



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 12:27 PM EST

PDB ID : 4U26  
Title : Crystal structure of the E. coli ribosome bound to dalfopristin and quinupristin.  
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.  
Deposited on : 2014-07-16  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

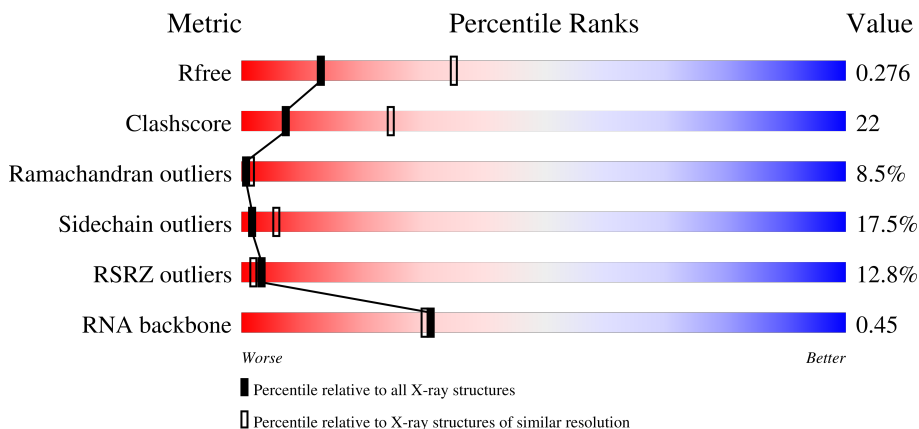
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| $R_{free}$            | 130704                   | 3140 (2.80-2.80)                                   |
| Clashscore            | 141614                   | 3569 (2.80-2.80)                                   |
| Ramachandran outliers | 138981                   | 3498 (2.80-2.80)                                   |
| Sidechain outliers    | 138945                   | 3500 (2.80-2.80)                                   |
| RSRZ outliers         | 127900                   | 3078 (2.80-2.80)                                   |
| RNA backbone          | 3102                     | 1227 (3.10-2.50)                                   |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AA    | 1539   |                  |
| 1   | CA    | 1539   |                  |
| 2   | AB    | 218    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | CB    | 218    |                  |
| 3   | AC    | 206    |                  |
| 3   | CC    | 206    |                  |
| 4   | AD    | 205    |                  |
| 4   | CD    | 205    |                  |
| 5   | AE    | 150    |                  |
| 5   | CE    | 150    |                  |
| 6   | AF    | 100    |                  |
| 6   | CF    | 100    |                  |
| 7   | AG    | 151    |                  |
| 7   | CG    | 151    |                  |
| 8   | AH    | 129    |                  |
| 8   | CH    | 129    |                  |
| 9   | AI    | 127    |                  |
| 9   | CI    | 127    |                  |
| 10  | AJ    | 98     |                  |
| 10  | CJ    | 98     |                  |
| 11  | AK    | 117    |                  |
| 11  | CK    | 117    |                  |
| 12  | AL    | 123    |                  |
| 12  | CL    | 123    |                  |
| 13  | AM    | 114    |                  |
| 13  | CM    | 114    |                  |
| 14  | AN    | 100    |                  |
| 14  | CN    | 100    |                  |


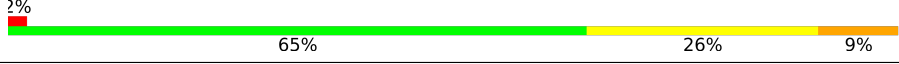

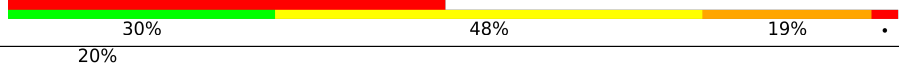


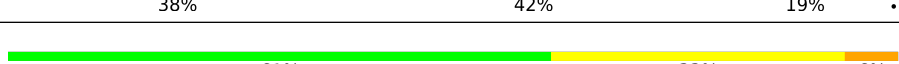
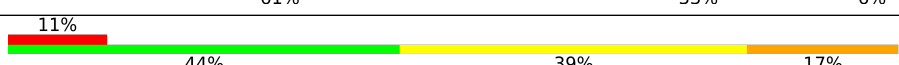
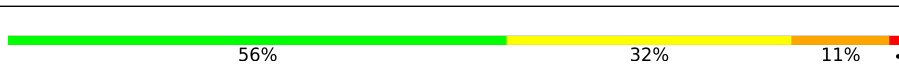
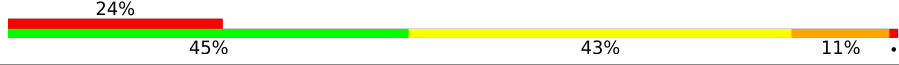

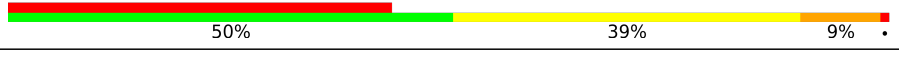


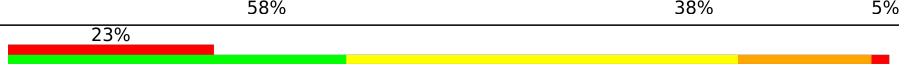


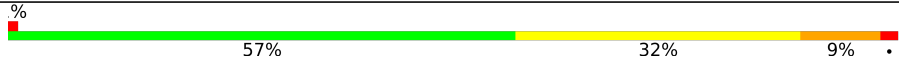







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | AO    | 88     |                  |
| 15  | CO    | 88     |                  |
| 16  | AP    | 82     |                  |
| 16  | CP    | 82     |   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





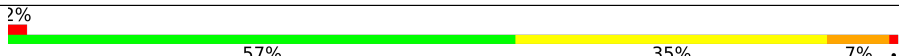

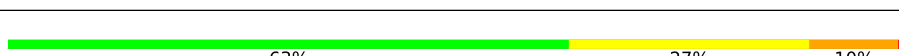
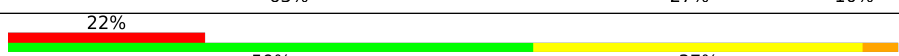
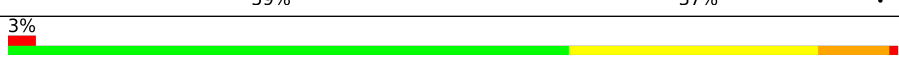

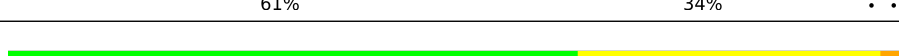
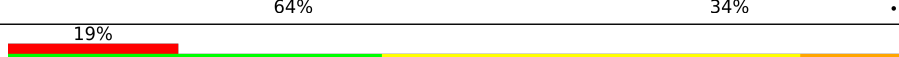
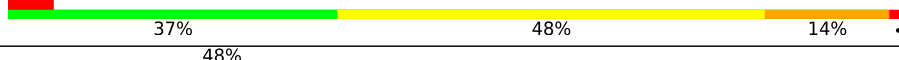



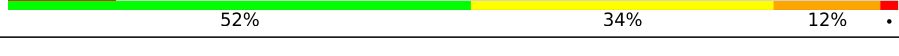


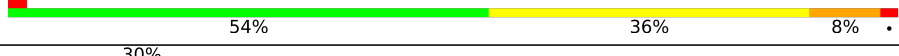
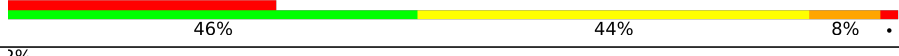
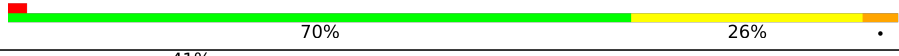



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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 27  | DF    | 177    |    |
| 28  | BG    | 176    |    |
| 28  | DG    | 176    |    |
| 29  | BH    | 149    |    |
| 29  | DH    | 149    |    |
| 30  | BI    | 141    |    |
| 30  | DI    | 141    |    |
| 31  | BJ    | 142    |    |
| 31  | DJ    | 142    |    |
| 32  | BK    | 122    |    |
| 32  | DK    | 122    |   |
| 33  | BL    | 143    |  |
| 33  | DL    | 143    |  |
| 34  | BM    | 136    |  |
| 34  | DM    | 136    |  |
| 35  | BN    | 120    |  |
| 35  | DN    | 120    |  |
| 36  | BO    | 116    |  |
| 36  | DO    | 116    |  |
| 37  | BP    | 114    |  |
| 37  | DP    | 114    |  |
| 38  | BQ    | 117    |  |
| 38  | DQ    | 117    |  |
| 39  | BR    | 103    |  |
| 39  | DR    | 103    |  |

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

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | D4    | 38     |                  |
| 53  | B5    | 228    |                  |
| 54  | B6    | 8      |                  |
| 54  | D6    | 8      |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | AA    | 1659 | -         | -        | -       | X                |
| 55  | MG   | AM    | 201  | -         | -        | -       | X                |
| 55  | MG   | BA    | 3134 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3003 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3005 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3026 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3028 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3041 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3048 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3056 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3062 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3071 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3072 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3077 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3131 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3133 | -         | -        | -       | X                |
| 55  | MG   | DA    | 3155 | -         | -        | -       | X                |
| 56  | DOL  | DA    | 3001 | -         | -        | X       | -                |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 288423 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 |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
|     |       |          | Total | C     | N    | O     | P    |         |         |       |
| 1   | AA    | 1538     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32995 | 14716 | 6050 | 10691 | 1538 |         |         |       |
| 1   | CA    | 1539     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 33015 | 14725 | 6052 | 10699 | 1539 |         |         |       |

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

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

- Molecule 5 is a protein called 30S ribosomal protein S5.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1106  | 687 | 211 | 202 | 6 |         |         |       |
| 5   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1106  | 687 | 211 | 202 | 6 |         |         |       |

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 15  | AO    | 88       | 710   | 437 | 143 | 129 | 1 | 0       | 0       | 0     |
| 15  | CO    | 88       | 710   | 437 | 143 | 129 | 1 | 0       | 0       | 0     |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

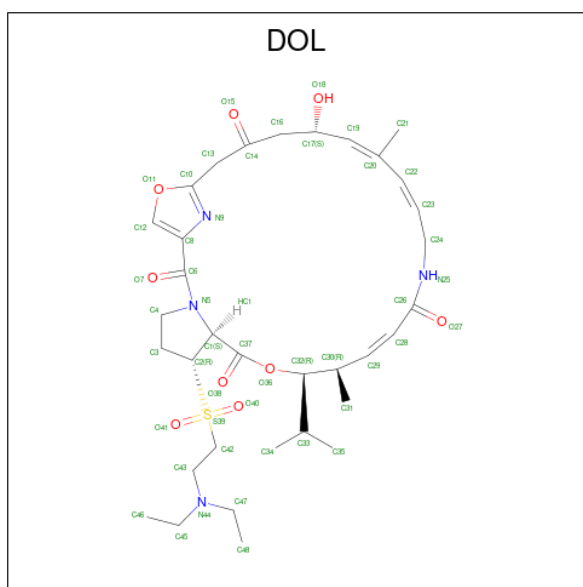
- Molecule 54 is a protein called Quinupristin.

| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---|---------|---------|-------|
|     |       |          | Total | C  | N | O  | S |         |         |       |
| 54  | B6    | 8        | 73    | 53 | 9 | 10 | 1 | 0       | 0       | 0     |
| 54  | D6    | 8        | 73    | 53 | 9 | 10 | 1 | 0       | 0       | 0     |

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55  | AA    | 71       | Total | Mg  | 0       | 0       |
|     |       |          | 71    | 71  |         |         |
| 55  | AM    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | BA    | 194      | Total | Mg  | 0       | 0       |
|     |       |          | 194   | 194 |         |         |
| 55  | BB    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 55  | BQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | CA    | 56       | Total | Mg  | 0       | 0       |
|     |       |          | 56    | 56  |         |         |
| 55  | DA    | 166      | Total | Mg  | 0       | 0       |
|     |       |          | 166   | 166 |         |         |
| 55  | DB    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 55  | DQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | D2    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 56 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C<sub>34</sub>H<sub>50</sub>N<sub>4</sub>O<sub>9</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 56  | BA    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 48    | 34 | 4 | 9 | 1 |         |         |
| 56  | DA    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 48    | 34 | 4 | 9 | 1 |         |         |

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | D4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 58 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 58  | AA    | 194      | Total | O   | 0       | 0       |
|     |       |          | 194   | 194 |         |         |
| 58  | AE    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 58  | AL    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 58  | AN    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 58  | AT    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 58  | AU    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BA    | 617      | Total O<br>617 617 | 0       | 0       |
| 58  | BB    | 14       | Total O<br>14 14   | 0       | 0       |
| 58  | BC    | 6        | Total O<br>6 6     | 0       | 0       |
| 58  | BD    | 4        | Total O<br>4 4     | 0       | 0       |
| 58  | BE    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BF    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BG    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BJ    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BL    | 7        | Total O<br>7 7     | 0       | 0       |
| 58  | BN    | 5        | Total O<br>5 5     | 0       | 0       |
| 58  | BQ    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BS    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | BT    | 2        | Total O<br>2 2     | 0       | 0       |
| 58  | B3    | 3        | Total O<br>3 3     | 0       | 0       |
| 58  | B4    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | CA    | 192      | Total O<br>192 192 | 0       | 0       |
| 58  | CL    | 1        | Total O<br>1 1     | 0       | 0       |
| 58  | CN    | 2        | Total O<br>2 2     | 0       | 0       |
| 58  | CT    | 2        | Total O<br>2 2     | 0       | 0       |
| 58  | CU    | 1        | Total O<br>1 1     | 0       | 0       |

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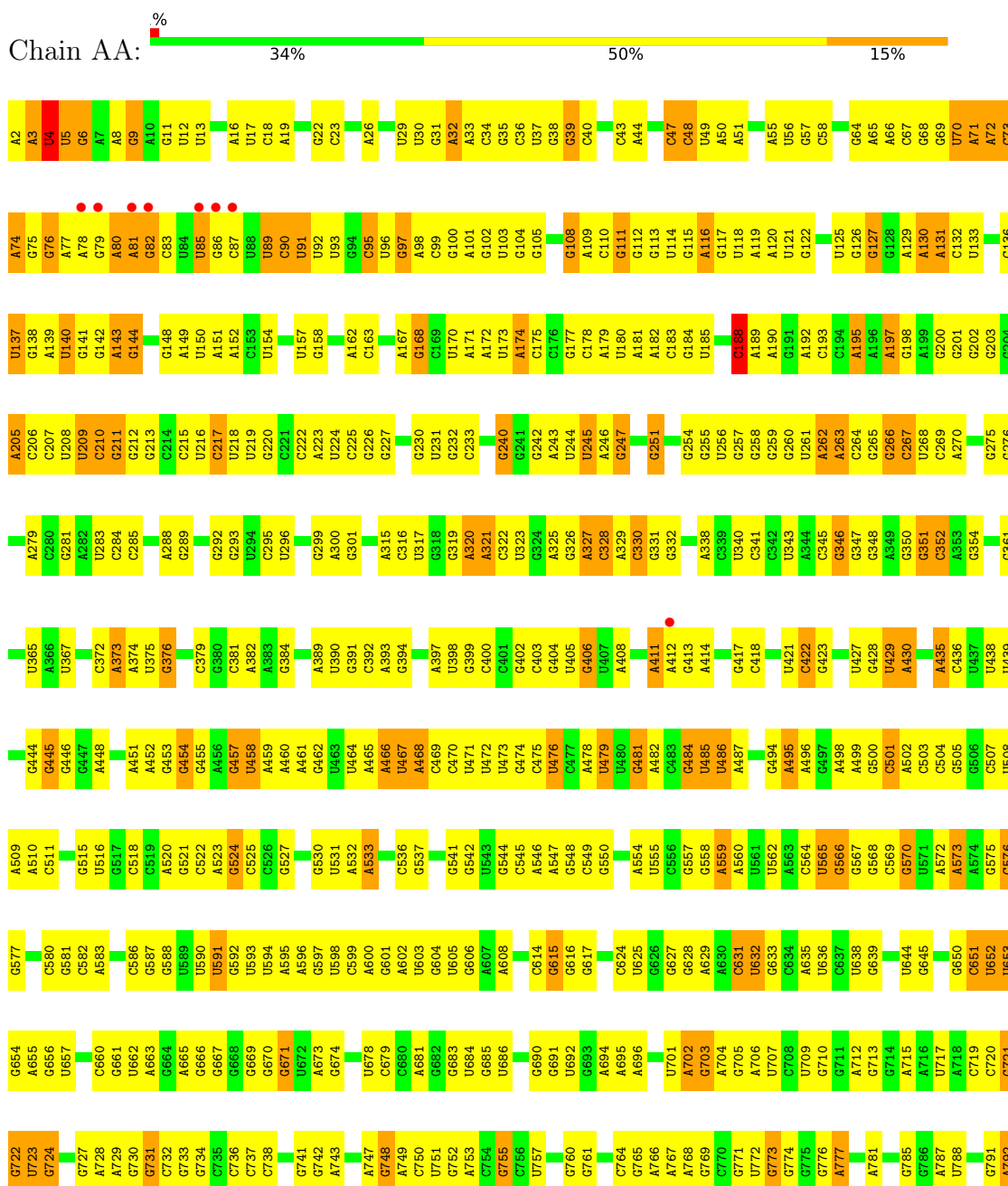
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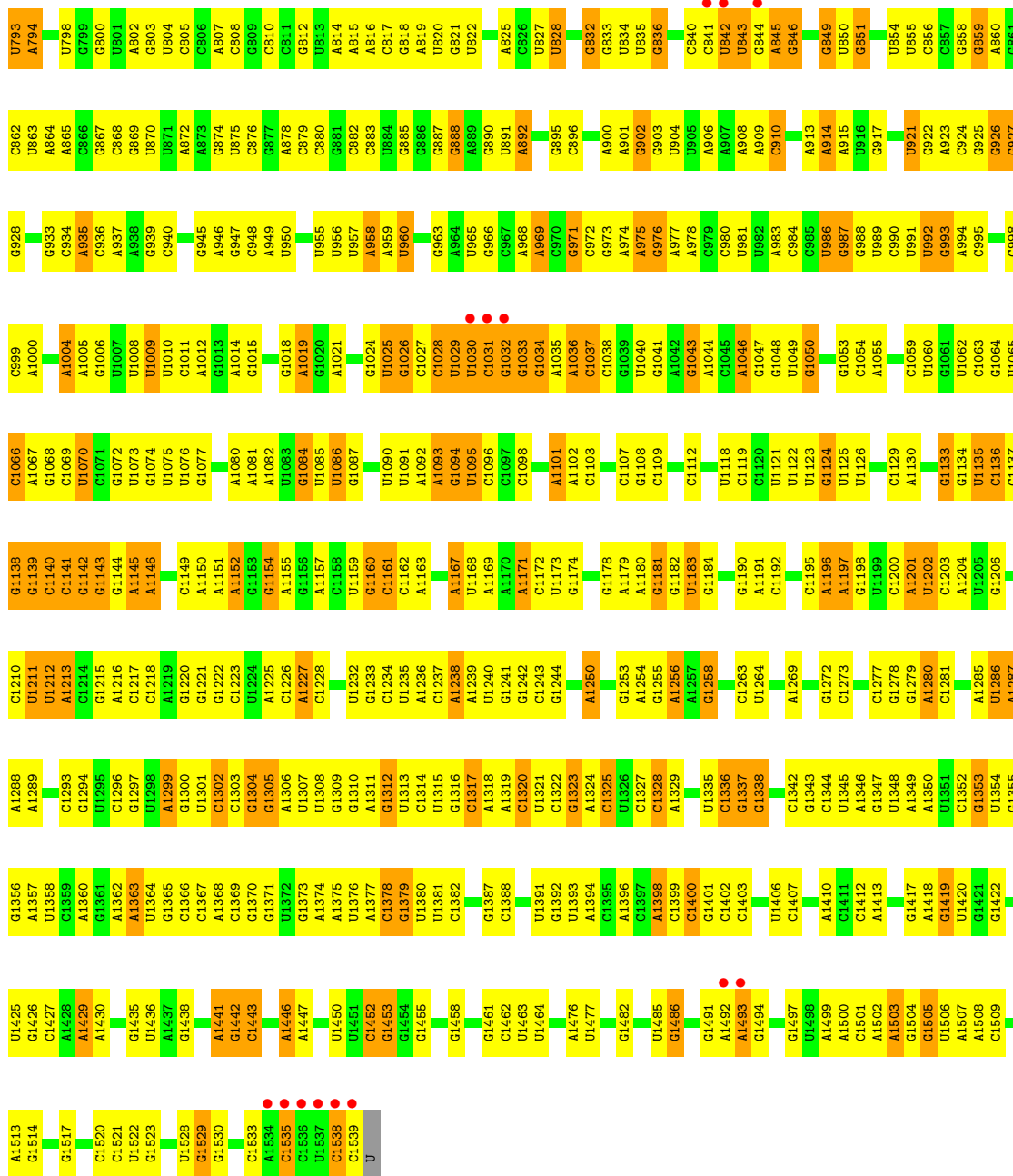
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 58  | DA    | 610      | Total<br>610 | O<br>610 | 0       | 0       |
| 58  | DB    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 58  | DC    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 58  | DD    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 58  | DE    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 58  | DJ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 58  | DL    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 58  | DN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 58  | DS    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 58  | DT    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 58  | DU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 58  | DV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 58  | D2    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 58  | D3    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 58  | D4    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

### 3 Residue-property plots [i](#)

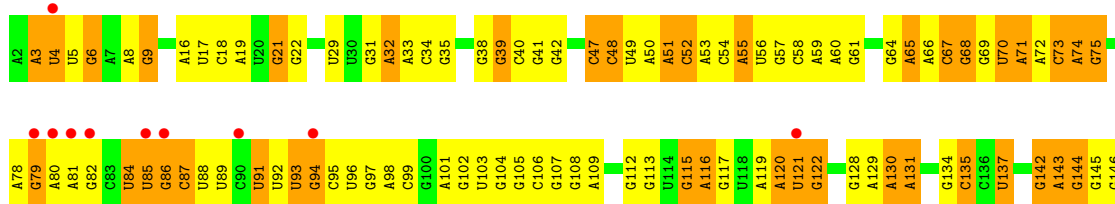
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 16S rRNA



