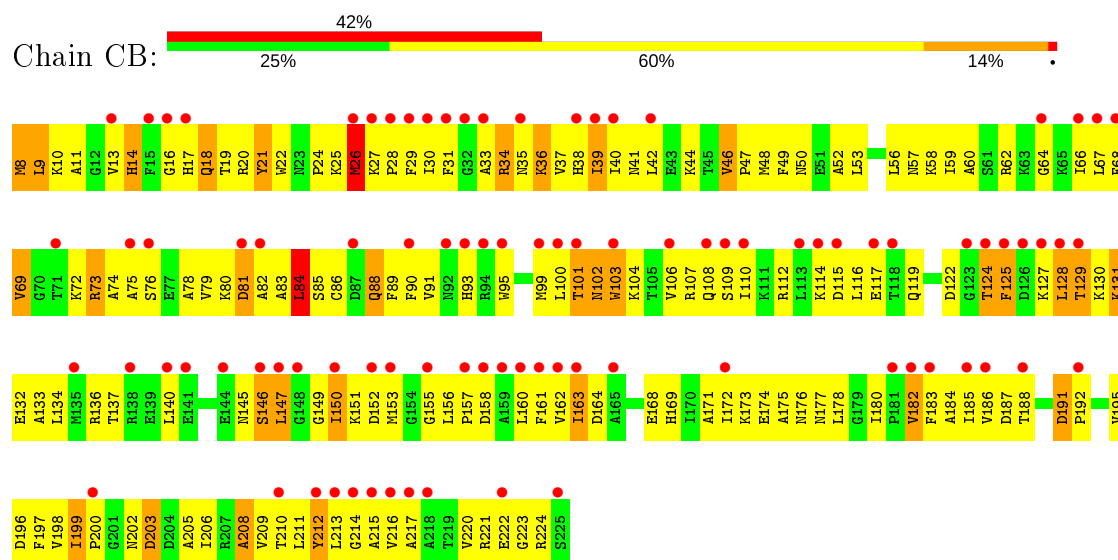
#### • Molecule 1: 16S rRNA



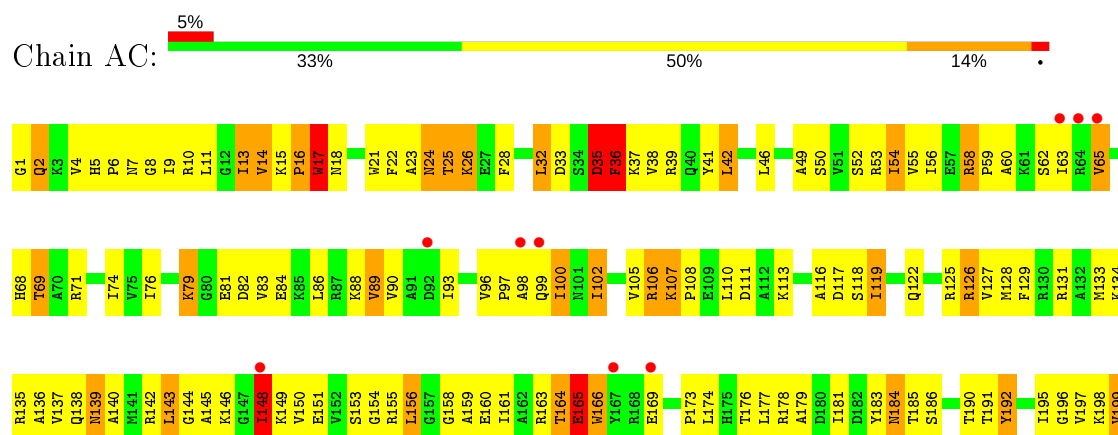




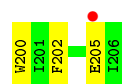
• Molecule 2: 30S ribosomal protein S2



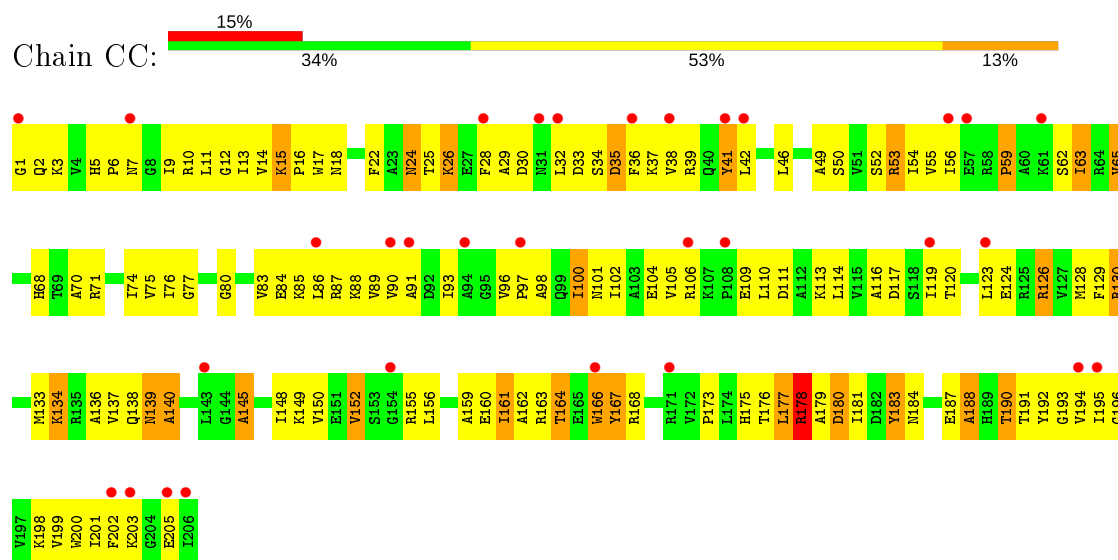
• Molecule 3: 30S ribosomal protein S3



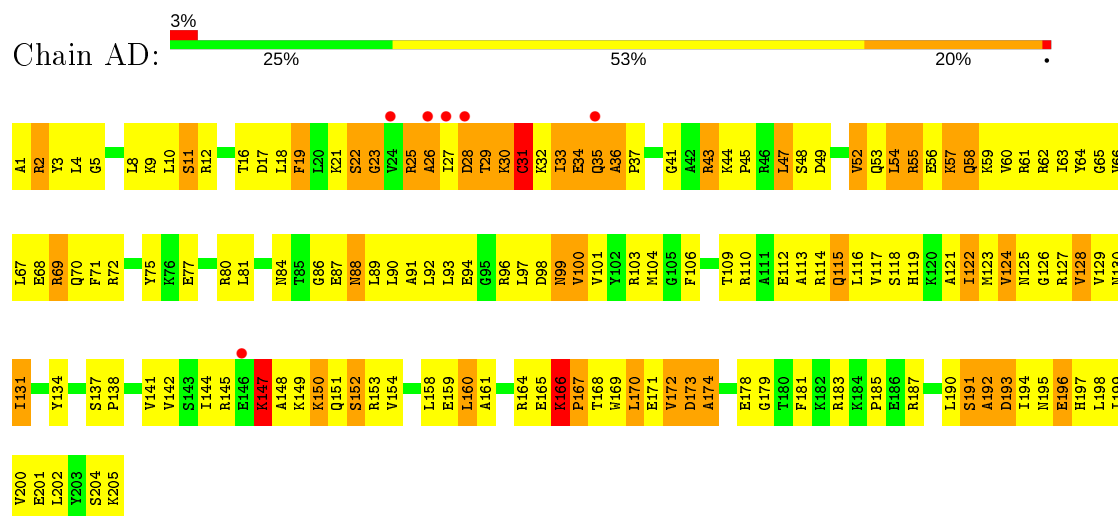




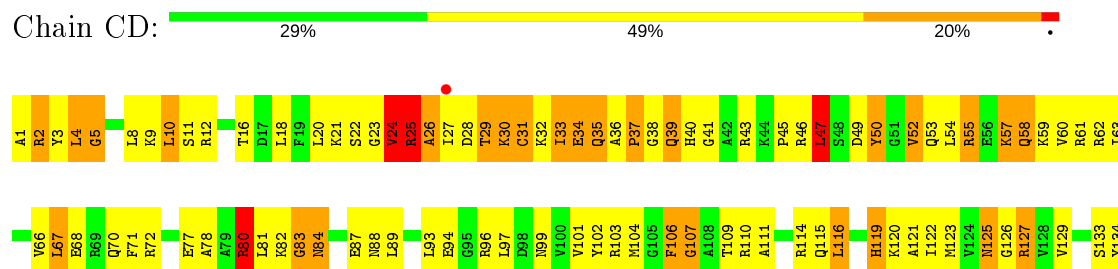
• Molecule 3: 30S ribosomal protein S3

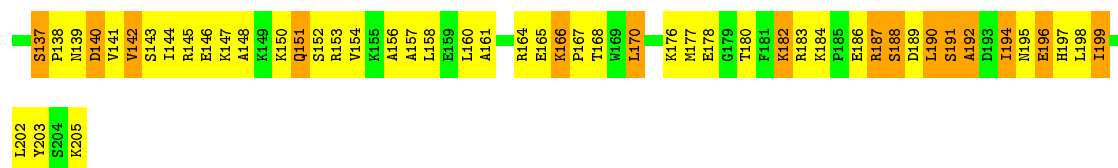


• Molecule 4: 30S ribosomal protein S4

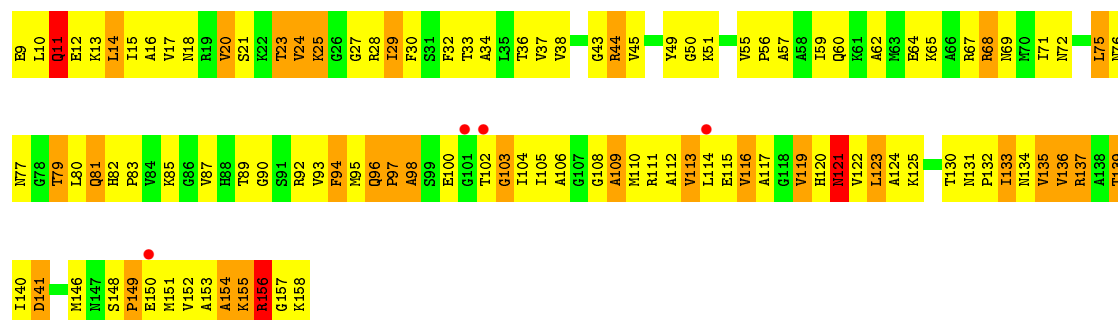


• Molecule 4: 30S ribosomal protein S4

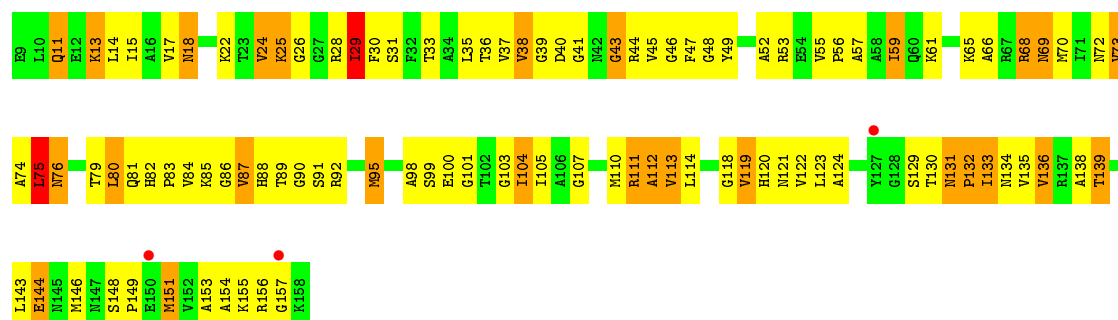




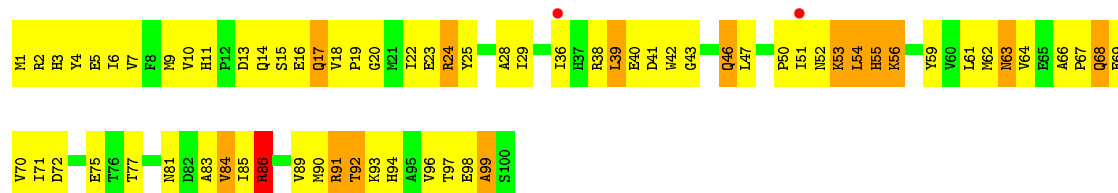
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

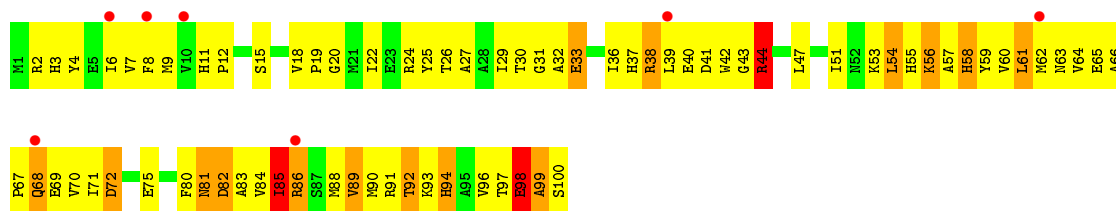


• Molecule 6: 30S ribosomal protein S6

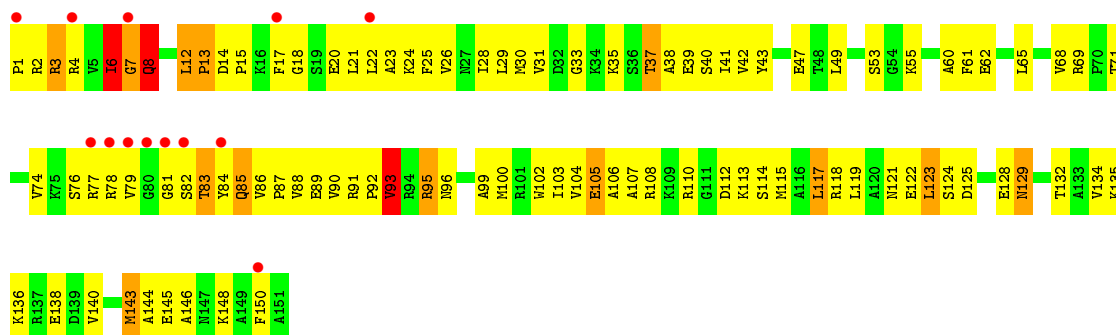


• Molecule 6: 30S ribosomal protein S6

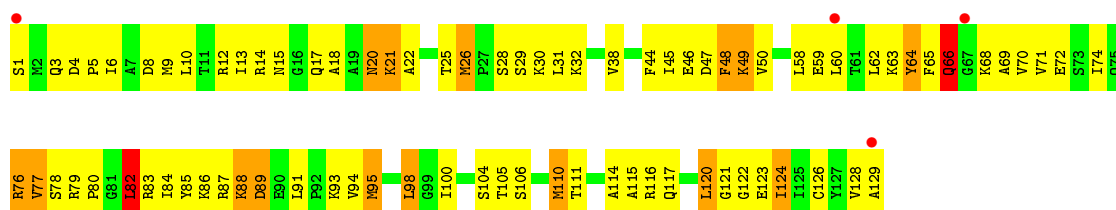




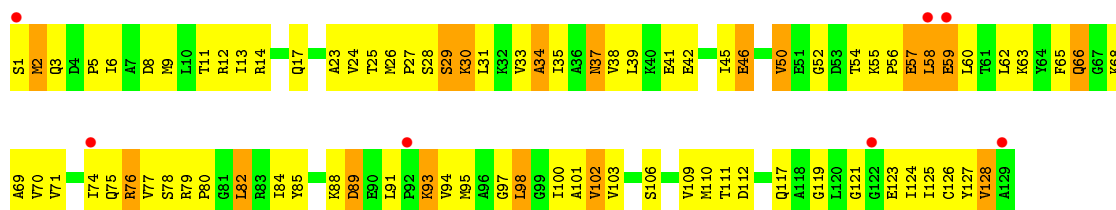
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

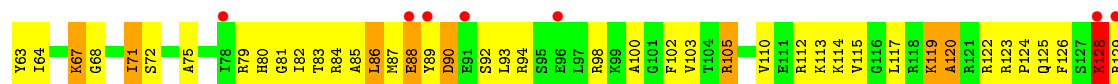


• Molecule 8: 30S ribosomal protein S8

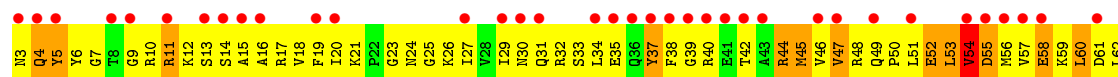


• Molecule 9: 30S ribosomal protein S9

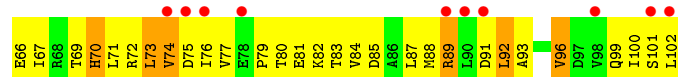
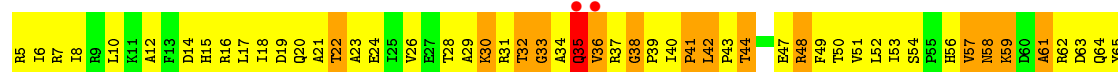




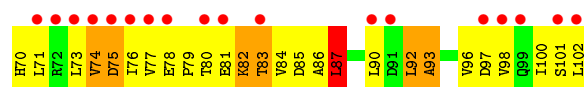
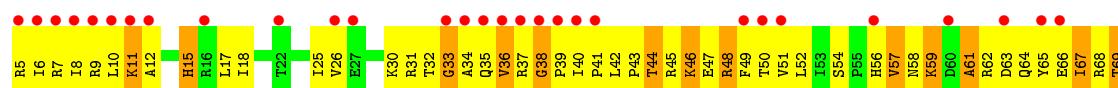
• Molecule 9: 30S ribosomal protein S9



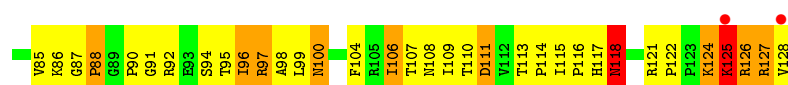
• Molecule 10: 30S ribosomal protein S10



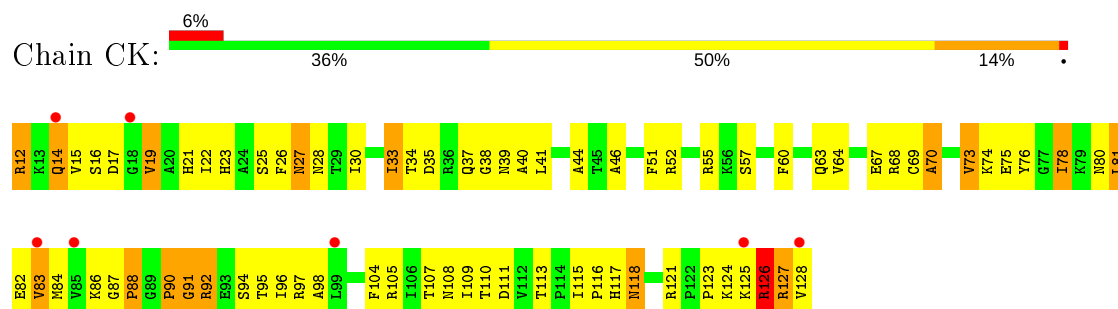
• Molecule 10: 30S ribosomal protein S10



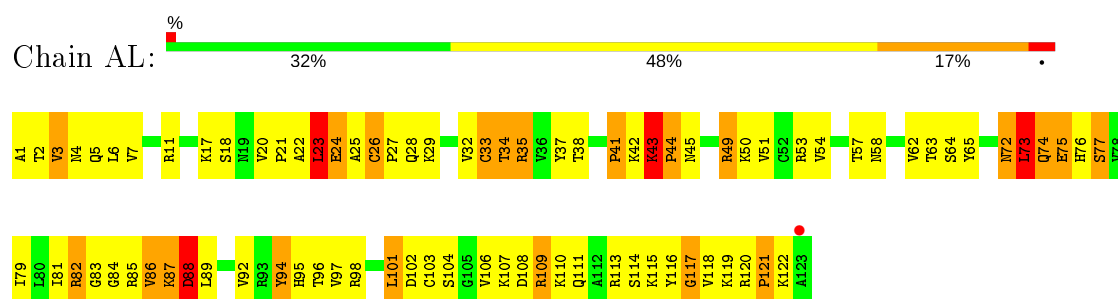
• Molecule 11: 30S ribosomal protein S11



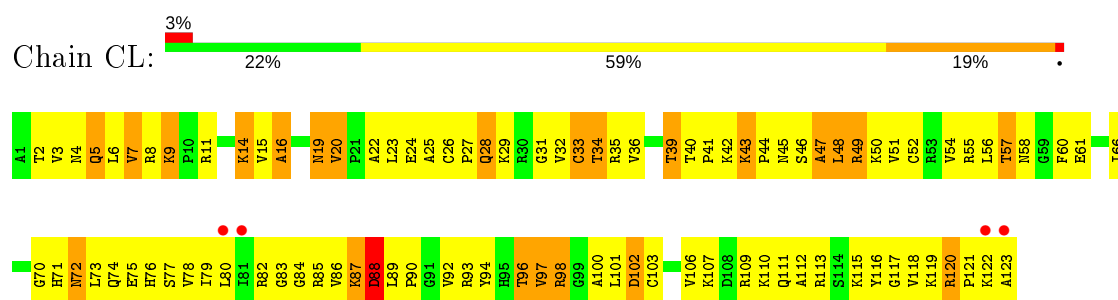
- Molecule 11: 30S ribosomal protein S11



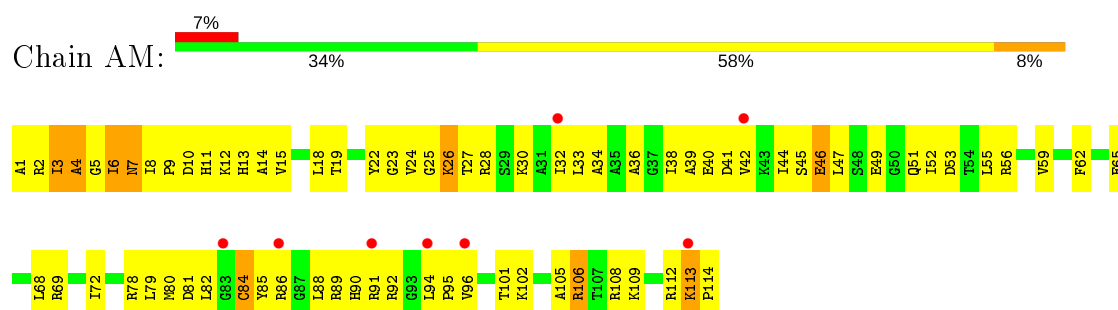
- Molecule 12: 30S ribosomal protein S12



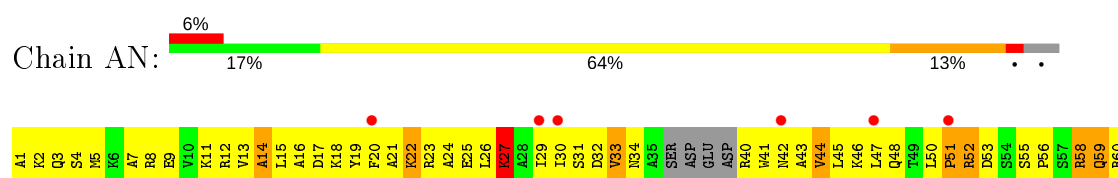
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

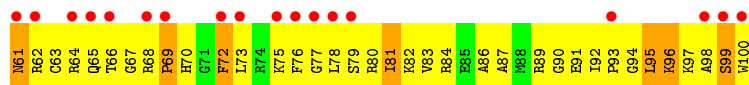
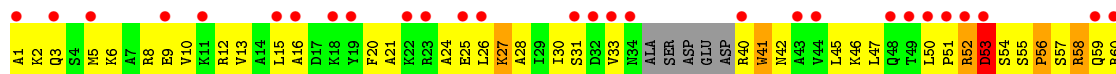


- Molecule 14: 30S ribosomal protein S14

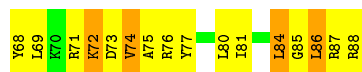
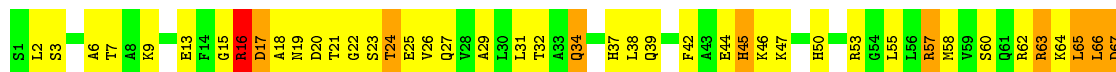
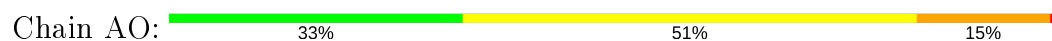




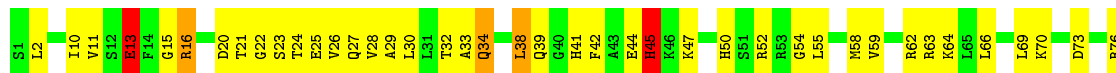
- Molecule 14: 30S ribosomal protein S14



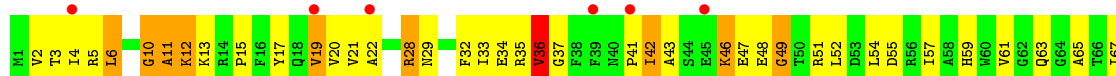
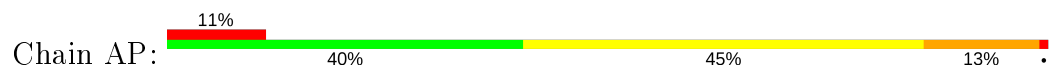
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

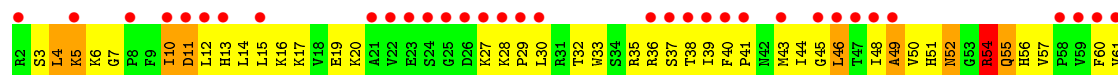


- Molecule 16: 30S ribosomal protein S16



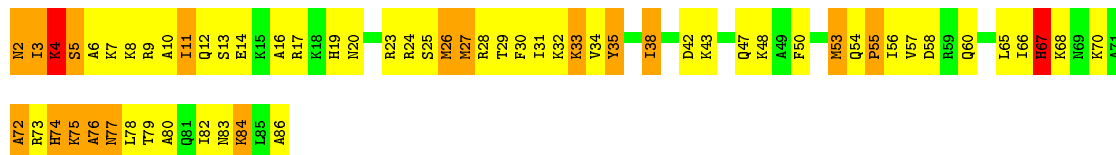
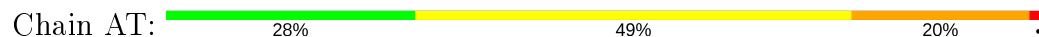
- Molecule 17: 30S ribosomal protein S17



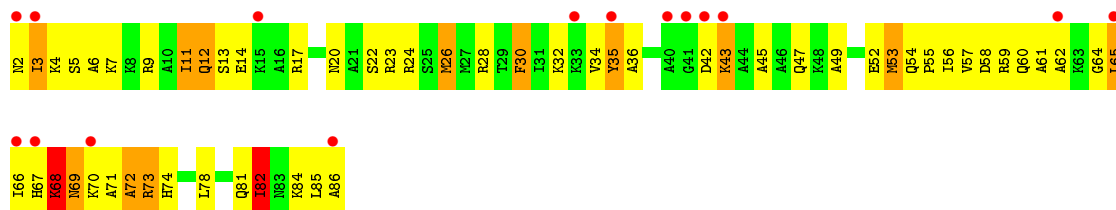




- Molecule 20: 30S ribosomal protein S20



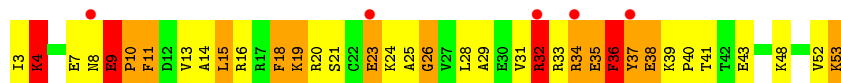
- Molecule 20: 30S ribosomal protein S20



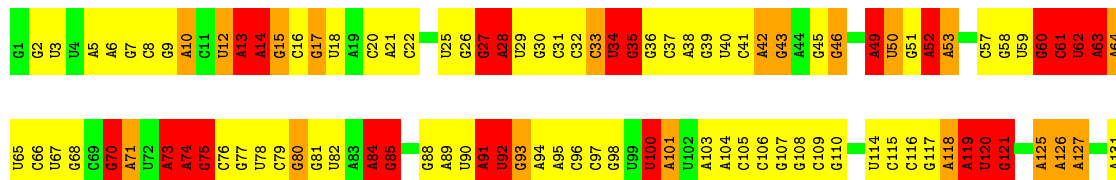
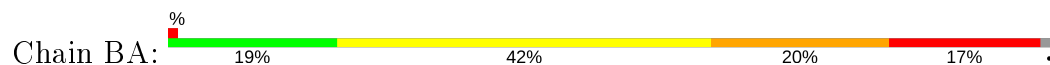
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA