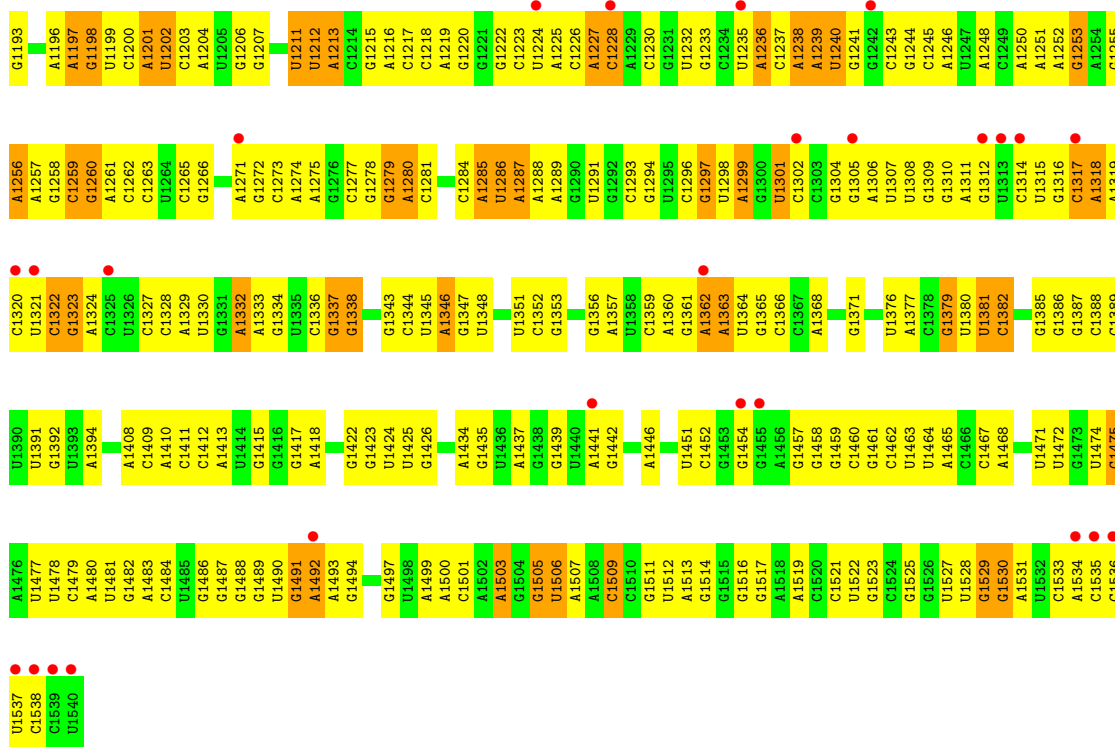


• Molecule 1: 16S rRNA

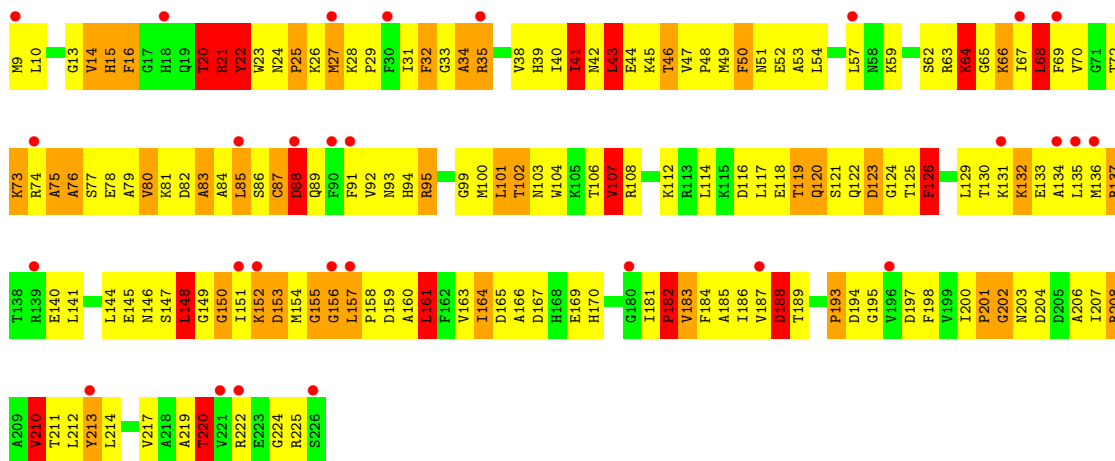


|       |       |       |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|
| U1125 | U1052 | U991  | C912 | C839 | G774 | G711 | A642 | A499 | U426 | A383 | C271 | U209 | G147 |
| U1126 | G1053 | U992  | A913 | C840 | G775 | A712 | G643 | A502 | U427 | G394 | G276 | C210 | G148 |
| G1127 | C1054 | G993  | A914 | C841 | G776 | G713 | C669 | A503 | G428 | C355 | G277 | G211 | C149 |
| A1128 | A1055 | A994  | U842 | U843 | A777 | G714 | G570 | C503 | U429 | A356 | G278 | G212 | U150 |
| C1129 | U1056 | C995  | U843 | U844 | G778 | A715 | U571 | C504 | A430 | G357 | A279 | G213 | A151 |
| A1130 | A1130 | A996  | U920 | A845 | C779 | A716 | A572 | G505 | A431 | U358 | C280 | C214 | A152 |
| G1133 | U1060 | C999  | U921 | G846 | A780 | U717 | A573 | G506 | A432 | G359 | G281 | C215 | C153 |
| G1134 | U1061 | A1000 | A923 | G847 | A781 | A718 | A574 | A509 | A435 | G362 | A282 | U216 | U154 |
| U1135 | G1063 | G1001 | C924 | C848 | C783 | C720 | C576 | A510 | A436 | U367 | U283 | U218 | C155 |
| C1136 | C1064 | G1002 | G925 | G849 | A784 | G721 | G577 | C511 | U437 | U368 | G284 | U219 | U157 |
| G1137 | U1065 | G1003 | G926 | U850 | G785 | G722 | C578 | U512 | U438 | C285 | C285 | G220 | G158 |
| C1138 | C1066 | A1004 | G927 | G851 | U723 | U723 | A579 | C513 | U439 | G369 | C286 | C221 | G159 |
| G1139 | A1067 | A1005 | C852 | A787 | G724 | G724 | C580 | C514 | C440 | C370 | G289 | G222 | A160 |
| C1140 | U1068 | G1006 | C853 | U790 | G725 | G725 | G581 | C517 | G445 | A371 | C290 | A223 | A161 |
| C1141 | C1069 | U1007 | U854 | A663 | A663 | A663 | C582 | U517 | G445 | C372 | C290 | U224 | A162 |
| G1142 | U1070 | C934  | G857 | G664 | G664 | A728 | A583 | C518 | G446 | A373 | U291 | U224 | C163 |
| G1143 | C1071 | U1009 | A935 | A665 | G665 | A729 | G584 | C519 | A374 | A374 | G227 | G227 | G164 |
| G1144 | U1072 | U1010 | G858 | G666 | G666 | G730 | G585 | A520 | A451 | U375 | U294 | U229 | G165 |
| A1145 | G1073 | C1011 | G859 | G667 | G667 | G731 | C586 | G524 | A452 | G376 | C295 | U229 | U166 |
| C1146 | U1074 | A1012 | A860 | G668 | G668 | G732 | U590 | C527 | G453 | G377 | U296 | G230 | G167 |
| U1147 | G1075 | G1013 | C940 | G669 | G670 | C735 | U591 | G527 | G454 | C378 | G297 | U231 | G168 |
| C1148 | A1014 | A1014 | G945 | G671 | G671 | C736 | G572 | C528 | G455 | C379 | A298 | U232 | C169 |
| G1149 | G1015 | G1015 | G946 | G672 | G672 | C737 | U592 | C529 | G456 | C380 | G299 | C233 | U170 |
| A1150 | A1016 | A1016 | A938 | U801 | U801 | C738 | U598 | G530 | G457 | G384 | A300 | C234 | A171 |
| A1151 | U1080 | U1037 | G947 | U802 | U802 | C739 | U599 | G531 | U458 | C385 | G301 | G237 | A172 |
| A1152 | A1081 | G1018 | C948 | G803 | G803 | U740 | U603 | U532 | A460 | C386 | G302 | G237 | U173 |
| C1153 | U1082 | A1019 | C949 | C868 | A675 | C741 | U604 | A533 | A460 | U387 | A303 | A238 | A174 |
| G1154 | G1084 | G1020 | U950 | U804 | A676 | G742 | G605 | A534 | A461 | C388 | U239 | U239 | C175 |
| A1157 | U1085 | A1021 | G951 | C905 | U677 | G742 | U606 | U534 | G462 | A389 | A306 | G240 | C176 |
| C1158 | U1086 | A1022 | U952 | C906 | U678 | A743 | G608 | A535 | U463 | U390 | C307 | G241 | G177 |
| C1159 | G1087 | U1023 | A872 | C873 | C679 | C744 | A607 | G536 | U464 | G391 | C308 | G242 | C178 |
| G1160 | U1088 | G1024 | A873 | C874 | C680 | G745 | A608 | G537 | A465 | C392 | A309 | A243 | A179 |
| C1161 | G1089 | U1025 | U875 | C810 | A681 | A746 | A609 | G538 | A466 | A393 | C312 | U244 | U180 |
| C1162 | U1090 | G1026 | C876 | G812 | G682 | U747 | U610 | A539 | U467 | A313 | U245 | U244 | A181 |
| A1167 | A1092 | A1028 | G877 | G813 | G683 | A748 | C611 | G540 | A468 | A313 | A246 | A246 | A182 |
| U1168 | U1093 | U1029 | C878 | A815 | U684 | A749 | C612 | G541 | C469 | C316 | G248 | G248 | C183 |
| C1169 | G1094 | U1030 | C880 | A816 | U685 | C750 | C613 | G542 | C470 | C316 | U249 | U249 | G184 |
| A1170 | U1095 | G1031 | G881 | C817 | G686 | U751 | G615 | U543 | U471 | C400 | A250 | A250 | U185 |
| C1171 | G1096 | G1032 | C882 | G818 | G688 | A752 | C618 | G544 | U472 | A401 | A320 | G251 | C187 |
| C1172 | C1097 | G1033 | C883 | G819 | C689 | C754 | C624 | A546 | U473 | A402 | A321 | G251 | C188 |
| G1175 | U1098 | G1034 | U884 | U820 | G690 | G755 | U619 | A547 | C475 | A404 | A327 | U252 | A189 |
| G1176 | G1099 | A1035 | G885 | G821 | G691 | C756 | C620 | G550 | U476 | U405 | G328 | G254 | A190 |
| G1177 | A1101 | C1036 | G888 | U822 | U692 | U757 | A621 | G551 | C477 | G406 | C328 | G255 | G191 |
| G1178 | U1102 | U1037 | A889 | C823 | G693 | C758 | A622 | U551 | A478 | U407 | A329 | U256 | A195 |
| A1179 | C1103 | G1038 | G890 | A825 | A694 | A759 | C623 | U552 | U479 | A408 | C330 | G257 | A196 |
| A1180 | G1104 | U1040 | U891 | G826 | A695 | G760 | C624 | A554 | U480 | U409 | G331 | G258 | A197 |
| G1181 | A1105 | G1041 | A892 | C826 | A696 | G761 | U625 | U555 | C481 | C410 | G332 | G259 | G198 |
| G1182 | G1106 | A1042 | C893 | U827 | G705 | G763 | G628 | C556 | G484 | A411 | G337 | G260 | A199 |
| U1183 | C1107 | G1043 | G894 | U828 | U701 | C764 | A629 | U556 | U485 | A412 | A338 | U261 | G200 |
| G1184 | G1108 | A1044 | A901 | G829 | U702 | A766 | A630 | A559 | U486 | A413 | C339 | A262 | G201 |
| G1187 | C1114 | U1045 | G832 | U833 | G703 | A767 | C631 | A560 | U486 | A414 | C339 | A262 | G202 |
| G1190 | A1117 | A1046 | U833 | A906 | A704 | A768 | U632 | U561 | C490 | U421 | C345 | G265 | G203 |
| A1191 | U1123 | G1047 | U834 | A907 | G705 | G769 | G633 | U562 | G346 | C422 | G347 | G267 | G204 |
| C1192 | G1124 | U1048 | U835 | A908 | A706 | C770 | G634 | A563 | A495 | C423 | G347 | G267 | A205 |
|       |       | U1049 | G836 | A909 | U707 | G771 | A635 | C564 | A496 | G423 | G347 | U268 | C206 |
|       |       | G1050 | U837 | A910 | U707 | U772 | A635 | U565 | A497 | G424 | G351 | U268 | C207 |
|       |       | C1051 | G838 | U911 | G773 | G773 | U636 | G566 | A498 | G425 | C352 | A270 | U208 |

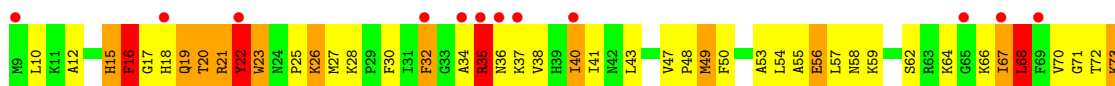


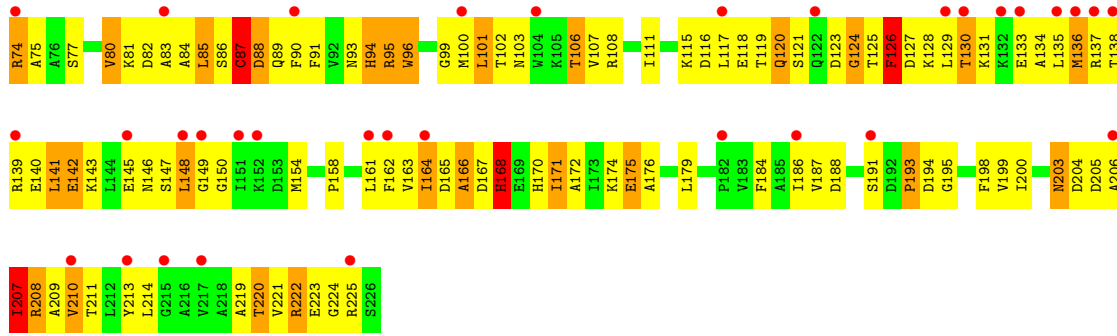


• Molecule 2: 30S ribosomal protein S2

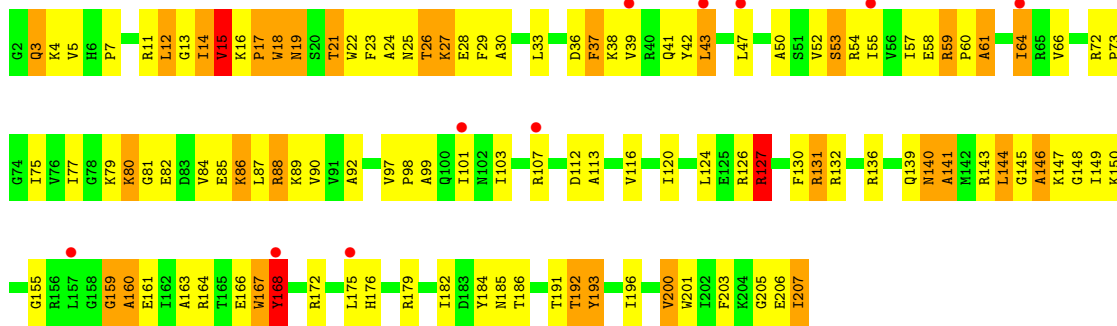


• Molecule 2: 30S ribosomal protein S2

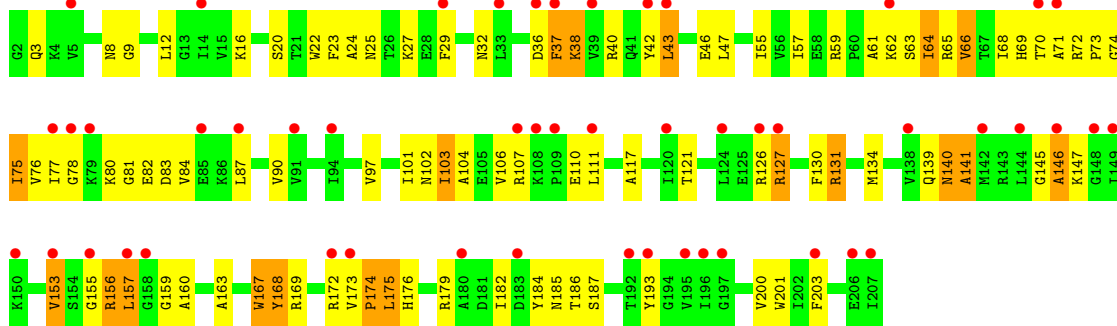




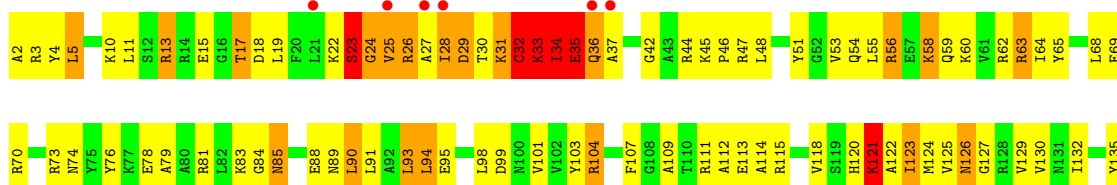
• Molecule 3: 30S ribosomal protein S3



• Molecule 3: 30S ribosomal protein S3

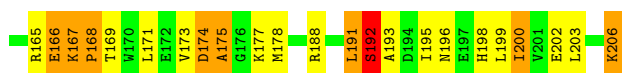
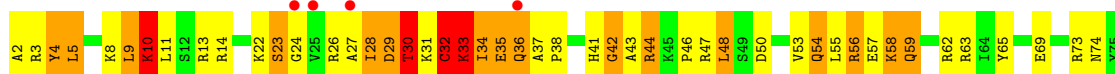
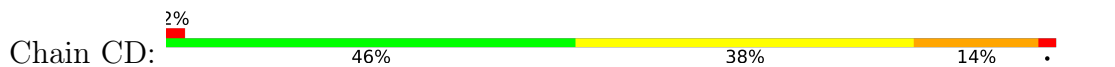


• Molecule 4: 30S ribosomal protein S4

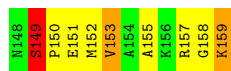
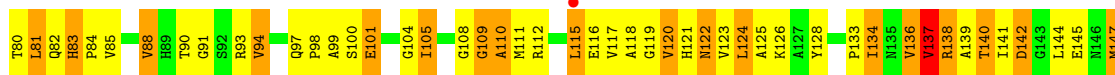
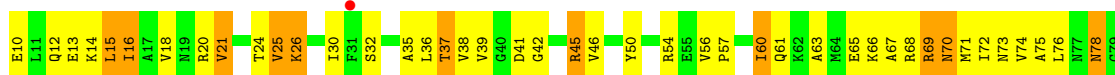




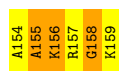
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

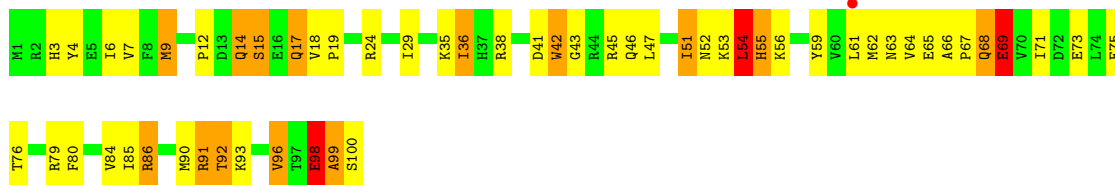


- Molecule 5: 30S ribosomal protein S5

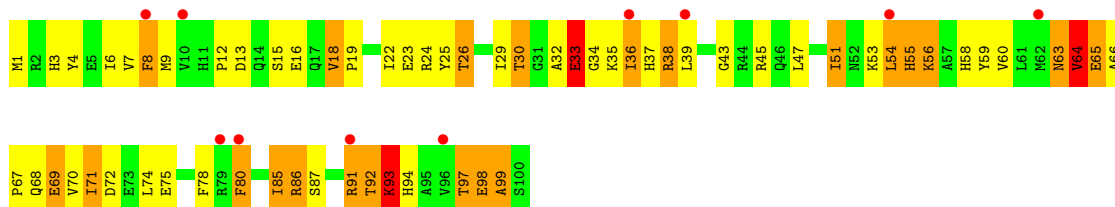


- Molecule 6: 30S ribosomal protein S6

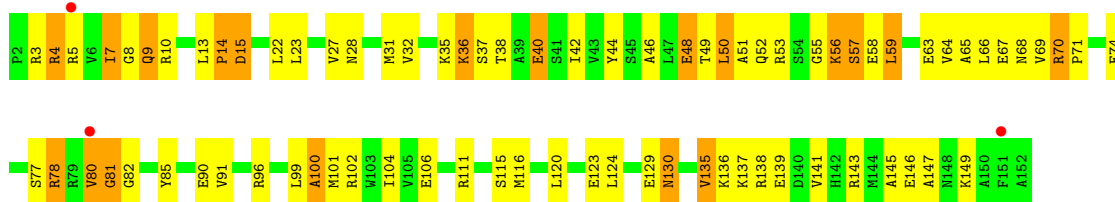




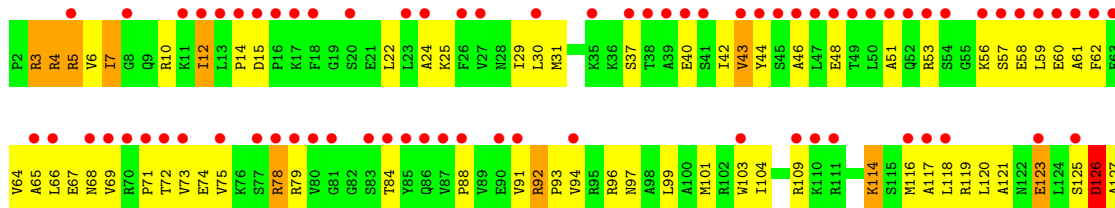
• Molecule 6: 30S ribosomal protein S6



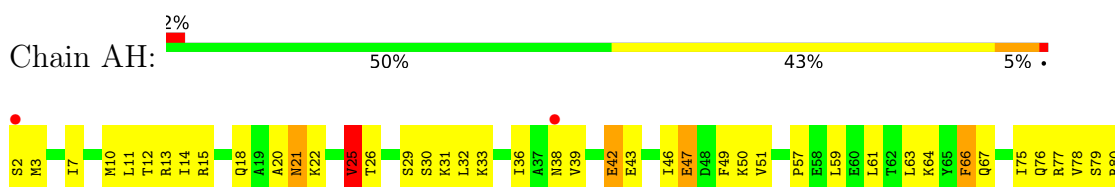
• Molecule 7: 30S ribosomal protein S7

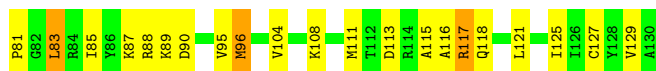


• Molecule 7: 30S ribosomal protein S7

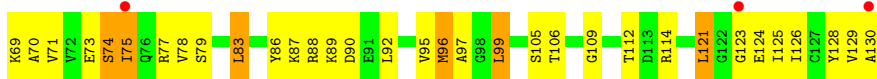
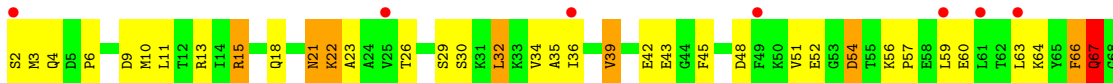


• Molecule 8: 30S ribosomal protein S8

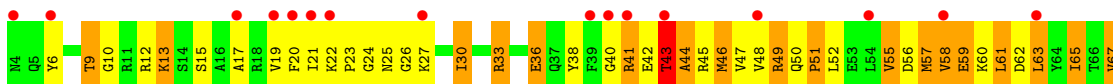




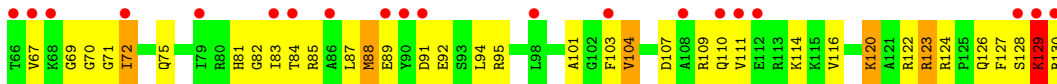
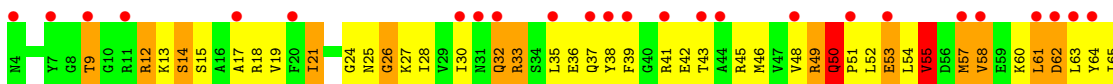
- Molecule 8: 30S ribosomal protein S8



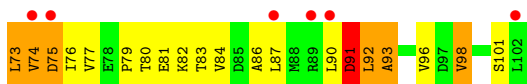
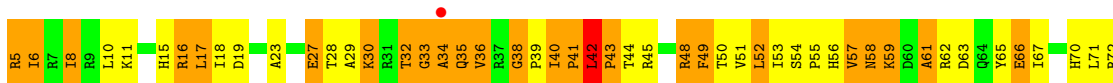
- Molecule 9: 30S ribosomal protein S9



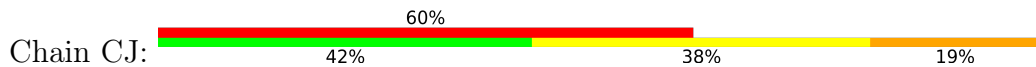
- Molecule 9: 30S ribosomal protein S9

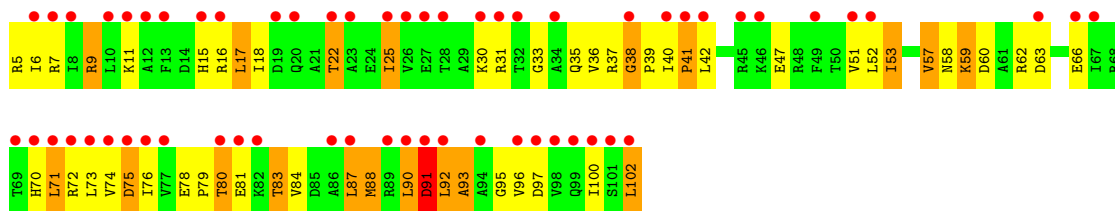


- Molecule 10: 30S ribosomal protein S10

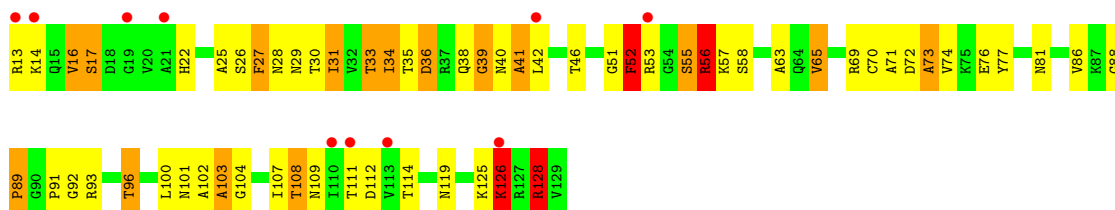


- Molecule 10: 30S ribosomal protein S10

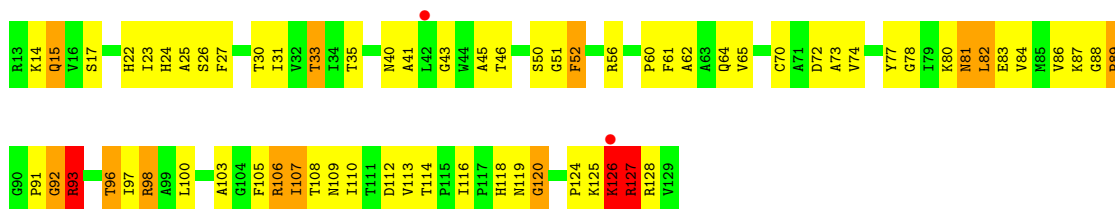




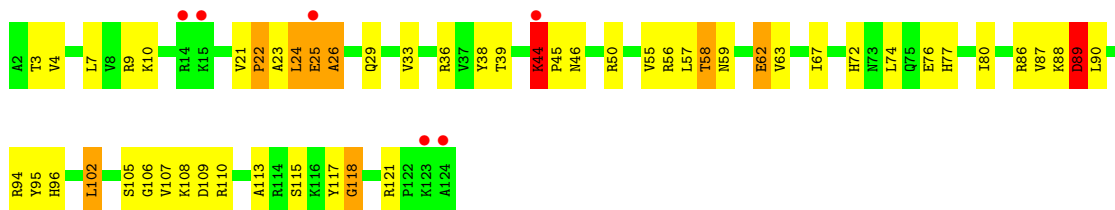
- Molecule 11: 30S ribosomal protein S11



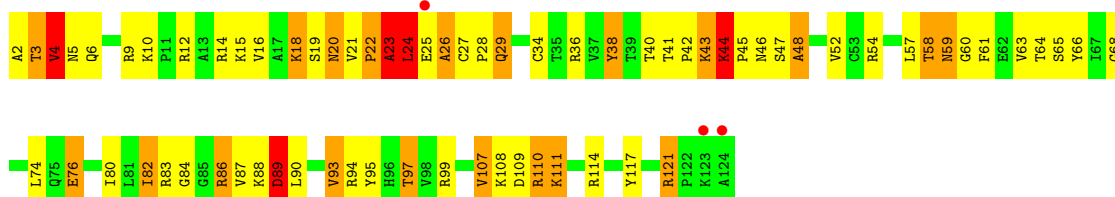
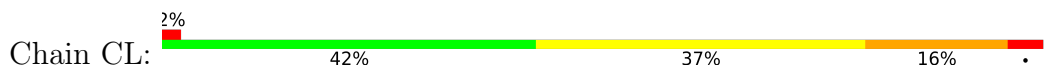
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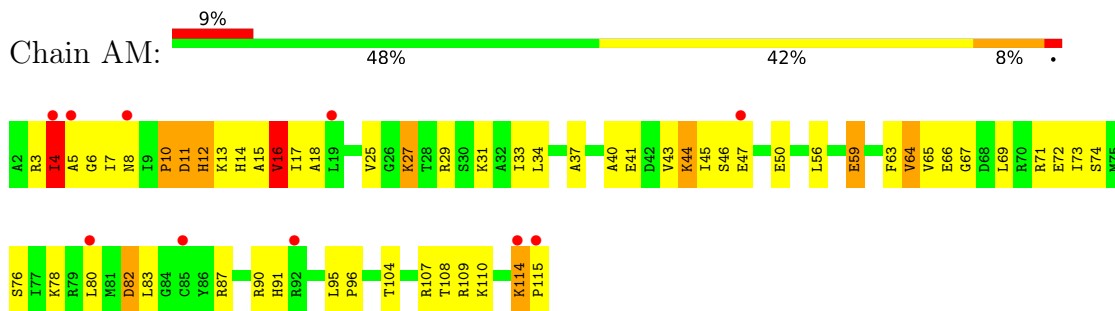
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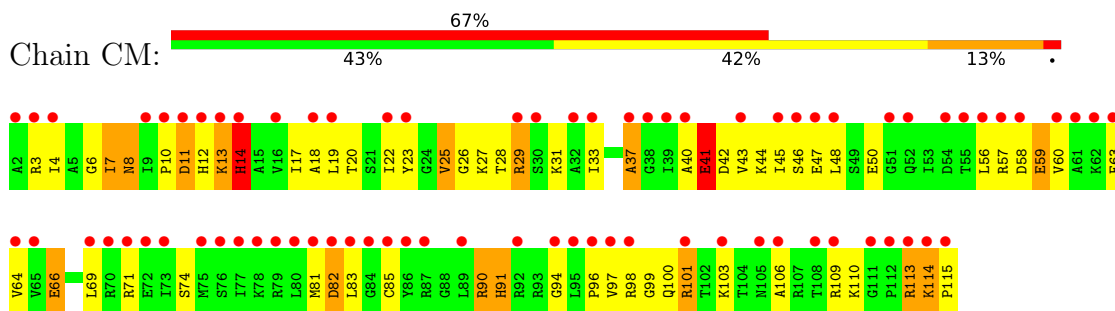
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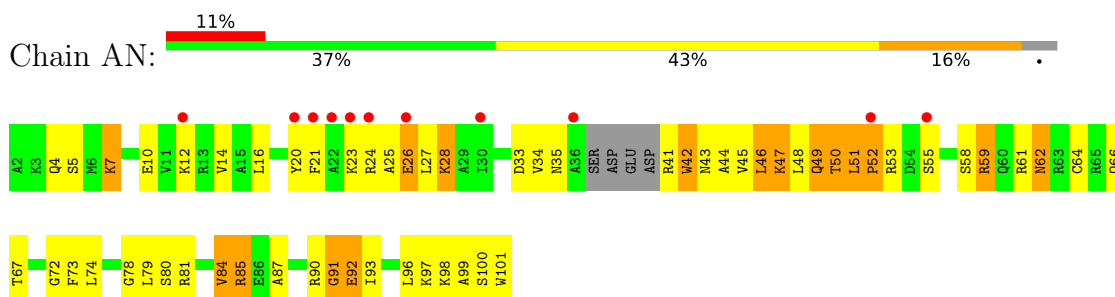
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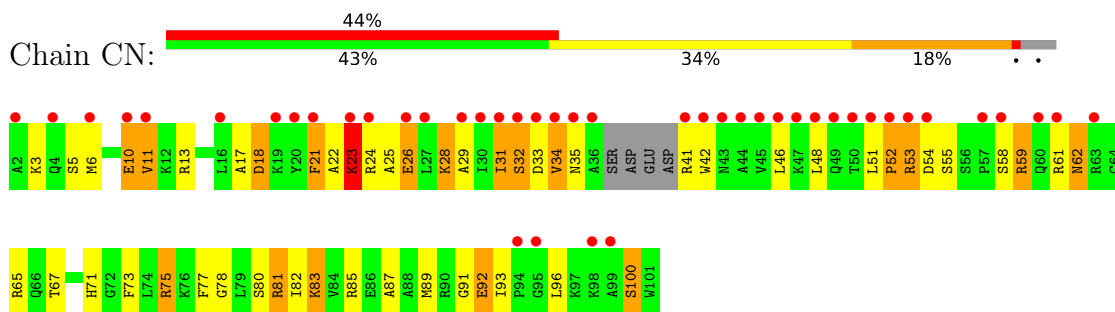
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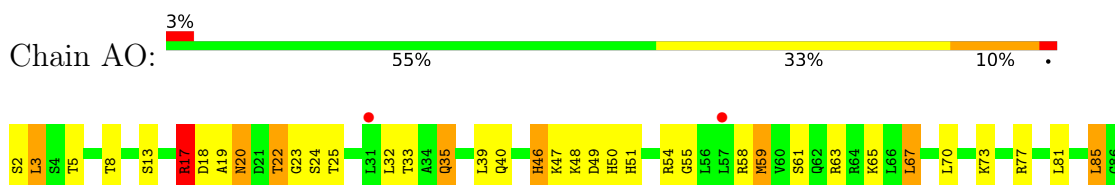
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

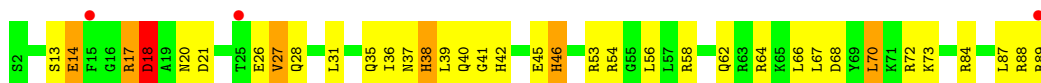


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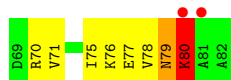
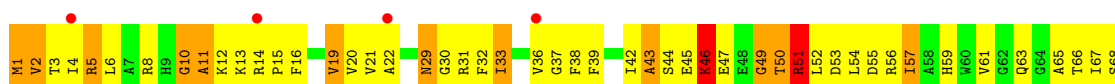




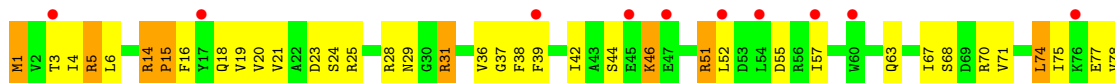
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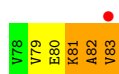
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- Molecule 16: 30S ribosomal protein S16



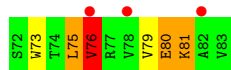
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- Molecule 17: 30S ribosomal protein S17







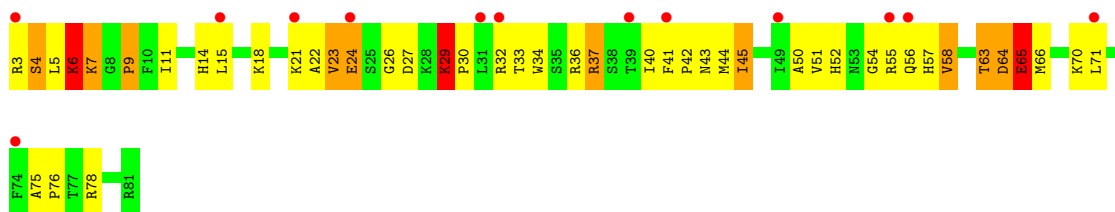
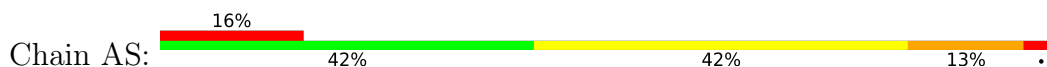
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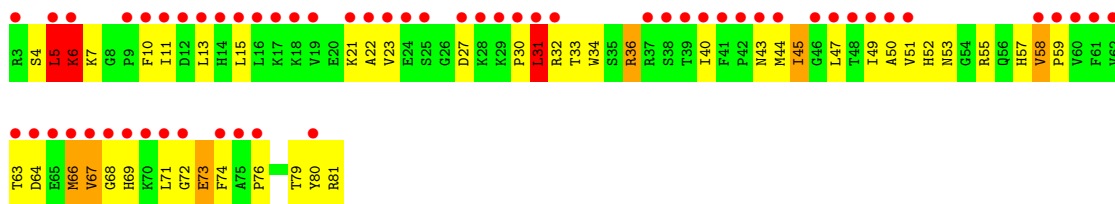
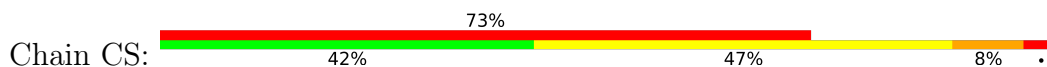
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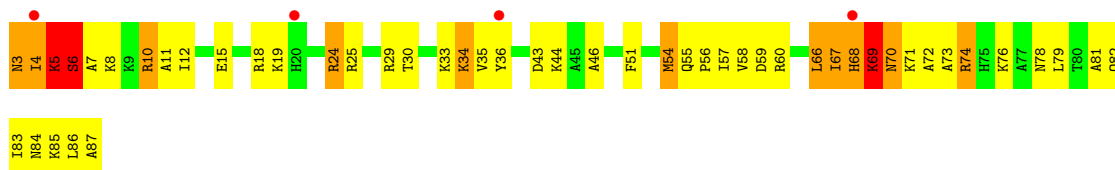
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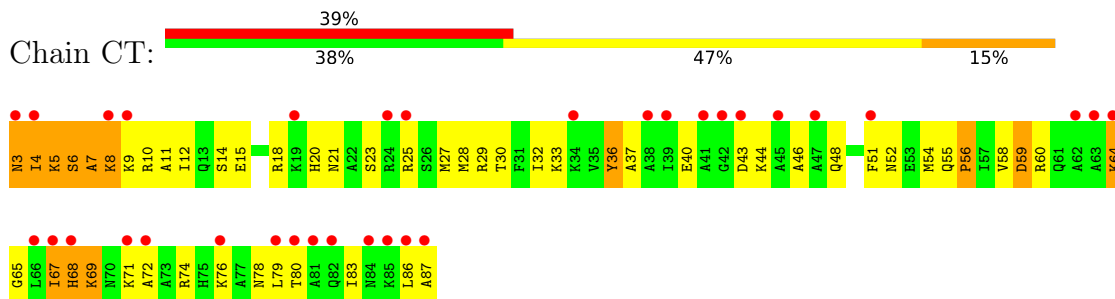
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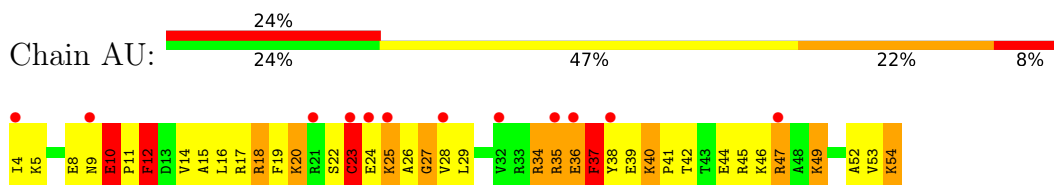
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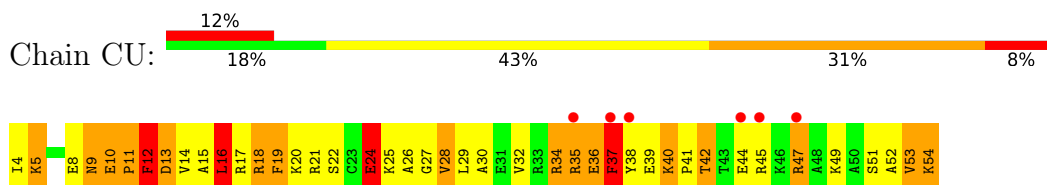
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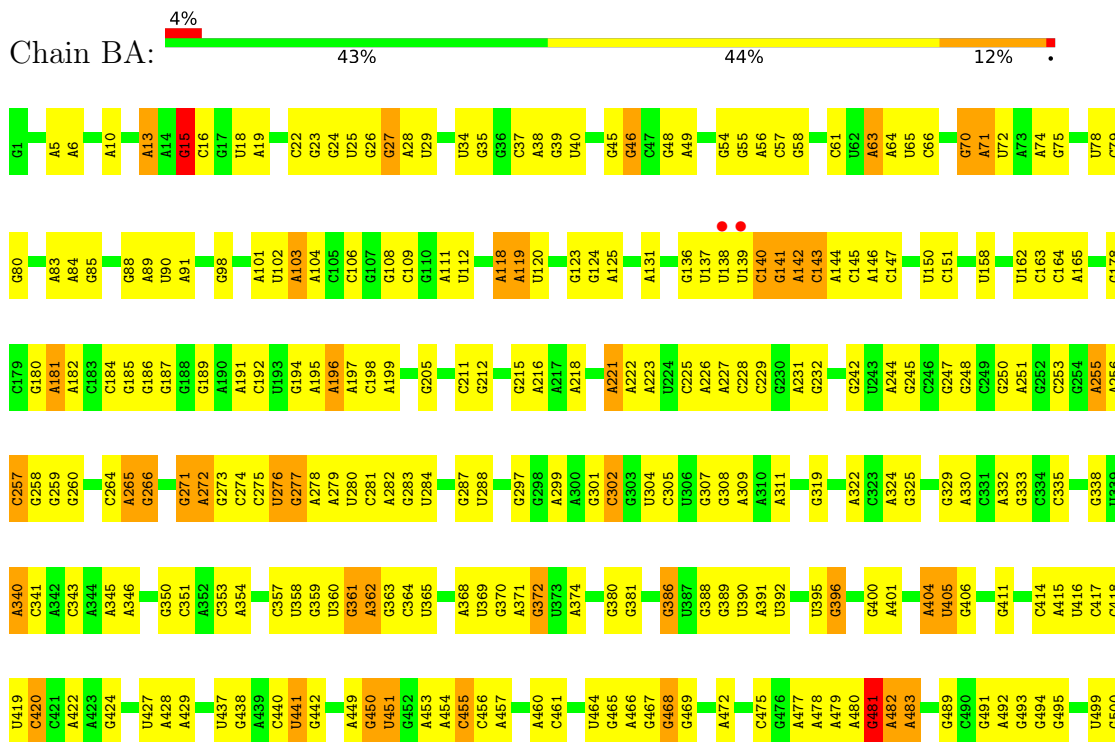
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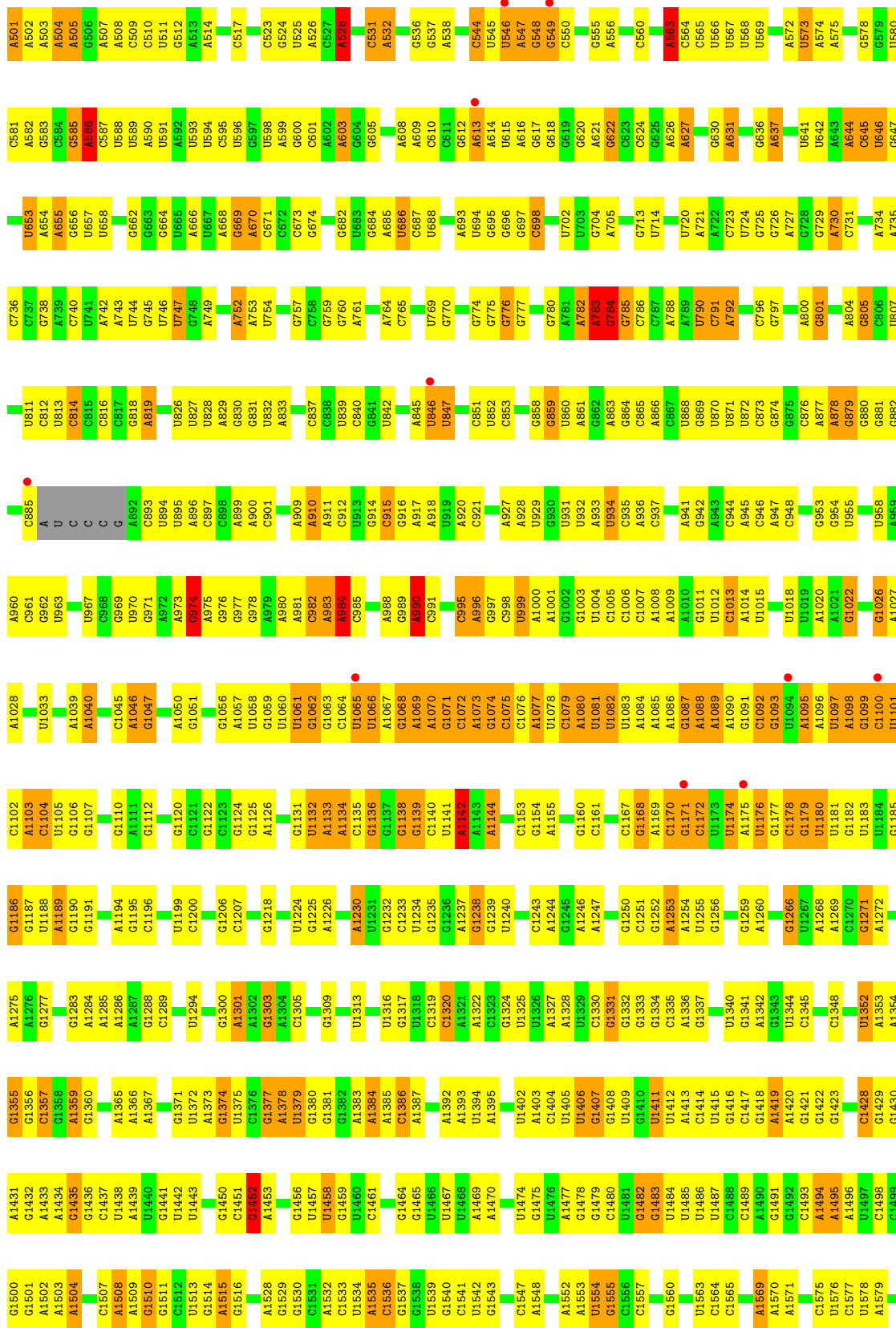


• Molecule 21: 30S ribosomal protein S21



• Molecule 22: 23S rRNA



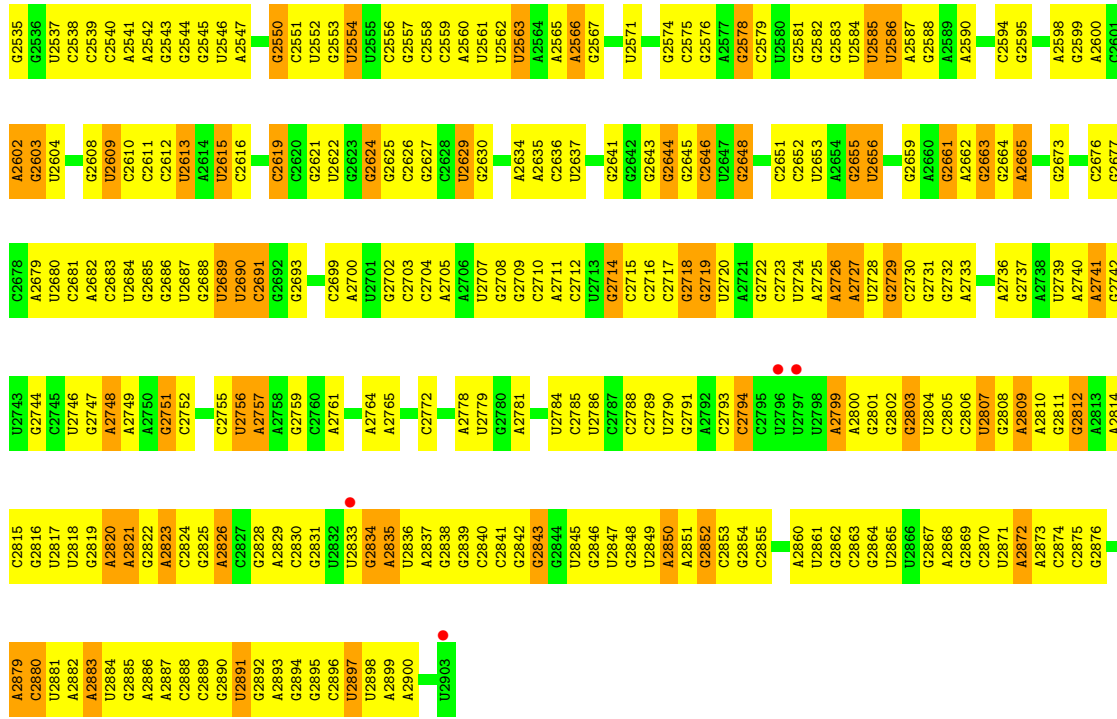


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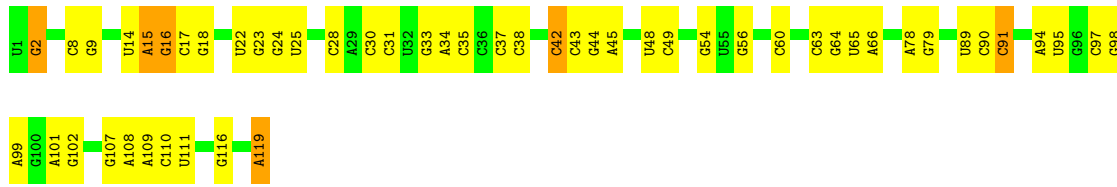


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| A905  | U906  | C908  | G909  | A909  | A910  | A911  | C912  | U913  | C914  | C915  | G916  | U919  | U920  | C921  | G922  | G923  | A927  | A928  | U931  | C932  | C933  | U934  | C935  | C936  | A937  | C938  | A941  | G942  | A943  | C944  | A945  | A946  | A947  | C948  | G949  | G950  | C951  | G952  | G953  | C957  | U958  | A959  | A960  | C961  | G962  | U963  | C964  | C965  | G966  | G969  | U970  | C971  | A972  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| A973  | G974  | G978  | A979  | A980  | A981  | C982  | A983  | A984  | C985  | C986  | G989  | A990  | G993  | C994  | C995  | A996  | G997  | C998  | U999  | A1000 | A1001 | G1002 | G1003 | C1006 | A1009 | A1010 | G1011 | C1012 | C1013 | G1016 | A1020 | G1022 | U1023 | G1024 | G1025 | G1026 | A1027 | A1028 | A1029 | C1030 | G1031 | A1032 | U1033 | G1034 | U1035 | G1036 | A1040 | G1041 | G1042 | G1043 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G636  | A637  | G638  | U639  | C640  | U641  | U642  | A643  | A644  | C645  | U646  | G647  | G648  | G649  | C650  | U653  | A654  | A655  | G656  | U657  | U658  | U659  | C660  | G661  | G662  | G663  | G664  | U667  | A668  | G669  | A670  | C671  | C672  | C673  | G674  | A675  | A676  | A677  | C678  | C679  | C680  | G681  | G682  | U683  | G684  | A685  | U686  | G687  | U688  | A689  | A693  | U694  | G695  | G696  | G697  | C698  | A699  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G700  | G701  | U702  | G703  | C704  | U705  | G708  | G711  | U714  | A715  | A716  | C717  | U720  | A721  | U724  | G725  | U726  | A727  | C728  | G729  | G730  | A730  | C731  | G732  | G733  | A734  | G738  | A739  | C740  | U744  | U745  | U746  | U747  | G748  | A749  | U750  | A751  | A752  | A753  | U754  | U755  | A756  | G757  | C758  | A761  | C765  | U766  | U767  | G768  | U769  | G770  | C771  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| C772  | U773  | G774  | G775  | G776  | G777  | G778  | U779  | A782  | A783  | G784  | G785  | A788  | A789  | U790  | U791  | C792  | A793  | A794  | C795  | C796  | G797  | G798  | G799  | A800  | G801  | A802  | G805  | G806  | U807  | G808  | G809  | U810  | C812  | U813  | C814  | C815  | C816  | A819  | A820  | A821  | G822  | A825  | U826  | U827  | U828  | A829  | C830  | C833  | G834  | C835  | C836  | C837  | G838  | C839  | G840  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| G841  | U842  | G843  | A844  | A845  | U846  | U847  | C848  | A849  | U852  | C853  | G856  | G857  | G858  | C859  | U860  | A861  | A862  | A863  | A864  | C865  | G866  | C867  | A868  | A869  | U871  | G874  | A877  | A878  | C880  | C881  | G882  | G883  | U884  | A     | U     | C     | C     | A892  | C893  | U894  | U895  | A896  | A897  | C898  | C899  | A899  | A900  | C901  | C902  | C903  | G904  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