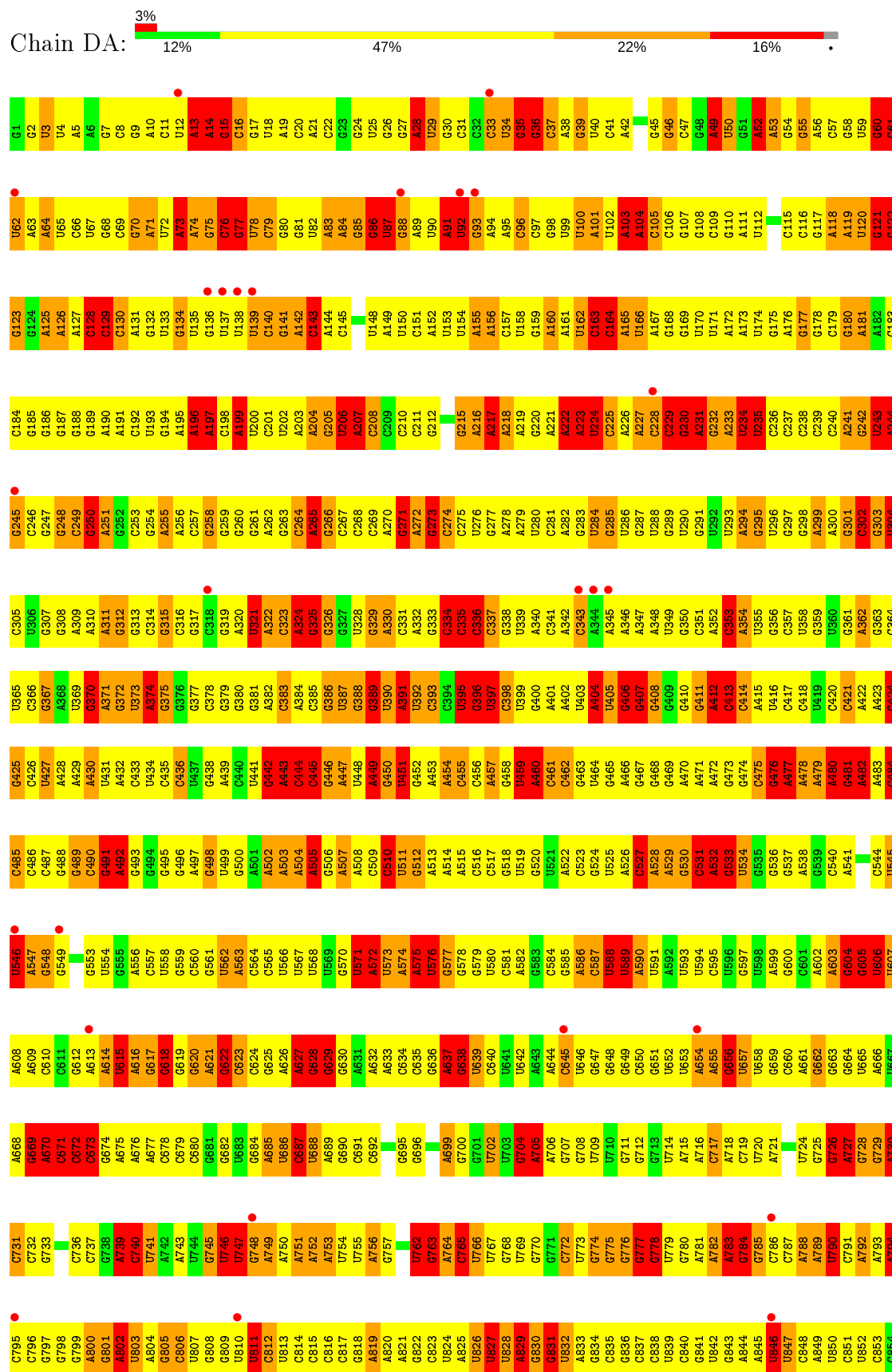




|       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A1046 | A983  | A917 | U850 | C787 | C723 | C560 | U598 | A538 | A471 | A402 | A332 | C267 | U202 | U135 |
| G1047 | A984  | A918 | C851 | A788 | U724 | A661 | A599 | G539 | A472 | U403 | G383 | C268 | A203 | U136 |
| A1048 | C985  | U919 | U852 | A789 | G726 | G662 | C540 | C540 | C473 | U404 | C334 | C269 | A204 | U137 |
| G1049 | C986  | A920 | C853 | U790 | G725 | G663 | C601 | A541 | G474 | U405 | C335 | C270 | A205 | U138 |
| A1050 | C987  | C921 | C854 | C791 | A727 | G664 | A602 | C542 | G475 | G406 | C336 | G271 | U206 | U139 |
| A1054 | A988  | G922 | G855 | A792 | G728 | U665 | A603 | G543 | G476 | G407 | U339 | G272 | A207 | U140 |
| G1055 | G989  | G923 | G856 | A793 | G729 | A666 | G604 | C544 | A477 | G408 | U340 | C273 | C208 | U141 |
| G1056 | A990  | G857 | G857 | A794 | A730 | U667 | G605 | U545 | A478 | G409 | A341 | C274 | C209 | G142 |
| A1057 | G993  | G858 | C858 | C795 | C731 | A668 | U606 | U546 | A479 | G410 | A342 | C275 | C210 | U143 |
| U1058 | A928  | G859 | U860 | C796 | G732 | G669 | U607 | A547 | A480 | G411 | A343 | U276 | C211 | U144 |
| C994  | U929  | G860 | C994 | C797 | G733 | A670 | A608 | A548 | G481 | A412 | A344 | U277 | G212 | U145 |
| G1059 | G995  | U930 | A861 | C798 | A734 | C671 | A609 | G549 | A482 | C413 | A345 | A278 | G213 | U146 |
| U1060 | A996  | G931 | G862 | G799 | A735 | C672 | C610 | C550 | A483 | C414 | A346 | A279 | G214 | U147 |
| U1061 | G997  | U932 | A863 | C736 | C673 | C673 | C611 | G551 | C484 | C415 | A347 | U280 | G215 | U148 |
| G1062 | C998  | A933 | G864 | C737 | G674 | G674 | G612 | U552 | C485 | C416 | U348 | C281 | A216 | U149 |
| G1063 | C1063 | U934 | C865 | G738 | A675 | A675 | A613 | U553 | C486 | C417 | U349 | A282 | A217 | U153 |
| C1064 | A1000 | C935 | A866 | A802 | A739 | A676 | A614 | U554 | G489 | C418 | C353 | U284 | A221 | U154 |
| U1065 | A936  | C937 | C867 | A804 | C740 | U679 | U615 | G555 | C490 | U419 | U353 | U285 | A222 | U155 |
| U1066 | G1002 | C937 | U868 | G805 | U741 | C679 | A616 | A856 | C491 | C420 | C357 | U286 | A223 | U156 |
| G1067 | G1003 | G938 | G869 | C806 | A742 | C680 | G617 | C557 | C492 | C421 | U358 | U287 | A226 | A161 |
| U1068 | U1004 | G939 | U870 | C807 | A743 | G681 | G618 | U558 | G493 | C422 | U359 | U288 | C228 | U162 |
| A1069 | C1005 | G940 | U871 | G808 | U744 | G682 | G619 | C559 | U499 | A423 | U360 | U289 | C229 | U163 |
| A1070 | U1006 | A941 | U872 | G809 | G745 | U688 | G620 | C560 | G495 | C424 | U361 | U290 | C230 | U164 |
| G1071 | A1008 | G942 | G875 | U810 | U746 | A885 | A621 | G561 | U496 | U434 | C362 | U291 | A227 | U165 |
| C1072 | U1009 | A943 | C876 | U811 | U747 | U686 | G622 | U562 | A497 | A438 | C363 | G295 | C231 | U166 |
| A1073 | A1010 | C944 | A877 | C812 | G748 | C887 | C623 | A563 | G498 | A439 | U364 | U296 | A232 | U170 |
| G1074 | U1012 | C946 | U878 | U813 | A749 | U688 | G624 | C564 | U499 | A440 | U365 | G302 | C236 | U171 |
| C1075 | C1013 | A947 | A878 | C815 | U750 | U689 | G625 | C565 | U500 | A441 | U366 | G303 | C237 | A172 |
| A1076 | U1014 | C947 | C885 | G816 | A751 | C691 | A626 | U566 | A501 | U442 | C366 | G304 | C238 | U173 |
| U1077 | U1015 | C948 | A879 | C817 | A752 | C692 | A627 | U567 | A502 | U443 | U367 | U306 | A241 | U174 |
| U1078 | G1017 | U954 | A880 | C818 | U754 | A693 | G628 | U568 | A503 | C436 | U368 | A300 | C240 | G177 |
| C1079 | U1018 | U955 | C876 | C819 | U755 | U694 | A631 | U569 | A504 | U437 | U369 | G307 | G242 | C179 |
| U1081 | U1019 | C957 | A881 | C820 | C758 | G695 | A632 | G570 | A505 | U444 | U370 | G308 | U243 | G180 |
| U1082 | C957  | C957 | C821 | A820 | U759 | G696 | A633 | U571 | G506 | U445 | A371 | A310 | A244 | A181 |
| U1083 | U1020 | U958 | C822 | G822 | G759 | C697 | A634 | A572 | G507 | U446 | U372 | A311 | G245 | A182 |
| A1084 | A1021 | A959 | C823 | G823 | G760 | A699 | C635 | U573 | A508 | U447 | U373 | G312 | G246 | C183 |
| U1085 | G1022 | A960 | U824 | C824 | A761 | G700 | G636 | A574 | G509 | U448 | A374 | G313 | G247 | C184 |
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| G1087 | G1024 | C962 | U826 | A826 | G763 | U702 | G638 | U576 | U511 | U450 | C378 | G315 | C249 | G186 |
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| G1094 | G1031 | G969 | G833 | C833 | G774 | U709 | U646 | G584 | C523 | U457 | U385 | A322 | G256 | U193 |
| A1095 | A1032 | U970 | G834 | C834 | G775 | U710 | U647 | G585 | G524 | U458 | U386 | A323 | G257 | G194 |
| U1096 | U1033 | G971 | A905 | C835 | G776 | G711 | G648 | U586 | U525 | U459 | U387 | A324 | G258 | A195 |
| U1097 | G1034 | A972 | U906 | C836 | G777 | G712 | G649 | A587 | A526 | U460 | U388 | G261 | A259 | A196 |
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| U1107 | C1043 | A980 | G914 | U847 | A783 | C719 | G656 | U594 | A533 | U467 | U395 | G268 | G269 |      |
| U1108 | C1044 | A981 | C915 | U848 | G784 | U720 | U657 | U595 | C595 | U468 | U396 | G269 | G270 |      |
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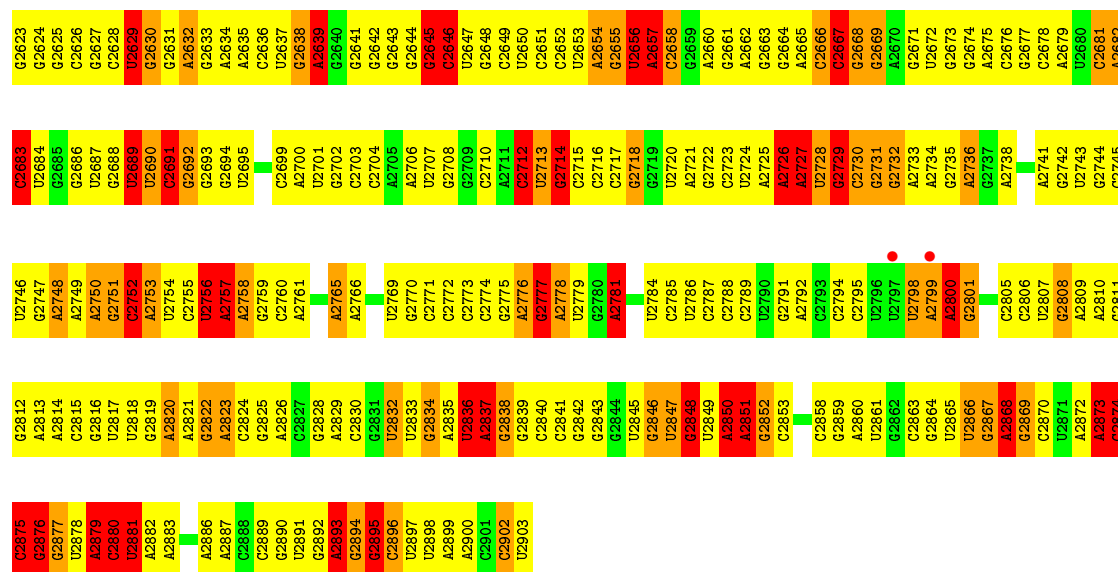
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| G1959 | U1886 | G1824 | G1763 | A1698 | A1634 | G1568 | U1497 | G1432 | G1371 | A1304 | U1242 | U1174 | A1111 |
| A1960 | G1887 | U1825 | G1764 | A1699 | A1635 | A1569 | C1498 | A1433 | A1372 | C1243 | C1243 | A1175 | G1112 |
| G1961 | G1888 | U1826 | U1765 | A1700 | A1636 | A1570 | C1499 | A1434 | A1370 | C1305 | C1244 | U1176 | G1113 |
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| C1964 | A1829 | A1829 | G1768 | G1703 |       |       | A1502 | G1437 | U1375 | G1310 | G1247 | G1179 | G1116 |
| C1965 | G1830 | G1830 | U1769 |       | A1641 |       | A1503 | U1438 | C1376 | G1311 | G1248 | U1180 | C1117 |
| C1966 | A1900 | G1831 | G1770 | C1706 | G1642 |       | A1504 | U1439 | C1377 | U1312 | G1249 | U1181 | C1118 |
| C1967 | A1901 | G1832 | G1771 | G1707 | G1643 |       | A1505 | U1440 | A1378 | U1313 | G1250 | U1182 | U1119 |
| C1968 | G1902 | C1833 | C1708 | A1580 | G1644 |       | U1506 |       | U1379 | C1314 | G1251 | U1183 | G1120 |
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| A1970 | G1904 | G1835 | A1774 | G1710 | G1646 |       | A1508 | G1445 | G1381 | U1315 | G1253 | G1185 |       |
| U1971 | C1775 |       | U1775 | A1711 | U1647 |       | A1509 | C1446 | G1382 | G1317 | A1254 | G1186 | A1126 |
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| C1974 | G1778 |       | U1714 | G1715 | A1650 |       | G1512 | G1450 | A1385 | C1320 | C1257 | A1189 | U1129 |
|       | U1779 |       | G1716 | G1716 | A1651 |       | C1513 | G1451 | A1386 | A1321 | U1258 | G1190 | U1130 |
|       | A1780 |       | U1717 | U1717 | A1652 |       | G1514 | G1452 | A1387 | A1322 | G1259 | G1191 | G1131 |
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|       | U1782 |       | G1718 | G1718 | A1654 |       | U1516 | G1454 | G1389 | G1324 | C1261 |       | A1133 |
|       | A1783 |       | U1719 | A1591 | A1655 |       |       | G1455 |       | U1325 |       |       | C1196 |
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|       | U1786 |       | G1722 | U1594 | G1658 |       | U1523 | U1458 |       | U1267 |       |       | G1136 |
|       | G1787 |       | G1723 | C1595 | G1659 |       | G1524 | G1459 |       | U1329 |       |       | G1137 |
|       | G1788 |       | G1724 | A1596 | G1660 |       | A1525 | U1460 |       | G1330 |       |       | G1138 |
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|       | C1790 |       | G1726 | A1598 | G1662 |       |       | C1462 |       | G1332 |       |       | C1140 |
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|       | A1794 |       | U1729 |       | A1665 |       |       | U1466 |       | C1335 |       |       | A1143 |
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|       | A1807 |       | A1744 |       | U1680 |       |       | G1479 |       | A1286 |       |       | A1156 |
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|       | G1821 |       | C1760 |       | G1695 |       |       | U1493 |       | G1300 |       |       | C1170 |
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| G2865 | G2866 | A2800 | A2753   | A2600 | C2538 | U2477 | C2416 | G2349 | A2288 | G2219 | A     | G2029 |
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| A2868 | A2869 | G2802 | G2741   | A2602 | C2540 | U2479 | A2419 | C2351 | G2290 | C2225 | G     | A2031 |
| C2869 | C2870 | G2803 | G2742   | G2603 | A2541 | A2480 | C2420 | A2352 | U2291 | C2226 | C     | G2032 |
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| C2872 | C2873 | G2805 | G2744   | U2605 | C2543 | G2482 | C2422 | C2354 | G2293 | U2228 | A     | U2034 |
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| A2885 | A2886 | G2812 | C2751   | C2612 | U2550 | G2490 | G2428 | G2361 | C2300 | G2235 | A     | U2041 |
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| A2893 | A2894 | G2816 | U2755   | U2616 | U2554 | G2494 | A2432 | G2365 | U2304 | U2240 | A     | G2045 |
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|       |       | G2823 | C2762   | U2623 | U2561 | C2501 | A2441 | C2379 | C2312 | G2258 | U     | G2054 |
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|       |       | C2825 | U2764   | U2625 | A2563 | U2503 | C2443 | C2381 | A2314 | G2260 | U     | G2056 |
|       |       | A2826 | U2765   | G2626 | C2564 | U2504 | U2444 | C2382 | G2315 | U2261 | G     | G2057 |
|       |       | U2827 | C2766   | U2627 | U2565 | C2505 | G2445 | G2383 | U2316 | U2262 | G     | A2058 |
|       |       | G2828 | A2767   | C2628 | U2566 | U2506 | G2446 | U2384 | A2317 | G2263 | A     | U2059 |
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|       |       | U2830 | U2769   | G2630 | U2568 | C2508 | A2448 | C2386 | G2319 | U2265 | C     | G2061 |
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|       |       | U2833 | U2772   | U2633 | U2571 | C2511 | A2451 | U2390 | G2322 | U2268 | U     | G2064 |
|       |       | A2834 | C2773   | A2634 | C2572 | C2512 | C2452 | U2391 | G2323 | U2269 | U     | G2065 |
|       |       | C2835 | U2774   | U2635 | U2573 | U2513 | A2453 | G2392 | G2324 | U2270 | U     | G2066 |
|       |       | U2836 | U2775   | C2636 | C2574 | C2514 | G2454 | U2393 | G2325 | U2271 | C     | G2067 |
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|       |       | C2860 | U2799   | U2660 | U2598 | G2538 | U2478 | G2417 | U2349 | G2288 | U     | G2091 |
|       |       | U2861 | C2799   | G2661 | C2599 | U2539 | U2479 | G2418 | G2350 | G2289 | U     | G2092 |
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|       |       | A2874 | U2812   | U2674 | U2612 | U2552 | U2492 | G2431 | U2363 | U2302 | U     | U2105 |
|       |       | C2875 | U2813   | U2675 | U2613 | U2553 | U2493 | G2432 | U2364 | U2303 | U     | G2106 |
|       |       | U2876 | U2814   | U2676 | U2614 | U2554 | U2494 | G2433 | U2365 | U2304 | U     | U2107 |
|       |       | A2877 | U2815   | U2677 | U2615 | U2555 | U2495 | G2434 | U2366 | U2305 | U     | G2108 |
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|       |       | A2886 | U2824   | U2686 | U2624 | U2564 | U2504 | G2443 | U2375 | U2314 | U     | U2117 |
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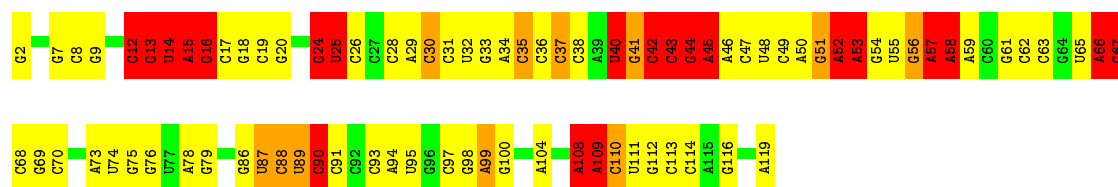




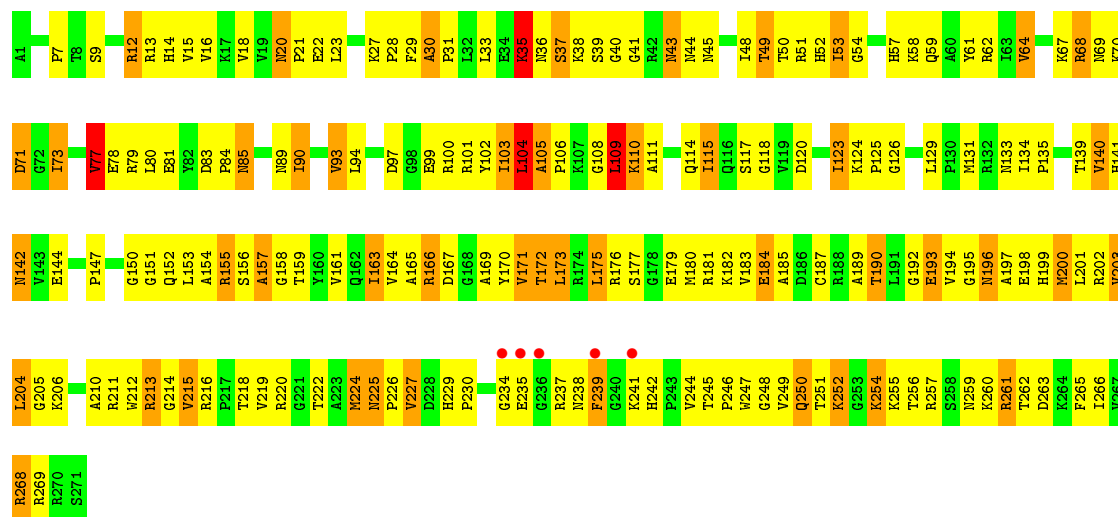
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| G2567 | U2506 | A2439 | G2375 | A2314 | C2254 | U     | C2066 | C2000 | G1930 | U1866 | G1799 | G1738 |
| U2568 | C2507 | G2440 | A2376 | G2315 | G2255 | U     | G2067 | C2001 | U1931 | G1867 | C1800 | A1739 |
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• Molecule 23: 5S rRNA

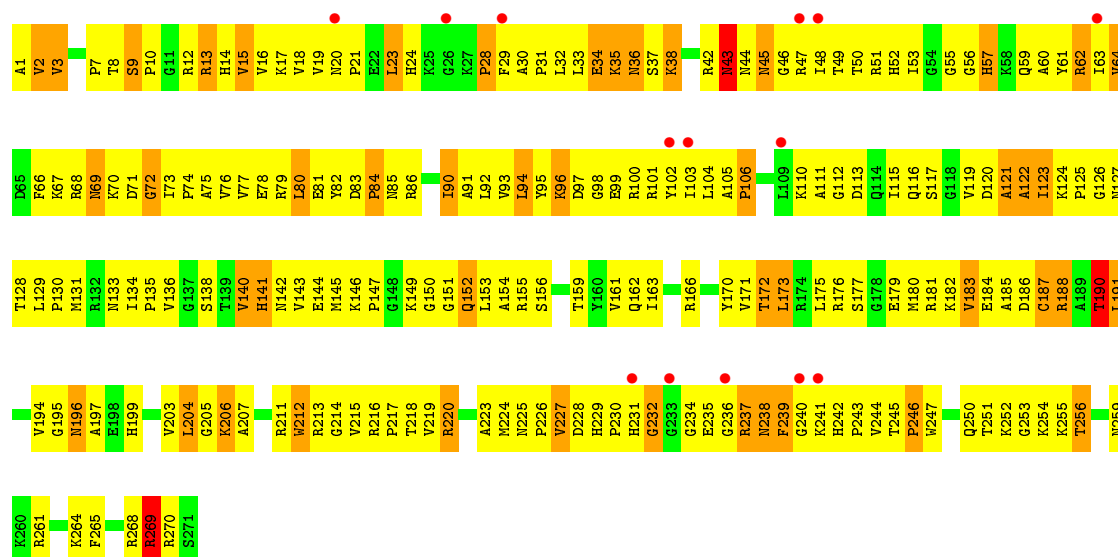


• Molecule 24: 50S ribosomal protein L2



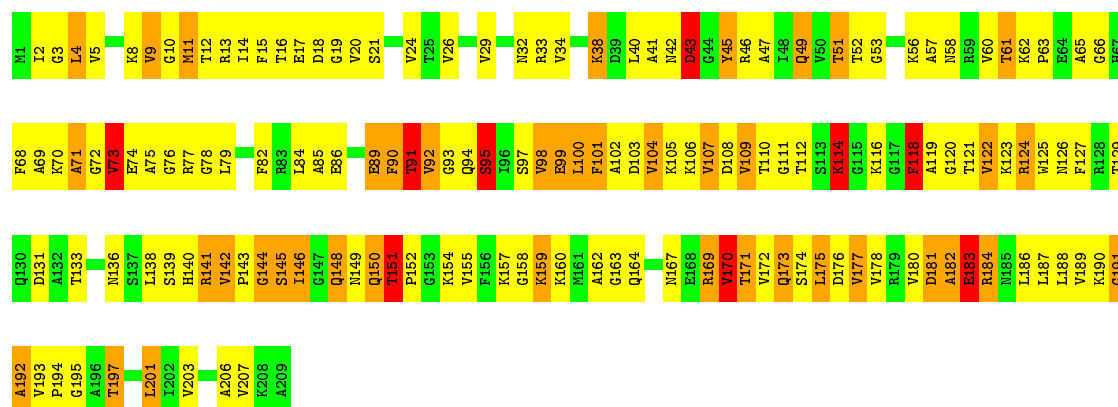
• Molecule 24: 50S ribosomal protein L2





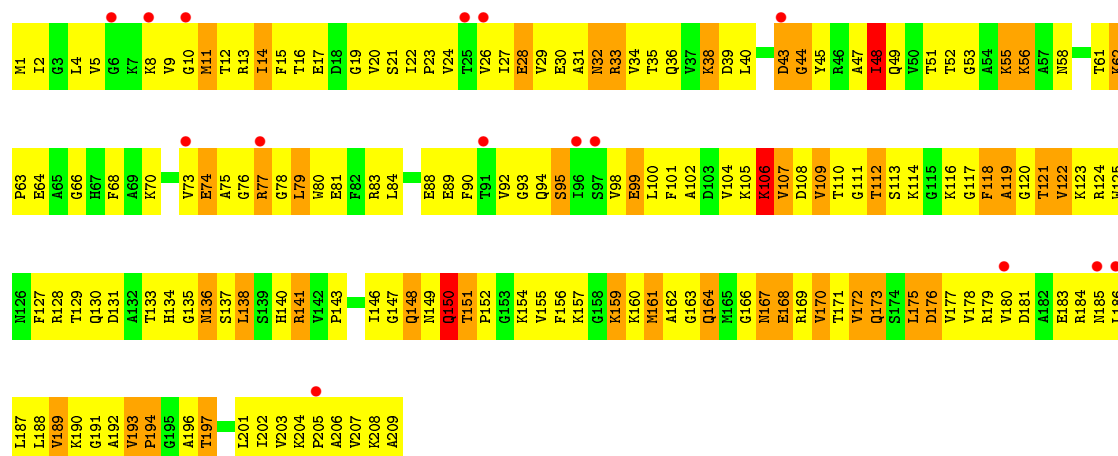
• Molecule 25: 50S ribosomal protein L3

Chain BD: 26% 50% 20% .