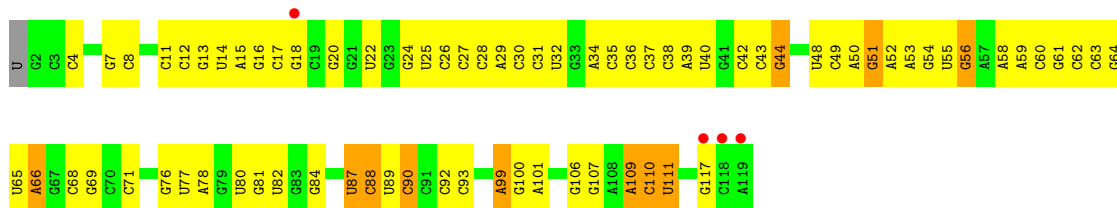
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| G2396 | G2396 | U2272 | G2203 | G2141 | C2065 | A1937 | U1865 | U1996 | C1728 | U1648 | U1578 |
| C2465 | A2273 | A2273 | A2205 | A2142 | C2066 | U1937 | U1866 | U1797 | U1729 | G1649 | U1579 |
| C2466 | A2274 | A2274 | G2206 | C2143 | U2068 | U1938 | G1867 | U1798 | G1730 | A1650 | G1581 |
| A2468 | C2275 | C2275 | C2207 | G2144 | G2069 | U1940 | G1868 | G1800 | G1731 | A1652 | C1582 |
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| A2406 | U2210 | U2210 | A2281 | A2147 | C2072 | A1947 | A1872 | A1803 | G1734 | A1655 | A1585 |
| A2407 | G2282 | G2282 | A2212 | C2148 | C2073 | C1947 | G1873 | C1804 | U1735 | C1658 | A1586 |
| A2408 | G2283 | G2283 | U2213 | U2149 | U2074 | G1948 | C1874 | A1805 | G1737 | G1659 | G1587 |
| G2409 | U2213 | U2213 | U2214 | U2150 | U2075 | U1949 | C1875 | C1806 | G1738 | G1660 | G1588 |
| G2410 | C2214 | C2214 | G2215 | U2151 | U2076 | G1950 | A1876 | G1807 | A1739 | G1661 | A1590 |
| A2411 | G2215 | G2215 | G2216 | G2156 | U2079 | U1951 | A1877 | A1808 | G1740 | U1662 | A1591 |
| A2412 | G2216 | G2216 | A2287 | C2157 | A2080 | U1952 | A1878 | A1809 | G1741 | G1663 | A1592 |
| A2413 | G2217 | G2217 | G2083 | A2158 | U2016 | A1953 | C1879 | A1810 | U1742 | A1664 | C1595 |
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| G2415 | G2219 | G2219 | C2085 | C2160 | G2018 | U1955 | C1881 | U1812 | A1744 | G1666 | A1597 |
| C2416 | G2220 | G2220 | G2086 | G2161 | A2019 | U1956 | U1882 | G1813 | A1745 | G1667 | A1598 |
| A2417 | G2221 | G2221 | G2087 | C2162 | A2020 | C1957 | U1883 | G1814 | G1750 | A1668 | A1599 |
| A2418 | G2222 | G2222 | C2091 | G2163 | A2021 | U1958 | G1884 | A1815 | A1749 | C1670 | C1600 |
| U2419 | G2223 | G2223 | U2092 | A2164 | C2022 | G1959 | G1885 | C1816 | G1751 | U1671 | G1601 |
| G2420 | G2224 | G2224 | G2093 | C2165 | G2023 | U1960 | A1889 | G1817 | U1752 | U1602 | U1602 |
| U2421 | G2225 | G2225 | A2094 | U2166 | C2025 | A1960 | A1890 | U1818 | G1753 | A1603 | A1603 |
| U2422 | G2226 | G2226 | G2094 | U2167 | U2026 | G1964 | A1891 | A1819 | G1754 | C1604 | C1604 |
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| A2425 | G2230 | G2230 | C2104 | C2168 | A2031 | U1966 | C1893 | G1826 | A1755 | A1676 | C1606 |
| A2426 | U2231 | U2231 | U2105 | A2169 | U2032 | C1967 | C1894 | U1827 | G1756 | A1677 | C1607 |
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| G2429 | G2303 | G2303 | U2108 | U2172 | A2034 | A1970 | U1897 | A1829 | A1759 | A1609 | A1609 |
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| G2502 | G2236 | G2236 | C2174 | C2175 | G2035 | G1972 | A1899 | G1831 | C1761 | C1611 | C1611 |
| G2503 | G2237 | G2237 | C2176 | C2177 | G2036 | U1973 | A1900 | G1832 | A1762 | C1612 | C1612 |
| U2504 | G2238 | G2238 | A2177 | C2178 | A2037 | G1974 | A1901 | G1833 | G1763 | G1613 | G1613 |
| U2505 | U2240 | U2240 | U2111 | U2112 | G2038 | U1975 | G1903 | U1834 | G1764 | A1614 | A1614 |
| A2435 | U2241 | U2241 | U2113 | U2113 | U2039 | U1976 | G1906 | G1835 | U1765 | C1615 | C1615 |
| G2436 | A2242 | A2242 | A2114 | U2114 | G2040 | A1977 | G1907 | C1836 | G1766 | A1616 | A1616 |
| G2437 | G2243 | G2243 | G2115 | U2115 | U2041 | A1978 | G1907 | C1837 | G1767 | C1617 | C1617 |
| U2438 | U2244 | U2244 | G2116 | U2116 | A2042 | U1979 | U1911 | G1838 | C1768 | A1618 | A1618 |
| A2439 | U2245 | U2245 | A2117 | U2117 | C2043 | U1980 | U1912 | C1839 | G1769 | G1619 | G1619 |
| G2440 | U2246 | U2246 | U2118 | U2118 | C2044 | A1981 | U1913 | G1840 | A1698 | A1620 | A1620 |
| G2441 | G2246 | G2246 | U2119 | U2119 | C2045 | U1982 | A1913 | C1841 | G1773 | U1621 | U1621 |
| G2442 | G2250 | G2250 | U2120 | U2120 | G2048 | G1983 | C1914 | C1844 | C1774 | G1622 | G1622 |
| G2443 | G2251 | G2251 | G2121 | G2121 | G2049 | G1984 | U1915 | G1845 | C1775 | G1623 | G1623 |
| G2444 | G2252 | G2252 | U2122 | U2122 | C2050 | C1985 | A1916 | G1846 | G1707 | U1624 | U1624 |
| G2445 | G2253 | G2253 | U2123 | U2123 | A2051 | U1986 | U1917 | A1847 | G1708 | C1625 | C1625 |
| G2446 | G2254 | G2254 | G2124 | U2124 | U2051 | A1987 | A1918 | A1847 | U1709 | A1626 | A1626 |
| G2447 | C2254 | C2254 | G2125 | U2125 | A2052 | G1988 | A1919 | G1849 | G1710 | G1627 | G1627 |
| G2448 | G2258 | G2258 | A2126 | U2126 | G2053 | G1989 | C1920 | G1850 | U1781 | G1628 | G1628 |
| A2450 | C2259 | C2259 | G2127 | U2127 | A2054 | C1990 | U1851 | U1851 | G1782 | G1715 | G1715 |
| A2451 | G2261 | G2261 | G2128 | U2128 | C2055 | U1991 | C1924 | U1852 | A1783 | U1716 | A1634 |
| A2452 | U2194 | U2194 | C2129 | U2129 | G2056 | U1992 | C1925 | A1853 | A1784 | A1717 | A1635 |
| A2453 | U2195 | U2195 | U2130 | U2130 | G2057 | U1993 | U1926 | U1854 | G1718 | G1718 | C1638 |
| G2454 | C2262 | C2262 | U2131 | U2131 | A2058 | C1994 | A1927 | U1855 | A1789 | C1639 | C1639 |
| G2455 | C2264 | C2264 | U2132 | U2132 | A2059 | U1995 | A1928 | U1856 | C1790 | A1640 | A1640 |
| G2456 | U2266 | U2266 | A2198 | U2198 | A2060 | U1996 | G1929 | G1857 | A1791 | A1641 | A1641 |
| A2457 | A2267 | A2267 | C2200 | C2200 | A2061 | C1997 | G1930 | A1858 | G1724 | G1724 | G1724 |
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• Molecule 23: 5S rRNA



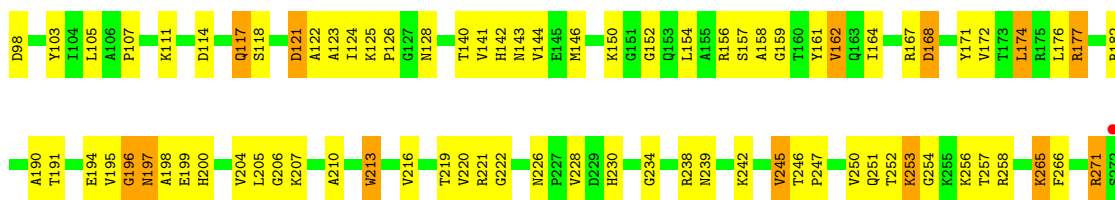
• Molecule 23: 5S rRNA



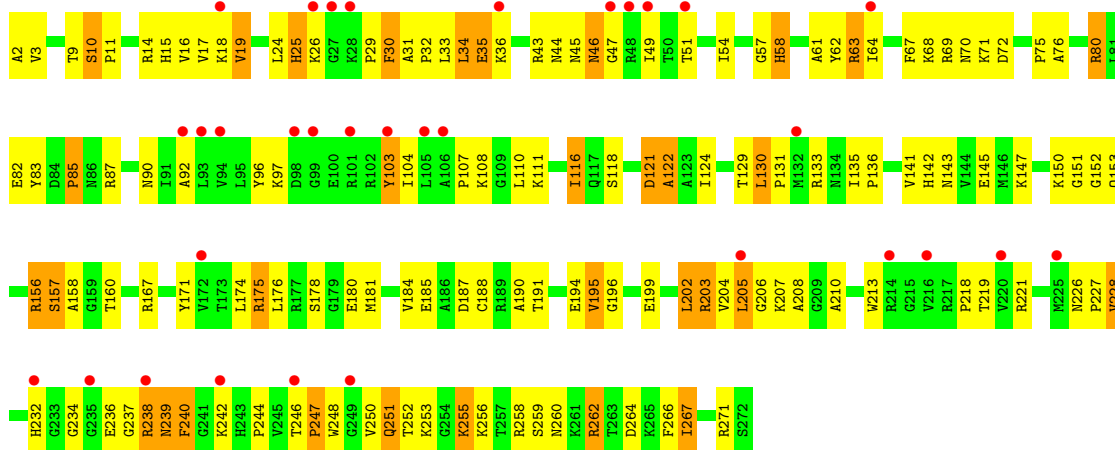
• Molecule 24: 50S ribosomal protein L2



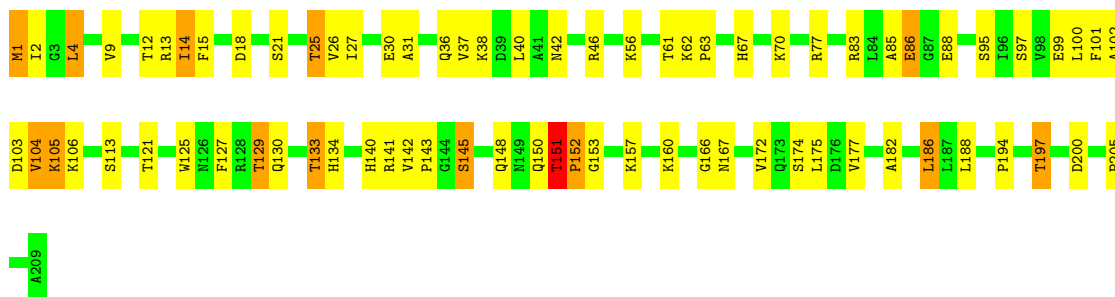




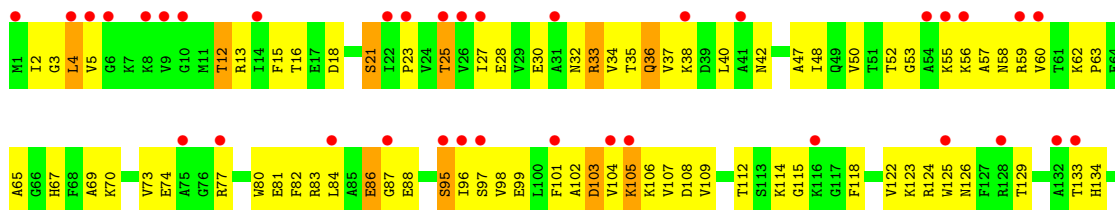
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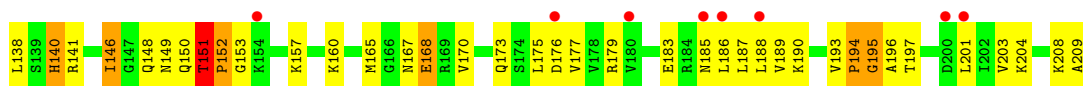


• Molecule 25: 50S ribosomal protein L3



• Molecule 25: 50S ribosomal protein L3





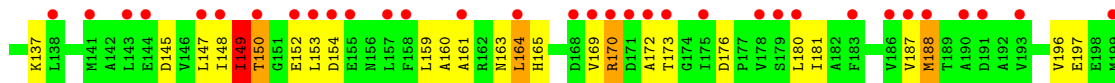
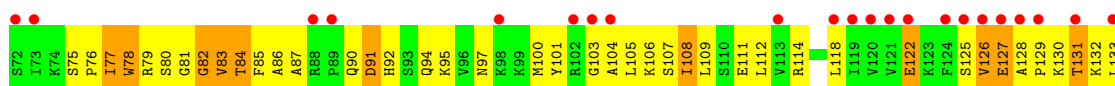
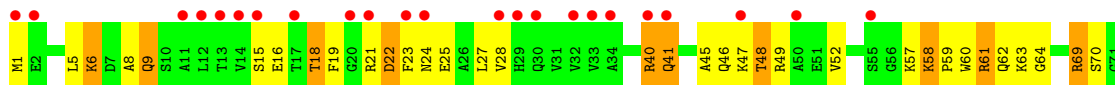
- Molecule 26: 50S ribosomal protein L4

Chain BE:  59% 34% 7%



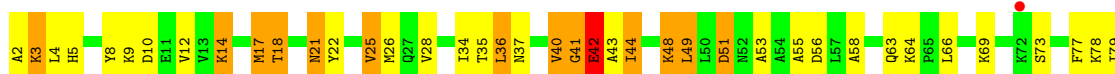
- Molecule 26: 50S ribosomal protein L4

Chain DE:  40% 49% 38% 12%

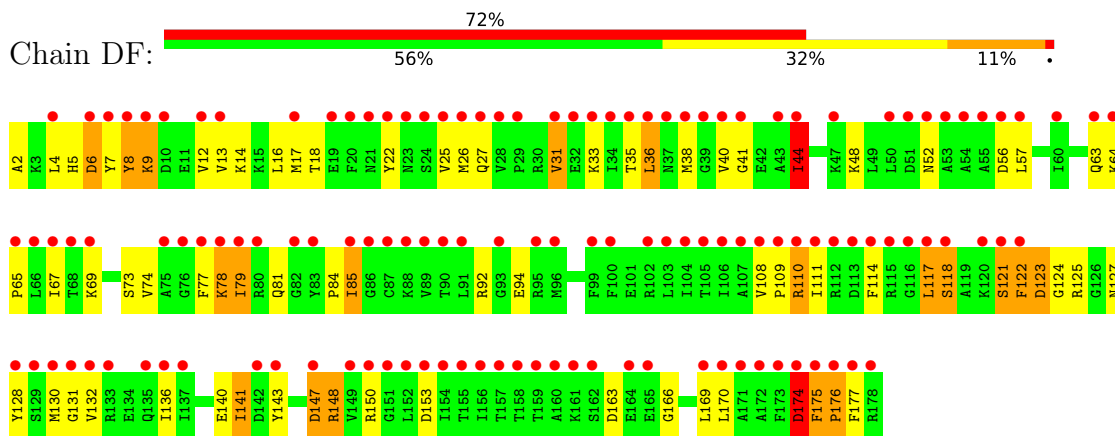


- Molecule 27: 50S ribosomal protein L5

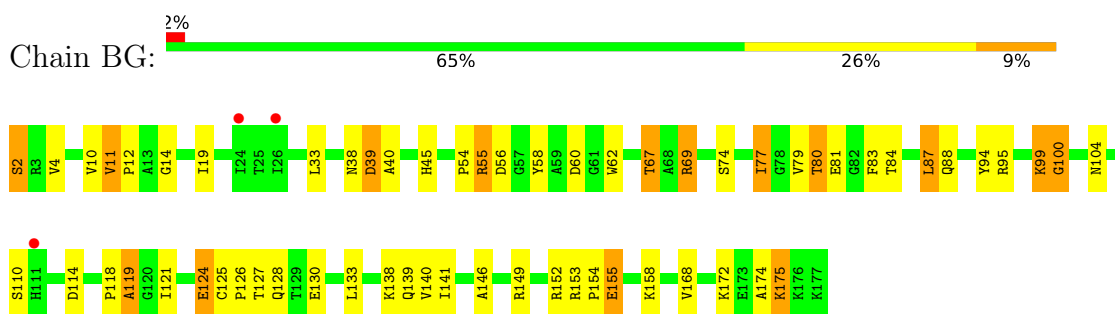
Chain BF:  2% 47% 37% 14%



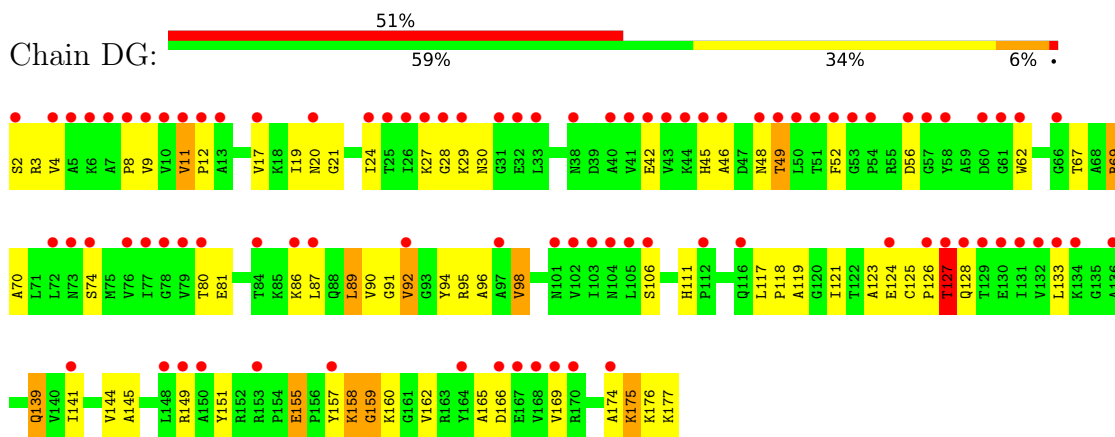
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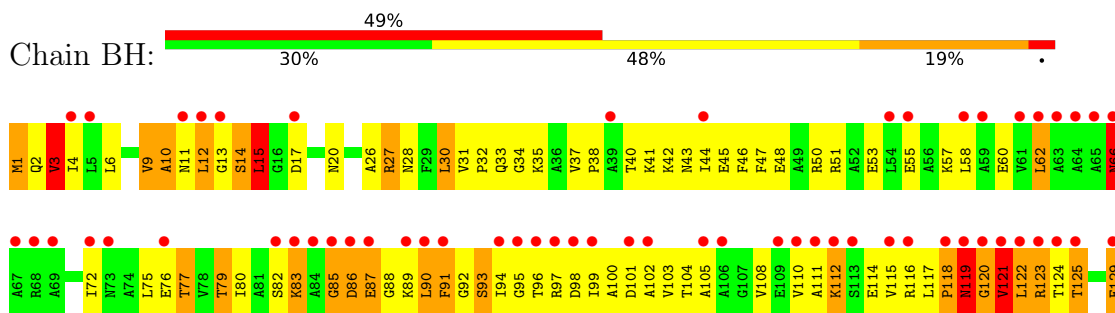
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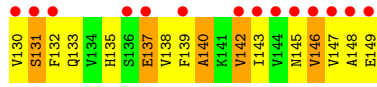


• Molecule 28: 50S ribosomal protein L6

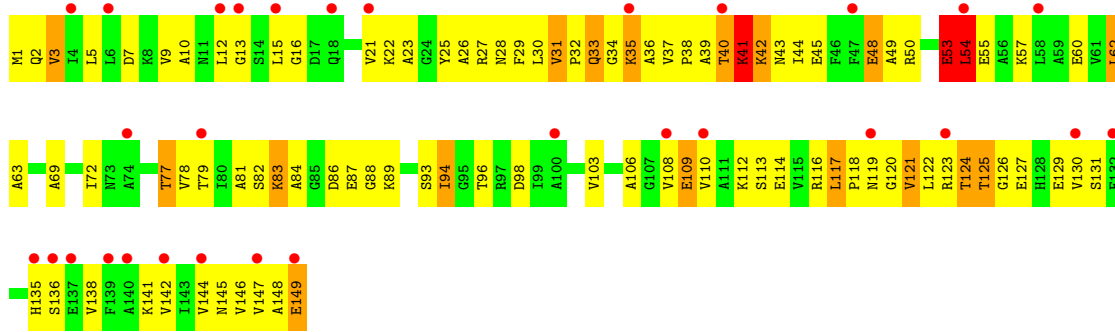


• Molecule 29: 50S ribosomal protein L9

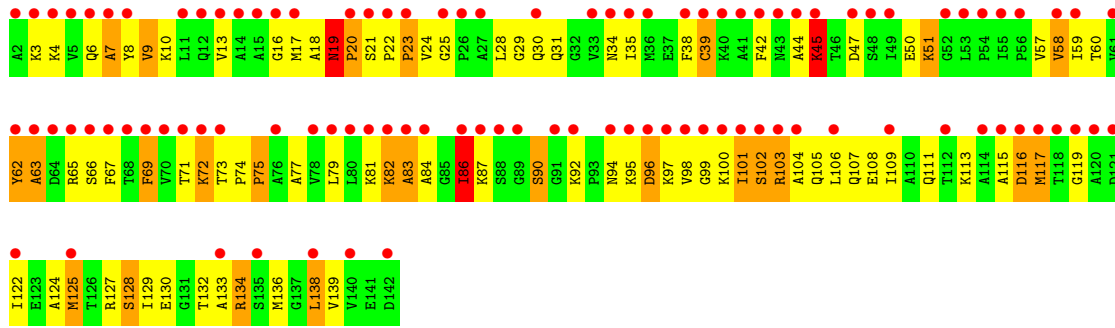
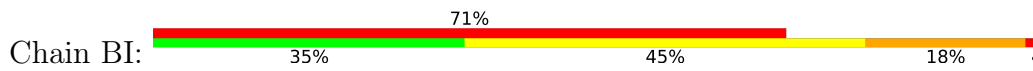




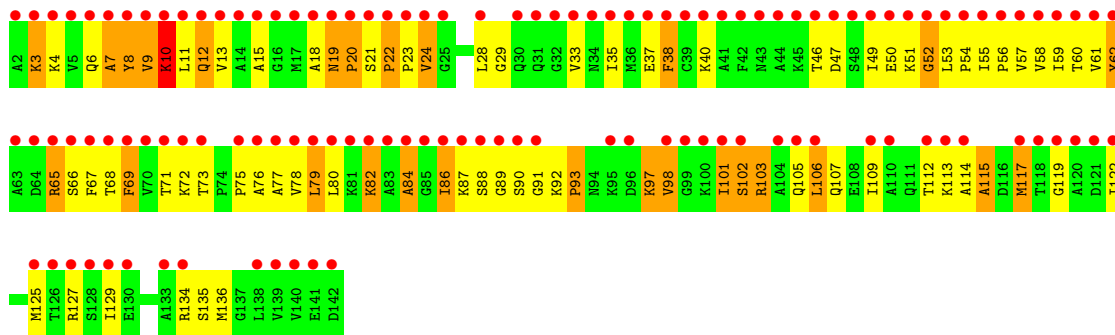
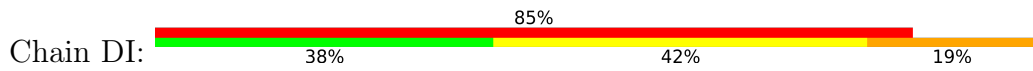
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

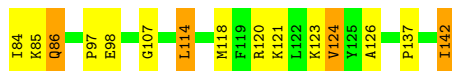


• Molecule 30: 50S ribosomal protein L11

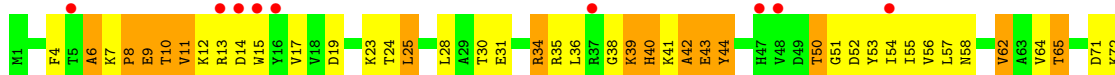


• Molecule 31: 50S ribosomal protein L13

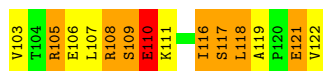
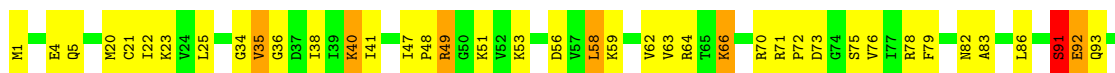




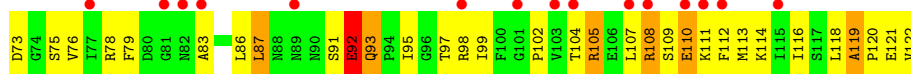
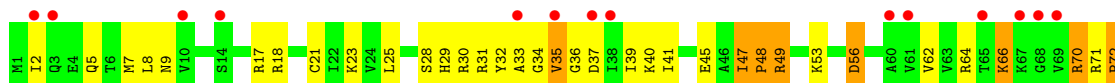
- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14



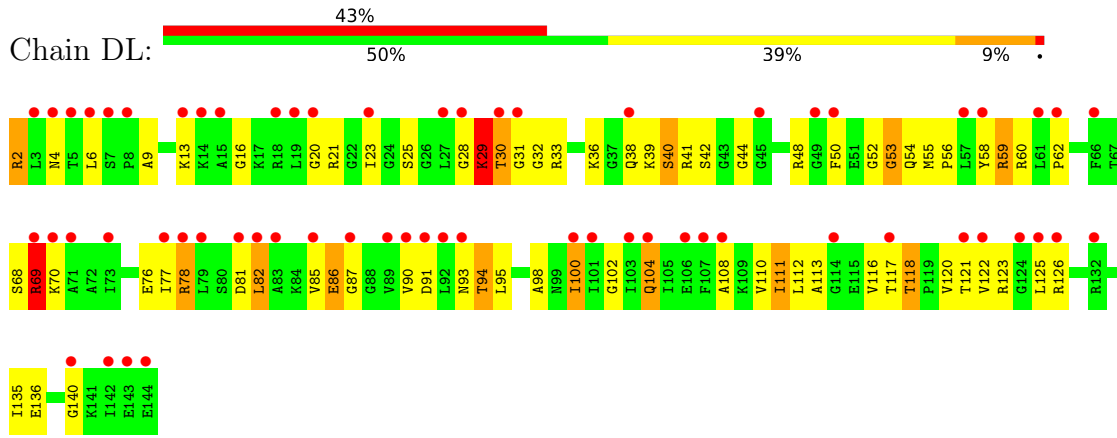
- Molecule 32: 50S ribosomal protein L14



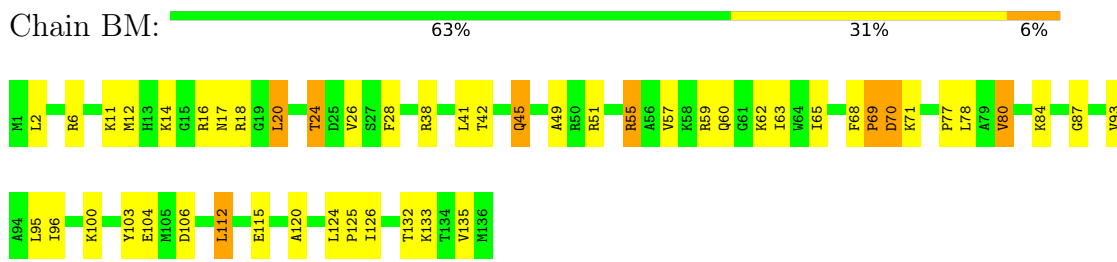
- Molecule 33: 50S ribosomal protein L15



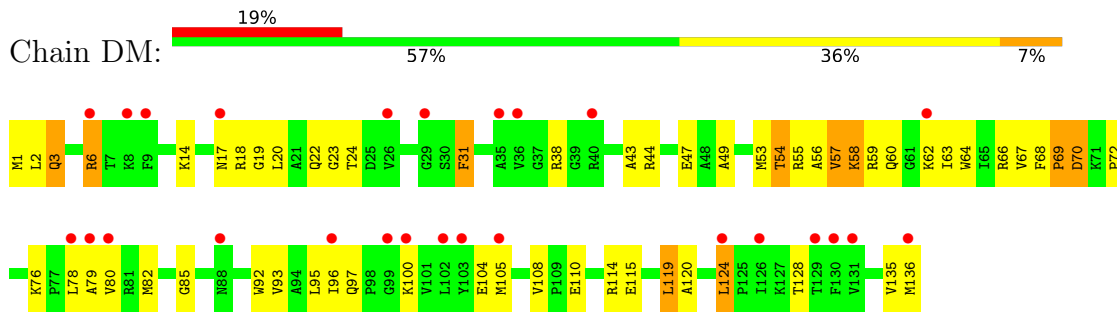
- Molecule 33: 50S ribosomal protein L15



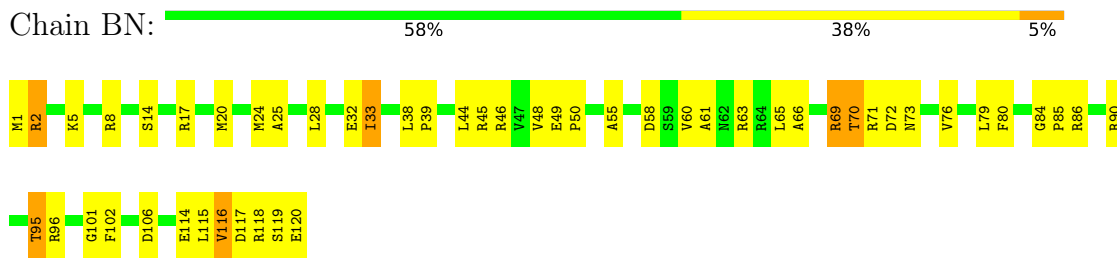
• Molecule 34: 50S ribosomal protein L16



• Molecule 34: 50S ribosomal protein L16

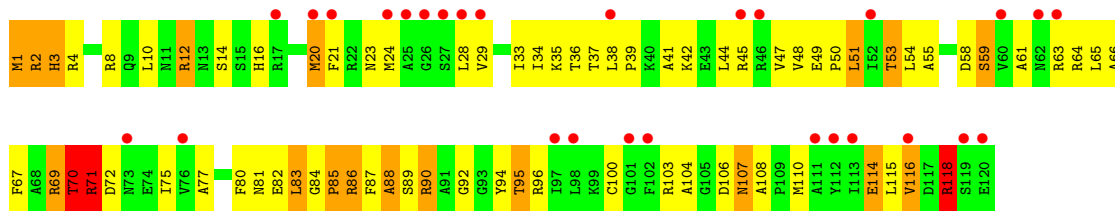


• Molecule 35: 50S ribosomal protein L17

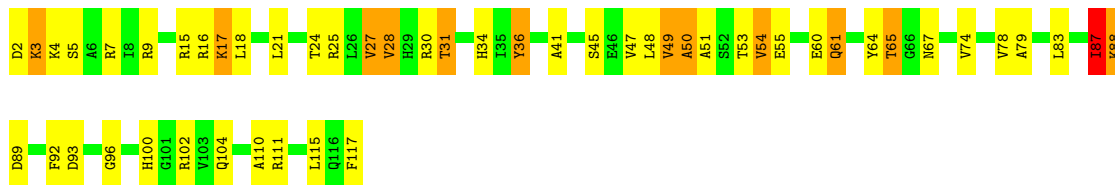


• Molecule 35: 50S ribosomal protein L17

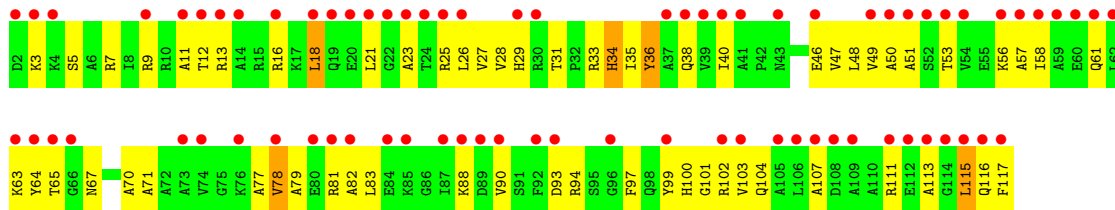




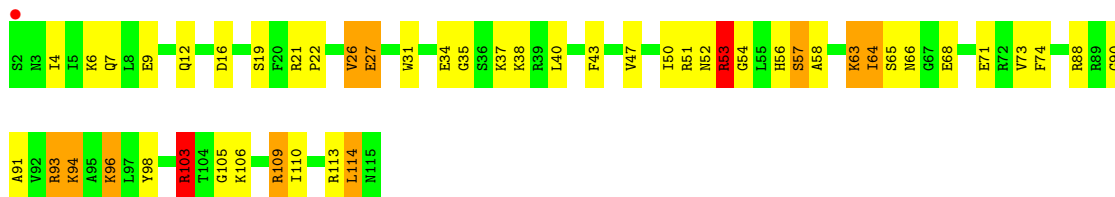
• Molecule 36: 50S ribosomal protein L18



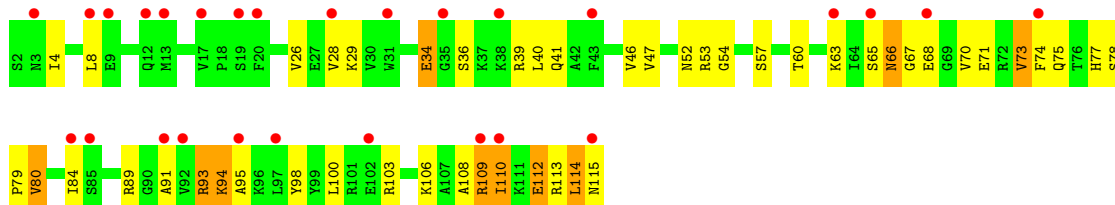
• Molecule 36: 50S ribosomal protein L18



• Molecule 37: 50S ribosomal protein L19

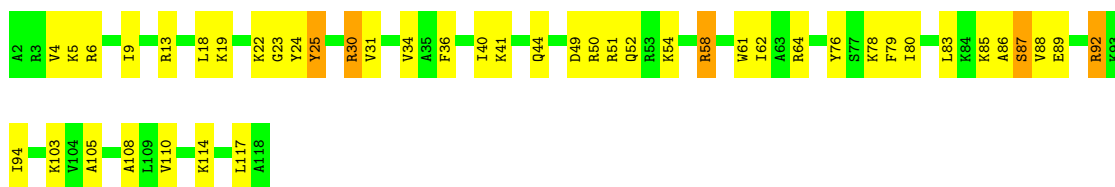


• Molecule 37: 50S ribosomal protein L19



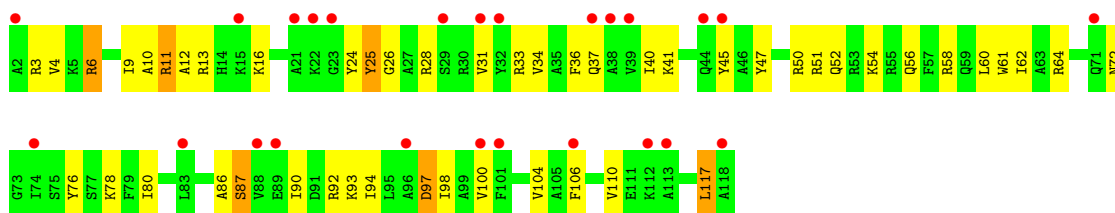
- Molecule 38: 50S ribosomal protein L20

Chain BQ:  62% 34%



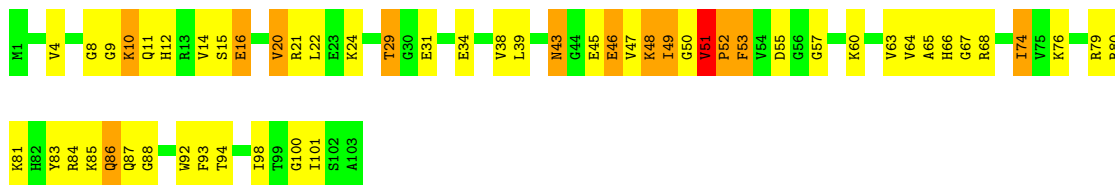
- Molecule 38: 50S ribosomal protein L20

Chain DQ:  21% 58% 37% 5%



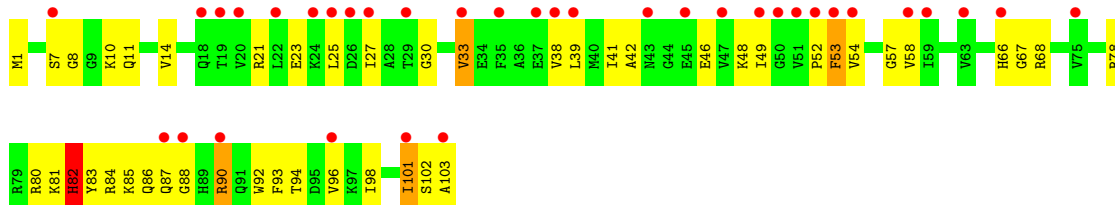
- Molecule 39: 50S ribosomal protein L21

Chain BR:  48% 40% 12%



- Molecule 39: 50S ribosomal protein L21

Chain DR:  34% 55% 40%



- Molecule 40: 50S ribosomal protein L22

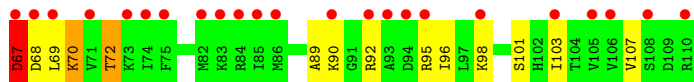
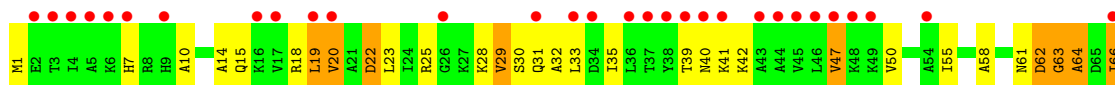
Chain BS:  59% 30% 11%



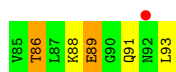




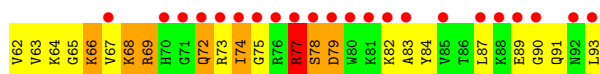
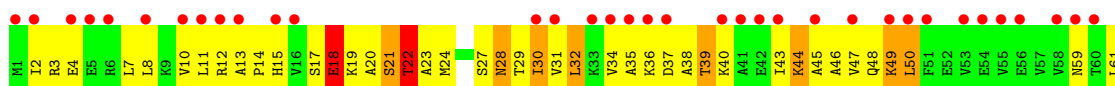
- Molecule 40: 50S ribosomal protein L22



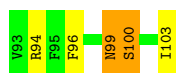
- Molecule 41: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L23

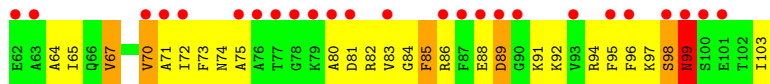
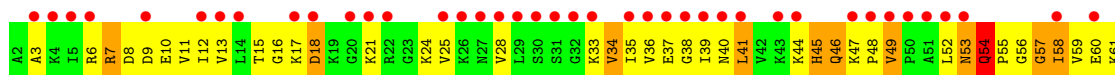


- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

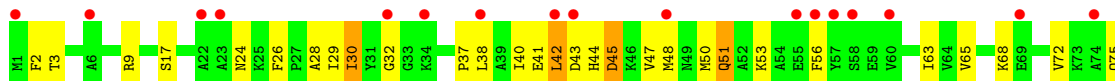




• Molecule 43: 50S ribosomal protein L25



• Molecule 43: 50S ribosomal protein L25



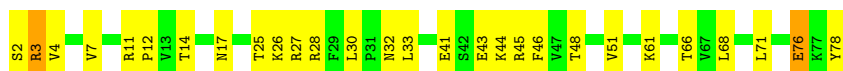
• Molecule 44: 50S ribosomal protein L27



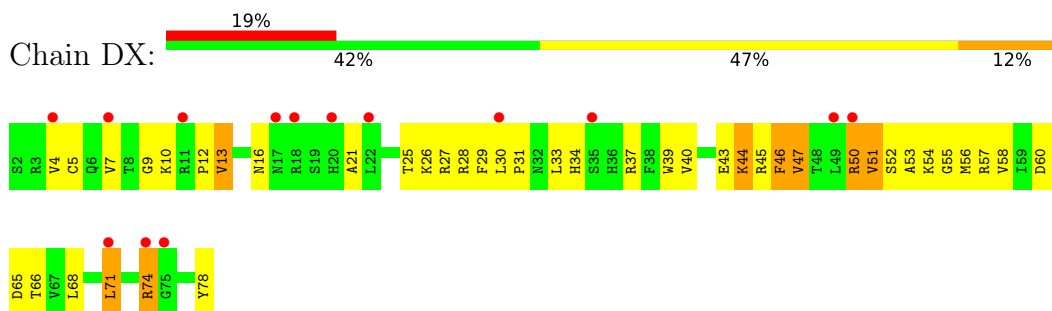
• Molecule 44: 50S ribosomal protein L27



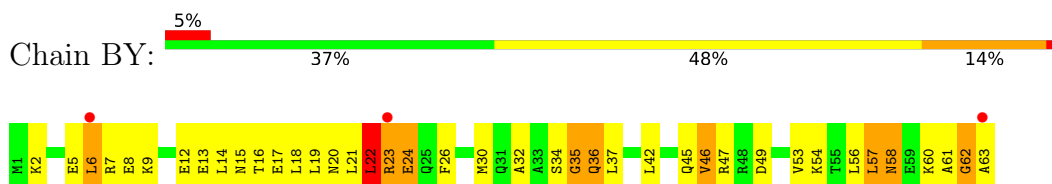
• Molecule 45: 50S ribosomal protein L28



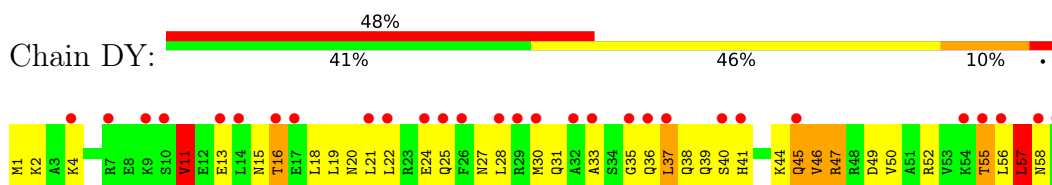
- Molecule 45: 50S ribosomal protein L28



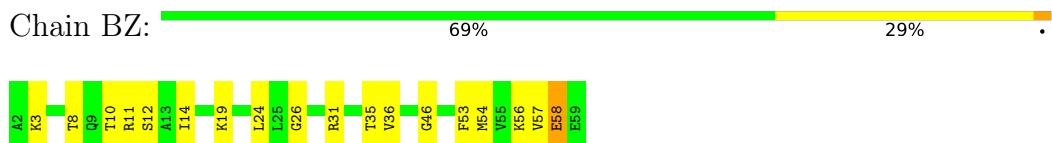
- Molecule 46: 50S ribosomal protein L29



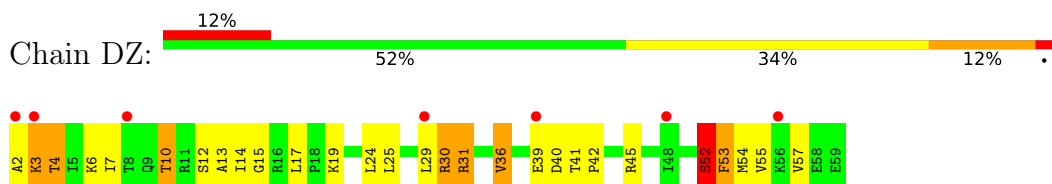
- Molecule 46: 50S ribosomal protein L29



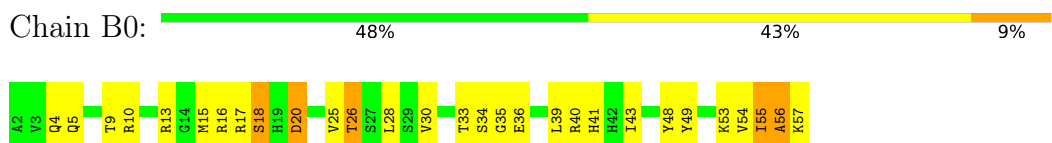
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30

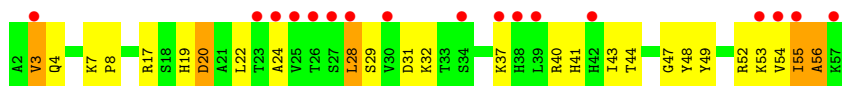


- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

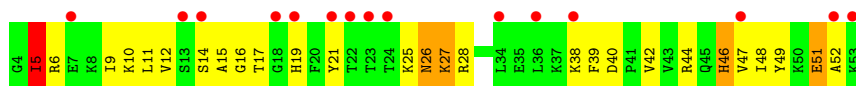




- Molecule 49: 50S ribosomal protein L33



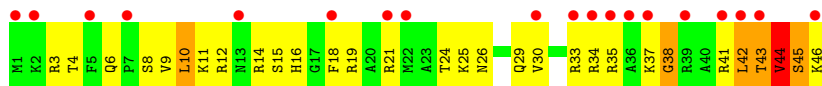
- Molecule 49: 50S ribosomal protein L33



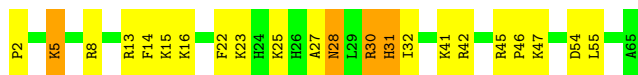
- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35



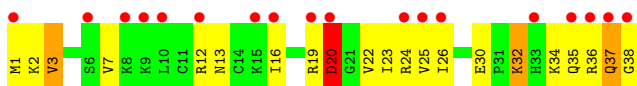
- Molecule 52: 50S ribosomal protein L36

Chain B4:  74% 24% .

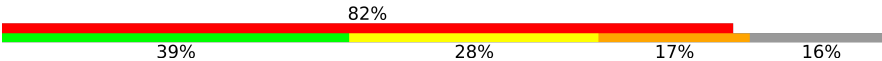


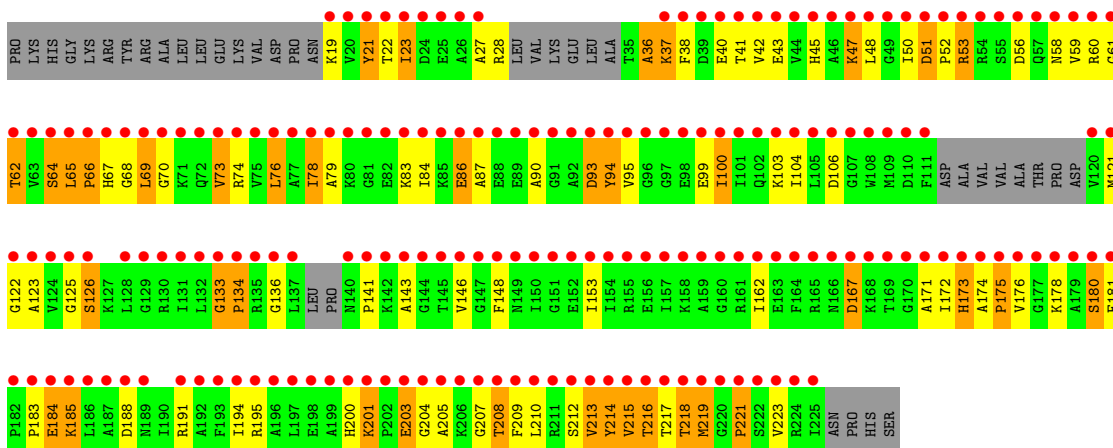
- Molecule 52: 50S ribosomal protein L36

Chain D4:  47% 45% 45% 8% .