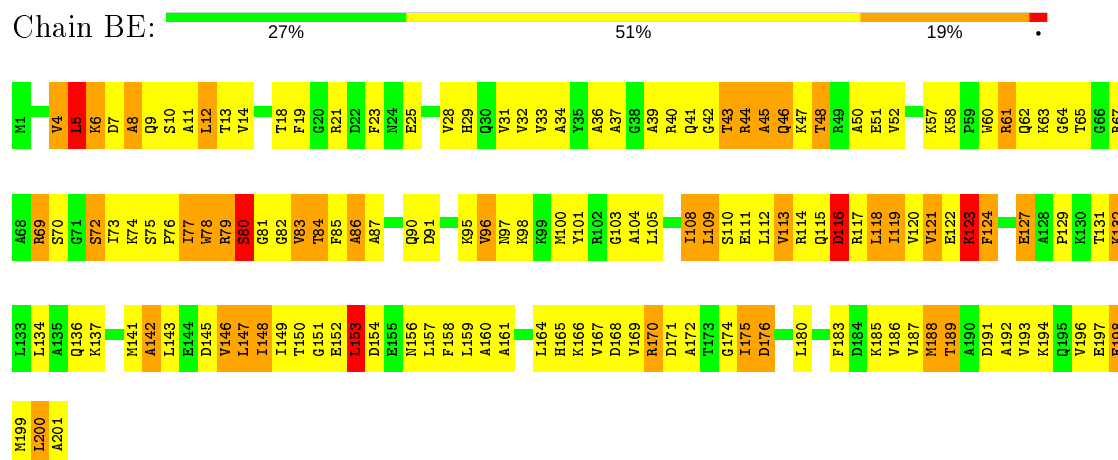
• Molecule 25: 50S ribosomal protein L3

Chain DD: 7% 21% 58% 20% .

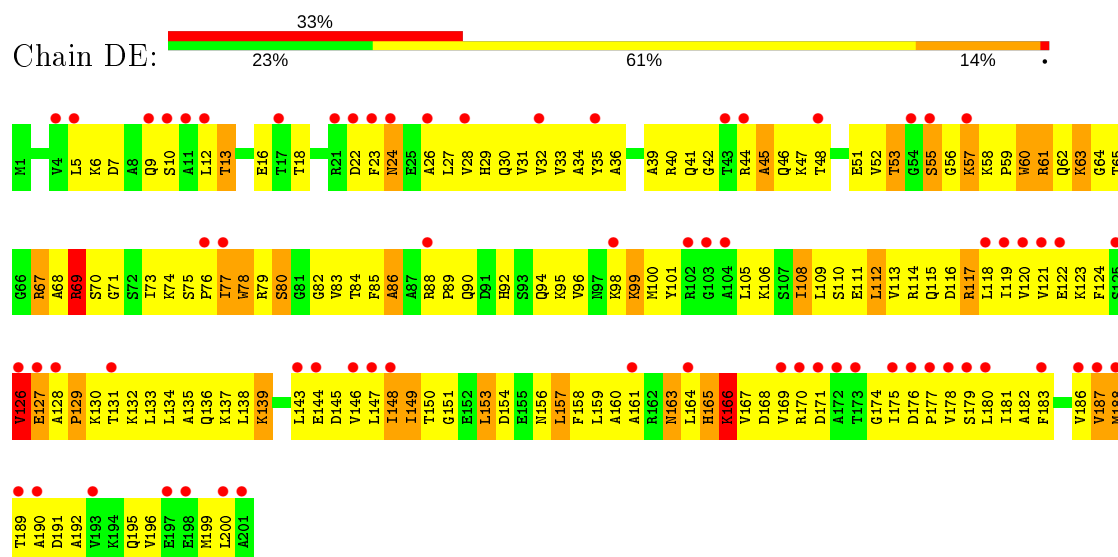




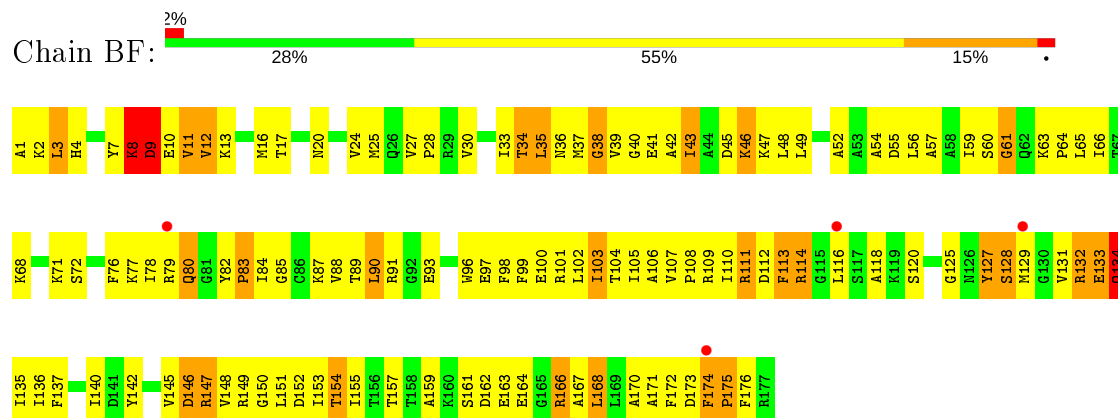
- Molecule 26: 50S ribosomal protein L4



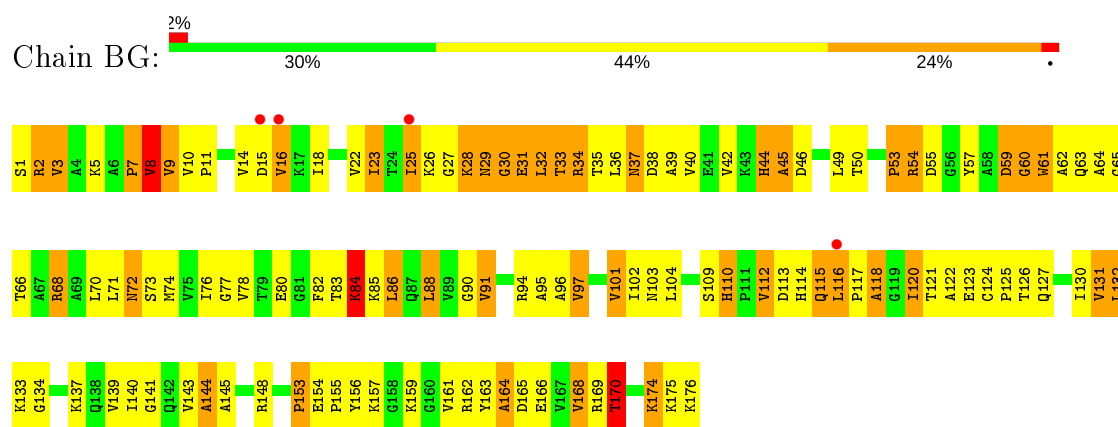
- Molecule 26: 50S ribosomal protein L4



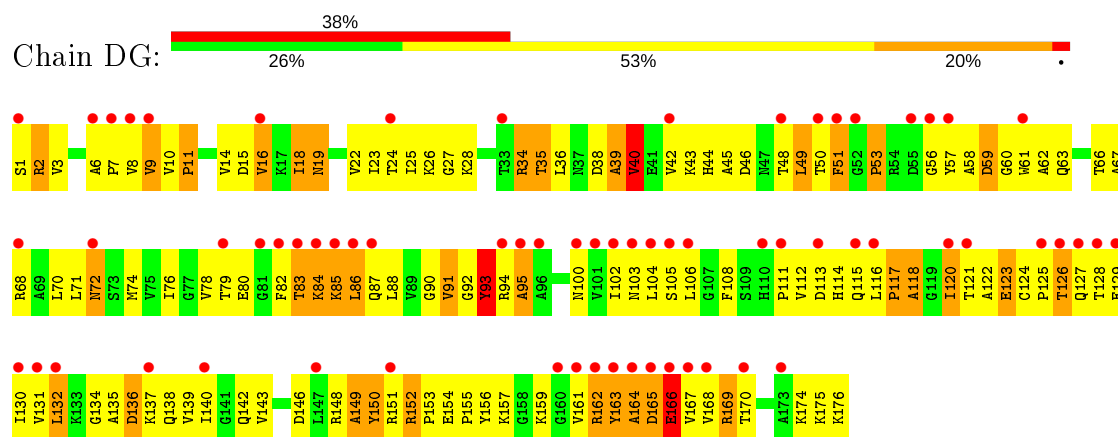
- Molecule 27: 50S ribosomal protein L5



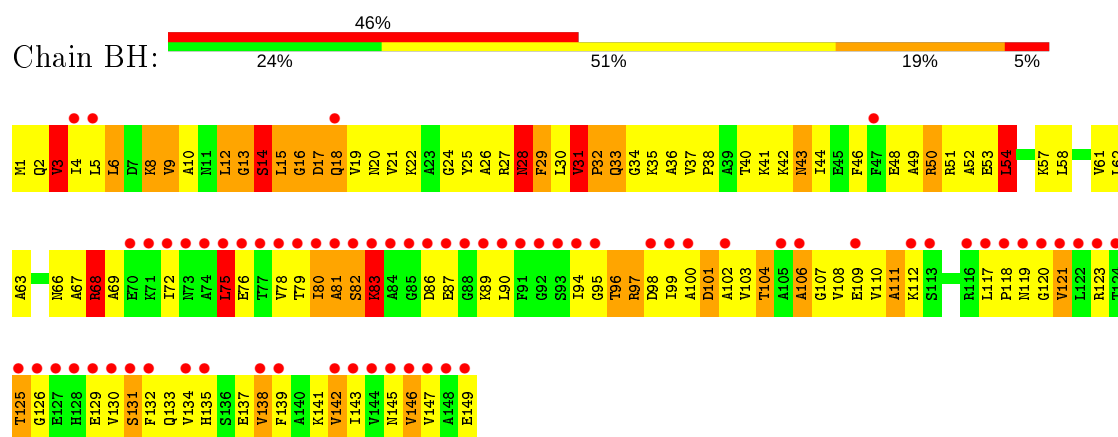
- Molecule 28: 50S ribosomal protein L6



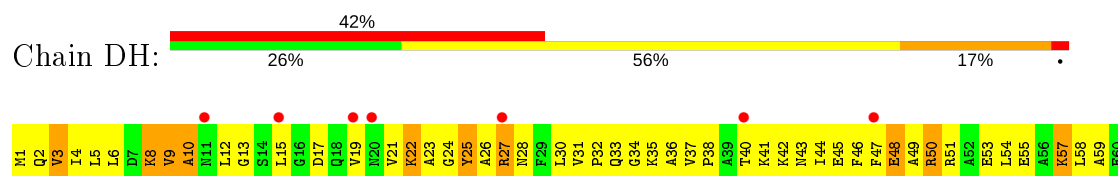
• Molecule 28: 50S ribosomal protein L6

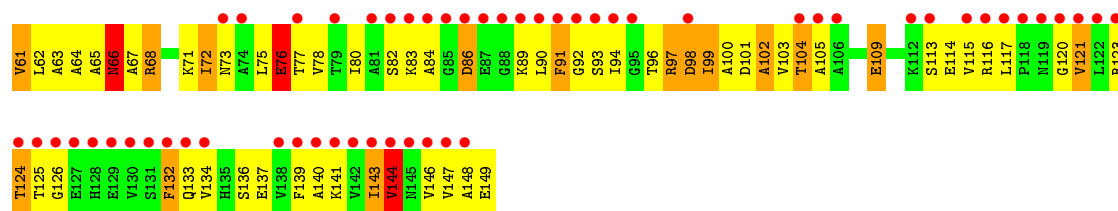


• Molecule 29: 50S ribosomal protein L9

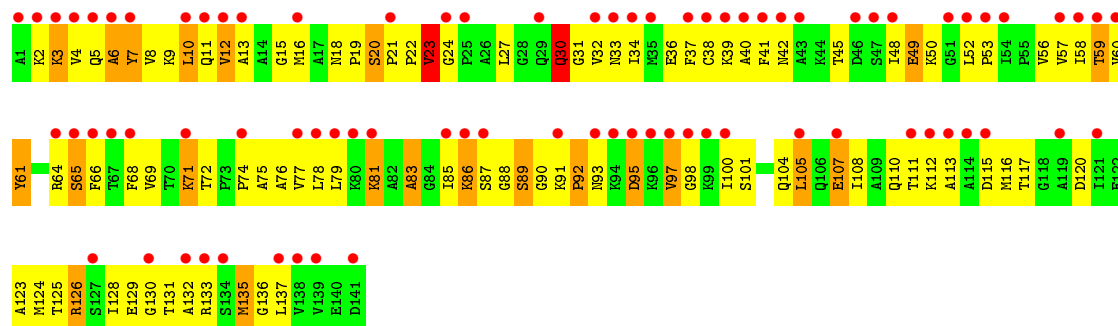


• Molecule 29: 50S ribosomal protein L9

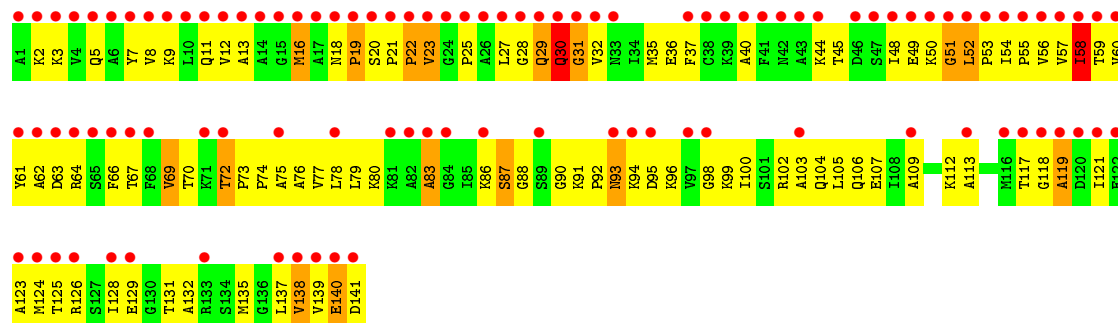
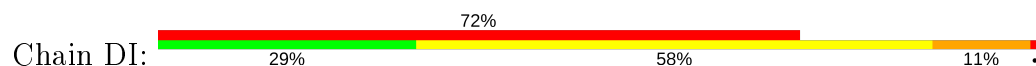




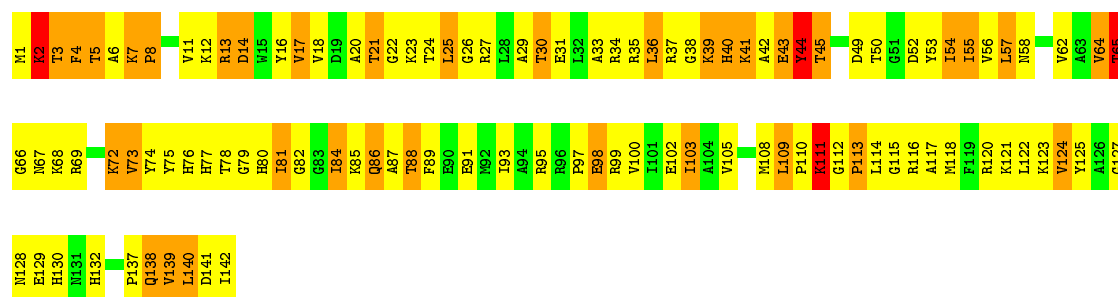
• Molecule 30: 50S ribosomal protein L11



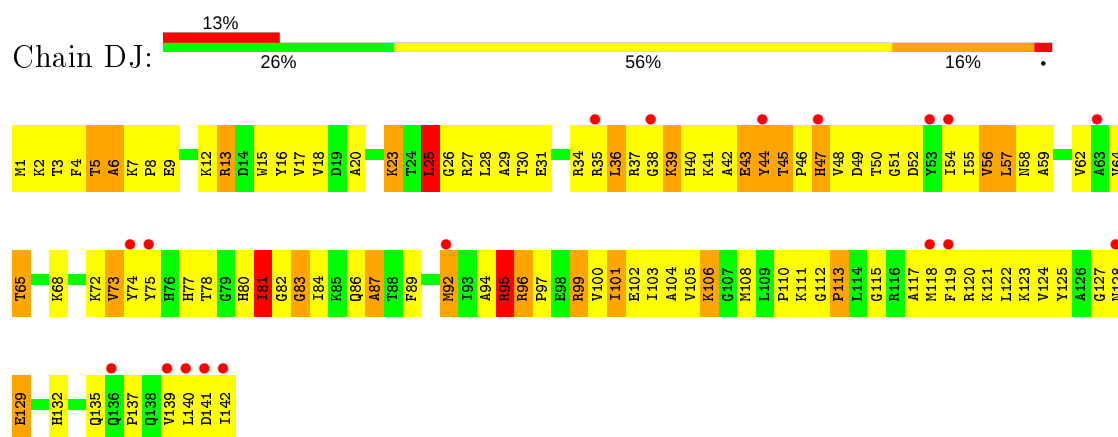
• Molecule 30: 50S ribosomal protein L11



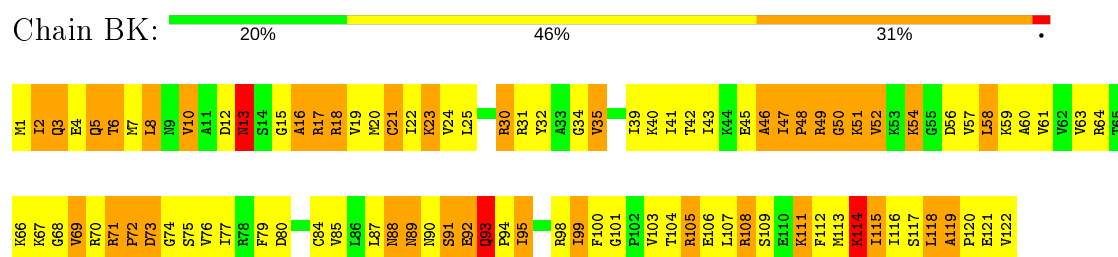
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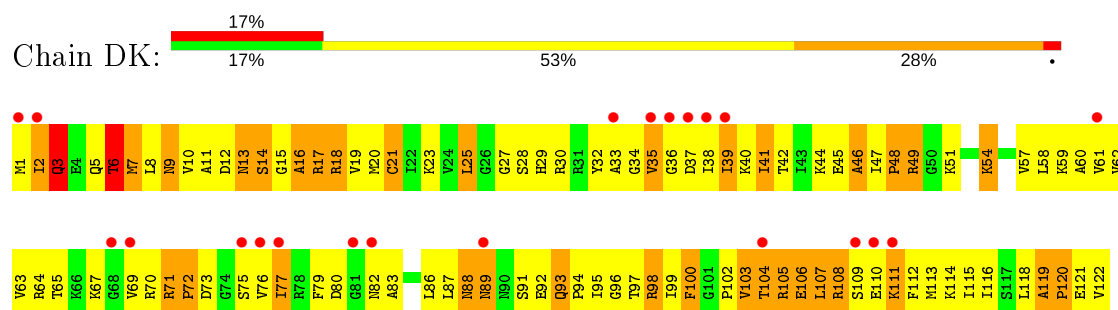
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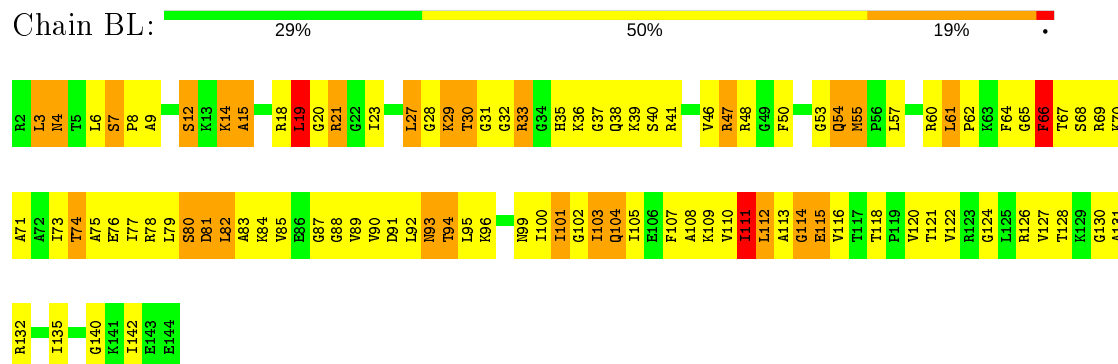
- Molecule 32: 50S ribosomal protein L14



- Molecule 32: 50S ribosomal protein L14

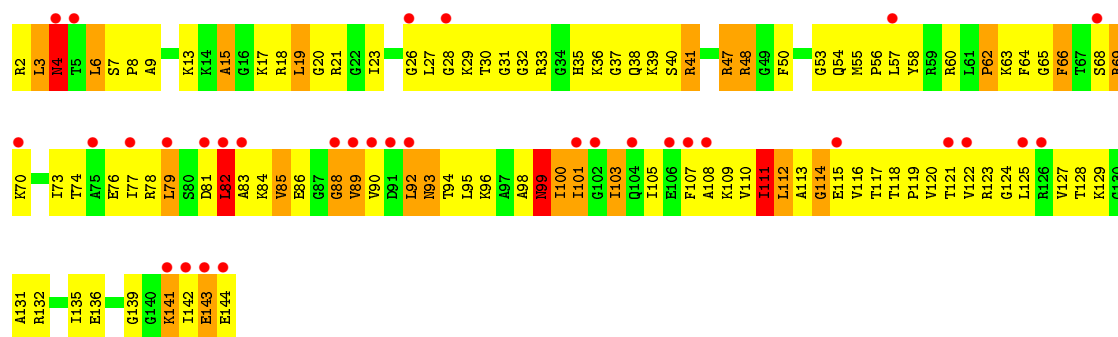


- Molecule 33: 50S ribosomal protein L15



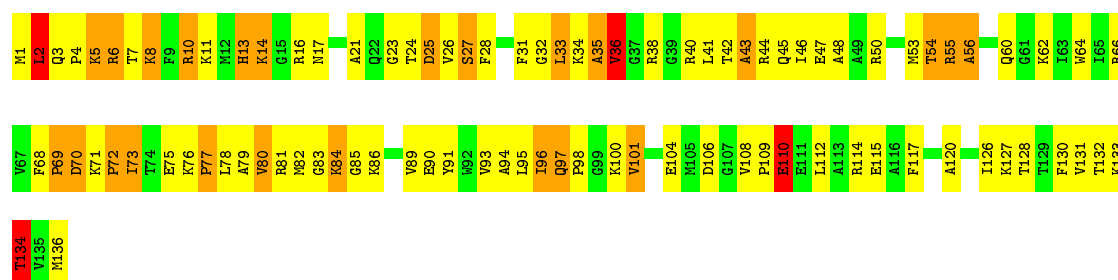
- Molecule 33: 50S ribosomal protein L15





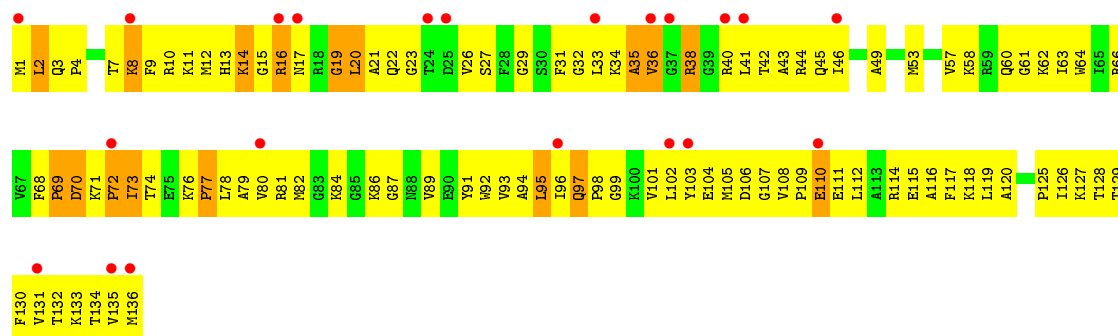
• Molecule 34: 50S ribosomal protein L16

Chain BM: 31% 49% 18%



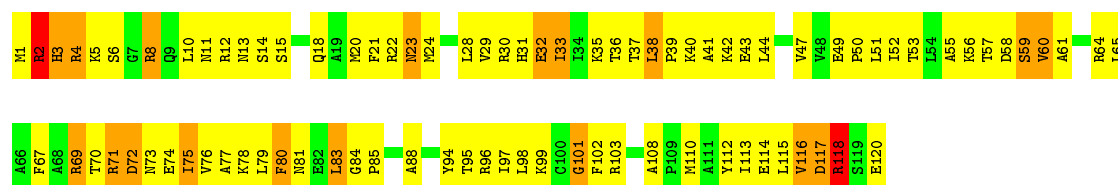
• Molecule 34: 50S ribosomal protein L16

Chain DM: 15% 23% 65% 13%

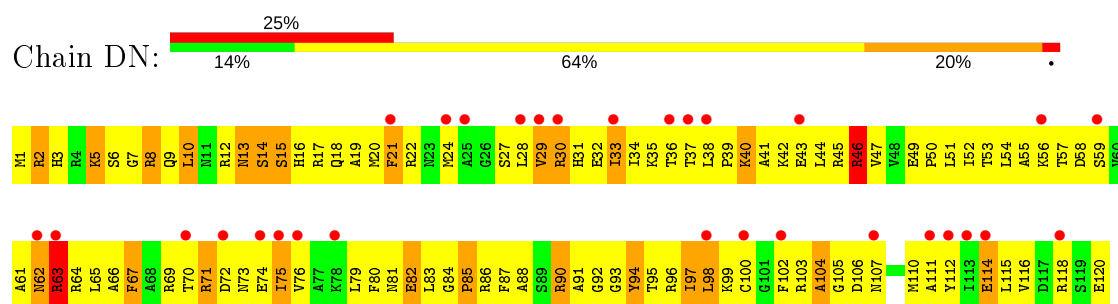


• Molecule 35: 50S ribosomal protein L17

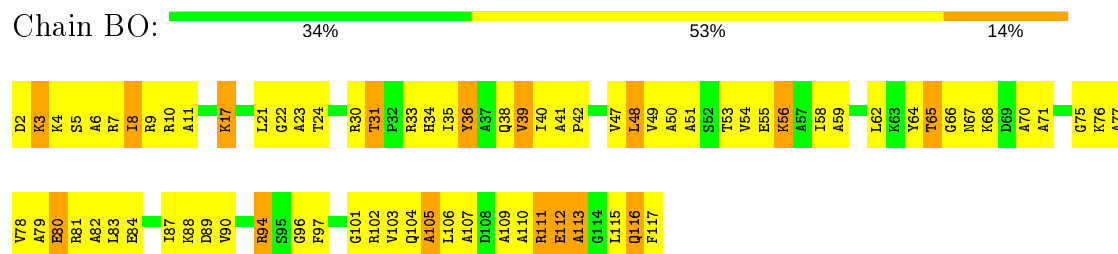
Chain BN: 28% 56% 15%



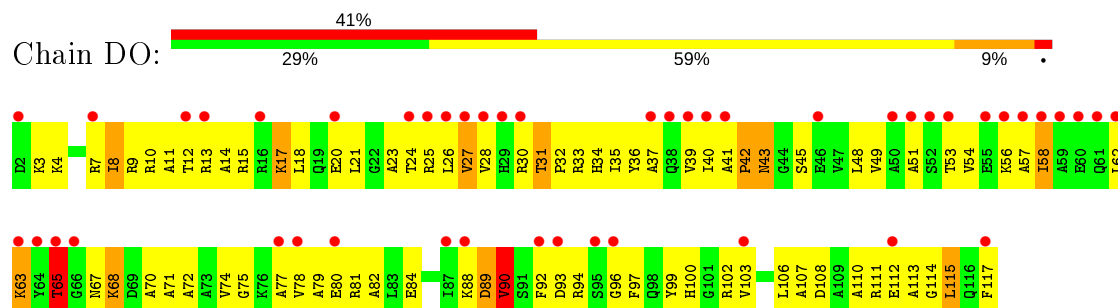
• Molecule 35: 50S ribosomal protein L17



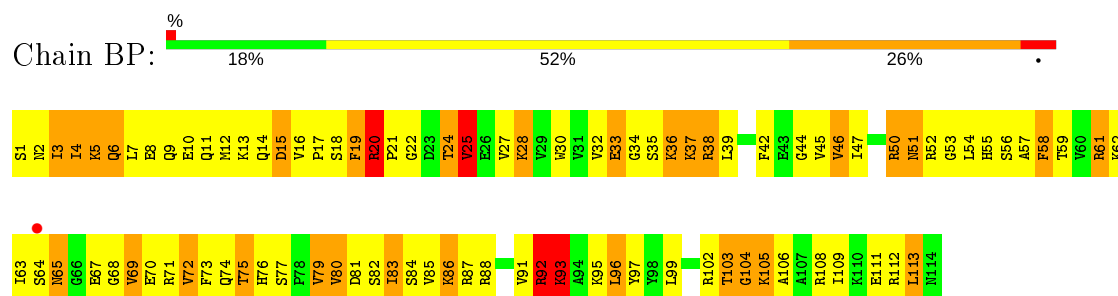
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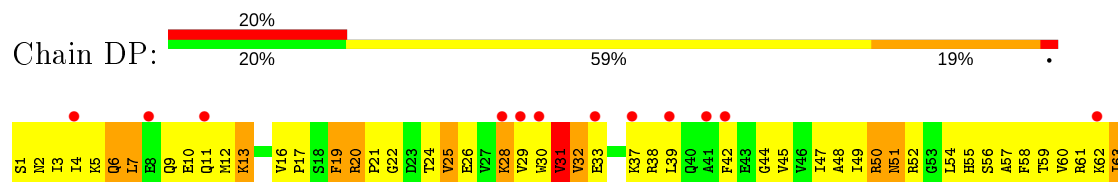
- Molecule 36: 50S ribosomal protein L18

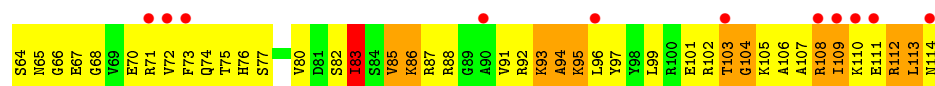


- Molecule 37: 50S ribosomal protein L19

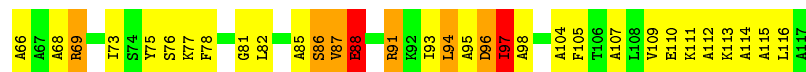
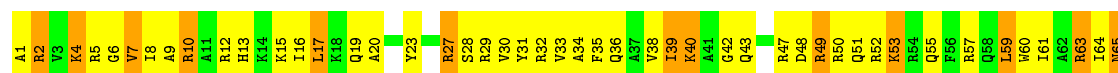
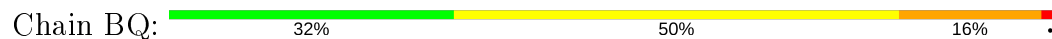


- Molecule 37: 50S ribosomal protein L19

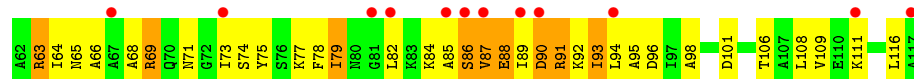
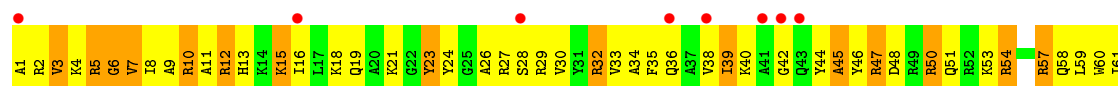




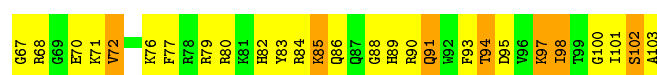
- Molecule 38: 50S ribosomal protein L20



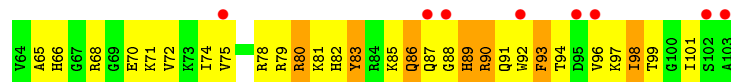
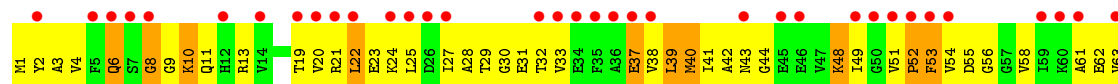
- Molecule 38: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L21

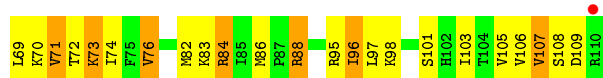


- Molecule 39: 50S ribosomal protein L21

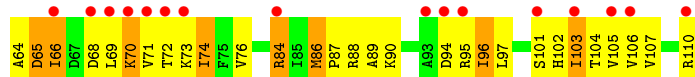


- Molecule 40: 50S ribosomal protein L22





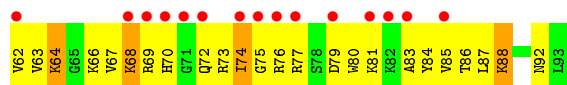
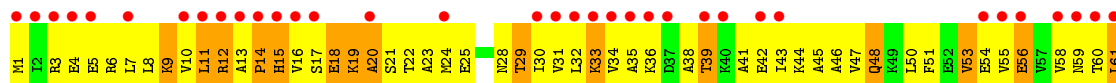
• Molecule 40: 50S ribosomal protein L22



• Molecule 41: 50S ribosomal protein L23



• Molecule 41: 50S ribosomal protein L23

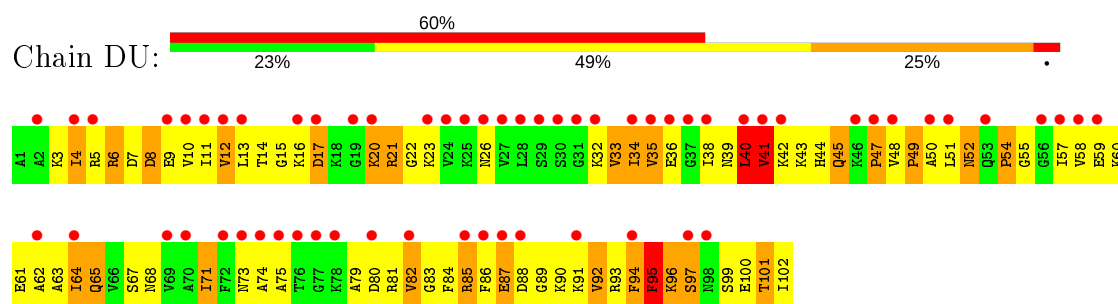


• Molecule 42: 50S ribosomal protein L24

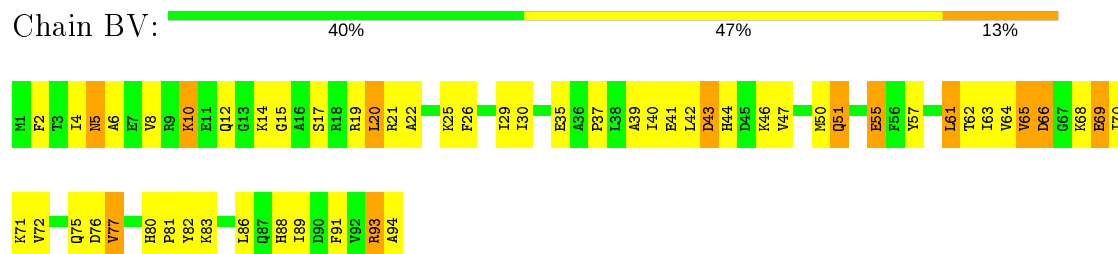


• Molecule 42: 50S ribosomal protein L24

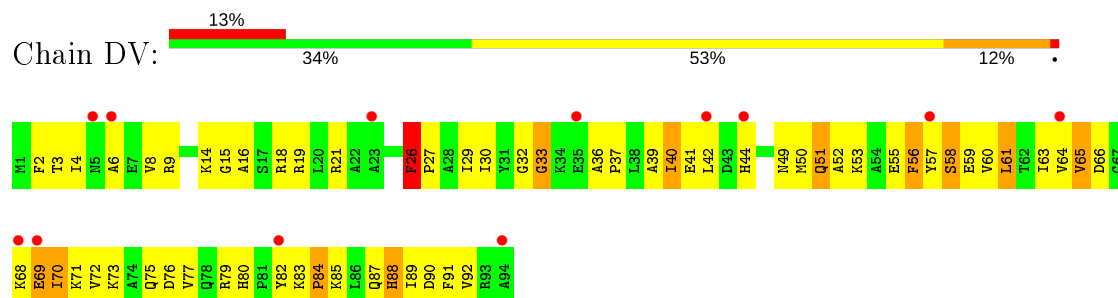




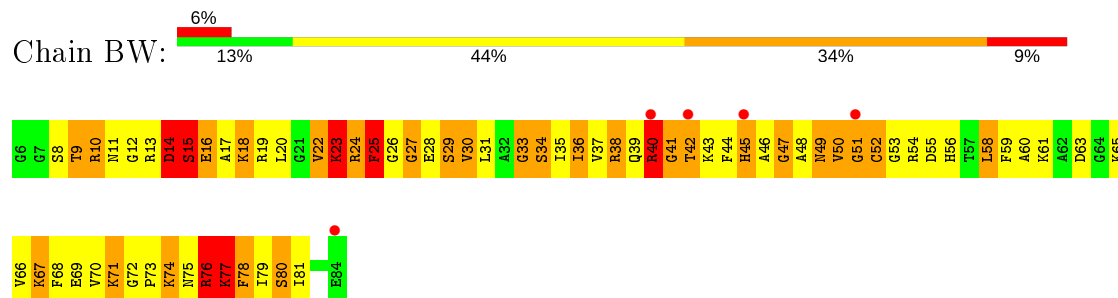
- Molecule 43: 50S ribosomal protein L25



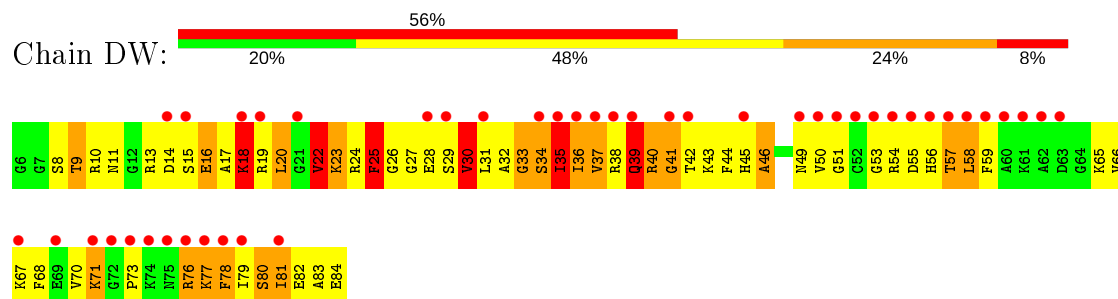
- Molecule 43: 50S ribosomal protein L25



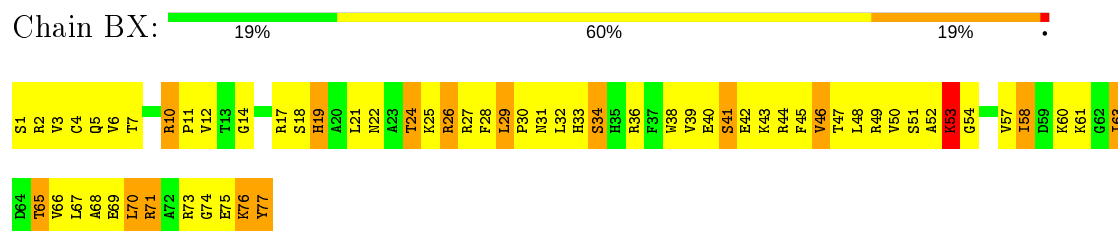
- Molecule 44: 50S ribosomal protein L27



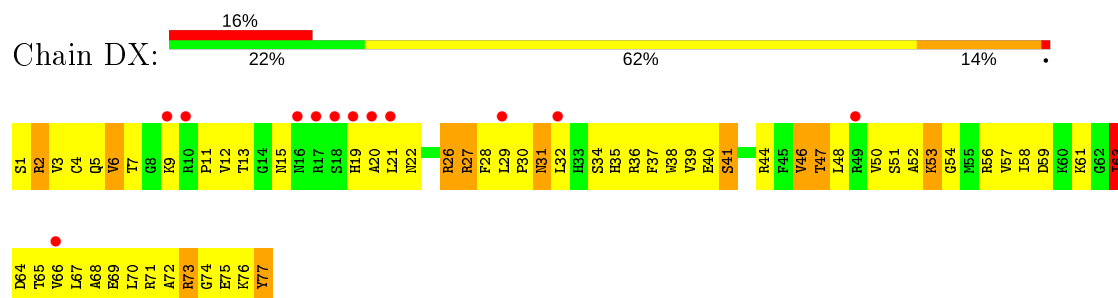
- Molecule 44: 50S ribosomal protein L27



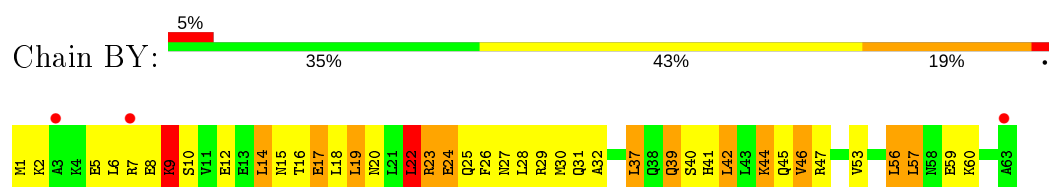
- Molecule 45: 50S ribosomal protein L28



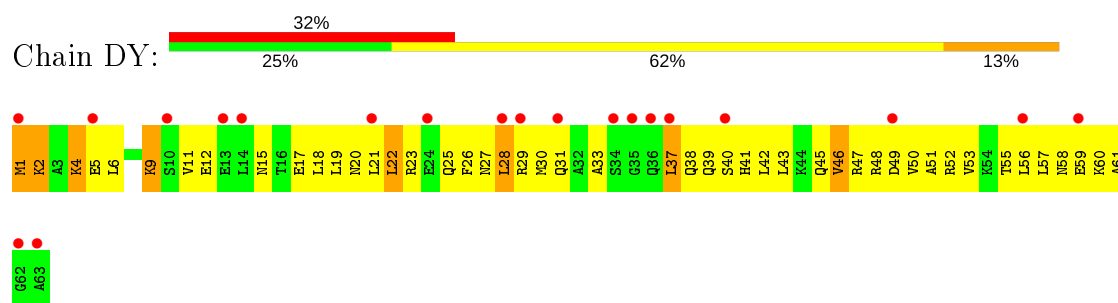
- Molecule 45: 50S ribosomal protein L28



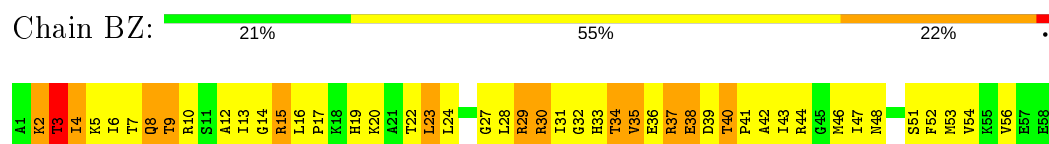
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29

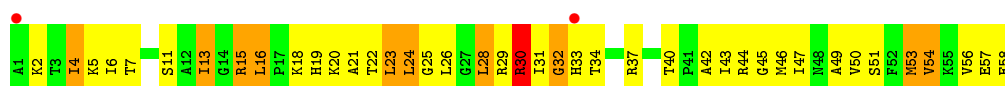


- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

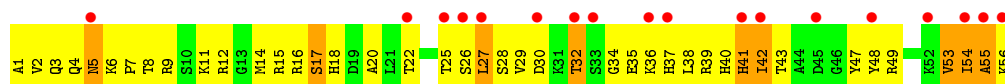




- Molecule 48: 50S ribosomal protein L32



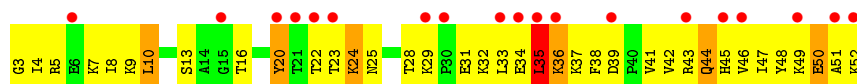
- Molecule 48: 50S ribosomal protein L32



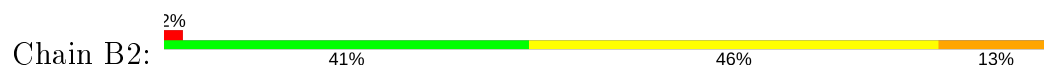
- Molecule 49: 50S ribosomal protein L33



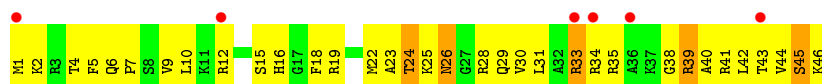
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



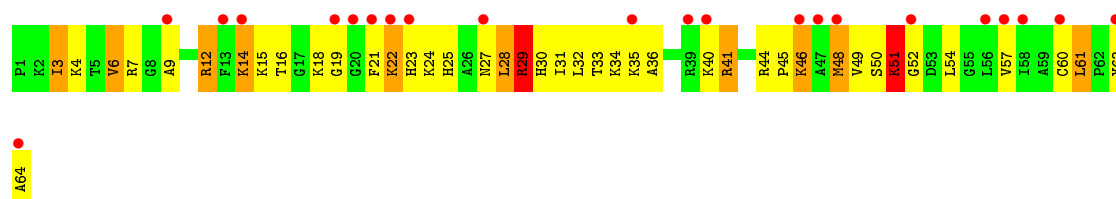
- Molecule 51: 50S ribosomal protein L35

Chain B3: 



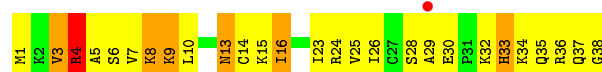
- Molecule 51: 50S ribosomal protein L35

Chain D3: 



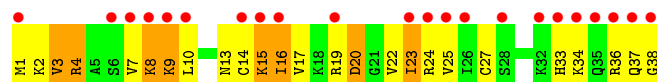
- Molecule 52: 50S ribosomal protein L36

Chain B4: 




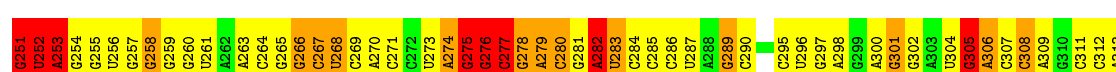
- Molecule 52: 50S ribosomal protein L36

Chain D4: 



- Molecule 53: 16S rRNA

Chain CA: 

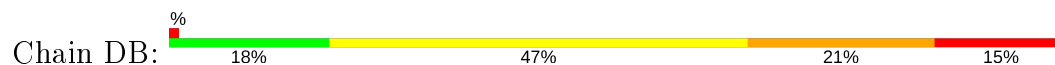


|       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|
| A1201 | G1138 | U1073 | G1013 | G953  | G888 | U822 | A759 | G700 | C634 | G566 | C594 | U439 | G376 | C314 |
| U1202 | G1139 | G1074 | A1014 | G954  | A889 | C823 | G760 | G700 | A635 | G567 | G505 | C440 | G377 | A315 |
| G1203 | C1140 | U1075 | G1015 | U955  | G890 | G824 | G761 | U701 | U636 | G568 | G506 | A441 | G378 | C316 |
| A1204 | C1141 | A1016 | G1016 | U956  | U891 | A825 | U762 | A702 | C637 | C569 | C507 | G442 | C379 | U317 |
| G1205 | G1142 | G1077 | U1017 | U957  | A892 | C826 | G763 | G703 |      | U508 | U508 | G443 | G380 | G318 |
| U1206 | G1143 | A958  | G1018 | A958  | C932 | U827 | G764 | A704 | A640 | U571 | A509 | G444 | C381 | G319 |
| G1207 | G1144 | G1079 | A1019 | A959  | G894 | U828 | G765 | G705 | U641 | U572 | A510 | G445 | A382 | A320 |
| C1208 | A1145 | A1080 | G1020 | U960  | G895 | G829 | A766 | A706 | A642 | A573 | C511 |      | A383 | A321 |
| G1209 | A1146 | A1081 | A1021 | U961  | C896 |      |      | U707 | C643 | A574 | U512 | A448 | G384 | C322 |
| C1210 | C1147 | A1082 | A1022 | C962  | C897 | G833 | G769 | U708 | U644 | C575 | C513 |      | A325 |      |
| U1211 | U1148 | U1083 | G1023 | G963  | G898 | U834 | C770 | U709 | G645 | C576 | C514 |      | C385 |      |
| U1212 | A1149 | G1084 | G1024 | A964  | C900 | U835 | G771 | G710 | G646 | G577 | G515 |      | C386 |      |
| A1213 | A1150 | U1085 | U1025 | U965  | C899 | U836 | U772 | G711 | C647 | C578 | U516 |      | U387 |      |
| C1214 | A1151 | U1086 | G1026 | G966  | A901 | U837 | G773 | A712 | A648 | A579 | G517 |      | G388 |      |
| G1215 | A1152 | G1087 | C1027 | C967  | G902 | G838 | G774 | G713 | A649 | C580 | C518 |      | A389 |      |
| A1216 | G1153 | G1088 | G1028 | A968  | G903 |      | G775 | G714 | G650 | C581 | C519 |      | U390 |      |
| G1217 | G1154 | U1089 | A1029 | A969  | C904 | C841 | G776 | A715 | C651 | C582 | A520 |      | G391 |      |
| C1218 | A1155 | U1090 | U1030 | C970  | C909 | U842 | A777 | A716 | U652 | C583 | G521 |      | C392 |      |
| U1219 | G1156 | U1091 | G1031 | G971  | A909 | U843 | G778 | U717 | U653 | C584 | C522 |      | A393 |      |
| G1220 | A1157 | A1092 | G1032 | G972  | C910 | G844 |      | A718 | G654 | C585 | A523 |      | G394 |      |
| G1221 | C1158 | A1093 | G1033 | G973  |      |      | A781 | C719 | A655 | A461 |      |      | C395 |      |
| G1222 | U1159 | G1094 | G1034 | A974  | A913 | G846 | A782 | C720 | G656 | G462 |      |      | A397 |      |
| C1223 | G1160 | A1035 | A1036 | A975  | A914 | U847 | C783 | G721 | U657 | U463 |      |      | A398 |      |
| U1224 | C1161 | A1036 | A1037 | G976  | A915 | C848 | A784 | G722 | C658 | U464 |      |      | G399 |      |
| A1225 | G1162 | C1096 | C1037 | A977  | U916 | G849 | G785 | U723 | U659 | A465 |      |      | C400 |      |
| C1226 | C1162 | C1097 | G1038 | A978  | G917 |      | G786 | G724 |      | A466 |      |      |      |      |
| A1227 | U1165 | G1099 | G1039 | C979  | A918 | C853 | A787 | C725 | A663 | U467 |      |      | G404 |      |
| G1228 | G1166 | C1100 | U1040 | C980  | A919 | U854 | U788 | C726 | G664 | A468 |      |      | U405 |      |
| A1229 | A1167 | A1101 | G1041 | U991  | U920 | U855 | U789 | G727 | A665 | C469 |      |      | A406 |      |
| C1230 | U1168 | A1102 | A1042 | U982  | U921 |      | A790 | A728 | G666 |      |      |      | U407 |      |
| G1231 | A1169 | C1103 | G1043 | A983  | G922 | G858 | G791 | A729 | G667 | U473 |      |      | A408 |      |
| U1232 | A1170 | G1104 | A1044 | C984  | A923 | U859 | A792 | C730 | G668 | G474 |      |      | U409 |      |
| G1233 | C1171 | A1105 | C1045 | C985  | C924 | A860 | U793 | C731 | G669 | C475 |      |      | G348 |      |
| U1234 | C1172 | G1106 | A1046 | U986  | G925 | G861 | A794 | G732 | G670 | U476 |      |      | A411 |      |
| U1235 | U1173 | C1107 | G1047 | G987  | G926 | C862 | C795 | G733 | G671 | C477 |      |      | G350 |      |
| A1236 | G1176 | G1108 | G1048 | G988  | G927 | U863 | C796 | G734 | U672 | A478 |      |      | G413 |      |
| C1237 | U1177 | U1049 | U1049 | U989  | G928 | A864 | C797 | C735 | A673 | U479 |      |      | A414 |      |
| A1238 | G1177 | G1050 | C1051 | C990  |      | A865 | U798 | C736 | G674 | U480 |      |      | A353 |      |
| A1239 | G1178 | C1051 | U1052 | U991  | C931 | C866 | G799 | C737 | A675 | G481 |      |      | G384 |      |
| U1240 | A1179 | C1113 | G1053 | U992  | C932 | G867 | G800 | C738 | A676 | A482 |      |      | G417 |      |
| G1241 | A1180 | C1114 | G1054 | G993  | C933 | C868 | U801 | C739 | U677 | C483 |      |      | C418 |      |
| C1242 | G1181 |       | C1054 | A994  | C934 | C869 | A802 | U740 |      | G484 |      |      |      |      |
| G1243 | U1182 | A1117 | A1055 | U995  | A935 | U870 | G803 | G741 | C680 | U485 |      |      | U421 |      |
| C1244 | U1183 | U1118 | U1056 | A996  | C936 | U871 | U804 | G742 | C681 | U486 |      |      | C422 |      |
| C1245 | G1184 | G1057 | G1057 | U997  | A937 | A872 |      | A743 | G682 | A487 |      |      | G423 |      |
| U1246 | G1186 | U1123 | C1058 | C998  | A938 | A873 | A807 | C744 | G683 | C488 |      |      | G424 |      |
| A1247 | G1187 | G1124 | U1059 | C999  | G939 | C874 | C808 | G745 | U684 | U551 |      |      | G425 |      |
| C1248 | U1126 | U1126 | U1060 | A1000 | C940 | U875 | G809 | A746 | G685 | U552 |      |      | U426 |      |
| U1249 | G1127 | G1127 | G1061 | C1001 | G941 | C876 | C810 | A747 | U686 | A554 |      |      | U427 |      |
| A1250 | C1128 | C1128 | U1062 | G1002 | G942 | G877 | C811 | G748 | A687 | U555 |      |      | G428 |      |
| C1251 | A1191 | C1129 | G1063 | G1003 | U943 | A878 | C812 | A749 | G688 | C494 |      |      | U429 |      |
| A1252 | C1192 | C1192 | U1064 | A1004 | G944 | C879 | U813 | C750 | C689 | A495 |      |      | A430 |      |
| G1253 | G1193 | A1130 | U1065 | A1005 | G945 | C880 | A814 | U751 | G690 | A496 |      |      | U367 |      |
| A1254 | U1194 | C1066 | G1066 | G1006 | A946 | C881 | A815 | G752 | C691 | G497 |      |      | A431 |      |
| G1255 | C1195 | G1132 | A1067 | U1007 | G947 | C882 | A816 | A753 | U692 | A560 |      |      | A498 |      |
| A1256 | U1196 | G1068 | G1068 | U1008 | C948 | C883 | C817 | C754 | G693 | U561 |      |      | U434 |      |
| C1257 | A1197 | G1133 | C1069 | U1009 | A949 | U884 | G818 | G755 | A694 | G500 |      |      | A435 |      |
| G1258 | U1198 | U1135 | U1070 | U1010 | U950 | C885 | A819 | C756 | A695 | C501 |      |      | C436 |      |
| C1259 | G1199 | C1136 | C1071 | C1011 | U951 | G886 | U820 | U757 | C696 | A502 |      |      | U437 |      |
|       | C1200 | C1137 | G1072 | A1012 | U952 | G887 | G821 | C758 | U697 | C503 |      |      | U438 |      |

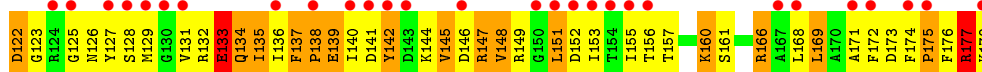
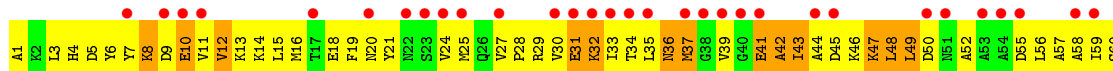




• Molecule 57: 5S rRNA



• Molecule 58: 50S ribosomal protein L5



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.08 Å   434.46 Å   618.92 Å<br>90.00°   90.00°   90.00°  | Depositor        |
| Resolution (Å)  | 76.35 – 3.29<br>76.35 – 3.29                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 77.5 (76.35-3.29)<br>77.5 (76.35-3.29)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.65 (at 3.26 Å)  | Xtriage          |
| Refinement program  | PHENIX ?, PHENIX (phenix.refine)                            | Depositor        |
| R, $R_{free}$   | 0.189 , 0.241<br>0.202 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set   | 14080 reflections (2.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 66.6  | Xtriage          |
| Anisotropy  | 0.324   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.23 , 77.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 284501  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 103.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, CLY