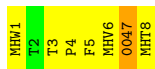
- Molecule 53: 50S ribosomal protein L1

Chain B5:  82% 39% 28% 17% 16%



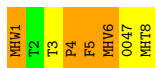
- Molecule 54: Quinupristin

Chain B6:  12% 75% 12%



- Molecule 54: Quinupristin

Chain D6:  12% 38% 50%



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.26Å 432.34Å 621.39Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 69.08 – 2.80<br>69.08 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.1 (69.08-2.80)<br>94.1 (69.08-2.80)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.14  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.40 (at 2.81Å)   | Xtrriage         |
| Refinement program  | PHENIX (phenix.refine: 1.8.1_1160)                          | Depositor        |
| R, $R_{free}$   | 0.225 , 0.271<br>0.230 , 0.276                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5217 reflections (0.40%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 48.8  | Xtrriage         |
| Anisotropy  | 0.379   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 54.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 288423  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MHU, ZN, MG, MHT, 004, DOL, MHW, DBB, MHV

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    | 0.34         | 0/36944 | 0.80        | 3/57632 (0.0%) |
| 1   | CA    | 0.28         | 0/36966 | 0.78        | 1/57666 (0.0%) |
| 2   | AB    | 0.28         | 0/1736  | 0.56        | 0/2338         |
| 2   | CB    | 0.26         | 0/1736  | 0.50        | 0/2338         |
| 3   | AC    | 0.28         | 0/1652  | 0.53        | 0/2225         |
| 3   | CC    | 0.25         | 0/1652  | 0.48        | 0/2225         |
| 4   | AD    | 0.29         | 0/1665  | 0.55        | 0/2227         |
| 4   | CD    | 0.31         | 0/1665  | 0.55        | 0/2227         |
| 5   | AE    | 0.31         | 0/1119  | 0.61        | 0/1504         |
| 5   | CE    | 0.29         | 0/1119  | 0.59        | 0/1504         |
| 6   | AF    | 0.30         | 0/836   | 0.55        | 0/1128         |
| 6   | CF    | 0.27         | 0/836   | 0.57        | 1/1128 (0.1%)  |
| 7   | AG    | 0.26         | 0/1196  | 0.48        | 0/1602         |
| 7   | CG    | 0.25         | 0/1196  | 0.49        | 0/1602         |
| 8   | AH    | 0.31         | 0/989   | 0.50        | 0/1326         |
| 8   | CH    | 0.25         | 0/989   | 0.48        | 0/1326         |
| 9   | AI    | 0.26         | 0/1034  | 0.54        | 0/1375         |
| 9   | CI    | 0.26         | 0/1034  | 0.52        | 0/1375         |
| 10  | AJ    | 0.29         | 0/797   | 0.55        | 0/1077         |
| 10  | CJ    | 0.25         | 0/797   | 0.50        | 0/1077         |
| 11  | AK    | 0.29         | 0/893   | 0.63        | 1/1205 (0.1%)  |
| 11  | CK    | 0.26         | 0/893   | 0.52        | 0/1205         |
| 12  | AL    | 0.31         | 0/969   | 0.58        | 0/1300         |
| 12  | CL    | 0.29         | 0/969   | 0.60        | 0/1300         |
| 13  | AM    | 0.27         | 0/893   | 0.55        | 0/1193         |
| 13  | CM    | 0.26         | 0/893   | 0.50        | 0/1193         |
| 14  | AN    | 0.28         | 0/785   | 0.55        | 0/1043         |
| 14  | CN    | 0.25         | 0/785   | 0.46        | 0/1043         |
| 15  | AO    | 0.28         | 0/718   | 0.53        | 0/959          |
| 15  | CO    | 0.26         | 0/718   | 0.46        | 0/959          |
| 16  | AP    | 0.30         | 0/659   | 0.66        | 1/884 (0.1%)   |
| 16  | CP    | 0.27         | 0/659   | 0.49        | 0/884          |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 17  | AQ    | 0.30         | 0/658          | 0.58        | 0/881            |
| 17  | CQ    | 0.28         | 0/658          | 0.51        | 0/881            |
| 18  | AR    | 0.26         | 0/463          | 0.53        | 0/621            |
| 18  | CR    | 0.26         | 0/463          | 0.49        | 0/621            |
| 19  | AS    | 0.27         | 0/653          | 0.50        | 0/877            |
| 19  | CS    | 0.27         | 0/653          | 0.54        | 0/877            |
| 20  | AT    | 0.31         | 0/671          | 0.55        | 0/888            |
| 20  | CT    | 0.25         | 0/671          | 0.50        | 0/888            |
| 21  | AU    | 0.36         | 0/431          | 0.62        | 0/570            |
| 21  | CU    | 0.33         | 0/431          | 0.56        | 0/570            |
| 22  | BA    | 0.59         | 5/69659 (0.0%) | 0.99        | 92/108672 (0.1%) |
| 22  | DA    | 0.27         | 0/69659        | 0.79        | 4/108672 (0.0%)  |
| 23  | BB    | 0.52         | 0/2850         | 0.93        | 0/4444           |
| 23  | DB    | 0.23         | 0/2828         | 0.76        | 0/4410           |
| 24  | BC    | 0.38         | 0/2122         | 0.60        | 0/2852           |
| 24  | DC    | 0.27         | 0/2122         | 0.52        | 0/2852           |
| 25  | BD    | 0.42         | 0/1586         | 0.63        | 1/2134 (0.0%)    |
| 25  | DD    | 0.26         | 0/1586         | 0.51        | 0/2134           |
| 26  | BE    | 0.37         | 0/1571         | 0.60        | 0/2113           |
| 26  | DE    | 0.26         | 0/1571         | 0.51        | 0/2113           |
| 27  | BF    | 0.30         | 0/1435         | 0.52        | 0/1926           |
| 27  | DF    | 0.24         | 0/1435         | 0.46        | 0/1926           |
| 28  | BG    | 0.30         | 0/1343         | 0.53        | 0/1816           |
| 28  | DG    | 0.25         | 0/1343         | 0.46        | 0/1816           |
| 29  | BH    | 0.36         | 0/1121         | 0.66        | 1/1515 (0.1%)    |
| 29  | DH    | 0.35         | 0/1121         | 0.56        | 0/1515           |
| 30  | BI    | 0.29         | 0/1046         | 0.54        | 0/1410           |
| 30  | DI    | 0.28         | 0/1046         | 0.52        | 0/1410           |
| 31  | BJ    | 0.42         | 0/1152         | 0.58        | 0/1551           |
| 31  | DJ    | 0.25         | 0/1152         | 0.51        | 0/1551           |
| 32  | BK    | 0.41         | 0/948          | 0.64        | 0/1268           |
| 32  | DK    | 0.27         | 0/948          | 0.51        | 0/1268           |
| 33  | BL    | 0.39         | 0/1054         | 0.64        | 0/1403           |
| 33  | DL    | 0.26         | 0/1054         | 0.51        | 0/1403           |
| 34  | BM    | 0.42         | 0/1093         | 0.63        | 0/1460           |
| 34  | DM    | 0.25         | 0/1093         | 0.46        | 0/1460           |
| 35  | BN    | 0.43         | 0/974          | 0.68        | 0/1301           |
| 35  | DN    | 0.27         | 0/974          | 0.56        | 1/1301 (0.1%)    |
| 36  | BO    | 0.34         | 0/902          | 0.55        | 0/1209           |
| 36  | DO    | 0.24         | 0/902          | 0.45        | 0/1209           |
| 37  | BP    | 0.42         | 0/929          | 0.69        | 2/1242 (0.2%)    |
| 37  | DP    | 0.26         | 0/929          | 0.47        | 0/1242           |
| 38  | BQ    | 0.50         | 0/960          | 0.66        | 0/1278           |



| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 38  | DQ    | 0.26         | 0/960           | 0.47        | 0/1278            |
| 39  | BR    | 0.47         | 0/829           | 0.73        | 1/1107 (0.1%)     |
| 39  | DR    | 0.25         | 0/829           | 0.50        | 0/1107            |
| 40  | BS    | 0.51         | 0/864           | 0.64        | 0/1156            |
| 40  | DS    | 0.26         | 0/864           | 0.50        | 0/1156            |
| 41  | BT    | 0.36         | 0/745           | 0.60        | 0/994             |
| 41  | DT    | 0.25         | 0/745           | 0.49        | 0/994             |
| 42  | BU    | 0.36         | 0/788           | 0.57        | 0/1051            |
| 42  | DU    | 0.28         | 0/788           | 0.52        | 0/1051            |
| 43  | BV    | 0.37         | 0/766           | 0.58        | 0/1025            |
| 43  | DV    | 0.24         | 0/766           | 0.44        | 0/1025            |
| 44  | BW    | 0.44         | 0/587           | 0.71        | 2/776 (0.3%)      |
| 44  | DW    | 0.25         | 0/576           | 0.47        | 0/762             |
| 45  | BX    | 0.34         | 0/635           | 0.57        | 0/848             |
| 45  | DX    | 0.28         | 0/635           | 0.53        | 0/848             |
| 46  | BY    | 0.32         | 0/510           | 0.63        | 0/677             |
| 46  | DY    | 0.25         | 0/510           | 0.50        | 0/677             |
| 47  | BZ    | 0.43         | 0/453           | 0.61        | 0/605             |
| 47  | DZ    | 0.26         | 0/453           | 0.48        | 0/605             |
| 48  | B0    | 0.44         | 0/450           | 0.64        | 0/599             |
| 48  | D0    | 0.27         | 0/450           | 0.50        | 0/599             |
| 49  | B1    | 0.37         | 0/417           | 0.53        | 0/554             |
| 49  | D1    | 0.28         | 0/417           | 0.49        | 0/554             |
| 50  | B2    | 0.44         | 0/380           | 0.69        | 0/498             |
| 50  | D2    | 0.28         | 0/380           | 0.51        | 0/498             |
| 51  | B3    | 0.38         | 0/513           | 0.57        | 0/676             |
| 51  | D3    | 0.25         | 0/513           | 0.44        | 0/676             |
| 52  | B4    | 0.43         | 0/303           | 0.63        | 0/397             |
| 52  | D4    | 0.25         | 0/303           | 0.49        | 0/397             |
| 53  | B5    | 0.25         | 0/1145          | 0.49        | 0/1556            |
| 54  | B6    | 1.77         | 0/13            | 2.40        | 1/15 (6.7%)       |
| 54  | D6    | 1.44         | 0/13            | 2.02        | 1/15 (6.7%)       |
| All | All   | 0.39         | 5/310652 (0.0%) | 0.79        | 113/464396 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | CF    | 0                   | 1                   |
| 11  | AK    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12  | CL    | 0                   | 2                   |
| 25  | BD    | 0                   | 1                   |
| 25  | DD    | 0                   | 1                   |
| All | All   | 0                   | 6                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22  | BA    | 984  | A    | N9-C4 | -8.33 | 1.32        | 1.37     |
| 22  | BA    | 1142 | A    | N9-C4 | -7.64 | 1.33        | 1.37     |
| 22  | BA    | 1936 | A    | N9-C4 | -7.63 | 1.33        | 1.37     |
| 22  | BA    | 528  | A    | N9-C4 | -7.62 | 1.33        | 1.37     |
| 22  | BA    | 528  | A    | N3-C4 | -5.47 | 1.31        | 1.34     |

The worst 5 of 113 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 22  | BA    | 974 | G    | C4-C5-N7 | 10.83  | 115.13      | 110.80   |
| 22  | BA    | 974 | G    | C6-C5-N7 | -10.21 | 124.27      | 130.40   |
| 25  | BD    | 151 | THR  | C-N-CD   | -9.98  | 98.64       | 120.60   |
| 22  | BA    | 984 | A    | C2-N3-C4 | -9.95  | 105.62      | 110.60   |
| 22  | BA    | 974 | G    | C5-N7-C8 | -9.65  | 99.48       | 104.30   |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 11  | AK    | 126 | LYS  | Peptide |
| 25  | BD    | 151 | THR  | Peptide |
| 6   | CF    | 54  | LEU  | Peptide |
| 12  | CL    | 23  | ALA  | Peptide |
| 12  | CL    | 24  | LEU  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 32995 | 0        | 16607    | 962     | 0            |
| 1   | CA    | 33015 | 0        | 16617    | 1107    | 1            |
| 2   | AB    | 1705  | 0        | 1732     | 164     | 0            |
| 2   | CB    | 1705  | 0        | 1732     | 135     | 0            |
| 3   | AC    | 1625  | 0        | 1696     | 78      | 0            |
| 3   | CC    | 1625  | 0        | 1696     | 69      | 0            |
| 4   | AD    | 1643  | 0        | 1707     | 116     | 0            |
| 4   | CD    | 1643  | 0        | 1707     | 116     | 0            |
| 5   | AE    | 1106  | 0        | 1148     | 88      | 0            |
| 5   | CE    | 1106  | 0        | 1148     | 99      | 0            |
| 6   | AF    | 818   | 0        | 808      | 47      | 0            |
| 6   | CF    | 818   | 0        | 808      | 60      | 0            |
| 7   | AG    | 1182  | 0        | 1238     | 58      | 0            |
| 7   | CG    | 1182  | 0        | 1238     | 66      | 0            |
| 8   | AH    | 979   | 0        | 1031     | 49      | 0            |
| 8   | CH    | 979   | 0        | 1031     | 52      | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 87      | 0            |
| 9   | CI    | 1022  | 0        | 1070     | 66      | 0            |
| 10  | AJ    | 787   | 0        | 828      | 81      | 0            |
| 10  | CJ    | 787   | 0        | 828      | 56      | 0            |
| 11  | AK    | 877   | 0        | 887      | 68      | 0            |
| 11  | CK    | 877   | 0        | 887      | 55      | 0            |
| 12  | AL    | 955   | 0        | 1016     | 44      | 0            |
| 12  | CL    | 955   | 0        | 1016     | 74      | 0            |
| 13  | AM    | 884   | 0        | 941      | 44      | 0            |
| 13  | CM    | 884   | 0        | 941      | 51      | 0            |
| 14  | AN    | 774   | 0        | 824      | 58      | 0            |
| 14  | CN    | 774   | 0        | 824      | 51      | 0            |
| 15  | AO    | 710   | 0        | 728      | 31      | 0            |
| 15  | CO    | 710   | 0        | 728      | 29      | 0            |
| 16  | AP    | 649   | 0        | 666      | 53      | 0            |
| 16  | CP    | 649   | 0        | 666      | 36      | 0            |
| 17  | AQ    | 649   | 0        | 691      | 63      | 0            |
| 17  | CQ    | 649   | 0        | 691      | 53      | 0            |
| 18  | AR    | 456   | 0        | 478      | 17      | 0            |
| 18  | CR    | 456   | 0        | 478      | 25      | 0            |
| 19  | AS    | 638   | 0        | 665      | 39      | 0            |
| 19  | CS    | 638   | 0        | 665      | 42      | 0            |
| 20  | AT    | 665   | 0        | 714      | 65      | 0            |
| 20  | CT    | 665   | 0        | 714      | 46      | 0            |
| 21  | AU    | 426   | 0        | 449      | 52      | 0            |
| 21  | CU    | 426   | 0        | 449      | 53      | 0            |
| 22  | BA    | 62195 | 0        | 31280    | 1486    | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22  | DA    | 62195 | 0        | 31280    | 2451    | 1            |
| 23  | BB    | 2549  | 0        | 1291     | 37      | 0            |
| 23  | DB    | 2529  | 0        | 1281     | 66      | 0            |
| 24  | BC    | 2083  | 0        | 2154     | 102     | 0            |
| 24  | DC    | 2083  | 0        | 2154     | 128     | 0            |
| 25  | BD    | 1565  | 0        | 1616     | 66      | 0            |
| 25  | DD    | 1565  | 0        | 1616     | 97      | 0            |
| 26  | BE    | 1552  | 0        | 1619     | 67      | 0            |
| 26  | DE    | 1552  | 0        | 1619     | 91      | 0            |
| 27  | BF    | 1411  | 0        | 1444     | 84      | 0            |
| 27  | DF    | 1411  | 0        | 1444     | 54      | 0            |
| 28  | BG    | 1323  | 0        | 1371     | 41      | 0            |
| 28  | DG    | 1323  | 0        | 1371     | 42      | 0            |
| 29  | BH    | 1110  | 0        | 1147     | 139     | 0            |
| 29  | DH    | 1110  | 0        | 1148     | 87      | 0            |
| 30  | BI    | 1032  | 0        | 1085     | 76      | 0            |
| 30  | DI    | 1032  | 0        | 1085     | 85      | 0            |
| 31  | BJ    | 1129  | 0        | 1162     | 48      | 0            |
| 31  | DJ    | 1129  | 0        | 1162     | 62      | 0            |
| 32  | BK    | 939   | 0        | 1012     | 45      | 0            |
| 32  | DK    | 939   | 0        | 1012     | 53      | 0            |
| 33  | BL    | 1045  | 0        | 1117     | 54      | 0            |
| 33  | DL    | 1045  | 0        | 1117     | 75      | 0            |
| 34  | BM    | 1074  | 0        | 1157     | 43      | 0            |
| 34  | DM    | 1074  | 0        | 1157     | 41      | 0            |
| 35  | BN    | 961   | 0        | 1000     | 39      | 0            |
| 35  | DN    | 961   | 0        | 1000     | 71      | 0            |
| 36  | BO    | 892   | 0        | 923      | 38      | 0            |
| 36  | DO    | 892   | 0        | 923      | 41      | 0            |
| 37  | BP    | 917   | 0        | 962      | 45      | 0            |
| 37  | DP    | 917   | 0        | 962      | 42      | 0            |
| 38  | BQ    | 947   | 0        | 1019     | 39      | 0            |
| 38  | DQ    | 947   | 0        | 1019     | 47      | 0            |
| 39  | BR    | 816   | 0        | 839      | 66      | 0            |
| 39  | DR    | 816   | 0        | 839      | 36      | 0            |
| 40  | BS    | 857   | 0        | 922      | 33      | 0            |
| 40  | DS    | 857   | 0        | 922      | 37      | 0            |
| 41  | BT    | 739   | 0        | 807      | 41      | 0            |
| 41  | DT    | 739   | 0        | 807      | 60      | 0            |
| 42  | BU    | 780   | 0        | 831      | 37      | 0            |
| 42  | DU    | 780   | 0        | 831      | 68      | 0            |
| 43  | BV    | 753   | 0        | 780      | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | DV    | 753   | 0        | 780      | 21      | 0            |
| 44  | BW    | 580   | 0        | 594      | 20      | 0            |
| 44  | DW    | 569   | 0        | 581      | 23      | 0            |
| 45  | BX    | 625   | 0        | 652      | 15      | 0            |
| 45  | DX    | 625   | 0        | 652      | 46      | 0            |
| 46  | BY    | 509   | 0        | 543      | 34      | 0            |
| 46  | DY    | 509   | 0        | 543      | 26      | 0            |
| 47  | BZ    | 449   | 0        | 488      | 9       | 0            |
| 47  | DZ    | 449   | 0        | 488      | 24      | 0            |
| 48  | B0    | 444   | 0        | 458      | 27      | 0            |
| 48  | D0    | 444   | 0        | 458      | 23      | 0            |
| 49  | B1    | 410   | 0        | 440      | 19      | 0            |
| 49  | D1    | 410   | 0        | 440      | 22      | 0            |
| 50  | B2    | 377   | 0        | 418      | 10      | 0            |
| 50  | D2    | 377   | 0        | 418      | 31      | 0            |
| 51  | B3    | 504   | 0        | 572      | 28      | 0            |
| 51  | D3    | 504   | 0        | 572      | 22      | 0            |
| 52  | B4    | 302   | 0        | 340      | 7       | 0            |
| 52  | D4    | 302   | 0        | 340      | 15      | 0            |
| 53  | B5    | 1142  | 0        | 865      | 69      | 0            |
| 54  | B6    | 73    | 0        | 64       | 3       | 0            |
| 54  | D6    | 73    | 0        | 65       | 12      | 0            |
| 55  | AA    | 71    | 0        | 0        | 0       | 0            |
| 55  | AM    | 1     | 0        | 0        | 0       | 0            |
| 55  | BA    | 194   | 0        | 0        | 0       | 0            |
| 55  | BB    | 4     | 0        | 0        | 0       | 0            |
| 55  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 55  | CA    | 56    | 0        | 0        | 0       | 0            |
| 55  | D2    | 1     | 0        | 0        | 0       | 0            |
| 55  | DA    | 166   | 0        | 0        | 0       | 0            |
| 55  | DB    | 3     | 0        | 0        | 0       | 0            |
| 55  | DQ    | 1     | 0        | 0        | 0       | 0            |
| 56  | BA    | 48    | 0        | 50       | 15      | 0            |
| 56  | DA    | 48    | 0        | 50       | 25      | 0            |
| 57  | B4    | 1     | 0        | 0        | 0       | 0            |
| 57  | D4    | 1     | 0        | 0        | 0       | 0            |
| 58  | AA    | 194   | 0        | 0        | 18      | 0            |
| 58  | AE    | 2     | 0        | 0        | 0       | 0            |
| 58  | AL    | 1     | 0        | 0        | 0       | 0            |
| 58  | AN    | 3     | 0        | 0        | 0       | 0            |
| 58  | AT    | 2     | 0        | 0        | 0       | 0            |
| 58  | AU    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 58  | B3    | 3      | 0        | 0        | 0       | 0            |
| 58  | B4    | 1      | 0        | 0        | 0       | 0            |
| 58  | BA    | 617    | 0        | 0        | 66      | 0            |
| 58  | BB    | 14     | 0        | 0        | 1       | 0            |
| 58  | BC    | 6      | 0        | 0        | 1       | 0            |
| 58  | BD    | 4      | 0        | 0        | 2       | 0            |
| 58  | BE    | 1      | 0        | 0        | 0       | 0            |
| 58  | BF    | 1      | 0        | 0        | 1       | 0            |
| 58  | BG    | 1      | 0        | 0        | 1       | 0            |
| 58  | BJ    | 1      | 0        | 0        | 0       | 0            |
| 58  | BL    | 7      | 0        | 0        | 0       | 0            |
| 58  | BN    | 5      | 0        | 0        | 0       | 0            |
| 58  | BQ    | 1      | 0        | 0        | 0       | 0            |
| 58  | BS    | 1      | 0        | 0        | 0       | 0            |
| 58  | BT    | 2      | 0        | 0        | 0       | 0            |
| 58  | CA    | 192    | 0        | 0        | 12      | 0            |
| 58  | CL    | 1      | 0        | 0        | 0       | 0            |
| 58  | CN    | 2      | 0        | 0        | 0       | 0            |
| 58  | CT    | 2      | 0        | 0        | 0       | 0            |
| 58  | CU    | 1      | 0        | 0        | 1       | 0            |
| 58  | D2    | 1      | 0        | 0        | 1       | 0            |
| 58  | D3    | 1      | 0        | 0        | 0       | 0            |
| 58  | D4    | 1      | 0        | 0        | 0       | 0            |
| 58  | DA    | 610    | 0        | 0        | 84      | 0            |
| 58  | DB    | 13     | 0        | 0        | 1       | 0            |
| 58  | DC    | 8      | 0        | 0        | 1       | 0            |
| 58  | DD    | 4      | 0        | 0        | 2       | 0            |
| 58  | DE    | 4      | 0        | 0        | 0       | 0            |
| 58  | DJ    | 1      | 0        | 0        | 0       | 0            |
| 58  | DL    | 4      | 0        | 0        | 1       | 0            |
| 58  | DN    | 2      | 0        | 0        | 0       | 0            |
| 58  | DS    | 2      | 0        | 0        | 0       | 0            |
| 58  | DT    | 3      | 0        | 0        | 1       | 0            |
| 58  | DU    | 1      | 0        | 0        | 0       | 0            |
| 58  | DV    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 288423 | 0        | 193016   | 10587   | 1            |

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 22.

The worst 5 of 10587 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) |
|------------------|--------------------|--------------------------|-------------------|
| 29:BH:117:LEU:O  | 29:BH:121:VAL:HG23 | 1.34                     | 1.22              |
| 22:BA:730:A:OP2  | 58:BA:3693:HOH:O   | 1.58                     | 1.21              |
| 1:AA:533:A:OP1   | 58:AA:1848:HOH:O   | 1.65                     | 1.15              |
| 29:BH:117:LEU:O  | 29:BH:121:VAL:CG2  | 1.95                     | 1.14              |
| 22:BA:2498:C:OP2 | 58:BA:3684:HOH:O   | 1.64                     | 1.13              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:CA:204:G:OP1 | 22:DA:289:G:O2'[3_545] | 2.12                     | 0.08              |

### 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 2   | AB    | 216/218 (99%) | 126 (58%) | 45 (21%) | 45 (21%) | 0           | 0 |
| 2   | CB    | 216/218 (99%) | 140 (65%) | 51 (24%) | 25 (12%) | 0           | 1 |
| 3   | AC    | 204/206 (99%) | 148 (72%) | 35 (17%) | 21 (10%) | 0           | 1 |
| 3   | CC    | 204/206 (99%) | 154 (76%) | 39 (19%) | 11 (5%)  | 2           | 5 |
| 4   | AD    | 203/205 (99%) | 137 (68%) | 39 (19%) | 27 (13%) | 0           | 0 |
| 4   | CD    | 203/205 (99%) | 152 (75%) | 32 (16%) | 19 (9%)  | 0           | 1 |
| 5   | AE    | 148/150 (99%) | 102 (69%) | 27 (18%) | 19 (13%) | 0           | 1 |
| 5   | CE    | 148/150 (99%) | 100 (68%) | 33 (22%) | 15 (10%) | 0           | 1 |
| 6   | AF    | 98/100 (98%)  | 73 (74%)  | 15 (15%) | 10 (10%) | 0           | 1 |
| 6   | CF    | 98/100 (98%)  | 68 (69%)  | 15 (15%) | 15 (15%) | 0           | 0 |
| 7   | AG    | 149/151 (99%) | 107 (72%) | 29 (20%) | 13 (9%)  | 1           | 1 |
| 7   | CG    | 149/151 (99%) | 119 (80%) | 22 (15%) | 8 (5%)   | 2           | 5 |
| 8   | AH    | 127/129 (98%) | 90 (71%)  | 28 (22%) | 9 (7%)   | 1           | 2 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8   | CH    | 127/129 (98%) | 98 (77%)  | 19 (15%) | 10 (8%)  | 1           | 2   |
| 9   | AI    | 125/127 (98%) | 87 (70%)  | 24 (19%) | 14 (11%) | 0           | 1   |
| 9   | CI    | 125/127 (98%) | 89 (71%)  | 18 (14%) | 18 (14%) | 0           | 0   |
| 10  | AJ    | 96/98 (98%)   | 64 (67%)  | 11 (12%) | 21 (22%) | 0           | 0   |
| 10  | CJ    | 96/98 (98%)   | 73 (76%)  | 11 (12%) | 12 (12%) | 0           | 1   |
| 11  | AK    | 115/117 (98%) | 81 (70%)  | 17 (15%) | 17 (15%) | 0           | 0   |
| 11  | CK    | 115/117 (98%) | 82 (71%)  | 24 (21%) | 9 (8%)   | 1           | 2   |
| 12  | AL    | 121/123 (98%) | 91 (75%)  | 21 (17%) | 9 (7%)   | 1           | 2   |
| 12  | CL    | 121/123 (98%) | 92 (76%)  | 18 (15%) | 11 (9%)  | 1           | 1   |
| 13  | AM    | 112/114 (98%) | 81 (72%)  | 21 (19%) | 10 (9%)  | 1           | 1   |
| 13  | CM    | 112/114 (98%) | 80 (71%)  | 18 (16%) | 14 (12%) | 0           | 1   |
| 14  | AN    | 92/100 (92%)  | 61 (66%)  | 21 (23%) | 10 (11%) | 0           | 1   |
| 14  | CN    | 92/100 (92%)  | 58 (63%)  | 20 (22%) | 14 (15%) | 0           | 0   |
| 15  | AO    | 86/88 (98%)   | 65 (76%)  | 14 (16%) | 7 (8%)   | 1           | 2   |
| 15  | CO    | 86/88 (98%)   | 64 (74%)  | 17 (20%) | 5 (6%)   | 1           | 4   |
| 16  | AP    | 80/82 (98%)   | 55 (69%)  | 15 (19%) | 10 (12%) | 0           | 1   |
| 16  | CP    | 80/82 (98%)   | 59 (74%)  | 13 (16%) | 8 (10%)  | 0           | 1   |
| 17  | AQ    | 78/80 (98%)   | 53 (68%)  | 18 (23%) | 7 (9%)   | 1           | 1   |
| 17  | CQ    | 78/80 (98%)   | 56 (72%)  | 15 (19%) | 7 (9%)   | 1           | 1   |
| 18  | AR    | 53/55 (96%)   | 42 (79%)  | 11 (21%) | 0        | 100         | 100 |
| 18  | CR    | 53/55 (96%)   | 37 (70%)  | 12 (23%) | 4 (8%)   | 1           | 2   |
| 19  | AS    | 77/79 (98%)   | 57 (74%)  | 11 (14%) | 9 (12%)  | 0           | 1   |
| 19  | CS    | 77/79 (98%)   | 55 (71%)  | 11 (14%) | 11 (14%) | 0           | 0   |
| 20  | AT    | 83/85 (98%)   | 59 (71%)  | 19 (23%) | 5 (6%)   | 1           | 4   |
| 20  | CT    | 83/85 (98%)   | 62 (75%)  | 12 (14%) | 9 (11%)  | 0           | 1   |
| 21  | AU    | 49/51 (96%)   | 26 (53%)  | 8 (16%)  | 15 (31%) | 0           | 0   |
| 21  | CU    | 49/51 (96%)   | 21 (43%)  | 16 (33%) | 12 (24%) | 0           | 0   |
| 24  | BC    | 269/271 (99%) | 218 (81%) | 39 (14%) | 12 (4%)  | 2           | 8   |
| 24  | DC    | 269/271 (99%) | 196 (73%) | 48 (18%) | 25 (9%)  | 0           | 1   |
| 25  | BD    | 207/209 (99%) | 180 (87%) | 21 (10%) | 6 (3%)   | 4           | 15  |
| 25  | DD    | 207/209 (99%) | 153 (74%) | 43 (21%) | 11 (5%)  | 2           | 6   |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 26  | BE    | 199/201 (99%) | 165 (83%) | 30 (15%) | 4 (2%)   | 7           | 24 |
| 26  | DE    | 199/201 (99%) | 154 (77%) | 27 (14%) | 18 (9%)  | 1           | 1  |
| 27  | BF    | 175/177 (99%) | 142 (81%) | 24 (14%) | 9 (5%)   | 2           | 6  |
| 27  | DF    | 175/177 (99%) | 135 (77%) | 27 (15%) | 13 (7%)  | 1           | 2  |
| 28  | BG    | 174/176 (99%) | 148 (85%) | 16 (9%)  | 10 (6%)  | 1           | 5  |
| 28  | DG    | 174/176 (99%) | 127 (73%) | 36 (21%) | 11 (6%)  | 1           | 3  |
| 29  | BH    | 147/149 (99%) | 89 (60%)  | 37 (25%) | 21 (14%) | 0           | 0  |
| 29  | DH    | 147/149 (99%) | 100 (68%) | 32 (22%) | 15 (10%) | 0           | 1  |
| 30  | BI    | 139/141 (99%) | 78 (56%)  | 37 (27%) | 24 (17%) | 0           | 0  |
| 30  | DI    | 139/141 (99%) | 82 (59%)  | 38 (27%) | 19 (14%) | 0           | 0  |
| 31  | BJ    | 140/142 (99%) | 125 (89%) | 14 (10%) | 1 (1%)   | 22          | 53 |
| 31  | DJ    | 140/142 (99%) | 104 (74%) | 23 (16%) | 13 (9%)  | 0           | 1  |
| 32  | BK    | 120/122 (98%) | 97 (81%)  | 14 (12%) | 9 (8%)   | 1           | 2  |
| 32  | DK    | 120/122 (98%) | 95 (79%)  | 15 (12%) | 10 (8%)  | 1           | 2  |
| 33  | BL    | 141/143 (99%) | 112 (79%) | 21 (15%) | 8 (6%)   | 1           | 5  |
| 33  | DL    | 141/143 (99%) | 98 (70%)  | 31 (22%) | 12 (8%)  | 1           | 1  |
| 34  | BM    | 134/136 (98%) | 120 (90%) | 11 (8%)  | 3 (2%)   | 6           | 22 |
| 34  | DM    | 134/136 (98%) | 112 (84%) | 17 (13%) | 5 (4%)   | 3           | 11 |
| 35  | BN    | 118/120 (98%) | 95 (80%)  | 21 (18%) | 2 (2%)   | 9           | 29 |
| 35  | DN    | 118/120 (98%) | 90 (76%)  | 18 (15%) | 10 (8%)  | 1           | 1  |
| 36  | BO    | 114/116 (98%) | 96 (84%)  | 14 (12%) | 4 (4%)   | 3           | 12 |
| 36  | DO    | 114/116 (98%) | 82 (72%)  | 24 (21%) | 8 (7%)   | 1           | 3  |
| 37  | BP    | 112/114 (98%) | 99 (88%)  | 8 (7%)   | 5 (4%)   | 2           | 8  |
| 37  | DP    | 112/114 (98%) | 88 (79%)  | 18 (16%) | 6 (5%)   | 2           | 5  |
| 38  | BQ    | 115/117 (98%) | 102 (89%) | 12 (10%) | 1 (1%)   | 17          | 46 |
| 38  | DQ    | 115/117 (98%) | 92 (80%)  | 22 (19%) | 1 (1%)   | 17          | 46 |
| 39  | BR    | 101/103 (98%) | 81 (80%)  | 10 (10%) | 10 (10%) | 0           | 1  |
| 39  | DR    | 101/103 (98%) | 72 (71%)  | 23 (23%) | 6 (6%)   | 1           | 4  |
| 40  | BS    | 108/110 (98%) | 94 (87%)  | 10 (9%)  | 4 (4%)   | 3           | 11 |
| 40  | DS    | 108/110 (98%) | 83 (77%)  | 17 (16%) | 8 (7%)   | 1           | 2  |
| 41  | BT    | 91/93 (98%)   | 74 (81%)  | 9 (10%)  | 8 (9%)   | 1           | 1  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 41  | DT    | 91/93 (98%)       | 53 (58%)   | 28 (31%)   | 10 (11%) | 0           | 1   |
| 42  | BU    | 100/102 (98%)     | 77 (77%)   | 19 (19%)   | 4 (4%)   | 3           | 9   |
| 42  | DU    | 100/102 (98%)     | 69 (69%)   | 19 (19%)   | 12 (12%) | 0           | 1   |
| 43  | BV    | 92/94 (98%)       | 84 (91%)   | 7 (8%)     | 1 (1%)   | 14          | 41  |
| 43  | DV    | 92/94 (98%)       | 76 (83%)   | 14 (15%)   | 2 (2%)   | 6           | 22  |
| 44  | BW    | 74/76 (97%)       | 68 (92%)   | 4 (5%)     | 2 (3%)   | 5           | 17  |
| 44  | DW    | 73/76 (96%)       | 61 (84%)   | 12 (16%)   | 0        | 100         | 100 |
| 45  | BX    | 75/77 (97%)       | 68 (91%)   | 6 (8%)     | 1 (1%)   | 12          | 36  |
| 45  | DX    | 75/77 (97%)       | 58 (77%)   | 12 (16%)   | 5 (7%)   | 1           | 3   |
| 46  | BY    | 61/63 (97%)       | 43 (70%)   | 10 (16%)   | 8 (13%)  | 0           | 1   |
| 46  | DY    | 61/63 (97%)       | 44 (72%)   | 12 (20%)   | 5 (8%)   | 1           | 2   |
| 47  | BZ    | 56/58 (97%)       | 54 (96%)   | 2 (4%)     | 0        | 100         | 100 |
| 47  | DZ    | 56/58 (97%)       | 41 (73%)   | 10 (18%)   | 5 (9%)   | 1           | 1   |
| 48  | B0    | 54/56 (96%)       | 46 (85%)   | 4 (7%)     | 4 (7%)   | 1           | 2   |
| 48  | D0    | 54/56 (96%)       | 37 (68%)   | 12 (22%)   | 5 (9%)   | 0           | 1   |
| 49  | B1    | 48/50 (96%)       | 40 (83%)   | 4 (8%)     | 4 (8%)   | 1           | 2   |
| 49  | D1    | 48/50 (96%)       | 36 (75%)   | 8 (17%)    | 4 (8%)   | 1           | 2   |
| 50  | B2    | 44/46 (96%)       | 37 (84%)   | 5 (11%)    | 2 (4%)   | 2           | 8   |
| 50  | D2    | 44/46 (96%)       | 34 (77%)   | 6 (14%)    | 4 (9%)   | 1           | 1   |
| 51  | B3    | 62/64 (97%)       | 56 (90%)   | 5 (8%)     | 1 (2%)   | 9           | 31  |
| 51  | D3    | 62/64 (97%)       | 52 (84%)   | 6 (10%)    | 4 (6%)   | 1           | 3   |
| 52  | B4    | 36/38 (95%)       | 31 (86%)   | 4 (11%)    | 1 (3%)   | 5           | 17  |
| 52  | D4    | 36/38 (95%)       | 32 (89%)   | 2 (6%)     | 2 (6%)   | 2           | 5   |
| 53  | B5    | 183/228 (80%)     | 87 (48%)   | 53 (29%)   | 43 (24%) | 0           | 0   |
| 54  | B6    | 2/8 (25%)         | 2 (100%)   | 0          | 0        | 100         | 100 |
| 54  | D6    | 2/8 (25%)         | 0          | 2 (100%)   | 0        | 100         | 100 |
| All | All   | 11422/11688 (98%) | 8528 (75%) | 1918 (17%) | 976 (8%) | 1           | 1   |

5 of 976 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 16  | PHE  |
| 2   | AB    | 20  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 22  | TYR  |
| 2   | AB    | 25  | PRO  |
| 2   | AB    | 34  | ALA  |

### 5.3.2 Protein sidechains [i](#)

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%) | 132 (73%) | 48 (27%) | 0           | 1  |
| 2   | CB    | 180/180 (100%) | 130 (72%) | 50 (28%) | 0           | 1  |
| 3   | AC    | 170/170 (100%) | 135 (79%) | 35 (21%) | 1           | 3  |
| 3   | CC    | 170/170 (100%) | 144 (85%) | 26 (15%) | 2           | 8  |
| 4   | AD    | 172/172 (100%) | 139 (81%) | 33 (19%) | 1           | 4  |
| 4   | CD    | 172/172 (100%) | 143 (83%) | 29 (17%) | 2           | 6  |
| 5   | AE    | 113/113 (100%) | 84 (74%)  | 29 (26%) | 0           | 1  |
| 5   | CE    | 113/113 (100%) | 86 (76%)  | 27 (24%) | 0           | 2  |
| 6   | AF    | 87/87 (100%)   | 69 (79%)  | 18 (21%) | 1           | 3  |
| 6   | CF    | 87/87 (100%)   | 61 (70%)  | 26 (30%) | 0           | 1  |
| 7   | AG    | 124/124 (100%) | 101 (82%) | 23 (18%) | 1           | 5  |
| 7   | CG    | 124/124 (100%) | 99 (80%)  | 25 (20%) | 1           | 4  |
| 8   | AH    | 104/104 (100%) | 84 (81%)  | 20 (19%) | 1           | 4  |
| 8   | CH    | 104/104 (100%) | 82 (79%)  | 22 (21%) | 1           | 3  |
| 9   | AI    | 105/105 (100%) | 77 (73%)  | 28 (27%) | 0           | 1  |
| 9   | CI    | 105/105 (100%) | 88 (84%)  | 17 (16%) | 2           | 7  |
| 10  | AJ    | 86/86 (100%)   | 67 (78%)  | 19 (22%) | 1           | 3  |
| 10  | CJ    | 86/86 (100%)   | 68 (79%)  | 18 (21%) | 1           | 3  |
| 11  | AK    | 90/90 (100%)   | 76 (84%)  | 14 (16%) | 2           | 8  |
| 11  | CK    | 90/90 (100%)   | 71 (79%)  | 19 (21%) | 1           | 3  |
| 12  | AL    | 103/103 (100%) | 89 (86%)  | 14 (14%) | 3           | 11 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 12  | CL    | 103/103 (100%) | 82 (80%)  | 21 (20%) | 1           | 4  |
| 13  | AM    | 92/92 (100%)   | 74 (80%)  | 18 (20%) | 1           | 4  |
| 13  | CM    | 92/92 (100%)   | 75 (82%)  | 17 (18%) | 1           | 5  |
| 14  | AN    | 79/83 (95%)    | 64 (81%)  | 15 (19%) | 1           | 4  |
| 14  | CN    | 79/83 (95%)    | 70 (89%)  | 9 (11%)  | 5           | 18 |
| 15  | AO    | 75/76 (99%)    | 63 (84%)  | 12 (16%) | 2           | 7  |
| 15  | CO    | 75/76 (99%)    | 65 (87%)  | 10 (13%) | 4           | 12 |
| 16  | AP    | 65/65 (100%)   | 50 (77%)  | 15 (23%) | 1           | 2  |
| 16  | CP    | 65/65 (100%)   | 54 (83%)  | 11 (17%) | 2           | 6  |
| 17  | AQ    | 74/74 (100%)   | 50 (68%)  | 24 (32%) | 0           | 0  |
| 17  | CQ    | 74/74 (100%)   | 51 (69%)  | 23 (31%) | 0           | 0  |
| 18  | AR    | 48/48 (100%)   | 38 (79%)  | 10 (21%) | 1           | 3  |
| 18  | CR    | 48/48 (100%)   | 38 (79%)  | 10 (21%) | 1           | 3  |
| 19  | AS    | 70/70 (100%)   | 55 (79%)  | 15 (21%) | 1           | 3  |
| 19  | CS    | 70/70 (100%)   | 58 (83%)  | 12 (17%) | 2           | 6  |
| 20  | AT    | 65/65 (100%)   | 51 (78%)  | 14 (22%) | 1           | 3  |
| 20  | CT    | 65/65 (100%)   | 57 (88%)  | 8 (12%)  | 4           | 15 |
| 21  | AU    | 44/44 (100%)   | 29 (66%)  | 15 (34%) | 0           | 0  |
| 21  | CU    | 44/44 (100%)   | 29 (66%)  | 15 (34%) | 0           | 0  |
| 24  | BC    | 216/216 (100%) | 189 (88%) | 27 (12%) | 4           | 14 |
| 24  | DC    | 216/216 (100%) | 197 (91%) | 19 (9%)  | 10          | 29 |
| 25  | BD    | 164/164 (100%) | 148 (90%) | 16 (10%) | 8           | 24 |
| 25  | DD    | 164/164 (100%) | 145 (88%) | 19 (12%) | 5           | 17 |
| 26  | BE    | 165/165 (100%) | 136 (82%) | 29 (18%) | 2           | 5  |
| 26  | DE    | 165/165 (100%) | 137 (83%) | 28 (17%) | 2           | 6  |
| 27  | BF    | 148/148 (100%) | 116 (78%) | 32 (22%) | 1           | 3  |
| 27  | DF    | 148/148 (100%) | 119 (80%) | 29 (20%) | 1           | 4  |
| 28  | BG    | 137/137 (100%) | 118 (86%) | 19 (14%) | 3           | 11 |
| 28  | DG    | 137/137 (100%) | 114 (83%) | 23 (17%) | 2           | 6  |
| 29  | BH    | 114/114 (100%) | 88 (77%)  | 26 (23%) | 1           | 2  |
| 29  | DH    | 114/114 (100%) | 88 (77%)  | 26 (23%) | 1           | 2  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 30  | BI    | 109/109 (100%) | 82 (75%)  | 27 (25%) | 0           | 2  |
| 30  | DI    | 109/109 (100%) | 80 (73%)  | 29 (27%) | 0           | 1  |
| 31  | BJ    | 116/116 (100%) | 105 (90%) | 11 (10%) | 8           | 25 |
| 31  | DJ    | 116/116 (100%) | 94 (81%)  | 22 (19%) | 1           | 4  |
| 32  | BK    | 103/103 (100%) | 89 (86%)  | 14 (14%) | 3           | 11 |
| 32  | DK    | 103/103 (100%) | 90 (87%)  | 13 (13%) | 4           | 14 |
| 33  | BL    | 102/102 (100%) | 91 (89%)  | 11 (11%) | 6           | 19 |
| 33  | DL    | 102/102 (100%) | 86 (84%)  | 16 (16%) | 2           | 8  |
| 34  | BM    | 109/109 (100%) | 99 (91%)  | 10 (9%)  | 9           | 27 |
| 34  | DM    | 109/109 (100%) | 95 (87%)  | 14 (13%) | 4           | 13 |
| 35  | BN    | 100/100 (100%) | 94 (94%)  | 6 (6%)   | 19          | 48 |
| 35  | DN    | 100/100 (100%) | 76 (76%)  | 24 (24%) | 0           | 2  |
| 36  | BO    | 86/86 (100%)   | 65 (76%)  | 21 (24%) | 0           | 2  |
| 36  | DO    | 86/86 (100%)   | 70 (81%)  | 16 (19%) | 1           | 5  |
| 37  | BP    | 99/99 (100%)   | 81 (82%)  | 18 (18%) | 1           | 5  |
| 37  | DP    | 99/99 (100%)   | 90 (91%)  | 9 (9%)   | 9           | 27 |
| 38  | BQ    | 89/89 (100%)   | 78 (88%)  | 11 (12%) | 4           | 14 |
| 38  | DQ    | 89/89 (100%)   | 78 (88%)  | 11 (12%) | 4           | 14 |
| 39  | BR    | 84/84 (100%)   | 74 (88%)  | 10 (12%) | 5           | 16 |
| 39  | DR    | 84/84 (100%)   | 76 (90%)  | 8 (10%)  | 8           | 25 |
| 40  | BS    | 93/93 (100%)   | 76 (82%)  | 17 (18%) | 1           | 5  |
| 40  | DS    | 93/93 (100%)   | 83 (89%)  | 10 (11%) | 6           | 19 |
| 41  | BT    | 80/80 (100%)   | 68 (85%)  | 12 (15%) | 3           | 9  |
| 41  | DT    | 80/80 (100%)   | 66 (82%)  | 14 (18%) | 2           | 6  |
| 42  | BU    | 83/83 (100%)   | 72 (87%)  | 11 (13%) | 4           | 12 |
| 42  | DU    | 83/83 (100%)   | 68 (82%)  | 15 (18%) | 1           | 5  |
| 43  | BV    | 78/78 (100%)   | 63 (81%)  | 15 (19%) | 1           | 4  |
| 43  | DV    | 78/78 (100%)   | 65 (83%)  | 13 (17%) | 2           | 6  |
| 44  | BW    | 57/58 (98%)    | 47 (82%)  | 10 (18%) | 2           | 6  |
| 44  | DW    | 56/58 (97%)    | 50 (89%)  | 6 (11%)  | 6           | 20 |
| 45  | BX    | 67/67 (100%)   | 61 (91%)  | 6 (9%)   | 9           | 28 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |     |
|-----|-------|-----------------|------------|------------|-------------|-----|
| 45  | DX    | 67/67 (100%)    | 58 (87%)   | 9 (13%)    | 4           | 12  |
| 46  | BY    | 55/55 (100%)    | 50 (91%)   | 5 (9%)     | 9           | 27  |
| 46  | DY    | 55/55 (100%)    | 43 (78%)   | 12 (22%)   | 1           | 3   |
| 47  | BZ    | 48/48 (100%)    | 41 (85%)   | 7 (15%)    | 3           | 9   |
| 47  | DZ    | 48/48 (100%)    | 38 (79%)   | 10 (21%)   | 1           | 3   |
| 48  | B0    | 47/47 (100%)    | 42 (89%)   | 5 (11%)    | 6           | 20  |
| 48  | D0    | 47/47 (100%)    | 43 (92%)   | 4 (8%)     | 10          | 31  |
| 49  | B1    | 45/45 (100%)    | 42 (93%)   | 3 (7%)     | 16          | 43  |
| 49  | D1    | 45/45 (100%)    | 39 (87%)   | 6 (13%)    | 4           | 12  |
| 50  | B2    | 38/38 (100%)    | 34 (90%)   | 4 (10%)    | 7           | 20  |
| 50  | D2    | 38/38 (100%)    | 31 (82%)   | 7 (18%)    | 1           | 5   |
| 51  | B3    | 51/51 (100%)    | 45 (88%)   | 6 (12%)    | 5           | 16  |
| 51  | D3    | 51/51 (100%)    | 46 (90%)   | 5 (10%)    | 8           | 24  |
| 52  | B4    | 34/34 (100%)    | 32 (94%)   | 2 (6%)     | 19          | 49  |
| 52  | D4    | 34/34 (100%)    | 26 (76%)   | 8 (24%)    | 1           | 2   |
| 53  | B5    | 61/180 (34%)    | 48 (79%)   | 13 (21%)   | 1           | 3   |
| 54  | B6    | 2/2 (100%)      | 2 (100%)   | 0          | 100         | 100 |
| 54  | D6    | 2/2 (100%)      | 2 (100%)   | 0          | 100         | 100 |
| All | All   | 9390/9522 (99%) | 7747 (82%) | 1643 (18%) | 2           | 6   |

5 of 1643 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CD    | 200 | ILE  |
| 16  | CP    | 55  | ASP  |
| 46  | DY    | 49  | ASP  |
| 5   | CE    | 153 | VAL  |
| 4   | CD    | 192 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DC    | 251 | GLN  |
| 39  | DR    | 89  | HIS  |
| 25  | DD    | 140 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | DH    | 128 | HIS  |
| 42  | DU    | 74  | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1537/1539 (99%) | 324 (21%)         | 11 (0%)         |
| 1   | CA    | 1538/1539 (99%) | 342 (22%)         | 10 (0%)         |
| 22  | BA    | 2895/2903 (99%) | 579 (20%)         | 24 (0%)         |
| 22  | DA    | 2895/2903 (99%) | 704 (24%)         | 32 (1%)         |
| 23  | BB    | 118/119 (99%)   | 16 (13%)          | 0               |
| 23  | DB    | 117/119 (98%)   | 20 (17%)          | 0               |
| All | All   | 9100/9122 (99%) | 1985 (21%)        | 77 (0%)         |

5 of 1985 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 3   | A    |
| 1   | AA    | 4   | U    |
| 1   | AA    | 5   | U    |
| 1   | AA    | 6   | G    |
| 1   | AA    | 9   | G    |

5 of 77 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1514 | G    |
| 22  | DA    | 2326 | C    |
| 22  | DA    | 1847 | A    |
| 22  | DA    | 2157 | G    |
| 22  | DA    | 2756 | U    |

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 54  | DBB  | D6    | 3   | 54   | 4,5,6        | 1.18 | 0           | 1,5,7       | 1.37 | 0           |
| 54  | MHV  | B6    | 6   | 54   | 7,9,10       | 1.59 | 1 (14%)     | 7,11,13     | 3.44 | 4 (57%)     |
| 54  | DBB  | B6    | 3   | 54   | 4,5,6        | 1.31 | 0           | 1,5,7       | 2.61 | 1 (100%)    |
| 54  | MHW  | B6    | 1   | 54   | 9,9,10       | 1.64 | 1 (11%)     | 10,11,13    | 2.86 | 4 (40%)     |
| 54  | MHU  | D6    | 5   | 54   | 14,15,16     | 1.63 | 3 (21%)     | 18,19,21    | 1.15 | 2 (11%)     |
| 54  | MHW  | D6    | 1   | 54   | 9,9,10       | 1.95 | 1 (11%)     | 10,11,13    | 3.07 | 4 (40%)     |
| 54  | MHU  | B6    | 5   | 54   | 14,15,16     | 1.80 | 3 (21%)     | 18,19,21    | 1.27 | 3 (16%)     |
| 54  | 004  | B6    | 7   | 54   | 9,10,11      | 1.52 | 1 (11%)     | 9,12,14     | 2.03 | 3 (33%)     |
| 54  | 004  | D6    | 7   | 54   | 9,10,11      | 0.78 | 0           | 9,12,14     | 0.60 | 0           |
| 54  | MHV  | D6    | 6   | 54   | 7,9,10       | 1.19 | 0           | 7,11,13     | 3.21 | 4 (57%)     |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 54  | DBB  | D6    | 3   | 54   | -       | 0/3/4/6   | -       |
| 54  | MHV  | B6    | 6   | 54   | -       | 0/1/12/14 | 0/1/1/1 |
| 54  | DBB  | B6    | 3   | 54   | -       | 1/3/4/6   | -       |
| 54  | MHW  | B6    | 1   | 54   | -       | 0/2/2/4   | 0/1/1/1 |
| 54  | MHU  | D6    | 5   | 54   | -       | 0/9/12/14 | 0/1/1/1 |
| 54  | MHW  | D6    | 1   | 54   | -       | 0/2/2/4   | 0/1/1/1 |
| 54  | MHU  | B6    | 5   | 54   | -       | 0/9/12/14 | 0/1/1/1 |
| 54  | 004  | B6    | 7   | 54   | -       | 1/4/6/8   | 0/1/1/1 |
| 54  | 004  | D6    | 7   | 54   | -       | 2/4/6/8   | 0/1/1/1 |
| 54  | MHV  | D6    | 6   | 54   | -       | 0/1/12/14 | 0/1/1/1 |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 54  | D6    | 1   | MHW  | CA-C  | 5.22  | 1.54        | 1.48     |
| 54  | B6    | 5   | MHU  | CZ-NZ | 5.22  | 1.49        | 1.37     |
| 54  | D6    | 5   | MHU  | CZ-NZ | 4.69  | 1.48        | 1.37     |
| 54  | B6    | 7   | 004  | CB-CA | -4.30 | 1.48        | 1.52     |
| 54  | B6    | 1   | MHW  | CA-C  | 3.99  | 1.52        | 1.48     |

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



| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 54  | D6    | 1   | MHW  | CD-CE-N   | 6.55  | 134.13      | 123.43   |
| 54  | B6    | 1   | MHW  | CD-CE-N   | 5.89  | 133.04      | 123.43   |
| 54  | B6    | 6   | MHV  | CD2-CG-CB | 5.52  | 124.11      | 115.89   |
| 54  | D6    | 6   | MHV  | CD2-CE-N  | -5.22 | 98.62       | 110.03   |
| 54  | D6    | 6   | MHV  | CD2-CG-CB | 5.13  | 123.53      | 115.89   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 54  | B6    | 3   | DBB  | N-CA-CB-CG  |
| 54  | D6    | 7   | 004  | C-CA-CB-CG1 |
| 54  | D6    | 7   | 004  | C-CA-CB-CG2 |
| 54  | B6    | 7   | 004  | C-CA-CB-CG1 |

There are no ring outliers.