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    | 0.50         | 2/36834 (0.0%) | 1.24        | 439/57462 (0.8%) |
| 2   | AB    | 0.24         | 0/1736         | 0.44        | 0/2338           |
| 2   | CB    | 0.23         | 0/1736         | 0.44        | 0/2338           |
| 3   | AC    | 0.26         | 0/1652         | 0.48        | 0/2225           |
| 3   | CC    | 0.22         | 0/1652         | 0.42        | 0/2225           |
| 4   | AD    | 0.29         | 0/1665         | 0.50        | 0/2227           |
| 4   | CD    | 0.32         | 0/1665         | 0.55        | 0/2227           |
| 5   | AE    | 0.31         | 0/1119         | 0.56        | 0/1504           |
| 5   | CE    | 0.35         | 1/1119 (0.1%)  | 0.53        | 0/1504           |
| 6   | AF    | 0.28         | 0/836          | 0.47        | 0/1128           |
| 6   | CF    | 0.26         | 0/836          | 0.48        | 0/1128           |
| 7   | AG    | 0.23         | 0/1196         | 0.45        | 0/1602           |
| 8   | AH    | 0.30         | 0/989          | 0.52        | 0/1326           |
| 8   | CH    | 0.26         | 0/989          | 0.49        | 0/1326           |
| 9   | AI    | 0.24         | 0/1034         | 0.45        | 0/1375           |
| 9   | CI    | 0.21         | 0/1034         | 0.41        | 0/1375           |
| 10  | AJ    | 0.24         | 0/797          | 0.47        | 0/1077           |
| 10  | CJ    | 0.21         | 0/797          | 0.45        | 0/1077           |
| 11  | AK    | 0.26         | 0/893          | 0.51        | 0/1205           |
| 11  | CK    | 0.26         | 0/893          | 0.50        | 0/1205           |
| 12  | AL    | 0.35         | 0/969          | 0.66        | 1/1300 (0.1%)    |
| 12  | CL    | 0.29         | 0/969          | 0.54        | 0/1300           |
| 13  | AM    | 0.23         | 0/893          | 0.47        | 0/1193           |
| 14  | AN    | 0.26         | 0/785          | 0.46        | 0/1043           |
| 14  | CN    | 0.21         | 0/780          | 0.37        | 0/1036           |
| 15  | AO    | 0.29         | 0/722          | 0.45        | 0/964            |
| 15  | CO    | 0.25         | 0/722          | 0.42        | 0/964            |
| 16  | AP    | 0.30         | 0/659          | 0.48        | 0/884            |
| 17  | AQ    | 0.35         | 0/658          | 0.56        | 0/881            |
| 17  | CQ    | 0.27         | 0/658          | 0.49        | 0/881            |
| 18  | AR    | 0.28         | 0/463          | 0.47        | 0/621            |
| 18  | CR    | 0.26         | 0/463          | 0.45        | 0/621            |

| Mol | Chain | Bond lengths |                | Bond angles |                    |
|-----|-------|--------------|----------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5            |
| 19  | AS    | 0.24         | 0/653          | 0.43        | 0/877              |
| 19  | CS    | 0.20         | 0/653          | 0.41        | 0/877              |
| 20  | AT    | 0.31         | 0/671          | 0.52        | 0/888              |
| 20  | CT    | 0.25         | 0/671          | 0.49        | 0/888              |
| 21  | AU    | 0.27         | 0/431          | 0.45        | 0/570              |
| 21  | CU    | 0.32         | 0/431          | 0.57        | 0/570              |
| 22  | BA    | 0.73         | 7/68626 (0.0%) | 1.54        | 1278/107056 (1.2%) |
| 22  | DA    | 0.45         | 2/68314 (0.0%) | 1.23        | 934/106569 (0.9%)  |
| 23  | BB    | 0.68         | 0/2828         | 1.42        | 40/4410 (0.9%)     |
| 24  | BC    | 0.40         | 0/2122         | 0.67        | 0/2852             |
| 24  | DC    | 0.29         | 0/2122         | 0.51        | 0/2852             |
| 25  | BD    | 0.51         | 0/1586         | 0.72        | 1/2134 (0.0%)      |
| 25  | DD    | 0.28         | 0/1586         | 0.54        | 0/2134             |
| 26  | BE    | 0.42         | 0/1571         | 0.63        | 0/2113             |
| 26  | DE    | 0.24         | 0/1571         | 0.46        | 0/2113             |
| 27  | BF    | 0.32         | 0/1435         | 0.52        | 0/1926             |
| 28  | BG    | 0.36         | 0/1343         | 0.59        | 0/1816             |
| 28  | DG    | 0.22         | 0/1343         | 0.44        | 0/1816             |
| 29  | BH    | 0.27         | 0/1122         | 0.47        | 0/1515             |
| 29  | DH    | 0.25         | 0/1122         | 0.51        | 2/1515 (0.1%)      |
| 30  | BI    | 0.23         | 0/1046         | 0.47        | 0/1410             |
| 30  | DI    | 0.20         | 0/1046         | 0.42        | 0/1410             |
| 31  | BJ    | 0.52         | 0/1152         | 0.77        | 0/1551             |
| 31  | DJ    | 0.26         | 0/1152         | 0.55        | 1/1551 (0.1%)      |
| 32  | BK    | 0.49         | 0/948          | 0.71        | 0/1268             |
| 32  | DK    | 0.29         | 0/948          | 0.52        | 0/1268             |
| 33  | BL    | 0.41         | 0/1054         | 0.71        | 1/1403 (0.1%)      |
| 33  | DL    | 0.25         | 0/1054         | 0.50        | 0/1403             |
| 34  | BM    | 0.46         | 0/1093         | 0.68        | 0/1460             |
| 34  | DM    | 0.27         | 0/1093         | 0.46        | 0/1460             |
| 35  | BN    | 0.42         | 0/974          | 0.68        | 0/1301             |
| 35  | DN    | 0.26         | 0/974          | 0.48        | 0/1301             |
| 36  | BO    | 0.39         | 0/902          | 0.59        | 0/1209             |
| 36  | DO    | 0.21         | 0/902          | 0.40        | 0/1209             |
| 37  | BP    | 0.45         | 0/929          | 0.71        | 0/1242             |
| 37  | DP    | 0.27         | 0/929          | 0.47        | 0/1242             |
| 38  | BQ    | 0.55         | 0/960          | 0.69        | 0/1278             |
| 38  | DQ    | 0.27         | 0/960          | 0.44        | 0/1278             |
| 39  | BR    | 0.54         | 0/829          | 0.72        | 0/1107             |
| 39  | DR    | 0.26         | 0/829          | 0.49        | 0/1107             |
| 40  | BS    | 0.51         | 0/864          | 0.73        | 0/1156             |
| 40  | DS    | 0.26         | 0/864          | 0.50        | 0/1156             |
| 41  | BT    | 0.43         | 0/745          | 0.68        | 0/994              |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 41  | DT    | 0.22         | 0/745            | 0.45        | 0/994              |
| 42  | BU    | 0.39         | 0/788            | 0.67        | 0/1051             |
| 42  | DU    | 0.22         | 0/788            | 0.45        | 0/1051             |
| 43  | BV    | 0.41         | 0/766            | 0.60        | 0/1025             |
| 43  | DV    | 0.23         | 0/766            | 0.42        | 0/1025             |
| 44  | BW    | 0.49         | 0/603            | 0.77        | 0/797              |
| 44  | DW    | 0.25         | 0/603            | 0.46        | 0/797              |
| 45  | BX    | 0.39         | 0/635            | 0.66        | 0/848              |
| 45  | DX    | 0.26         | 0/635            | 0.52        | 0/848              |
| 46  | BY    | 0.36         | 0/510            | 0.60        | 0/677              |
| 46  | DY    | 0.21         | 0/510            | 0.42        | 0/677              |
| 47  | BZ    | 0.51         | 0/453            | 0.73        | 0/605              |
| 47  | DZ    | 0.25         | 0/453            | 0.50        | 0/605              |
| 48  | B0    | 0.44         | 0/450            | 0.69        | 0/599              |
| 48  | D0    | 0.26         | 0/450            | 0.48        | 0/599              |
| 49  | B1    | 0.36         | 0/417            | 0.54        | 0/554              |
| 49  | D1    | 0.24         | 0/417            | 0.44        | 0/554              |
| 50  | B2    | 0.45         | 0/380            | 0.62        | 0/498              |
| 50  | D2    | 0.25         | 0/380            | 0.47        | 0/498              |
| 51  | B3    | 0.44         | 0/513            | 0.62        | 0/676              |
| 51  | D3    | 0.25         | 0/513            | 0.49        | 0/676              |
| 52  | B4    | 0.47         | 0/303            | 0.74        | 0/397              |
| 52  | D4    | 0.32         | 0/303            | 0.45        | 0/397              |
| 53  | CA    | 0.46         | 3/36762 (0.0%)   | 1.18        | 421/57350 (0.7%)   |
| 54  | CG    | 0.21         | 0/1188           | 0.42        | 0/1591             |
| 55  | CM    | 0.19         | 0/885            | 0.39        | 0/1181             |
| 56  | CP    | 0.27         | 0/649            | 0.49        | 0/870              |
| 57  | DB    | 0.43         | 1/2803 (0.0%)    | 1.07        | 30/4371 (0.7%)     |
| 58  | DF    | 0.22         | 0/1444           | 0.45        | 0/1937             |
| All | All   | 0.51         | 16/306773 (0.0%) | 1.17        | 3148/458565 (0.7%) |

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 |
|-----|-------|---------------------|---------------------|
| 25  | BD    | 0                   | 1                   |
| 31  | BJ    | 0                   | 1                   |
| 35  | BN    | 0                   | 1                   |
| 58  | DF    | 0                   | 1                   |
| All | All   | 0                   | 4                   |

The worst 5 of 16 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 53  | CA    | 1396 | A    | O3'-P | -16.33 | 1.41        | 1.61     |
| 1   | AA    | 1047 | G    | O3'-P | -13.54 | 1.45        | 1.61     |
| 22  | BA    | 1905 | C    | O3'-P | -12.21 | 1.46        | 1.61     |
| 22  | BA    | 2197 | U    | O3'-P | -9.98  | 1.49        | 1.61     |
| 22  | BA    | 876  | C    | O3'-P | -9.54  | 1.49        | 1.61     |

The worst 5 of 3148 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22  | DA    | 2586 | U    | N1-C1'-C2' | -16.52 | 92.53       | 114.00   |
| 22  | BA    | 627  | A    | P-O3'-C3'  | 15.92  | 138.81      | 119.70   |
| 22  | BA    | 531  | C    | P-O3'-C3'  | 15.89  | 138.77      | 119.70   |
| 1   | AA    | 1047 | G    | P-O3'-C3'  | -15.60 | 100.98      | 119.70   |
| 22  | BA    | 2068 | U    | N1-C1'-C2' | -15.16 | 94.30       | 114.00   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 25  | BD    | 9   | VAL  | Peptide   |
| 31  | BJ    | 43  | GLU  | Peptide   |
| 35  | BN    | 101 | GLY  | Peptide   |
| 58  | DF    | 177 | ARG  | Mainchain |

## 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    | 32895 | 0        | 16553    | 1994    | 0            |
| 2   | AB    | 1705  | 0        | 1731     | 279     | 0            |
| 2   | CB    | 1705  | 0        | 1732     | 233     | 0            |
| 3   | AC    | 1625  | 0        | 1699     | 178     | 0            |
| 3   | CC    | 1625  | 0        | 1699     | 193     | 0            |
| 4   | AD    | 1643  | 0        | 1710     | 243     | 0            |
| 4   | CD    | 1643  | 0        | 1710     | 224     | 0            |
| 5   | AE    | 1106  | 0        | 1148     | 206     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | CE    | 1106  | 0        | 1148     | 145     | 0            |
| 6   | AF    | 818   | 0        | 808      | 111     | 0            |
| 6   | CF    | 818   | 0        | 808      | 117     | 0            |
| 7   | AG    | 1182  | 0        | 1240     | 130     | 0            |
| 8   | AH    | 979   | 0        | 1034     | 136     | 0            |
| 8   | CH    | 979   | 0        | 1034     | 126     | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 133     | 0            |
| 9   | CI    | 1022  | 0        | 1070     | 164     | 0            |
| 10  | AJ    | 787   | 0        | 828      | 141     | 0            |
| 10  | CJ    | 787   | 0        | 828      | 148     | 0            |
| 11  | AK    | 877   | 0        | 887      | 140     | 0            |
| 11  | CK    | 877   | 0        | 887      | 128     | 0            |
| 12  | AL    | 955   | 0        | 1019     | 127     | 0            |
| 12  | CL    | 955   | 0        | 1019     | 156     | 0            |
| 13  | AM    | 884   | 0        | 944      | 94      | 0            |
| 14  | AN    | 774   | 0        | 827      | 136     | 0            |
| 14  | CN    | 769   | 0        | 822      | 130     | 0            |
| 15  | AO    | 714   | 0        | 737      | 84      | 0            |
| 15  | CO    | 714   | 0        | 737      | 61      | 0            |
| 16  | AP    | 649   | 0        | 666      | 79      | 0            |
| 17  | AQ    | 649   | 0        | 691      | 100     | 0            |
| 17  | CQ    | 649   | 0        | 691      | 112     | 0            |
| 18  | AR    | 456   | 0        | 478      | 53      | 0            |
| 18  | CR    | 456   | 0        | 478      | 57      | 0            |
| 19  | AS    | 638   | 0        | 665      | 74      | 0            |
| 19  | CS    | 638   | 0        | 665      | 109     | 0            |
| 20  | AT    | 665   | 0        | 714      | 97      | 0            |
| 20  | CT    | 665   | 0        | 714      | 86      | 0            |
| 21  | AU    | 426   | 0        | 449      | 116     | 0            |
| 21  | CU    | 426   | 0        | 449      | 92      | 0            |
| 22  | BA    | 61274 | 0        | 30819    | 3248    | 0            |
| 22  | DA    | 60995 | 0        | 30679    | 5259    | 0            |
| 23  | BB    | 2529  | 0        | 1281     | 118     | 0            |
| 24  | BC    | 2083  | 0        | 2157     | 287     | 0            |
| 24  | DC    | 2083  | 0        | 2157     | 345     | 0            |
| 25  | BD    | 1565  | 0        | 1616     | 269     | 0            |
| 25  | DD    | 1565  | 0        | 1616     | 291     | 0            |
| 26  | BE    | 1552  | 0        | 1619     | 203     | 0            |
| 26  | DE    | 1552  | 0        | 1619     | 266     | 0            |
| 27  | BF    | 1411  | 0        | 1447     | 208     | 0            |
| 28  | BG    | 1323  | 0        | 1374     | 211     | 0            |
| 28  | DG    | 1323  | 0        | 1374     | 199     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | BH    | 1111  | 0        | 1148     | 166     | 0            |
| 29  | DH    | 1111  | 0        | 1148     | 175     | 0            |
| 30  | BI    | 1032  | 0        | 1088     | 114     | 0            |
| 30  | DI    | 1032  | 0        | 1088     | 120     | 0            |
| 31  | BJ    | 1129  | 0        | 1162     | 216     | 0            |
| 31  | DJ    | 1129  | 0        | 1162     | 202     | 0            |
| 32  | BK    | 939   | 0        | 1012     | 164     | 0            |
| 32  | DK    | 939   | 0        | 1012     | 183     | 0            |
| 33  | BL    | 1045  | 0        | 1117     | 169     | 0            |
| 33  | DL    | 1045  | 0        | 1117     | 192     | 0            |
| 34  | BM    | 1074  | 0        | 1157     | 146     | 0            |
| 34  | DM    | 1074  | 0        | 1157     | 150     | 0            |
| 35  | BN    | 961   | 0        | 1000     | 123     | 0            |
| 35  | DN    | 961   | 0        | 1000     | 207     | 0            |
| 36  | BO    | 892   | 0        | 923      | 92      | 0            |
| 36  | DO    | 892   | 0        | 923      | 107     | 0            |
| 37  | BP    | 917   | 0        | 965      | 195     | 0            |
| 37  | DP    | 917   | 0        | 965      | 172     | 0            |
| 38  | BQ    | 947   | 0        | 1022     | 191     | 0            |
| 38  | DQ    | 947   | 0        | 1022     | 180     | 0            |
| 39  | BR    | 816   | 0        | 839      | 138     | 0            |
| 39  | DR    | 816   | 0        | 839      | 137     | 0            |
| 40  | BS    | 857   | 0        | 922      | 110     | 0            |
| 40  | DS    | 857   | 0        | 922      | 131     | 0            |
| 41  | BT    | 739   | 0        | 807      | 156     | 0            |
| 41  | DT    | 739   | 0        | 807      | 159     | 0            |
| 42  | BU    | 780   | 0        | 834      | 84      | 0            |
| 42  | DU    | 780   | 0        | 834      | 133     | 0            |
| 43  | BV    | 753   | 0        | 780      | 76      | 0            |
| 43  | DV    | 753   | 0        | 780      | 108     | 0            |
| 44  | BW    | 596   | 0        | 610      | 229     | 0            |
| 44  | DW    | 596   | 0        | 610      | 174     | 0            |
| 45  | BX    | 625   | 0        | 655      | 104     | 0            |
| 45  | DX    | 625   | 0        | 655      | 114     | 0            |
| 46  | BY    | 509   | 0        | 543      | 69      | 0            |
| 46  | DY    | 509   | 0        | 543      | 102     | 0            |
| 47  | BZ    | 449   | 0        | 491      | 58      | 0            |
| 47  | DZ    | 449   | 0        | 491      | 58      | 0            |
| 48  | B0    | 444   | 0        | 461      | 32      | 0            |
| 48  | D0    | 444   | 0        | 461      | 75      | 0            |
| 49  | B1    | 410   | 0        | 440      | 57      | 0            |
| 49  | D1    | 410   | 0        | 440      | 53      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 50  | B2    | 377   | 0        | 418      | 36      | 0            |
| 50  | D2    | 377   | 0        | 418      | 66      | 0            |
| 51  | B3    | 504   | 0        | 574      | 53      | 0            |
| 51  | D3    | 504   | 0        | 574      | 67      | 0            |
| 52  | B4    | 302   | 0        | 340      | 47      | 0            |
| 52  | D4    | 302   | 0        | 342      | 41      | 0            |
| 53  | CA    | 32831 | 0        | 16521    | 2416    | 0            |
| 54  | CG    | 1175  | 0        | 1230     | 194     | 0            |
| 55  | CM    | 877   | 0        | 937      | 167     | 0            |
| 56  | CP    | 639   | 0        | 656      | 101     | 0            |
| 57  | DB    | 2507  | 0        | 1270     | 234     | 0            |
| 58  | DF    | 1420  | 0        | 1460     | 282     | 0            |
| 59  | AA    | 42    | 0        | 0        | 0       | 0            |
| 59  | AN    | 1     | 0        | 0        | 0       | 0            |
| 59  | BA    | 134   | 0        | 0        | 0       | 0            |
| 59  | BB    | 4     | 0        | 0        | 0       | 0            |
| 59  | BL    | 1     | 0        | 0        | 0       | 0            |
| 59  | CA    | 42    | 0        | 0        | 0       | 0            |
| 59  | DA    | 132   | 0        | 0        | 0       | 0            |
| 59  | DB    | 1     | 0        | 0        | 0       | 0            |
| 59  | DC    | 2     | 0        | 0        | 0       | 0            |
| 59  | DE    | 1     | 0        | 0        | 0       | 0            |
| 59  | DJ    | 1     | 0        | 0        | 0       | 0            |
| 60  | BA    | 27    | 0        | 32       | 2       | 0            |
| 61  | B4    | 1     | 0        | 0        | 0       | 0            |
| 61  | D4    | 1     | 0        | 0        | 0       | 0            |
| 62  | AA    | 197   | 0        | 0        | 5       | 0            |
| 62  | AE    | 1     | 0        | 0        | 0       | 0            |
| 62  | AL    | 1     | 0        | 0        | 0       | 0            |
| 62  | AN    | 6     | 0        | 0        | 2       | 0            |
| 62  | AT    | 2     | 0        | 0        | 0       | 0            |
| 62  | AU    | 1     | 0        | 0        | 0       | 0            |
| 62  | B2    | 2     | 0        | 0        | 0       | 0            |
| 62  | B3    | 2     | 0        | 0        | 1       | 0            |
| 62  | B4    | 1     | 0        | 0        | 0       | 0            |
| 62  | BA    | 601   | 0        | 0        | 48      | 0            |
| 62  | BB    | 20    | 0        | 0        | 1       | 0            |
| 62  | BC    | 8     | 0        | 0        | 0       | 0            |
| 62  | BD    | 4     | 0        | 0        | 1       | 0            |
| 62  | BE    | 1     | 0        | 0        | 1       | 0            |
| 62  | BL    | 3     | 0        | 0        | 1       | 0            |
| 62  | BN    | 3     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 62  | BQ    | 1      | 0        | 0        | 0       | 0            |
| 62  | BR    | 1      | 0        | 0        | 1       | 0            |
| 62  | BT    | 3      | 0        | 0        | 0       | 0            |
| 62  | CA    | 193    | 0        | 0        | 7       | 0            |
| 62  | CE    | 4      | 0        | 0        | 0       | 0            |
| 62  | CI    | 1      | 0        | 0        | 0       | 0            |
| 62  | CL    | 1      | 0        | 0        | 0       | 0            |
| 62  | CN    | 3      | 0        | 0        | 0       | 0            |
| 62  | CT    | 3      | 0        | 0        | 0       | 0            |
| 62  | CU    | 2      | 0        | 0        | 0       | 0            |
| 62  | D2    | 2      | 0        | 0        | 0       | 0            |
| 62  | D3    | 1      | 0        | 0        | 0       | 0            |
| 62  | D4    | 4      | 0        | 0        | 0       | 0            |
| 62  | DA    | 599    | 0        | 0        | 28      | 0            |
| 62  | DB    | 4      | 0        | 0        | 0       | 0            |
| 62  | DC    | 9      | 0        | 0        | 2       | 0            |
| 62  | DD    | 2      | 0        | 0        | 0       | 0            |
| 62  | DE    | 3      | 0        | 0        | 0       | 0            |
| 62  | DJ    | 5      | 0        | 0        | 0       | 0            |
| 62  | DL    | 5      | 0        | 0        | 1       | 0            |
| 62  | DN    | 3      | 0        | 0        | 0       | 0            |
| 62  | DT    | 3      | 0        | 0        | 1       | 0            |
| 62  | DU    | 2      | 0        | 0        | 0       | 0            |
| 62  | DV    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 284501 | 0        | 190871   | 25099   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

The worst 5 of 25099 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:900:A:C2'  | 22:BA:901:C:H5'   | 1.40                     | 1.46              |
| 2:AB:108:GLN:O   | 2:AB:110:ILE:N    | 1.58                     | 1.37              |
| 22:BA:1073:A:C2' | 22:BA:1074:G:H5'' | 1.54                     | 1.35              |
| 2:CB:93:HIS:CG   | 2:CB:145:ASN:O    | 1.88                     | 1.27              |
| 28:BG:84:LYS:HG3 | 28:BG:132:LEU:N   | 1.49                     | 1.26              |

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | AB    | 216/218 (99%) | 121 (56%) | 65 (30%) | 30 (14%) | 0           | 1  |
| 2   | CB    | 216/218 (99%) | 145 (67%) | 54 (25%) | 17 (8%)  | 1           | 6  |
| 3   | AC    | 204/206 (99%) | 154 (76%) | 33 (16%) | 17 (8%)  | 1           | 6  |
| 3   | CC    | 204/206 (99%) | 147 (72%) | 40 (20%) | 17 (8%)  | 1           | 6  |
| 4   | AD    | 203/205 (99%) | 134 (66%) | 42 (21%) | 27 (13%) | 0           | 1  |
| 4   | CD    | 203/205 (99%) | 139 (68%) | 38 (19%) | 26 (13%) | 0           | 1  |
| 5   | AE    | 148/150 (99%) | 105 (71%) | 26 (18%) | 17 (12%) | 0           | 2  |
| 5   | CE    | 148/150 (99%) | 110 (74%) | 23 (16%) | 15 (10%) | 0           | 3  |
| 6   | AF    | 98/100 (98%)  | 71 (72%)  | 19 (19%) | 8 (8%)   | 1           | 6  |
| 6   | CF    | 98/100 (98%)  | 62 (63%)  | 27 (28%) | 9 (9%)   | 1           | 4  |
| 7   | AG    | 149/151 (99%) | 107 (72%) | 34 (23%) | 8 (5%)   | 2           | 12 |
| 8   | AH    | 127/129 (98%) | 92 (72%)  | 27 (21%) | 8 (6%)   | 1           | 10 |
| 8   | CH    | 127/129 (98%) | 87 (68%)  | 30 (24%) | 10 (8%)  | 1           | 6  |
| 9   | AI    | 125/127 (98%) | 83 (66%)  | 31 (25%) | 11 (9%)  | 1           | 5  |
| 9   | CI    | 125/127 (98%) | 87 (70%)  | 29 (23%) | 9 (7%)   | 1           | 8  |
| 10  | AJ    | 96/98 (98%)   | 64 (67%)  | 19 (20%) | 13 (14%) | 0           | 1  |
| 10  | CJ    | 96/98 (98%)   | 58 (60%)  | 24 (25%) | 14 (15%) | 0           | 1  |
| 11  | AK    | 115/117 (98%) | 85 (74%)  | 18 (16%) | 12 (10%) | 0           | 3  |
| 11  | CK    | 115/117 (98%) | 89 (77%)  | 17 (15%) | 9 (8%)   | 1           | 6  |
| 12  | AL    | 121/123 (98%) | 84 (69%)  | 21 (17%) | 16 (13%) | 0           | 1  |
| 12  | CL    | 121/123 (98%) | 84 (69%)  | 25 (21%) | 12 (10%) | 0           | 3  |
| 13  | AM    | 112/114 (98%) | 87 (78%)  | 17 (15%) | 8 (7%)   | 1           | 8  |
| 14  | AN    | 92/100 (92%)  | 54 (59%)  | 23 (25%) | 15 (16%) | 0           | 1  |
| 14  | CN    | 91/100 (91%)  | 58 (64%)  | 27 (30%) | 6 (7%)   | 1           | 9  |
| 15  | AO    | 86/88 (98%)   | 58 (67%)  | 22 (26%) | 6 (7%)   | 1           | 8  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 15  | CO    | 86/88 (98%)   | 68 (79%)  | 15 (17%) | 3 (4%)   | 3           | 22 |
| 16  | AP    | 80/82 (98%)   | 58 (72%)  | 13 (16%) | 9 (11%)  | 0           | 2  |
| 17  | AQ    | 78/80 (98%)   | 46 (59%)  | 20 (26%) | 12 (15%) | 0           | 1  |
| 17  | CQ    | 78/80 (98%)   | 60 (77%)  | 8 (10%)  | 10 (13%) | 0           | 1  |
| 18  | AR    | 53/55 (96%)   | 39 (74%)  | 13 (24%) | 1 (2%)   | 8           | 35 |
| 18  | CR    | 53/55 (96%)   | 40 (76%)  | 11 (21%) | 2 (4%)   | 3           | 20 |
| 19  | AS    | 77/79 (98%)   | 56 (73%)  | 14 (18%) | 7 (9%)   | 1           | 4  |
| 19  | CS    | 77/79 (98%)   | 46 (60%)  | 24 (31%) | 7 (9%)   | 1           | 4  |
| 20  | AT    | 83/85 (98%)   | 54 (65%)  | 20 (24%) | 9 (11%)  | 0           | 3  |
| 20  | CT    | 83/85 (98%)   | 55 (66%)  | 21 (25%) | 7 (8%)   | 1           | 5  |
| 21  | AU    | 49/51 (96%)   | 25 (51%)  | 17 (35%) | 7 (14%)  | 0           | 1  |
| 21  | CU    | 49/51 (96%)   | 24 (49%)  | 11 (22%) | 14 (29%) | 0           | 0  |
| 24  | BC    | 269/271 (99%) | 197 (73%) | 53 (20%) | 19 (7%)  | 1           | 8  |
| 24  | DC    | 269/271 (99%) | 177 (66%) | 55 (20%) | 37 (14%) | 0           | 1  |
| 25  | BD    | 207/209 (99%) | 140 (68%) | 38 (18%) | 29 (14%) | 0           | 1  |
| 25  | DD    | 207/209 (99%) | 134 (65%) | 39 (19%) | 34 (16%) | 0           | 1  |
| 26  | BE    | 199/201 (99%) | 143 (72%) | 35 (18%) | 21 (11%) | 0           | 3  |
| 26  | DE    | 199/201 (99%) | 122 (61%) | 51 (26%) | 26 (13%) | 0           | 1  |
| 27  | BF    | 175/177 (99%) | 127 (73%) | 33 (19%) | 15 (9%)  | 1           | 5  |
| 28  | BG    | 174/176 (99%) | 115 (66%) | 32 (18%) | 27 (16%) | 0           | 1  |
| 28  | DG    | 174/176 (99%) | 100 (58%) | 43 (25%) | 31 (18%) | 0           | 1  |
| 29  | BH    | 147/149 (99%) | 67 (46%)  | 46 (31%) | 34 (23%) | 0           | 0  |
| 29  | DH    | 147/149 (99%) | 71 (48%)  | 58 (40%) | 18 (12%) | 0           | 2  |
| 30  | BI    | 139/141 (99%) | 84 (60%)  | 41 (30%) | 14 (10%) | 0           | 3  |
| 30  | DI    | 139/141 (99%) | 78 (56%)  | 43 (31%) | 18 (13%) | 0           | 1  |
| 31  | BJ    | 140/142 (99%) | 101 (72%) | 23 (16%) | 16 (11%) | 0           | 2  |
| 31  | DJ    | 140/142 (99%) | 90 (64%)  | 30 (21%) | 20 (14%) | 0           | 1  |
| 32  | BK    | 120/122 (98%) | 83 (69%)  | 15 (12%) | 22 (18%) | 0           | 1  |
| 32  | DK    | 120/122 (98%) | 83 (69%)  | 13 (11%) | 24 (20%) | 0           | 0  |
| 33  | BL    | 141/143 (99%) | 104 (74%) | 28 (20%) | 9 (6%)   | 1           | 9  |
| 33  | DL    | 141/143 (99%) | 81 (57%)  | 42 (30%) | 18 (13%) | 0           | 1  |

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| Mol | Chain | Analysed      | Favoured | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 34  | BM    | 134/136 (98%) | 91 (68%) | 25 (19%) | 18 (13%) | 0           | 1  |
| 34  | DM    | 134/136 (98%) | 93 (69%) | 24 (18%) | 17 (13%) | 0           | 1  |
| 35  | BN    | 118/120 (98%) | 87 (74%) | 21 (18%) | 10 (8%)  | 1           | 5  |
| 35  | DN    | 118/120 (98%) | 72 (61%) | 30 (25%) | 16 (14%) | 0           | 1  |
| 36  | BO    | 114/116 (98%) | 87 (76%) | 20 (18%) | 7 (6%)   | 1           | 10 |
| 36  | DO    | 114/116 (98%) | 76 (67%) | 26 (23%) | 12 (10%) | 0           | 3  |
| 37  | BP    | 112/114 (98%) | 75 (67%) | 21 (19%) | 16 (14%) | 0           | 1  |
| 37  | DP    | 112/114 (98%) | 65 (58%) | 27 (24%) | 20 (18%) | 0           | 1  |
| 38  | BQ    | 115/117 (98%) | 91 (79%) | 17 (15%) | 7 (6%)   | 1           | 10 |
| 38  | DQ    | 115/117 (98%) | 78 (68%) | 24 (21%) | 13 (11%) | 0           | 2  |
| 39  | BR    | 101/103 (98%) | 76 (75%) | 16 (16%) | 9 (9%)   | 1           | 5  |
| 39  | DR    | 101/103 (98%) | 67 (66%) | 25 (25%) | 9 (9%)   | 1           | 5  |
| 40  | BS    | 108/110 (98%) | 77 (71%) | 25 (23%) | 6 (6%)   | 2           | 12 |
| 40  | DS    | 108/110 (98%) | 75 (69%) | 21 (19%) | 12 (11%) | 0           | 2  |
| 41  | BT    | 91/93 (98%)   | 55 (60%) | 19 (21%) | 17 (19%) | 0           | 1  |
| 41  | DT    | 91/93 (98%)   | 47 (52%) | 28 (31%) | 16 (18%) | 0           | 1  |
| 42  | BU    | 100/102 (98%) | 63 (63%) | 22 (22%) | 15 (15%) | 0           | 1  |
| 42  | DU    | 100/102 (98%) | 50 (50%) | 23 (23%) | 27 (27%) | 0           | 0  |
| 43  | BV    | 92/94 (98%)   | 80 (87%) | 10 (11%) | 2 (2%)   | 6           | 31 |
| 43  | DV    | 92/94 (98%)   | 61 (66%) | 24 (26%) | 7 (8%)   | 1           | 7  |
| 44  | BW    | 77/79 (98%)   | 27 (35%) | 25 (32%) | 25 (32%) | 0           | 0  |
| 44  | DW    | 77/79 (98%)   | 34 (44%) | 22 (29%) | 21 (27%) | 0           | 0  |
| 45  | BX    | 75/77 (97%)   | 54 (72%) | 15 (20%) | 6 (8%)   | 1           | 6  |
| 45  | DX    | 75/77 (97%)   | 46 (61%) | 24 (32%) | 5 (7%)   | 1           | 9  |
| 46  | BY    | 61/63 (97%)   | 37 (61%) | 16 (26%) | 8 (13%)  | 0           | 1  |
| 46  | DY    | 61/63 (97%)   | 40 (66%) | 16 (26%) | 5 (8%)   | 1           | 6  |
| 47  | BZ    | 56/58 (97%)   | 44 (79%) | 10 (18%) | 2 (4%)   | 3           | 21 |
| 47  | DZ    | 56/58 (97%)   | 35 (62%) | 15 (27%) | 6 (11%)  | 0           | 3  |
| 48  | B0    | 54/56 (96%)   | 42 (78%) | 8 (15%)  | 4 (7%)   | 1           | 7  |
| 48  | D0    | 54/56 (96%)   | 37 (68%) | 12 (22%) | 5 (9%)   | 0           | 4  |
| 49  | B1    | 48/50 (96%)   | 37 (77%) | 6 (12%)  | 5 (10%)  | 0           | 3  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 49  | D1    | 48/50 (96%)       | 33 (69%)   | 10 (21%)   | 5 (10%)    | 0           | 3  |
| 50  | B2    | 44/46 (96%)       | 37 (84%)   | 6 (14%)    | 1 (2%)     | 6           | 30 |
| 50  | D2    | 44/46 (96%)       | 32 (73%)   | 6 (14%)    | 6 (14%)    | 0           | 1  |
| 51  | B3    | 62/64 (97%)       | 50 (81%)   | 8 (13%)    | 4 (6%)     | 1           | 9  |
| 51  | D3    | 62/64 (97%)       | 40 (64%)   | 17 (27%)   | 5 (8%)     | 1           | 6  |
| 52  | B4    | 36/38 (95%)       | 28 (78%)   | 4 (11%)    | 4 (11%)    | 0           | 2  |
| 52  | D4    | 36/38 (95%)       | 24 (67%)   | 6 (17%)    | 6 (17%)    | 0           | 1  |
| 54  | CG    | 148/150 (99%)     | 103 (70%)  | 34 (23%)   | 11 (7%)    | 1           | 7  |
| 55  | CM    | 111/113 (98%)     | 63 (57%)   | 36 (32%)   | 12 (11%)   | 0           | 3  |
| 56  | CP    | 78/80 (98%)       | 50 (64%)   | 19 (24%)   | 9 (12%)    | 0           | 2  |
| 58  | DF    | 176/178 (99%)     | 98 (56%)   | 46 (26%)   | 32 (18%)   | 0           | 1  |
| All | All   | 11238/11447 (98%) | 7490 (67%) | 2445 (22%) | 1303 (12%) | 0           | 2  |

5 of 1303 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 20  | ARG  |
| 2   | AB    | 21  | TYR  |
| 2   | AB    | 37  | VAL  |
| 2   | AB    | 40  | ILE  |
| 2   | AB    | 75  | ALA  |

### 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%) | 147 (82%) | 33 (18%) | 1           | 7  |
| 2   | CB    | 180/180 (100%) | 152 (84%) | 28 (16%) | 2           | 12 |
| 3   | AC    | 170/170 (100%) | 140 (82%) | 30 (18%) | 2           | 8  |
| 3   | CC    | 170/170 (100%) | 153 (90%) | 17 (10%) | 7           | 28 |
| 4   | AD    | 172/172 (100%) | 142 (83%) | 30 (17%) | 2           | 8  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4   | CD    | 172/172 (100%) | 140 (81%) | 32 (19%) | 1           | 7  |
| 5   | AE    | 113/113 (100%) | 87 (77%)  | 26 (23%) | 1           | 3  |
| 5   | CE    | 113/113 (100%) | 92 (81%)  | 21 (19%) | 1           | 7  |
| 6   | AF    | 87/87 (100%)   | 74 (85%)  | 13 (15%) | 3           | 13 |
| 6   | CF    | 87/87 (100%)   | 73 (84%)  | 14 (16%) | 2           | 11 |
| 7   | AG    | 124/124 (100%) | 109 (88%) | 15 (12%) | 5           | 21 |
| 8   | AH    | 104/104 (100%) | 90 (86%)  | 14 (14%) | 4           | 17 |
| 8   | CH    | 104/104 (100%) | 91 (88%)  | 13 (12%) | 4           | 19 |
| 9   | AI    | 105/105 (100%) | 87 (83%)  | 18 (17%) | 2           | 9  |
| 9   | CI    | 105/105 (100%) | 92 (88%)  | 13 (12%) | 4           | 20 |
| 10  | AJ    | 86/86 (100%)   | 74 (86%)  | 12 (14%) | 3           | 16 |
| 10  | CJ    | 86/86 (100%)   | 77 (90%)  | 9 (10%)  | 7           | 26 |
| 11  | AK    | 90/90 (100%)   | 72 (80%)  | 18 (20%) | 1           | 5  |
| 11  | CK    | 90/90 (100%)   | 77 (86%)  | 13 (14%) | 3           | 15 |
| 12  | AL    | 103/103 (100%) | 85 (82%)  | 18 (18%) | 2           | 8  |
| 12  | CL    | 103/103 (100%) | 86 (84%)  | 17 (16%) | 2           | 10 |
| 13  | AM    | 92/92 (100%)   | 88 (96%)  | 4 (4%)   | 29          | 59 |
| 14  | AN    | 79/83 (95%)    | 72 (91%)  | 7 (9%)   | 9           | 32 |
| 14  | CN    | 79/83 (95%)    | 68 (86%)  | 11 (14%) | 3           | 16 |
| 15  | AO    | 76/76 (100%)   | 67 (88%)  | 9 (12%)  | 5           | 21 |
| 15  | CO    | 76/76 (100%)   | 68 (90%)  | 8 (10%)  | 7           | 26 |
| 16  | AP    | 65/65 (100%)   | 58 (89%)  | 7 (11%)  | 6           | 25 |
| 17  | AQ    | 74/74 (100%)   | 60 (81%)  | 14 (19%) | 1           | 6  |
| 17  | CQ    | 74/74 (100%)   | 62 (84%)  | 12 (16%) | 2           | 10 |
| 18  | AR    | 48/48 (100%)   | 46 (96%)  | 2 (4%)   | 30          | 60 |
| 18  | CR    | 48/48 (100%)   | 44 (92%)  | 4 (8%)   | 11          | 35 |
| 19  | AS    | 70/70 (100%)   | 63 (90%)  | 7 (10%)  | 7           | 28 |
| 19  | CS    | 70/70 (100%)   | 63 (90%)  | 7 (10%)  | 7           | 28 |
| 20  | AT    | 65/65 (100%)   | 50 (77%)  | 15 (23%) | 1           | 3  |
| 20  | CT    | 65/65 (100%)   | 55 (85%)  | 10 (15%) | 2           | 12 |
| 21  | AU    | 44/44 (100%)   | 37 (84%)  | 7 (16%)  | 2           | 11 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 21  | CU    | 44/44 (100%)   | 36 (82%)  | 8 (18%)  | 1           | 7  |
| 24  | BC    | 216/216 (100%) | 166 (77%) | 50 (23%) | 1           | 3  |
| 24  | DC    | 216/216 (100%) | 189 (88%) | 27 (12%) | 4           | 19 |
| 25  | BD    | 164/164 (100%) | 131 (80%) | 33 (20%) | 1           | 5  |
| 25  | DD    | 164/164 (100%) | 139 (85%) | 25 (15%) | 3           | 12 |
| 26  | BE    | 165/165 (100%) | 126 (76%) | 39 (24%) | 1           | 2  |
| 26  | DE    | 165/165 (100%) | 148 (90%) | 17 (10%) | 7           | 26 |
| 27  | BF    | 148/148 (100%) | 124 (84%) | 24 (16%) | 2           | 10 |
| 28  | BG    | 137/137 (100%) | 107 (78%) | 30 (22%) | 1           | 3  |
| 28  | DG    | 137/137 (100%) | 121 (88%) | 16 (12%) | 5           | 22 |
| 29  | BH    | 114/114 (100%) | 96 (84%)  | 18 (16%) | 2           | 11 |
| 29  | DH    | 114/114 (100%) | 98 (86%)  | 16 (14%) | 3           | 16 |
| 30  | BI    | 109/109 (100%) | 91 (84%)  | 18 (16%) | 2           | 10 |
| 30  | DI    | 109/109 (100%) | 103 (94%) | 6 (6%)   | 21          | 52 |
| 31  | BJ    | 116/116 (100%) | 84 (72%)  | 32 (28%) | 0           | 1  |
| 31  | DJ    | 116/116 (100%) | 103 (89%) | 13 (11%) | 6           | 23 |
| 32  | BK    | 103/103 (100%) | 78 (76%)  | 25 (24%) | 0           | 2  |
| 32  | DK    | 103/103 (100%) | 82 (80%)  | 21 (20%) | 1           | 4  |
| 33  | BL    | 102/102 (100%) | 71 (70%)  | 31 (30%) | 0           | 1  |
| 33  | DL    | 102/102 (100%) | 89 (87%)  | 13 (13%) | 4           | 19 |
| 34  | BM    | 109/109 (100%) | 87 (80%)  | 22 (20%) | 1           | 5  |
| 34  | DM    | 109/109 (100%) | 103 (94%) | 6 (6%)   | 21          | 52 |
| 35  | BN    | 100/100 (100%) | 83 (83%)  | 17 (17%) | 2           | 9  |
| 35  | DN    | 100/100 (100%) | 80 (80%)  | 20 (20%) | 1           | 5  |
| 36  | BO    | 86/86 (100%)   | 71 (83%)  | 15 (17%) | 2           | 8  |
| 36  | DO    | 86/86 (100%)   | 78 (91%)  | 8 (9%)   | 9           | 30 |
| 37  | BP    | 99/99 (100%)   | 72 (73%)  | 27 (27%) | 0           | 1  |
| 37  | DP    | 99/99 (100%)   | 89 (90%)  | 10 (10%) | 7           | 27 |
| 38  | BQ    | 89/89 (100%)   | 72 (81%)  | 17 (19%) | 1           | 6  |
| 38  | DQ    | 89/89 (100%)   | 75 (84%)  | 14 (16%) | 2           | 12 |
| 39  | BR    | 84/84 (100%)   | 66 (79%)  | 18 (21%) | 1           | 4  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 39  | DR    | 84/84 (100%)   | 71 (84%)  | 13 (16%) | 2           | 12 |
| 40  | BS    | 93/93 (100%)   | 74 (80%)  | 19 (20%) | 1           | 4  |
| 40  | DS    | 93/93 (100%)   | 79 (85%)  | 14 (15%) | 3           | 13 |
| 41  | BT    | 80/80 (100%)   | 59 (74%)  | 21 (26%) | 0           | 1  |
| 41  | DT    | 80/80 (100%)   | 74 (92%)  | 6 (8%)   | 13          | 39 |
| 42  | BU    | 83/83 (100%)   | 66 (80%)  | 17 (20%) | 1           | 4  |
| 42  | DU    | 83/83 (100%)   | 73 (88%)  | 10 (12%) | 5           | 21 |
| 43  | BV    | 78/78 (100%)   | 61 (78%)  | 17 (22%) | 1           | 3  |
| 43  | DV    | 78/78 (100%)   | 70 (90%)  | 8 (10%)  | 7           | 26 |
| 44  | BW    | 59/59 (100%)   | 41 (70%)  | 18 (30%) | 0           | 1  |
| 44  | DW    | 59/59 (100%)   | 44 (75%)  | 15 (25%) | 0           | 2  |
| 45  | BX    | 67/67 (100%)   | 51 (76%)  | 16 (24%) | 0           | 2  |
| 45  | DX    | 67/67 (100%)   | 57 (85%)  | 10 (15%) | 3           | 13 |
| 46  | BY    | 55/55 (100%)   | 45 (82%)  | 10 (18%) | 1           | 7  |
| 46  | DY    | 55/55 (100%)   | 52 (94%)  | 3 (6%)   | 21          | 52 |
| 47  | BZ    | 48/48 (100%)   | 32 (67%)  | 16 (33%) | 0           | 0  |
| 47  | DZ    | 48/48 (100%)   | 40 (83%)  | 8 (17%)  | 2           | 10 |
| 48  | B0    | 47/47 (100%)   | 34 (72%)  | 13 (28%) | 0           | 1  |
| 48  | D0    | 47/47 (100%)   | 40 (85%)  | 7 (15%)  | 3           | 13 |
| 49  | B1    | 45/45 (100%)   | 38 (84%)  | 7 (16%)  | 2           | 12 |
| 49  | D1    | 45/45 (100%)   | 41 (91%)  | 4 (9%)   | 9           | 32 |
| 50  | B2    | 38/38 (100%)   | 31 (82%)  | 7 (18%)  | 1           | 7  |
| 50  | D2    | 38/38 (100%)   | 35 (92%)  | 3 (8%)   | 12          | 37 |
| 51  | B3    | 51/51 (100%)   | 45 (88%)  | 6 (12%)  | 5           | 21 |
| 51  | D3    | 51/51 (100%)   | 40 (78%)  | 11 (22%) | 1           | 4  |
| 52  | B4    | 34/34 (100%)   | 29 (85%)  | 5 (15%)  | 3           | 14 |
| 52  | D4    | 34/34 (100%)   | 29 (85%)  | 5 (15%)  | 3           | 14 |
| 54  | CG    | 123/123 (100%) | 104 (85%) | 19 (15%) | 2           | 12 |
| 55  | CM    | 91/91 (100%)   | 81 (89%)  | 10 (11%) | 6           | 24 |
| 56  | CP    | 65/65 (100%)   | 54 (83%)  | 11 (17%) | 2           | 9  |
| 58  | DF    | 149/149 (100%) | 127 (85%) | 22 (15%) | 3           | 14 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles        |
|-----|-------|------------------|------------|------------|--------------------|
| All | All   | 9331/9339 (100%) | 7816 (84%) | 1515 (16%) | <b>2</b> <b>10</b> |

5 of 1515 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | BQ    | 40  | LYS  |
| 47  | BZ    | 56  | VAL  |
| 39  | DR    | 13  | ARG  |
| 39  | BR    | 46  | GLU  |
| 42  | BU    | 86  | PHE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 355 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | BS    | 61  | ASN  |
| 3   | CC    | 18  | ASN  |
| 42  | DU    | 52  | ASN  |
| 42  | BU    | 52  | ASN  |
| 46  | BY    | 41  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1532/1533 (99%) | 482 (31%)         | 233 (15%)       |
| 22  | BA    | 2850/2903 (98%) | 900 (31%)         | 473 (16%)       |
| 22  | DA    | 2839/2903 (97%) | 1062 (37%)        | 506 (17%)       |
| 23  | BB    | 117/118 (99%)   | 32 (27%)          | 18 (15%)        |
| 53  | CA    | 1529/1530 (99%) | 548 (35%)         | 236 (15%)       |
| 57  | DB    | 116/117 (99%)   | 38 (32%)          | 15 (12%)        |
| All | All   | 8983/9104 (98%) | 3062 (34%)        | 1481 (16%)      |

5 of 3062 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 5   | U    |
| 1   | AA    | 6   | G    |
| 1   | AA    | 7   | A    |
| 1   | AA    | 8   | A    |
| 1   | AA    | 9   | G    |



5 of 1481 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 2654 | A    |
| 53  | CA    | 531  | U    |
| 22  | DA    | 2286 | G    |
| 22  | BA    | 2791 | G    |
| 53  | CA    | 116  | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 60  | CLY  | BA    | 3135 | -    | 25,28,28     | 1.49 | 4 (16%)     | 29,40,40    | 1.52 | 8 (27%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 60  | CLY  | BA    | 3135 | -    | -       | 2/21/53/53 | 0/2/2/2 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 60  | BA    | 3135 | CLY  | C14-N2 | 3.38 | 1.51        | 1.47     |
| 60  | BA    | 3135 | CLY  | C15-N2 | 2.88 | 1.52        | 1.46     |
| 60  | BA    | 3135 | CLY  | O5-C4  | 2.75 | 1.48        | 1.44     |
| 60  | BA    | 3135 | CLY  | C6-S1  | 2.24 | 1.84        | 1.79     |

The worst 5 of 8 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 60  | BA    | 3135 | CLY  | C11-C10-N1 | -3.28 | 109.28      | 116.58   |
| 60  | BA    | 3135 | CLY  | C10-C11-N2 | -2.62 | 107.53      | 112.40   |
| 60  | BA    | 3135 | CLY  | O4-C1-C2   | -2.38 | 104.84      | 110.35   |
| 60  | BA    | 3135 | CLY  | C9-C8-CL1  | -2.17 | 105.14      | 108.76   |
| 60  | BA    | 3135 | CLY  | C15-N2-C14 | 2.16  | 115.39      | 112.45   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

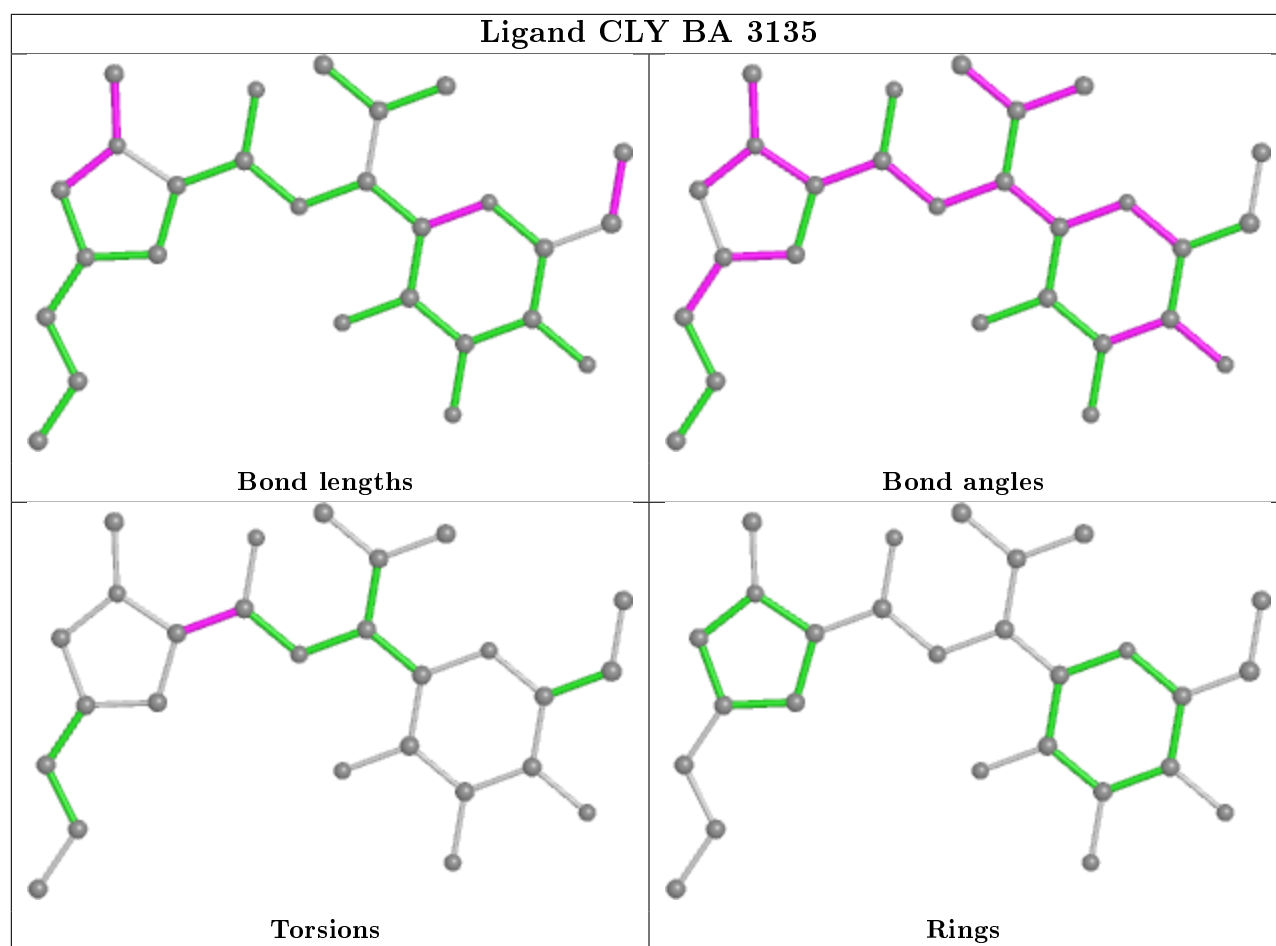
| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 60  | BA    | 3135 | CLY  | N1-C10-C11-C12 |
| 60  | BA    | 3135 | CLY  | N1-C10-C11-N2  |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60  | BA    | 3135 | CLY  | 2       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1533/1533 (100%) | -0.56  | 20 (1%) 77 76 | 26, 75, 180, 427      | 0     |
| 2   | AB    | 218/218 (100%)   | 1.35   | 47 (21%) 0 1  | 111, 151, 210, 294    | 0     |
| 2   | CB    | 218/218 (100%)   | 1.86   | 91 (41%) 0 0  | 125, 161, 248, 300    | 0     |
| 3   | AC    | 206/206 (100%)   | 0.38   | 10 (4%) 29 28 | 51, 97, 147, 208      | 0     |
| 3   | CC    | 206/206 (100%)   | 0.93   | 31 (15%) 2 2  | 74, 144, 225, 261     | 0     |
| 4   | AD    | 205/205 (100%)   | -0.02  | 6 (2%) 51 50  | 43, 83, 164, 311      | 0     |
| 4   | CD    | 205/205 (100%)   | -0.27  | 1 (0%) 91 91  | 31, 59, 113, 227      | 0     |
| 5   | AE    | 150/150 (100%)   | 0.15   | 4 (2%) 54 52  | 55, 78, 148, 255      | 0     |
| 5   | CE    | 150/150 (100%)   | 0.26   | 3 (2%) 65 63  | 55, 85, 149, 258      | 0     |
| 6   | AF    | 100/100 (100%)   | -0.06  | 2 (2%) 65 63  | 53, 90, 143, 171      | 0     |
| 6   | CF    | 100/100 (100%)   | 0.46   | 7 (7%) 16 16  | 72, 107, 167, 226     | 0     |
| 7   | AG    | 151/151 (100%)   | 0.39   | 13 (8%) 10 10 | 67, 129, 199, 248     | 0     |
| 8   | AH    | 129/129 (100%)   | 0.17   | 4 (3%) 49 48  | 38, 71, 123, 214      | 0     |
| 8   | CH    | 129/129 (100%)   | 0.46   | 7 (5%) 25 24  | 53, 100, 161, 214     | 0     |
| 9   | AI    | 127/127 (100%)   | 0.90   | 21 (16%) 1 2  | 66, 125, 243, 279     | 0     |
| 9   | CI    | 127/127 (100%)   | 2.01   | 51 (40%) 0 0  | 111, 184, 282, 308    | 0     |
| 10  | AJ    | 98/98 (100%)     | 0.62   | 12 (12%) 4 4  | 60, 114, 210, 262     | 0     |
| 10  | CJ    | 98/98 (100%)     | 2.43   | 47 (47%) 0 0  | 103, 188, 266, 292    | 0     |
| 11  | AK    | 117/117 (100%)   | 0.46   | 5 (4%) 35 33  | 36, 98, 174, 203      | 0     |
| 11  | CK    | 117/117 (100%)   | 0.38   | 7 (5%) 21 21  | 55, 104, 165, 196     | 0     |
| 12  | AL    | 123/123 (100%)   | -0.27  | 1 (0%) 86 86  | 15, 54, 116, 167      | 0     |
| 12  | CL    | 123/123 (100%)   | 0.28   | 4 (3%) 46 44  | 36, 73, 121, 188      | 0     |
| 13  | AM    | 114/114 (100%)   | 0.45   | 8 (7%) 16 16  | 76, 125, 196, 274     | 0     |
| 14  | AN    | 96/100 (96%)     | 0.27   | 6 (6%) 20 20  | 59, 102, 195, 267     | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 14  | CN    | 95/100 (95%)    | 2.30   | 46 (48%) 0 0  | 109, 221, 327, 373    | 0     |
| 15  | AO    | 88/88 (100%)    | -0.41  | 0 100 100     | 36, 70, 123, 182      | 0     |
| 15  | CO    | 88/88 (100%)    | 0.07   | 1 (1%) 80 80  | 59, 103, 158, 277     | 0     |
| 16  | AP    | 82/82 (100%)    | 0.51   | 9 (10%) 5 5   | 44, 74, 148, 243      | 0     |
| 17  | AQ    | 80/80 (100%)    | 0.48   | 7 (8%) 10 10  | 29, 78, 141, 267      | 0     |
| 17  | CQ    | 80/80 (100%)    | 0.86   | 13 (16%) 1 2  | 48, 106, 161, 199     | 0     |
| 18  | AR    | 55/55 (100%)    | 0.06   | 3 (5%) 25 24  | 60, 86, 161, 196      | 0     |
| 18  | CR    | 55/55 (100%)    | 0.16   | 1 (1%) 68 66  | 47, 92, 186, 230      | 0     |
| 19  | AS    | 79/79 (100%)    | 1.52   | 21 (26%) 0 0  | 79, 127, 199, 277     | 0     |
| 19  | CS    | 79/79 (100%)    | 3.17   | 48 (60%) 0 0  | 181, 371, 451, 469    | 0     |
| 20  | AT    | 85/85 (100%)    | -0.08  | 0 100 100     | 43, 76, 116, 143      | 0     |
| 20  | CT    | 85/85 (100%)    | 1.02   | 15 (17%) 1 1  | 58, 117, 197, 268     | 0     |
| 21  | AU    | 51/51 (100%)    | 1.78   | 21 (41%) 0 0  | 88, 157, 204, 230     | 0     |
| 21  | CU    | 51/51 (100%)    | 0.54   | 5 (9%) 7 7    | 58, 111, 182, 320     | 0     |
| 22  | BA    | 2854/2903 (98%) | -0.51  | 36 (1%) 77 76 | 4, 28, 155, 403       | 0     |
| 22  | DA    | 2841/2903 (97%) | 0.22   | 83 (2%) 51 50 | 49, 122, 252, 460     | 0     |
| 23  | BB    | 118/118 (100%)  | -0.61  | 0 100 100     | 13, 43, 77, 106       | 0     |
| 24  | BC    | 271/271 (100%)  | -0.34  | 5 (1%) 68 66  | 5, 39, 81, 171        | 0     |
| 24  | DC    | 271/271 (100%)  | 0.43   | 14 (5%) 27 25 | 51, 96, 147, 192      | 0     |
| 25  | BD    | 209/209 (100%)  | -0.43  | 0 100 100     | 3, 23, 72, 171        | 0     |
| 25  | DD    | 209/209 (100%)  | 0.54   | 15 (7%) 15 15 | 50, 111, 176, 290     | 0     |
| 26  | BE    | 201/201 (100%)  | -0.28  | 0 100 100     | 2, 37, 98, 185        | 0     |
| 26  | DE    | 201/201 (100%)  | 1.66   | 67 (33%) 0 0  | 62, 197, 395, 486     | 0     |
| 27  | BF    | 177/177 (100%)  | 0.09   | 4 (2%) 60 58  | 27, 70, 127, 197      | 0     |
| 28  | BG    | 176/176 (100%)  | -0.03  | 4 (2%) 60 58  | 23, 60, 119, 205      | 0     |
| 28  | DG    | 176/176 (100%)  | 1.63   | 67 (38%) 0 0  | 95, 195, 279, 335     | 0     |
| 29  | BH    | 149/149 (100%)  | 3.03   | 68 (45%) 0 0  | 40, 177, 291, 362     | 0     |
| 29  | DH    | 149/149 (100%)  | 3.28   | 63 (42%) 0 0  | 82, 181, 277, 319     | 0     |
| 30  | BI    | 141/141 (100%)  | 3.00   | 80 (56%) 0 0  | 162, 269, 338, 374    | 0     |
| 30  | DI    | 141/141 (100%)  | 3.53   | 101 (71%) 0 0 | 210, 324, 369, 408    | 0     |
| 31  | BJ    | 142/142 (100%)  | -0.50  | 0 100 100     | 6, 21, 60, 138        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 31  | DJ    | 142/142 (100%) | 0.83   | 18 (12%) 3 3 | 63, 102, 163, 184     | 0     |
| 32  | BK    | 122/122 (100%) | -0.45  | 0 100 100    | 7, 26, 74, 263        | 0     |
| 32  | DK    | 122/122 (100%) | 0.97   | 21 (17%) 1 1 | 52, 95, 164, 236      | 0     |
| 33  | BL    | 143/143 (100%) | -0.42  | 0 100 100    | 3, 35, 77, 103        | 0     |
| 33  | DL    | 143/143 (100%) | 1.35   | 33 (23%) 0 1 | 58, 159, 278, 348     | 0     |
| 34  | BM    | 136/136 (100%) | -0.47  | 0 100 100    | 4, 26, 66, 135        | 0     |
| 34  | DM    | 136/136 (100%) | 0.87   | 21 (15%) 2 2 | 44, 105, 164, 196     | 0     |
| 35  | BN    | 120/120 (100%) | -0.54  | 0 100 100    | 6, 20, 43, 151        | 0     |
| 35  | DN    | 120/120 (100%) | 1.33   | 30 (25%) 0 0 | 79, 127, 200, 268     | 0     |
| 36  | BO    | 116/116 (100%) | -0.24  | 0 100 100    | 26, 43, 77, 126       | 0     |
| 36  | DO    | 116/116 (100%) | 2.03   | 47 (40%) 0 0 | 124, 169, 240, 292    | 0     |
| 37  | BP    | 114/114 (100%) | -0.29  | 1 (0%) 84 84 | 9, 35, 83, 148        | 0     |
| 37  | DP    | 114/114 (100%) | 1.04   | 23 (20%) 1 1 | 62, 114, 174, 238     | 0     |
| 38  | BQ    | 117/117 (100%) | -0.57  | 0 100 100    | 3, 16, 43, 199        | 0     |
| 38  | DQ    | 117/117 (100%) | 1.03   | 20 (17%) 1 1 | 66, 103, 194, 288     | 0     |
| 39  | BR    | 103/103 (100%) | -0.45  | 1 (0%) 82 82 | 4, 31, 80, 180        | 0     |
| 39  | DR    | 103/103 (100%) | 2.02   | 43 (41%) 0 0 | 67, 130, 227, 316     | 0     |
| 40  | BS    | 110/110 (100%) | -0.50  | 1 (0%) 84 84 | 4, 17, 52, 175        | 0     |
| 40  | DS    | 110/110 (100%) | 1.79   | 43 (39%) 0 0 | 59, 130, 231, 279     | 0     |
| 41  | BT    | 93/93 (100%)   | -0.03  | 2 (2%) 62 59 | 19, 43, 128, 185      | 0     |
| 41  | DT    | 93/93 (100%)   | 2.64   | 50 (53%) 0 0 | 123, 205, 306, 347    | 0     |
| 42  | BU    | 102/102 (100%) | -0.11  | 1 (0%) 82 82 | 18, 49, 120, 241      | 0     |
| 42  | DU    | 102/102 (100%) | 3.05   | 61 (59%) 0 0 | 123, 285, 434, 557    | 0     |
| 43  | BV    | 94/94 (100%)   | -0.07  | 0 100 100    | 15, 43, 86, 142       | 0     |
| 43  | DV    | 94/94 (100%)   | 0.85   | 12 (12%) 3 3 | 97, 143, 194, 233     | 0     |
| 44  | BW    | 79/79 (100%)   | 0.02   | 5 (6%) 20 20 | 10, 30, 105, 223      | 0     |
| 44  | DW    | 79/79 (100%)   | 2.38   | 44 (55%) 0 0 | 82, 140, 238, 284     | 0     |
| 45  | BX    | 77/77 (100%)   | -0.41  | 0 100 100    | 11, 42, 84, 117       | 0     |
| 45  | DX    | 77/77 (100%)   | 0.95   | 12 (15%) 2 2 | 78, 117, 171, 236     | 0     |
| 46  | BY    | 63/63 (100%)   | 0.17   | 3 (4%) 30 29 | 30, 66, 136, 222      | 0     |
| 46  | DY    | 63/63 (100%)   | 1.97   | 20 (31%) 0 0 | 143, 309, 433, 440    | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 47  | BZ    | 58/58 (100%)      | -0.45  | 0 100 100      | 8, 22, 56, 111        | 0     |
| 47  | DZ    | 58/58 (100%)      | 0.30   | 2 (3%) 45 43   | 78, 119, 208, 217     | 0     |
| 48  | B0    | 56/56 (100%)      | -0.61  | 0 100 100      | 3, 24, 70, 159        | 0     |
| 48  | D0    | 56/56 (100%)      | 1.28   | 18 (32%) 0 0   | 63, 139, 242, 298     | 0     |
| 49  | B1    | 50/50 (100%)      | 0.29   | 2 (4%) 38 36   | 22, 48, 99, 165       | 0     |
| 49  | D1    | 50/50 (100%)      | 1.99   | 19 (38%) 0 0   | 99, 170, 210, 236     | 0     |
| 50  | B2    | 46/46 (100%)      | -0.54  | 1 (2%) 62 59   | 7, 26, 52, 155        | 0     |
| 50  | D2    | 46/46 (100%)      | 0.94   | 6 (13%) 3 3    | 81, 118, 175, 233     | 0     |
| 51  | B3    | 64/64 (100%)      | -0.58  | 0 100 100      | 5, 23, 44, 70         | 0     |
| 51  | D3    | 64/64 (100%)      | 1.61   | 22 (34%) 0 0   | 65, 128, 183, 257     | 0     |
| 52  | B4    | 38/38 (100%)      | 0.03   | 1 (2%) 56 52   | 21, 45, 86, 124       | 0     |
| 52  | D4    | 38/38 (100%)      | 2.45   | 22 (57%) 0 0   | 79, 137, 187, 227     | 0     |
| 53  | CA    | 1530/1530 (100%)  | -0.05  | 50 (3%) 46 44  | 34, 102, 281, 444     | 0     |
| 54  | CG    | 150/150 (100%)    | 2.27   | 76 (50%) 0 0   | 107, 224, 298, 322    | 0     |
| 55  | CM    | 113/113 (100%)    | 3.02   | 76 (67%) 0 0   | 182, 402, 494, 538    | 0     |
| 56  | CP    | 80/80 (100%)      | 0.90   | 11 (13%) 2 2   | 51, 94, 155, 236      | 0     |
| 57  | DB    | 117/117 (100%)    | -0.05  | 1 (0%) 84 84   | 95, 169, 224, 274     | 0     |
| 58  | DF    | 178/178 (100%)    | 2.03   | 84 (47%) 0 0   | 183, 225, 286, 338    | 0     |
| All | All   | 20431/20551 (99%) | 0.34   | 2108 (10%) 6 6 | 2, 94, 269, 557       | 0     |

The worst 5 of 2108 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 29  | DH    | 92  | GLY  | 29.7 |
| 29  | DH    | 124 | THR  | 23.0 |
| 29  | DH    | 91  | PHE  | 21.8 |
| 29  | DH    | 105 | ALA  | 21.1 |
| 30  | BI    | 67  | THR  | 15.3 |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|----------------------------|-------|
| 59  | MG   | DA    | 3129 | 1/1   | -0.39 | 1.35 | 233,233,233,233            | 0     |
| 59  | MG   | DA    | 3124 | 1/1   | -0.02 | 0.59 | 176,176,176,176            | 0     |
| 59  | MG   | DJ    | 201  | 1/1   | 0.01  | 2.07 | 230,230,230,230            | 0     |
| 59  | MG   | DA    | 3003 | 1/1   | 0.03  | 0.97 | 236,236,236,236            | 0     |
| 59  | MG   | DA    | 3013 | 1/1   | 0.26  | 0.24 | 126,126,126,126            | 0     |
| 59  | MG   | DA    | 3044 | 1/1   | 0.28  | 0.28 | 156,156,156,156            | 0     |
| 59  | MG   | DA    | 3017 | 1/1   | 0.28  | 0.18 | 204,204,204,204            | 0     |
| 59  | MG   | DA    | 3010 | 1/1   | 0.29  | 0.61 | 218,218,218,218            | 0     |
| 59  | MG   | DA    | 3025 | 1/1   | 0.34  | 1.37 | 278,278,278,278            | 0     |
| 59  | MG   | DA    | 3081 | 1/1   | 0.40  | 0.18 | 142,142,142,142            | 0     |
| 59  | MG   | DA    | 3019 | 1/1   | 0.40  | 2.04 | 247,247,247,247            | 0     |
| 59  | MG   | DA    | 3131 | 1/1   | 0.46  | 0.35 | 212,212,212,212            | 0     |
| 59  | MG   | DA    | 3001 | 1/1   | 0.49  | 0.19 | 151,151,151,151            | 0     |
| 59  | MG   | DA    | 3002 | 1/1   | 0.50  | 0.32 | 180,180,180,180            | 0     |
| 59  | MG   | DA    | 3110 | 1/1   | 0.51  | 0.27 | 153,153,153,153            | 0     |
| 59  | MG   | DA    | 3005 | 1/1   | 0.51  | 1.11 | 309,309,309,309            | 0     |
| 59  | MG   | DA    | 3061 | 1/1   | 0.52  | 1.00 | 229,229,229,229            | 0     |
| 59  | MG   | DA    | 3082 | 1/1   | 0.53  | 0.08 | 197,197,197,197            | 0     |
| 59  | MG   | DA    | 3098 | 1/1   | 0.54  | 0.16 | 172,172,172,172            | 0     |
| 59  | MG   | DA    | 3073 | 1/1   | 0.58  | 2.10 | 274,274,274,274            | 0     |
| 59  | MG   | DA    | 3007 | 1/1   | 0.59  | 0.65 | 254,254,254,254            | 0     |
| 59  | MG   | DA    | 3090 | 1/1   | 0.60  | 0.36 | 165,165,165,165            | 0     |
| 59  | MG   | CA    | 1602 | 1/1   | 0.64  | 0.15 | 175,175,175,175            | 0     |
| 59  | MG   | DA    | 3016 | 1/1   | 0.64  | 0.15 | 87,87,87,87                | 0     |
| 59  | MG   | AA    | 1629 | 1/1   | 0.64  | 0.20 | 180,180,180,180            | 0     |
| 59  | MG   | DA    | 3085 | 1/1   | 0.65  | 0.12 | 87,87,87,87                | 0     |
| 59  | MG   | CA    | 1619 | 1/1   | 0.66  | 0.38 | 214,214,214,214            | 0     |
| 59  | MG   | DA    | 3108 | 1/1   | 0.66  | 0.54 | 185,185,185,185            | 0     |
| 59  | MG   | DA    | 3030 | 1/1   | 0.66  | 0.13 | 68,68,68,68                | 0     |
| 59  | MG   | DA    | 3122 | 1/1   | 0.67  | 0.37 | 153,153,153,153            | 0     |
| 59  | MG   | DA    | 3046 | 1/1   | 0.68  | 0.17 | 151,151,151,151            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1616 | 1/1   | 0.69 | 0.39 | 254,254,254,254             | 0     |
| 59  | MG   | DA    | 3119 | 1/1   | 0.69 | 0.19 | 93,93,93,93                 | 0     |
| 59  | MG   | CA    | 1615 | 1/1   | 0.69 | 0.15 | 172,172,172,172             | 0     |
| 59  | MG   | DA    | 3015 | 1/1   | 0.70 | 0.24 | 183,183,183,183             | 0     |
| 59  | MG   | DA    | 3042 | 1/1   | 0.70 | 0.24 | 161,161,161,161             | 0     |
| 59  | MG   | CA    | 1627 | 1/1   | 0.70 | 0.38 | 181,181,181,181             | 0     |
| 59  | MG   | CA    | 1634 | 1/1   | 0.70 | 0.14 | 131,131,131,131             | 0     |
| 59  | MG   | DA    | 3132 | 1/1   | 0.70 | 0.35 | 174,174,174,174             | 0     |
| 59  | MG   | DA    | 3056 | 1/1   | 0.71 | 0.43 | 197,197,197,197             | 0     |
| 59  | MG   | DA    | 3117 | 1/1   | 0.71 | 0.22 | 71,71,71,71                 | 0     |
| 59  | MG   | CA    | 1636 | 1/1   | 0.71 | 0.29 | 181,181,181,181             | 0     |
| 59  | MG   | CA    | 1632 | 1/1   | 0.71 | 0.24 | 156,156,156,156             | 0     |
| 59  | MG   | CA    | 1629 | 1/1   | 0.71 | 0.12 | 197,197,197,197             | 0     |
| 59  | MG   | DA    | 3075 | 1/1   | 0.72 | 0.69 | 174,174,174,174             | 0     |
| 59  | MG   | DA    | 3027 | 1/1   | 0.72 | 0.61 | 253,253,253,253             | 0     |
| 59  | MG   | CA    | 1624 | 1/1   | 0.72 | 0.69 | 165,165,165,165             | 0     |
| 59  | MG   | DA    | 3048 | 1/1   | 0.72 | 0.32 | 218,218,218,218             | 0     |
| 59  | MG   | BA    | 3011 | 1/1   | 0.73 | 0.21 | 102,102,102,102             | 0     |
| 59  | MG   | DA    | 3109 | 1/1   | 0.73 | 0.31 | 174,174,174,174             | 0     |
| 59  | MG   | DA    | 3087 | 1/1   | 0.73 | 0.27 | 179,179,179,179             | 0     |
| 59  | MG   | DA    | 3004 | 1/1   | 0.74 | 0.12 | 114,114,114,114             | 0     |
| 59  | MG   | DA    | 3028 | 1/1   | 0.74 | 0.35 | 143,143,143,143             | 0     |
| 59  | MG   | CA    | 1618 | 1/1   | 0.74 | 0.29 | 113,113,113,113             | 0     |
| 59  | MG   | CA    | 1614 | 1/1   | 0.74 | 0.26 | 210,210,210,210             | 0     |
| 59  | MG   | DA    | 3105 | 1/1   | 0.74 | 0.23 | 262,262,262,262             | 0     |
| 59  | MG   | DE    | 301  | 1/1   | 0.76 | 0.47 | 131,131,131,131             | 0     |
| 59  | MG   | BA    | 3117 | 1/1   | 0.76 | 0.27 | 157,157,157,157             | 0     |
| 59  | MG   | DA    | 3049 | 1/1   | 0.76 | 0.23 | 172,172,172,172             | 0     |
| 59  | MG   | DA    | 3107 | 1/1   | 0.76 | 0.48 | 161,161,161,161             | 0     |
| 59  | MG   | CA    | 1637 | 1/1   | 0.77 | 0.22 | 74,74,74,74                 | 0     |
| 59  | MG   | CA    | 1623 | 1/1   | 0.77 | 0.16 | 124,124,124,124             | 0     |
| 59  | MG   | DA    | 3038 | 1/1   | 0.77 | 0.14 | 102,102,102,102             | 0     |
| 59  | MG   | DA    | 3029 | 1/1   | 0.77 | 0.19 | 112,112,112,112             | 0     |
| 59  | MG   | DA    | 3059 | 1/1   | 0.78 | 0.82 | 200,200,200,200             | 0     |
| 59  | MG   | CA    | 1628 | 1/1   | 0.78 | 1.37 | 260,260,260,260             | 0     |
| 59  | MG   | DA    | 3114 | 1/1   | 0.78 | 0.30 | 167,167,167,167             | 0     |
| 59  | MG   | DA    | 3072 | 1/1   | 0.78 | 0.07 | 187,187,187,187             | 0     |
| 59  | MG   | DA    | 3006 | 1/1   | 0.78 | 0.11 | 211,211,211,211             | 0     |
| 59  | MG   | DA    | 3062 | 1/1   | 0.79 | 1.49 | 211,211,211,211             | 0     |
| 59  | MG   | AA    | 1627 | 1/1   | 0.79 | 0.18 | 132,132,132,132             | 0     |
| 59  | MG   | DA    | 3018 | 1/1   | 0.79 | 0.17 | 226,226,226,226             | 0     |
| 59  | MG   | DC    | 301  | 1/1   | 0.80 | 0.25 | 145,145,145,145             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3077 | 1/1   | 0.80 | 0.54 | 222,222,222,222             | 0     |
| 59  | MG   | DA    | 3026 | 1/1   | 0.81 | 0.12 | 109,109,109,109             | 0     |
| 59  | MG   | CA    | 1620 | 1/1   | 0.81 | 0.13 | 168,168,168,168             | 0     |
| 59  | MG   | DA    | 3008 | 1/1   | 0.81 | 0.13 | 148,148,148,148             | 0     |
| 59  | MG   | BA    | 3131 | 1/1   | 0.81 | 0.27 | 154,154,154,154             | 0     |
| 59  | MG   | DA    | 3121 | 1/1   | 0.81 | 0.12 | 84,84,84,84                 | 0     |
| 59  | MG   | DA    | 3086 | 1/1   | 0.81 | 0.17 | 139,139,139,139             | 0     |
| 59  | MG   | DA    | 3094 | 1/1   | 0.82 | 0.20 | 107,107,107,107             | 0     |
| 59  | MG   | DA    | 3063 | 1/1   | 0.82 | 0.44 | 278,278,278,278             | 0     |
| 59  | MG   | BA    | 3003 | 1/1   | 0.83 | 0.11 | 69,69,69,69                 | 0     |
| 59  | MG   | AA    | 1610 | 1/1   | 0.83 | 0.09 | 190,190,190,190             | 0     |
| 59  | MG   | DA    | 3097 | 1/1   | 0.83 | 0.22 | 144,144,144,144             | 0     |
| 59  | MG   | AA    | 1618 | 1/1   | 0.83 | 0.60 | 197,197,197,197             | 0     |
| 59  | MG   | DA    | 3092 | 1/1   | 0.83 | 0.27 | 229,229,229,229             | 0     |
| 59  | MG   | DA    | 3021 | 1/1   | 0.83 | 0.38 | 199,199,199,199             | 0     |
| 59  | MG   | AA    | 1619 | 1/1   | 0.83 | 0.11 | 156,156,156,156             | 0     |
| 59  | MG   | DA    | 3093 | 1/1   | 0.83 | 0.13 | 114,114,114,114             | 0     |
| 59  | MG   | AN    | 201  | 1/1   | 0.83 | 0.25 | 159,159,159,159             | 0     |
| 59  | MG   | BB    | 201  | 1/1   | 0.83 | 0.32 | 222,222,222,222             | 0     |
| 59  | MG   | DA    | 3128 | 1/1   | 0.83 | 0.72 | 214,214,214,214             | 0     |
| 59  | MG   | AA    | 1607 | 1/1   | 0.83 | 0.15 | 103,103,103,103             | 0     |
| 59  | MG   | DA    | 3041 | 1/1   | 0.84 | 0.17 | 82,82,82,82                 | 0     |
| 59  | MG   | DA    | 3074 | 1/1   | 0.84 | 0.35 | 190,190,190,190             | 0     |
| 59  | MG   | BA    | 3001 | 1/1   | 0.84 | 0.13 | 116,116,116,116             | 0     |
| 59  | MG   | DA    | 3083 | 1/1   | 0.84 | 0.17 | 204,204,204,204             | 0     |
| 59  | MG   | BA    | 3091 | 1/1   | 0.84 | 0.07 | 32,32,32,32                 | 0     |
| 59  | MG   | CA    | 1622 | 1/1   | 0.84 | 0.14 | 226,226,226,226             | 0     |
| 59  | MG   | DA    | 3127 | 1/1   | 0.84 | 0.25 | 142,142,142,142             | 0     |
| 59  | MG   | AA    | 1603 | 1/1   | 0.84 | 0.10 | 111,111,111,111             | 0     |
| 59  | MG   | CA    | 1604 | 1/1   | 0.84 | 0.06 | 74,74,74,74                 | 0     |
| 59  | MG   | DA    | 3126 | 1/1   | 0.84 | 0.67 | 200,200,200,200             | 0     |
| 59  | MG   | BA    | 3096 | 1/1   | 0.85 | 0.16 | 102,102,102,102             | 0     |
| 59  | MG   | DA    | 3100 | 1/1   | 0.85 | 0.12 | 78,78,78,78                 | 0     |
| 59  | MG   | DA    | 3037 | 1/1   | 0.85 | 0.13 | 197,197,197,197             | 0     |
| 59  | MG   | DA    | 3070 | 1/1   | 0.85 | 0.13 | 56,56,56,56                 | 0     |
| 59  | MG   | DA    | 3058 | 1/1   | 0.85 | 0.18 | 204,204,204,204             | 0     |
| 59  | MG   | CA    | 1601 | 1/1   | 0.86 | 0.17 | 156,156,156,156             | 0     |
| 59  | MG   | BA    | 3085 | 1/1   | 0.86 | 0.22 | 100,100,100,100             | 0     |
| 59  | MG   | DA    | 3057 | 1/1   | 0.86 | 0.52 | 227,227,227,227             | 0     |
| 59  | MG   | CA    | 1639 | 1/1   | 0.86 | 0.14 | 165,165,165,165             | 0     |
| 59  | MG   | DC    | 302  | 1/1   | 0.86 | 0.27 | 129,129,129,129             | 0     |
| 59  | MG   | CA    | 1607 | 1/1   | 0.86 | 0.25 | 121,121,121,121             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | CA    | 1617 | 1/1   | 0.86 | 0.23 | 199,199,199,199             | 0     |
| 59  | MG   | CA    | 1603 | 1/1   | 0.86 | 0.29 | 162,162,162,162             | 0     |
| 59  | MG   | DA    | 3125 | 1/1   | 0.86 | 0.16 | 82,82,82,82                 | 0     |
| 59  | MG   | AA    | 1636 | 1/1   | 0.86 | 0.18 | 124,124,124,124             | 0     |
| 59  | MG   | DA    | 3045 | 1/1   | 0.86 | 0.20 | 78,78,78,78                 | 0     |
| 59  | MG   | BA    | 3074 | 1/1   | 0.87 | 0.24 | 93,93,93,93                 | 0     |
| 59  | MG   | BA    | 3090 | 1/1   | 0.87 | 0.18 | 128,128,128,128             | 0     |
| 59  | MG   | BA    | 3068 | 1/1   | 0.87 | 0.13 | 117,117,117,117             | 0     |
| 59  | MG   | DA    | 3091 | 1/1   | 0.88 | 0.20 | 116,116,116,116             | 0     |
| 59  | MG   | DA    | 3014 | 1/1   | 0.88 | 0.31 | 172,172,172,172             | 0     |
| 59  | MG   | BA    | 3069 | 1/1   | 0.88 | 0.33 | 151,151,151,151             | 0     |
| 59  | MG   | DA    | 3106 | 1/1   | 0.88 | 0.20 | 92,92,92,92                 | 0     |
| 59  | MG   | DA    | 3034 | 1/1   | 0.88 | 0.26 | 125,125,125,125             | 0     |
| 59  | MG   | DA    | 3064 | 1/1   | 0.88 | 0.14 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3071 | 1/1   | 0.88 | 0.11 | 133,133,133,133             | 0     |
| 59  | MG   | DA    | 3040 | 1/1   | 0.88 | 0.14 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3022 | 1/1   | 0.89 | 0.12 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3111 | 1/1   | 0.89 | 0.15 | 109,109,109,109             | 0     |
| 59  | MG   | BA    | 3110 | 1/1   | 0.89 | 0.25 | 92,92,92,92                 | 0     |
| 59  | MG   | AA    | 1614 | 1/1   | 0.89 | 0.25 | 194,194,194,194             | 0     |
| 59  | MG   | CA    | 1633 | 1/1   | 0.89 | 0.13 | 63,63,63,63                 | 0     |
| 59  | MG   | AA    | 1628 | 1/1   | 0.89 | 0.11 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3026 | 1/1   | 0.89 | 0.27 | 133,133,133,133             | 0     |
| 59  | MG   | DA    | 3096 | 1/1   | 0.89 | 0.16 | 102,102,102,102             | 0     |
| 59  | MG   | AA    | 1612 | 1/1   | 0.89 | 0.20 | 105,105,105,105             | 0     |
| 59  | MG   | BA    | 3024 | 1/1   | 0.89 | 0.58 | 166,166,166,166             | 0     |
| 59  | MG   | DA    | 3115 | 1/1   | 0.89 | 0.16 | 65,65,65,65                 | 0     |
| 59  | MG   | DA    | 3047 | 1/1   | 0.89 | 0.18 | 95,95,95,95                 | 0     |
| 59  | MG   | AA    | 1617 | 1/1   | 0.90 | 0.17 | 115,115,115,115             | 0     |
| 59  | MG   | CA    | 1625 | 1/1   | 0.90 | 0.22 | 100,100,100,100             | 0     |
| 59  | MG   | AA    | 1622 | 1/1   | 0.90 | 0.06 | 76,76,76,76                 | 0     |
| 59  | MG   | AA    | 1631 | 1/1   | 0.90 | 0.12 | 91,91,91,91                 | 0     |
| 59  | MG   | DA    | 3099 | 1/1   | 0.90 | 0.14 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3032 | 1/1   | 0.90 | 0.18 | 121,121,121,121             | 0     |
| 59  | MG   | DA    | 3035 | 1/1   | 0.90 | 0.41 | 194,194,194,194             | 0     |
| 59  | MG   | DA    | 3011 | 1/1   | 0.90 | 0.17 | 127,127,127,127             | 0     |
| 59  | MG   | AA    | 1635 | 1/1   | 0.90 | 0.18 | 194,194,194,194             | 0     |
| 59  | MG   | AA    | 1626 | 1/1   | 0.90 | 0.30 | 117,117,117,117             | 0     |
| 59  | MG   | AA    | 1639 | 1/1   | 0.90 | 0.08 | 108,108,108,108             | 0     |
| 59  | MG   | DA    | 3101 | 1/1   | 0.90 | 0.10 | 67,67,67,67                 | 0     |
| 59  | MG   | CA    | 1612 | 1/1   | 0.91 | 0.35 | 136,136,136,136             | 0     |
| 59  | MG   | DA    | 3039 | 1/1   | 0.91 | 0.20 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | DA    | 3130 | 1/1   | 0.91 | 0.15 | 85,85,85,85                 | 0     |
| 59  | MG   | DB    | 201  | 1/1   | 0.91 | 0.09 | 104,104,104,104             | 0     |
| 59  | MG   | DA    | 3068 | 1/1   | 0.91 | 0.39 | 209,209,209,209             | 0     |
| 59  | MG   | DA    | 3066 | 1/1   | 0.91 | 0.12 | 61,61,61,61                 | 0     |
| 59  | MG   | BA    | 3089 | 1/1   | 0.91 | 0.12 | 80,80,80,80                 | 0     |
| 59  | MG   | AA    | 1608 | 1/1   | 0.91 | 0.26 | 68,68,68,68                 | 0     |
| 59  | MG   | DA    | 3053 | 1/1   | 0.91 | 0.07 | 67,67,67,67                 | 0     |
| 59  | MG   | DA    | 3095 | 1/1   | 0.91 | 0.09 | 95,95,95,95                 | 0     |
| 59  | MG   | BA    | 3072 | 1/1   | 0.91 | 0.16 | 139,139,139,139             | 0     |
| 59  | MG   | DA    | 3050 | 1/1   | 0.91 | 0.14 | 106,106,106,106             | 0     |
| 59  | MG   | CA    | 1610 | 1/1   | 0.91 | 0.14 | 152,152,152,152             | 0     |
| 59  | MG   | BB    | 202  | 1/1   | 0.91 | 0.09 | 50,50,50,50                 | 0     |
| 59  | MG   | BA    | 3129 | 1/1   | 0.91 | 1.04 | 214,214,214,214             | 0     |
| 59  | MG   | CA    | 1631 | 1/1   | 0.92 | 0.23 | 93,93,93,93                 | 0     |
| 59  | MG   | DA    | 3112 | 1/1   | 0.92 | 0.14 | 131,131,131,131             | 0     |
| 59  | MG   | DA    | 3023 | 1/1   | 0.92 | 0.10 | 87,87,87,87                 | 0     |
| 59  | MG   | AA    | 1604 | 1/1   | 0.92 | 0.12 | 124,124,124,124             | 0     |
| 59  | MG   | BA    | 3082 | 1/1   | 0.92 | 0.16 | 114,114,114,114             | 0     |
| 59  | MG   | AA    | 1640 | 1/1   | 0.92 | 0.09 | 154,154,154,154             | 0     |
| 59  | MG   | DA    | 3123 | 1/1   | 0.92 | 0.13 | 61,61,61,61                 | 0     |
| 59  | MG   | CA    | 1638 | 1/1   | 0.92 | 0.10 | 130,130,130,130             | 0     |
| 59  | MG   | DA    | 3036 | 1/1   | 0.92 | 0.17 | 82,82,82,82                 | 0     |
| 59  | MG   | CA    | 1640 | 1/1   | 0.92 | 0.15 | 157,157,157,157             | 0     |
| 59  | MG   | CA    | 1609 | 1/1   | 0.93 | 0.11 | 83,83,83,83                 | 0     |
| 59  | MG   | DA    | 3089 | 1/1   | 0.93 | 0.09 | 99,99,99,99                 | 0     |
| 59  | MG   | BA    | 3133 | 1/1   | 0.93 | 0.12 | 139,139,139,139             | 0     |
| 59  | MG   | BA    | 3124 | 1/1   | 0.93 | 0.11 | 25,25,25,25                 | 0     |
| 59  | MG   | CA    | 1611 | 1/1   | 0.93 | 0.22 | 112,112,112,112             | 0     |
| 59  | MG   | BA    | 3088 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 61  | ZN   | D4    | 101  | 1/1   | 0.93 | 0.07 | 161,161,161,161             | 0     |
| 59  | MG   | DA    | 3020 | 1/1   | 0.93 | 0.22 | 49,49,49,49                 | 0     |
| 59  | MG   | CA    | 1606 | 1/1   | 0.93 | 0.09 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3086 | 1/1   | 0.93 | 0.16 | 131,131,131,131             | 0     |
| 59  | MG   | DA    | 3009 | 1/1   | 0.93 | 0.10 | 69,69,69,69                 | 0     |
| 59  | MG   | DA    | 3118 | 1/1   | 0.93 | 0.12 | 76,76,76,76                 | 0     |
| 59  | MG   | BA    | 3105 | 1/1   | 0.93 | 0.15 | 42,42,42,42                 | 0     |
| 59  | MG   | DA    | 3079 | 1/1   | 0.93 | 0.12 | 142,142,142,142             | 0     |
| 59  | MG   | BA    | 3103 | 1/1   | 0.93 | 0.15 | 4,4,4,4                     | 0     |
| 59  | MG   | DA    | 3076 | 1/1   | 0.93 | 0.17 | 93,93,93,93                 | 0     |
| 59  | MG   | BA    | 3014 | 1/1   | 0.93 | 0.13 | 68,68,68,68                 | 0     |
| 59  | MG   | BA    | 3046 | 1/1   | 0.94 | 0.07 | 149,149,149,149             | 0     |
| 59  | MG   | AA    | 1642 | 1/1   | 0.94 | 0.10 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | AA    | 1615 | 1/1   | 0.94 | 0.06 | 120,120,120,120             | 0     |
| 59  | MG   | BA    | 3111 | 1/1   | 0.94 | 0.21 | 77,77,77,77                 | 0     |
| 59  | MG   | DA    | 3067 | 1/1   | 0.94 | 0.10 | 83,83,83,83                 | 0     |
| 59  | MG   | DA    | 3084 | 1/1   | 0.94 | 0.40 | 144,144,144,144             | 0     |
| 59  | MG   | AA    | 1625 | 1/1   | 0.94 | 0.23 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3070 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | DA    | 3033 | 1/1   | 0.94 | 0.10 | 95,95,95,95                 | 0     |
| 59  | MG   | AA    | 1630 | 1/1   | 0.94 | 0.16 | 189,189,189,189             | 0     |
| 59  | MG   | CA    | 1621 | 1/1   | 0.94 | 0.22 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3060 | 1/1   | 0.94 | 0.11 | 105,105,105,105             | 0     |
| 59  | MG   | DA    | 3080 | 1/1   | 0.94 | 0.20 | 108,108,108,108             | 0     |
| 59  | MG   | DA    | 3024 | 1/1   | 0.94 | 0.14 | 89,89,89,89                 | 0     |
| 59  | MG   | BA    | 3033 | 1/1   | 0.94 | 0.32 | 162,162,162,162             | 0     |
| 59  | MG   | DA    | 3043 | 1/1   | 0.94 | 0.19 | 100,100,100,100             | 0     |
| 59  | MG   | DA    | 3088 | 1/1   | 0.94 | 0.20 | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3056 | 1/1   | 0.94 | 0.16 | 169,169,169,169             | 0     |
| 59  | MG   | DA    | 3031 | 1/1   | 0.94 | 0.17 | 105,105,105,105             | 0     |
| 59  | MG   | BA    | 3134 | 1/1   | 0.95 | 0.20 | 219,219,219,219             | 0     |
| 59  | MG   | CA    | 1642 | 1/1   | 0.95 | 0.07 | 82,82,82,82                 | 0     |
| 59  | MG   | AA    | 1606 | 1/1   | 0.95 | 0.11 | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1602 | 1/1   | 0.95 | 0.10 | 152,152,152,152             | 0     |
| 59  | MG   | DA    | 3103 | 1/1   | 0.95 | 0.20 | 44,44,44,44                 | 0     |
| 59  | MG   | BA    | 3060 | 1/1   | 0.95 | 0.31 | 210,210,210,210             | 0     |
| 59  | MG   | BA    | 3049 | 1/1   | 0.95 | 0.13 | 66,66,66,66                 | 0     |
| 59  | MG   | DA    | 3052 | 1/1   | 0.95 | 0.18 | 89,89,89,89                 | 0     |
| 59  | MG   | AA    | 1609 | 1/1   | 0.95 | 0.13 | 46,46,46,46                 | 0     |
| 59  | MG   | DA    | 3065 | 1/1   | 0.95 | 0.09 | 49,49,49,49                 | 0     |
| 59  | MG   | BA    | 3007 | 1/1   | 0.95 | 0.10 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3058 | 1/1   | 0.95 | 0.18 | 107,107,107,107             | 0     |
| 59  | MG   | DA    | 3055 | 1/1   | 0.95 | 0.12 | 120,120,120,120             | 0     |
| 59  | MG   | BA    | 3102 | 1/1   | 0.95 | 0.17 | 3,3,3,3                     | 0     |
| 59  | MG   | AA    | 1620 | 1/1   | 0.95 | 0.08 | 117,117,117,117             | 0     |
| 59  | MG   | BA    | 3054 | 1/1   | 0.95 | 0.33 | 189,189,189,189             | 0     |
| 59  | MG   | DA    | 3054 | 1/1   | 0.95 | 0.10 | 96,96,96,96                 | 0     |
| 59  | MG   | DA    | 3120 | 1/1   | 0.95 | 0.19 | 109,109,109,109             | 0     |
| 59  | MG   | BA    | 3093 | 1/1   | 0.95 | 0.09 | 36,36,36,36                 | 0     |
| 59  | MG   | BA    | 3078 | 1/1   | 0.96 | 0.13 | 20,20,20,20                 | 0     |
| 59  | MG   | CA    | 1630 | 1/1   | 0.96 | 0.06 | 131,131,131,131             | 0     |
| 59  | MG   | AA    | 1616 | 1/1   | 0.96 | 0.14 | 98,98,98,98                 | 0     |
| 59  | MG   | BA    | 3012 | 1/1   | 0.96 | 0.10 | 1,1,1,1                     | 0     |
| 59  | MG   | BA    | 3132 | 1/1   | 0.96 | 0.15 | 1,1,1,1                     | 0     |
| 59  | MG   | DA    | 3051 | 1/1   | 0.96 | 0.11 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3116 | 1/1   | 0.96 | 0.10 | 76,76,76,76                 | 0     |
| 59  | MG   | BA    | 3106 | 1/1   | 0.96 | 0.12 | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3027 | 1/1   | 0.96 | 0.18 | 46,46,46,46                 | 0     |
| 59  | MG   | CA    | 1641 | 1/1   | 0.96 | 0.22 | 79,79,79,79                 | 0     |
| 59  | MG   | BA    | 3035 | 1/1   | 0.96 | 0.53 | 171,171,171,171             | 0     |
| 59  | MG   | AA    | 1613 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3077 | 1/1   | 0.96 | 0.10 | 30,30,30,30                 | 0     |
| 59  | MG   | BA    | 3022 | 1/1   | 0.96 | 0.07 | 8,8,8,8                     | 0     |
| 59  | MG   | BA    | 3050 | 1/1   | 0.96 | 0.11 | 10,10,10,10                 | 0     |
| 59  | MG   | DA    | 3113 | 1/1   | 0.96 | 0.07 | 148,148,148,148             | 0     |
| 59  | MG   | CA    | 1635 | 1/1   | 0.96 | 0.13 | 95,95,95,95                 | 0     |
| 59  | MG   | BA    | 3016 | 1/1   | 0.96 | 0.07 | 2,2,2,2                     | 0     |
| 59  | MG   | BA    | 3123 | 1/1   | 0.96 | 0.15 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3010 | 1/1   | 0.96 | 0.08 | 29,29,29,29                 | 0     |
| 59  | MG   | AA    | 1638 | 1/1   | 0.96 | 0.10 | 116,116,116,116             | 0     |
| 59  | MG   | BA    | 3030 | 1/1   | 0.96 | 0.09 | 21,21,21,21                 | 0     |
| 59  | MG   | BA    | 3002 | 1/1   | 0.96 | 0.15 | 85,85,85,85                 | 0     |
| 59  | MG   | BA    | 3055 | 1/1   | 0.96 | 0.23 | 205,205,205,205             | 0     |
| 59  | MG   | DA    | 3078 | 1/1   | 0.96 | 0.34 | 180,180,180,180             | 0     |
| 59  | MG   | DA    | 3012 | 1/1   | 0.96 | 0.15 | 64,64,64,64                 | 0     |
| 59  | MG   | BA    | 3108 | 1/1   | 0.96 | 0.09 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3015 | 1/1   | 0.96 | 0.06 | 55,55,55,55                 | 0     |
| 59  | MG   | BA    | 3039 | 1/1   | 0.96 | 0.22 | 6,6,6,6                     | 0     |
| 59  | MG   | BL    | 201  | 1/1   | 0.96 | 0.13 | 53,53,53,53                 | 0     |
| 59  | MG   | BA    | 3104 | 1/1   | 0.97 | 0.13 | 3,3,3,3                     | 0     |
| 59  | MG   | BA    | 3118 | 1/1   | 0.97 | 0.16 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3126 | 1/1   | 0.97 | 0.10 | 9,9,9,9                     | 0     |
| 59  | MG   | BA    | 3107 | 1/1   | 0.97 | 0.18 | 5,5,5,5                     | 0     |
| 59  | MG   | AA    | 1605 | 1/1   | 0.97 | 0.14 | 39,39,39,39                 | 0     |
| 59  | MG   | BA    | 3020 | 1/1   | 0.97 | 0.11 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3099 | 1/1   | 0.97 | 0.16 | 1,1,1,1                     | 0     |
| 59  | MG   | BA    | 3084 | 1/1   | 0.97 | 0.12 | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3047 | 1/1   | 0.97 | 0.18 | 111,111,111,111             | 0     |
| 59  | MG   | BA    | 3066 | 1/1   | 0.97 | 0.12 | 10,10,10,10                 | 0     |
| 59  | MG   | BA    | 3130 | 1/1   | 0.97 | 0.26 | 97,97,97,97                 | 0     |
| 59  | MG   | BA    | 3008 | 1/1   | 0.97 | 0.13 | 7,7,7,7                     | 0     |
| 59  | MG   | BA    | 3119 | 1/1   | 0.97 | 0.07 | 51,51,51,51                 | 0     |
| 59  | MG   | CA    | 1608 | 1/1   | 0.97 | 0.22 | 41,41,41,41                 | 0     |
| 59  | MG   | AA    | 1623 | 1/1   | 0.97 | 0.06 | 102,102,102,102             | 0     |
| 59  | MG   | DA    | 3069 | 1/1   | 0.97 | 0.14 | 69,69,69,69                 | 0     |
| 59  | MG   | BA    | 3034 | 1/1   | 0.97 | 0.10 | 5,5,5,5                     | 0     |
| 59  | MG   | BA    | 3121 | 1/1   | 0.97 | 0.13 | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3021 | 1/1   | 0.97 | 0.14 | 7,7,7,7                     | 0     |
| 59  | MG   | BA    | 3037 | 1/1   | 0.97 | 0.11 | 5,5,5,5                     | 0     |
| 59  | MG   | AA    | 1611 | 1/1   | 0.97 | 0.07 | 62,62,62,62                 | 0     |
| 59  | MG   | AA    | 1624 | 1/1   | 0.97 | 0.11 | 82,82,82,82                 | 0     |
| 59  | MG   | BA    | 3004 | 1/1   | 0.97 | 0.12 | 138,138,138,138             | 0     |
| 59  | MG   | BA    | 3036 | 1/1   | 0.97 | 0.14 | 4,4,4,4                     | 0     |
| 59  | MG   | DA    | 3102 | 1/1   | 0.97 | 0.18 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3097 | 1/1   | 0.97 | 0.15 | 45,45,45,45                 | 0     |
| 59  | MG   | AA    | 1634 | 1/1   | 0.97 | 0.06 | 72,72,72,72                 | 0     |
| 59  | MG   | CA    | 1613 | 1/1   | 0.97 | 0.10 | 105,105,105,105             | 0     |
| 59  | MG   | BA    | 3009 | 1/1   | 0.97 | 0.13 | 6,6,6,6                     | 0     |
| 59  | MG   | CA    | 1626 | 1/1   | 0.97 | 0.22 | 23,23,23,23                 | 0     |
| 59  | MG   | AA    | 1637 | 1/1   | 0.97 | 0.14 | 27,27,27,27                 | 0     |
| 59  | MG   | BA    | 3076 | 1/1   | 0.97 | 0.11 | 114,114,114,114             | 0     |
| 59  | MG   | BA    | 3019 | 1/1   | 0.98 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | BA    | 3081 | 1/1   | 0.98 | 0.19 | 86,86,86,86                 | 0     |
| 59  | MG   | BA    | 3065 | 1/1   | 0.98 | 0.11 | 17,17,17,17                 | 0     |
| 59  | MG   | BA    | 3087 | 1/1   | 0.98 | 0.11 | 35,35,35,35                 | 0     |
| 59  | MG   | BA    | 3044 | 1/1   | 0.98 | 0.13 | 12,12,12,12                 | 0     |
| 59  | MG   | DA    | 3116 | 1/1   | 0.98 | 0.23 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3023 | 1/1   | 0.98 | 0.10 | 5,5,5,5                     | 0     |
| 59  | MG   | BA    | 3073 | 1/1   | 0.98 | 0.18 | 8,8,8,8                     | 0     |
| 59  | MG   | BA    | 3029 | 1/1   | 0.98 | 0.18 | 3,3,3,3                     | 0     |
| 59  | MG   | BA    | 3098 | 1/1   | 0.98 | 0.07 | 15,15,15,15                 | 0     |
| 59  | MG   | BB    | 204  | 1/1   | 0.98 | 0.12 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3071 | 1/1   | 0.98 | 0.10 | 7,7,7,7                     | 0     |
| 59  | MG   | BA    | 3101 | 1/1   | 0.98 | 0.06 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3053 | 1/1   | 0.98 | 0.09 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3057 | 1/1   | 0.98 | 0.06 | 48,48,48,48                 | 0     |
| 59  | MG   | BA    | 3018 | 1/1   | 0.98 | 0.29 | 6,6,6,6                     | 0     |
| 60  | CLY  | BA    | 3135 | 27/27 | 0.98 | 0.20 | 11,17,22,22                 | 0     |
| 59  | MG   | BA    | 3048 | 1/1   | 0.98 | 0.10 | 6,6,6,6                     | 0     |
| 59  | MG   | BA    | 3112 | 1/1   | 0.98 | 0.10 | 47,47,47,47                 | 0     |
| 59  | MG   | AA    | 1632 | 1/1   | 0.98 | 0.11 | 76,76,76,76                 | 0     |
| 59  | MG   | AA    | 1601 | 1/1   | 0.98 | 0.11 | 70,70,70,70                 | 0     |
| 59  | MG   | DA    | 3104 | 1/1   | 0.98 | 0.15 | 47,47,47,47                 | 0     |
| 59  | MG   | BA    | 3062 | 1/1   | 0.98 | 0.12 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3080 | 1/1   | 0.98 | 0.06 | 34,34,34,34                 | 0     |
| 59  | MG   | BA    | 3045 | 1/1   | 0.98 | 0.12 | 17,17,17,17                 | 0     |
| 59  | MG   | BA    | 3094 | 1/1   | 0.98 | 0.08 | 9,9,9,9                     | 0     |
| 59  | MG   | BA    | 3051 | 1/1   | 0.98 | 0.12 | 58,58,58,58                 | 0     |
| 59  | MG   | BA    | 3100 | 1/1   | 0.98 | 0.27 | 89,89,89,89                 | 0     |

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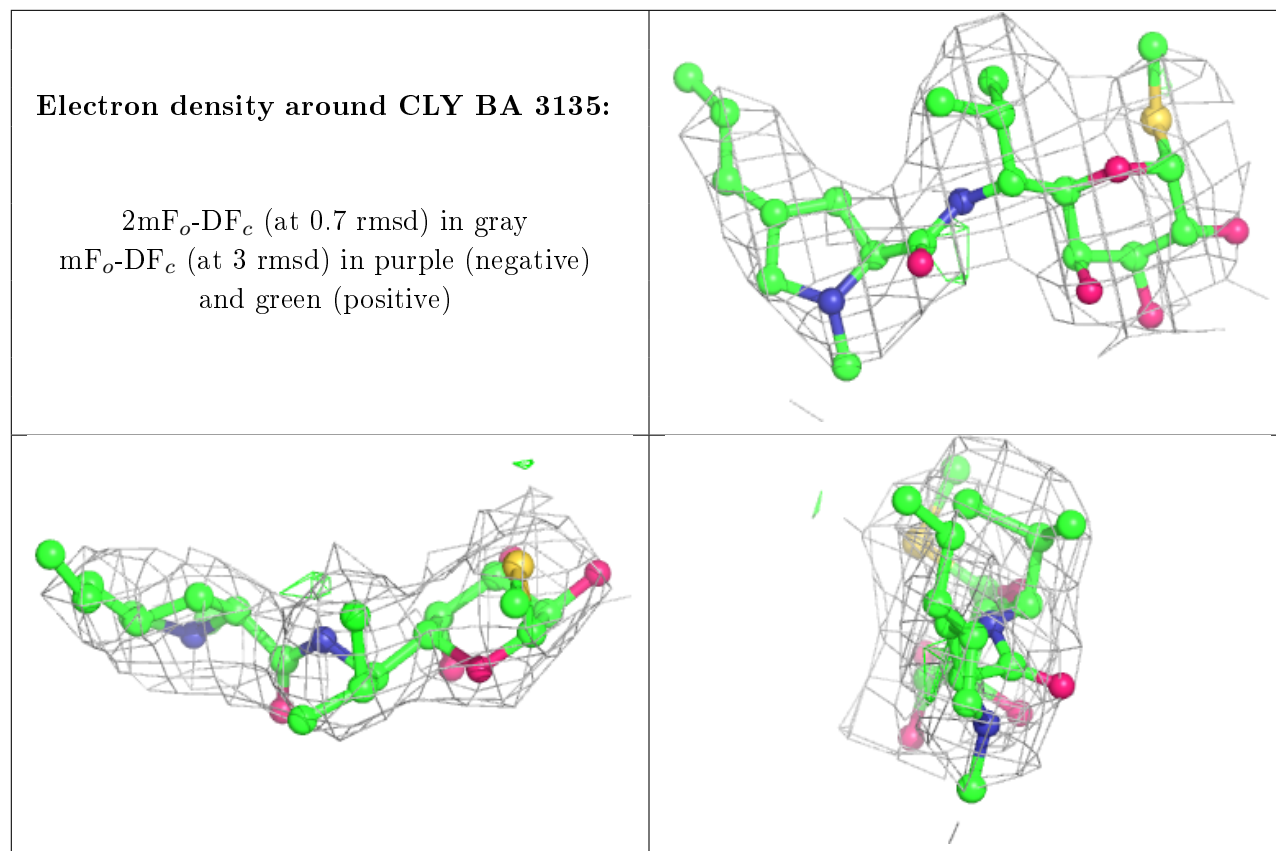
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 59  | MG   | BA    | 3075 | 1/1   | 0.98 | 0.07 | 29,29,29,29                 | 0     |
| 59  | MG   | BA    | 3061 | 1/1   | 0.98 | 0.16 | 20,20,20,20                 | 0     |
| 59  | MG   | BA    | 3122 | 1/1   | 0.98 | 0.16 | 137,137,137,137             | 0     |
| 59  | MG   | BA    | 3042 | 1/1   | 0.98 | 0.06 | 41,41,41,41                 | 0     |
| 59  | MG   | BA    | 3013 | 1/1   | 0.98 | 0.13 | 1,1,1,1                     | 0     |
| 59  | MG   | BA    | 3028 | 1/1   | 0.98 | 0.10 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3025 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 59  | MG   | BA    | 3114 | 1/1   | 0.98 | 0.15 | 4,4,4,4                     | 0     |
| 59  | MG   | BA    | 3052 | 1/1   | 0.98 | 0.07 | 5,5,5,5                     | 0     |
| 59  | MG   | BA    | 3059 | 1/1   | 0.98 | 0.12 | 190,190,190,190             | 0     |
| 59  | MG   | CA    | 1605 | 1/1   | 0.98 | 0.16 | 37,37,37,37                 | 0     |
| 59  | MG   | BB    | 203  | 1/1   | 0.98 | 0.06 | 17,17,17,17                 | 0     |
| 59  | MG   | BA    | 3113 | 1/1   | 0.98 | 0.08 | 114,114,114,114             | 0     |
| 59  | MG   | BA    | 3127 | 1/1   | 0.98 | 0.09 | 3,3,3,3                     | 0     |
| 59  | MG   | AA    | 1633 | 1/1   | 0.98 | 0.10 | 51,51,51,51                 | 0     |
| 59  | MG   | BA    | 3006 | 1/1   | 0.98 | 0.06 | 39,39,39,39                 | 0     |
| 59  | MG   | AA    | 1621 | 1/1   | 0.98 | 0.13 | 25,25,25,25                 | 0     |
| 59  | MG   | BA    | 3079 | 1/1   | 0.99 | 0.13 | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3115 | 1/1   | 0.99 | 0.10 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3125 | 1/1   | 0.99 | 0.13 | 27,27,27,27                 | 0     |
| 59  | MG   | AA    | 1641 | 1/1   | 0.99 | 0.18 | 22,22,22,22                 | 0     |
| 59  | MG   | BA    | 3032 | 1/1   | 0.99 | 0.21 | 3,3,3,3                     | 0     |
| 59  | MG   | BA    | 3063 | 1/1   | 0.99 | 0.12 | 1,1,1,1                     | 0     |
| 59  | MG   | BA    | 3005 | 1/1   | 0.99 | 0.09 | 87,87,87,87                 | 0     |
| 59  | MG   | BA    | 3109 | 1/1   | 0.99 | 0.17 | 124,124,124,124             | 0     |
| 59  | MG   | BA    | 3017 | 1/1   | 0.99 | 0.10 | 24,24,24,24                 | 0     |
| 61  | ZN   | B4    | 101  | 1/1   | 0.99 | 0.06 | 80,80,80,80                 | 0     |
| 59  | MG   | BA    | 3067 | 1/1   | 0.99 | 0.06 | 18,18,18,18                 | 0     |
| 59  | MG   | BA    | 3120 | 1/1   | 0.99 | 0.17 | 4,4,4,4                     | 0     |
| 59  | MG   | BA    | 3040 | 1/1   | 0.99 | 0.15 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3031 | 1/1   | 0.99 | 0.13 | 12,12,12,12                 | 0     |
| 59  | MG   | BA    | 3083 | 1/1   | 0.99 | 0.09 | 28,28,28,28                 | 0     |
| 59  | MG   | BA    | 3092 | 1/1   | 0.99 | 0.10 | 56,56,56,56                 | 0     |
| 59  | MG   | BA    | 3043 | 1/1   | 0.99 | 0.18 | 11,11,11,11                 | 0     |
| 59  | MG   | BA    | 3128 | 1/1   | 0.99 | 0.12 | 19,19,19,19                 | 0     |
| 59  | MG   | BA    | 3095 | 1/1   | 0.99 | 0.09 | 77,77,77,77                 | 0     |
| 59  | MG   | BA    | 3041 | 1/1   | 0.99 | 0.13 | 13,13,13,13                 | 0     |
| 59  | MG   | BA    | 3038 | 1/1   | 0.99 | 0.16 | 31,31,31,31                 | 0     |
| 59  | MG   | BA    | 3064 | 1/1   | 1.00 | 0.08 | 18,18,18,18                 | 0     |

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



orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.