6 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 54  | D6    | 3   | DBB  | 1       | 0            |
| 54  | D6    | 5   | MHU  | 3       | 0            |
| 54  | D6    | 1   | MHW  | 2       | 0            |
| 54  | B6    | 7   | 004  | 1       | 0            |
| 54  | D6    | 7   | 004  | 4       | 0            |
| 54  | D6    | 6   | MHV  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 56  | DOL  | BA    | 3001 | -    | 43,50,50     | 2.86 | 13 (30%) | 51,70,70    | 2.88 | 14 (27%) |
| 56  | DOL  | DA    | 3001 | -    | 43,50,50     | 2.90 | 13 (30%) | 51,70,70    | 2.81 | 13 (25%) |

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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 56  | DOL  | BA    | 3001 | -    | -       | 18/58/77/77 | 0/2/3/3 |
| 56  | DOL  | DA    | 3001 | -    | -       | 10/58/77/77 | 0/2/3/3 |

The worst 5 of 26 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 56  | DA    | 3001 | DOL  | O15-C14 | 9.27 | 1.37        | 1.21     |
| 56  | BA    | 3001 | DOL  | O15-C14 | 8.90 | 1.36        | 1.21     |
| 56  | DA    | 3001 | DOL  | C22-C23 | 8.04 | 1.53        | 1.32     |
| 56  | BA    | 3001 | DOL  | C22-C23 | 7.76 | 1.52        | 1.32     |
| 56  | DA    | 3001 | DOL  | O38-C37 | 6.42 | 1.37        | 1.21     |

The worst 5 of 27 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 56  | DA    | 3001 | DOL  | O40-S39-O41 | -15.45 | 100.57      | 118.19   |
| 56  | BA    | 3001 | DOL  | O40-S39-O41 | -14.66 | 101.47      | 118.19   |
| 56  | BA    | 3001 | DOL  | C8-C6-N5    | 6.55   | 127.31      | 119.76   |
| 56  | BA    | 3001 | DOL  | C29-C28-C26 | -5.90  | 107.93      | 122.69   |
| 56  | DA    | 3001 | DOL  | C4-N5-C1    | -5.06  | 106.22      | 112.45   |

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

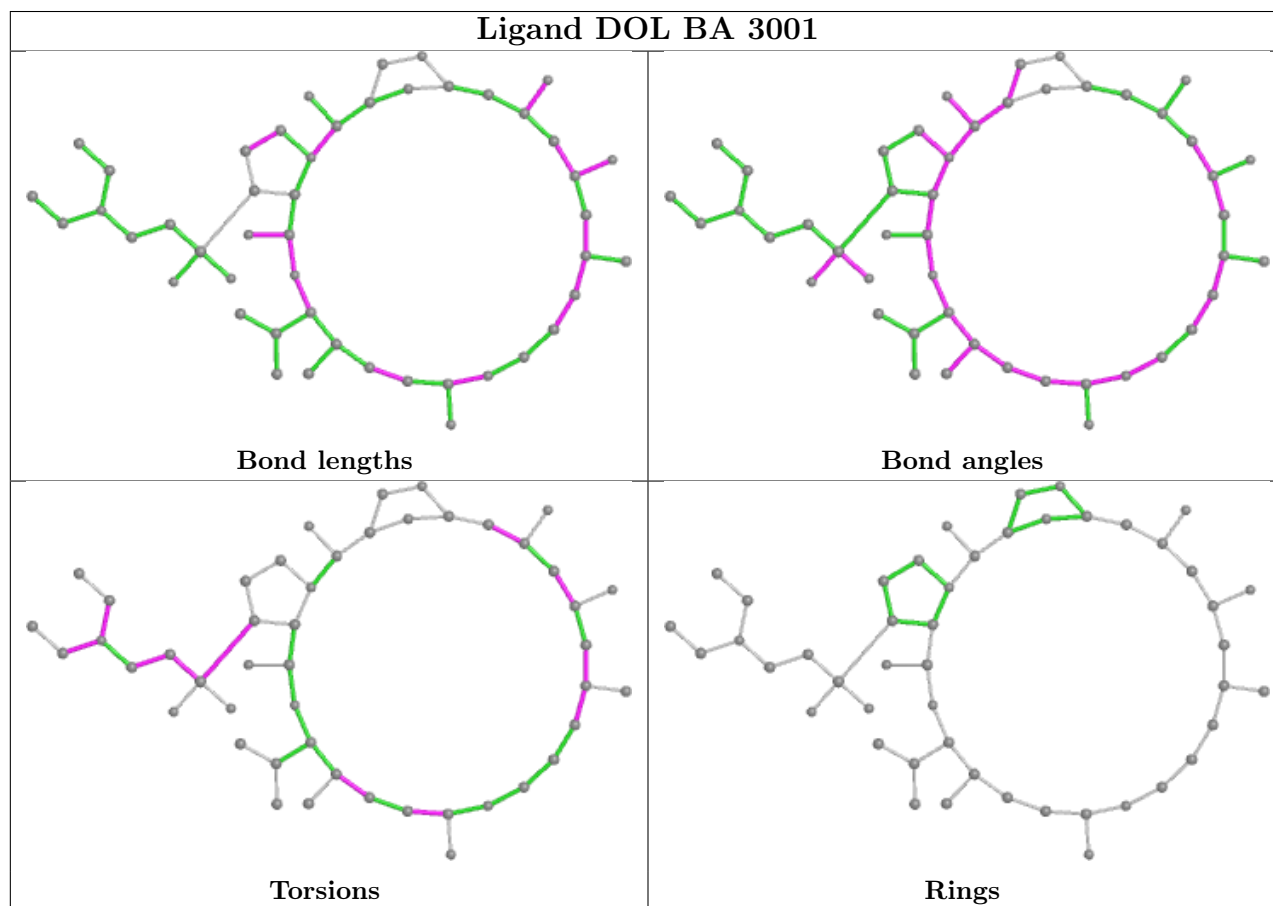
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 56  | BA    | 3001 | DOL  | C1-C2-S39-O40   |
| 56  | BA    | 3001 | DOL  | C1-C2-S39-C42   |
| 56  | BA    | 3001 | DOL  | S39-C42-C43-N44 |
| 56  | BA    | 3001 | DOL  | C14-C16-C17-O18 |
| 56  | BA    | 3001 | DOL  | C17-C19-C20-C22 |

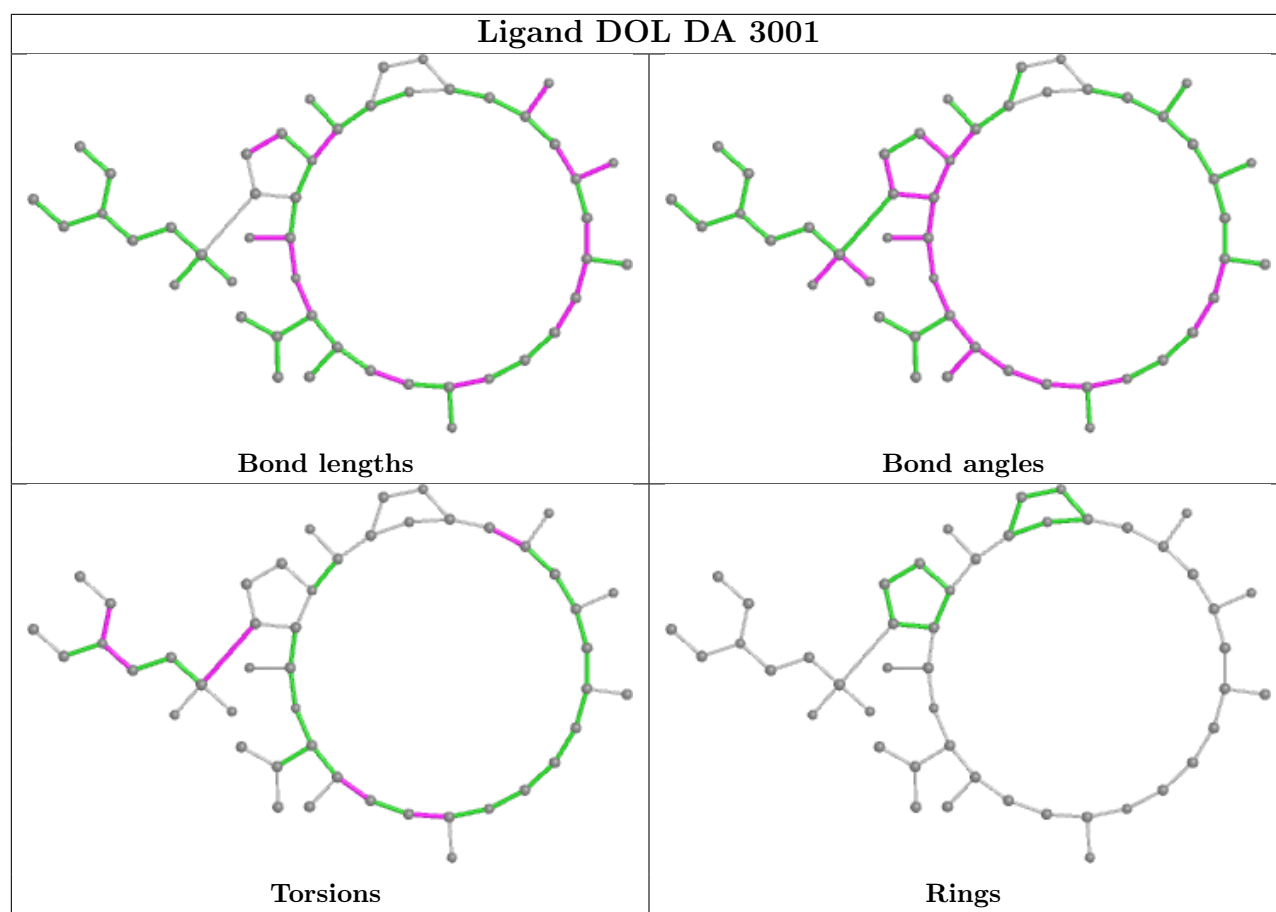
There are no ring outliers.

2 monomers are involved in 40 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 56  | BA    | 3001 | DOL  | 15      | 0            |
| 56  | DA    | 3001 | DOL  | 25      | 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1538/1539 (99%)  | -0.16  | 22 (1%) 75 70 | 10, 49, 132, 182      | 0     |
| 1   | CA    | 1539/1539 (100%) | 0.16   | 55 (3%) 42 32 | 22, 70, 146, 178      | 0     |
| 2   | AB    | 218/218 (100%)   | 0.80   | 29 (13%) 3 2  | 36, 73, 100, 117      | 0     |
| 2   | CB    | 218/218 (100%)   | 1.05   | 45 (20%) 1 0  | 57, 86, 108, 121      | 0     |
| 3   | AC    | 206/206 (100%)   | 0.15   | 10 (4%) 29 20 | 33, 57, 78, 95        | 0     |
| 3   | CC    | 206/206 (100%)   | 1.19   | 50 (24%) 0 0  | 55, 80, 96, 107       | 0     |
| 4   | AD    | 205/205 (100%)   | 0.36   | 8 (3%) 39 29  | 31, 56, 79, 99        | 0     |
| 4   | CD    | 205/205 (100%)   | -0.03  | 5 (2%) 59 49  | 13, 35, 60, 82        | 0     |
| 5   | AE    | 150/150 (100%)   | 0.10   | 2 (1%) 77 72  | 26, 47, 78, 93        | 0     |
| 5   | CE    | 150/150 (100%)   | 0.18   | 1 (0%) 87 84  | 25, 52, 84, 104       | 0     |
| 6   | AF    | 100/100 (100%)   | -0.18  | 1 (1%) 82 77  | 32, 54, 73, 77        | 0     |
| 6   | CF    | 100/100 (100%)   | 0.53   | 10 (10%) 7 4  | 41, 74, 92, 103       | 0     |
| 7   | AG    | 151/151 (100%)   | 0.26   | 3 (1%) 65 56  | 51, 75, 92, 100       | 0     |
| 7   | CG    | 151/151 (100%)   | 2.56   | 85 (56%) 0 0  | 82, 106, 114, 118     | 0     |
| 8   | AH    | 129/129 (100%)   | 0.18   | 2 (1%) 72 66  | 29, 46, 67, 79        | 0     |
| 8   | CH    | 129/129 (100%)   | 0.45   | 10 (7%) 13 7  | 46, 64, 80, 94        | 0     |
| 9   | AI    | 127/127 (100%)   | 0.93   | 22 (17%) 1 1  | 40, 74, 98, 107       | 0     |
| 9   | CI    | 127/127 (100%)   | 1.84   | 45 (35%) 0 0  | 79, 96, 112, 121      | 0     |
| 10  | AJ    | 98/98 (100%)     | 0.64   | 7 (7%) 16 9   | 38, 66, 86, 116       | 0     |
| 10  | CJ    | 98/98 (100%)     | 2.70   | 59 (60%) 0 0  | 72, 97, 115, 123      | 0     |
| 11  | AK    | 117/117 (100%)   | 0.49   | 10 (8%) 10 5  | 25, 60, 89, 119       | 0     |
| 11  | CK    | 117/117 (100%)   | 0.23   | 2 (1%) 70 63  | 35, 68, 79, 90        | 0     |
| 12  | AL    | 123/123 (100%)   | 0.15   | 6 (4%) 29 20  | 20, 34, 65, 97        | 0     |
| 12  | CL    | 123/123 (100%)   | 0.32   | 3 (2%) 59 49  | 30, 50, 74, 95        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13  | AM    | 114/114 (100%)  | 0.42   | 10 (8%) 10 5   | 47, 69, 91, 103       | 0     |
| 13  | CM    | 114/114 (100%)  | 3.11   | 76 (66%) 0 0   | 93, 113, 122, 125     | 0     |
| 14  | AN    | 96/100 (96%)    | 0.67   | 11 (11%) 4 2   | 36, 60, 96, 105       | 0     |
| 14  | CN    | 96/100 (96%)    | 2.16   | 44 (45%) 0 0   | 70, 96, 115, 122      | 0     |
| 15  | AO    | 88/88 (100%)    | 0.35   | 3 (3%) 45 35   | 29, 47, 64, 91        | 0     |
| 15  | CO    | 88/88 (100%)    | 0.32   | 3 (3%) 45 35   | 36, 64, 80, 102       | 0     |
| 16  | AP    | 82/82 (100%)    | 0.69   | 6 (7%) 15 8    | 34, 47, 83, 109       | 0     |
| 16  | CP    | 82/82 (100%)    | 0.98   | 11 (13%) 3 1   | 45, 62, 91, 112       | 0     |
| 17  | AQ    | 80/80 (100%)    | 0.26   | 3 (3%) 40 30   | 27, 48, 75, 111       | 0     |
| 17  | CQ    | 80/80 (100%)    | 1.14   | 19 (23%) 0 0   | 42, 77, 97, 99        | 0     |
| 18  | AR    | 55/55 (100%)    | 0.22   | 3 (5%) 25 16   | 40, 52, 77, 102       | 0     |
| 18  | CR    | 55/55 (100%)    | 0.28   | 4 (7%) 15 8    | 36, 54, 78, 108       | 0     |
| 19  | AS    | 79/79 (100%)    | 0.70   | 13 (16%) 1 1   | 54, 70, 88, 97        | 0     |
| 19  | CS    | 79/79 (100%)    | 3.96   | 58 (73%) 0 0   | 95, 114, 122, 128     | 0     |
| 20  | AT    | 85/85 (100%)    | 0.43   | 4 (4%) 31 22   | 35, 48, 68, 96        | 0     |
| 20  | CT    | 85/85 (100%)    | 1.81   | 33 (38%) 0 0   | 53, 78, 96, 101       | 0     |
| 21  | AU    | 51/51 (100%)    | 1.26   | 12 (23%) 0 0   | 41, 74, 95, 105       | 0     |
| 21  | CU    | 51/51 (100%)    | 0.68   | 6 (11%) 4 2    | 42, 69, 98, 102       | 0     |
| 22  | BA    | 2897/2903 (99%) | 0.14   | 106 (3%) 41 31 | 0, 14, 129, 195       | 0     |
| 22  | DA    | 2897/2903 (99%) | 0.40   | 129 (4%) 33 23 | 41, 85, 148, 181      | 0     |
| 23  | BB    | 119/119 (100%)  | -0.36  | 0 100 100      | 2, 23, 46, 81         | 0     |
| 23  | DB    | 118/119 (99%)   | 0.19   | 4 (3%) 45 35   | 69, 115, 134, 142     | 0     |
| 24  | BC    | 271/271 (100%)  | -0.18  | 1 (0%) 92 91   | 2, 18, 35, 55         | 0     |
| 24  | DC    | 271/271 (100%)  | 0.73   | 32 (11%) 4 2   | 46, 64, 77, 95        | 0     |
| 25  | BD    | 209/209 (100%)  | -0.25  | 0 100 100      | 0, 9, 34, 65          | 0     |
| 25  | DD    | 209/209 (100%)  | 1.16   | 44 (21%) 1 0   | 53, 72, 87, 97        | 0     |
| 26  | BE    | 201/201 (100%)  | -0.30  | 0 100 100      | 1, 23, 54, 88         | 0     |
| 26  | DE    | 201/201 (100%)  | 1.86   | 80 (39%) 0 0   | 52, 89, 105, 113      | 0     |
| 27  | BF    | 177/177 (100%)  | 0.19   | 4 (2%) 60 51   | 21, 40, 74, 88        | 0     |
| 27  | DF    | 177/177 (100%)  | 3.27   | 128 (72%) 0 0  | 94, 113, 124, 131     | 0     |
| 28  | BG    | 176/176 (100%)  | 0.04   | 3 (1%) 70 63   | 15, 35, 58, 72        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | DG    | 176/176 (100%) | 2.22   | 89 (50%) 0 0  | 78, 96, 110, 121      | 0     |
| 29  | BH    | 149/149 (100%) | 3.01   | 73 (48%) 0 0  | 25, 102, 121, 129     | 0     |
| 29  | DH    | 149/149 (100%) | 1.18   | 30 (20%) 1 0  | 25, 92, 107, 115      | 0     |
| 30  | BI    | 141/141 (100%) | 3.56   | 100 (70%) 0 0 | 89, 116, 126, 134     | 0     |
| 30  | DI    | 141/141 (100%) | 4.83   | 120 (85%) 0 0 | 105, 124, 135, 142    | 0     |
| 31  | BJ    | 142/142 (100%) | -0.27  | 0 100 100     | 1, 6, 26, 35          | 0     |
| 31  | DJ    | 142/142 (100%) | 0.84   | 16 (11%) 5 3  | 49, 69, 83, 91        | 0     |
| 32  | BK    | 122/122 (100%) | -0.34  | 0 100 100     | 3, 11, 28, 60         | 0     |
| 32  | DK    | 122/122 (100%) | 1.12   | 29 (23%) 0 0  | 48, 66, 84, 95        | 0     |
| 33  | BL    | 143/143 (100%) | -0.13  | 0 100 100     | 1, 18, 42, 65         | 0     |
| 33  | DL    | 143/143 (100%) | 1.95   | 62 (43%) 0 0  | 43, 87, 98, 115       | 0     |
| 34  | BM    | 136/136 (100%) | -0.38  | 0 100 100     | 1, 10, 24, 85         | 0     |
| 34  | DM    | 136/136 (100%) | 1.01   | 26 (19%) 1 1  | 44, 70, 85, 99        | 0     |
| 35  | BN    | 120/120 (100%) | -0.25  | 0 100 100     | 2, 7, 17, 65          | 0     |
| 35  | DN    | 120/120 (100%) | 1.29   | 28 (23%) 0 0  | 58, 78, 92, 112       | 0     |
| 36  | BO    | 116/116 (100%) | -0.21  | 0 100 100     | 14, 24, 42, 54        | 0     |
| 36  | DO    | 116/116 (100%) | 2.77   | 75 (64%) 0 0  | 85, 99, 110, 117      | 0     |
| 37  | BP    | 114/114 (100%) | -0.22  | 1 (0%) 84 80  | 6, 16, 41, 71         | 0     |
| 37  | DP    | 114/114 (100%) | 1.07   | 27 (23%) 0 0  | 61, 74, 86, 94        | 0     |
| 38  | BQ    | 117/117 (100%) | -0.31  | 0 100 100     | 0, 3, 12, 30          | 0     |
| 38  | DQ    | 117/117 (100%) | 1.15   | 25 (21%) 0 0  | 55, 70, 81, 89        | 0     |
| 39  | BR    | 103/103 (100%) | -0.29  | 0 100 100     | 0, 11, 31, 56         | 0     |
| 39  | DR    | 103/103 (100%) | 1.66   | 35 (33%) 0 0  | 57, 80, 92, 103       | 0     |
| 40  | BS    | 110/110 (100%) | -0.22  | 0 100 100     | 1, 4, 21, 68          | 0     |
| 40  | DS    | 110/110 (100%) | 2.12   | 53 (48%) 0 0  | 60, 79, 94, 105       | 0     |
| 41  | BT    | 93/93 (100%)   | 0.19   | 3 (3%) 47 37  | 10, 24, 68, 98        | 0     |
| 41  | DT    | 93/93 (100%)   | 2.71   | 57 (61%) 0 0  | 73, 91, 106, 115      | 0     |
| 42  | BU    | 102/102 (100%) | -0.22  | 2 (1%) 65 56  | 10, 25, 58, 77        | 0     |
| 42  | DU    | 102/102 (100%) | 3.20   | 65 (63%) 0 0  | 77, 95, 109, 120      | 0     |
| 43  | BV    | 94/94 (100%)   | -0.27  | 0 100 100     | 4, 18, 39, 52         | 0     |
| 43  | DV    | 94/94 (100%)   | 1.14   | 21 (22%) 0 0  | 72, 86, 98, 105       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | BW    | 76/76 (100%)      | -0.15  | 2 (2%) 56 46   | 4, 11, 27, 57         | 0     |
| 44  | DW    | 75/76 (98%)       | 2.04   | 39 (52%) 0 0   | 58, 83, 93, 104       | 0     |
| 45  | BX    | 77/77 (100%)      | -0.24  | 0 100 100      | 8, 22, 48, 68         | 0     |
| 45  | DX    | 77/77 (100%)      | 1.11   | 15 (19%) 1 0   | 47, 72, 87, 91        | 0     |
| 46  | BY    | 63/63 (100%)      | 0.23   | 3 (4%) 30 21   | 18, 38, 71, 94        | 0     |
| 46  | DY    | 63/63 (100%)      | 1.95   | 30 (47%) 0 0   | 81, 99, 106, 109      | 0     |
| 47  | BZ    | 58/58 (100%)      | -0.22  | 0 100 100      | 2, 6, 25, 34          | 0     |
| 47  | DZ    | 58/58 (100%)      | 0.83   | 7 (12%) 4 2    | 60, 73, 85, 103       | 0     |
| 48  | B0    | 56/56 (100%)      | -0.30  | 0 100 100      | 0, 7, 33, 60          | 0     |
| 48  | D0    | 56/56 (100%)      | 1.49   | 17 (30%) 0 0   | 51, 82, 95, 103       | 0     |
| 49  | B1    | 50/50 (100%)      | -0.23  | 1 (2%) 65 56   | 13, 25, 49, 57        | 0     |
| 49  | D1    | 50/50 (100%)      | 1.73   | 15 (30%) 0 0   | 73, 89, 94, 106       | 0     |
| 50  | B2    | 46/46 (100%)      | -0.14  | 1 (2%) 62 52   | 4, 8, 15, 79          | 0     |
| 50  | D2    | 46/46 (100%)      | 1.94   | 19 (41%) 0 0   | 58, 72, 86, 101       | 0     |
| 51  | B3    | 64/64 (100%)      | -0.18  | 0 100 100      | 4, 9, 17, 29          | 0     |
| 51  | D3    | 64/64 (100%)      | 1.69   | 26 (40%) 0 0   | 60, 75, 84, 94        | 0     |
| 52  | B4    | 38/38 (100%)      | -0.13  | 0 100 100      | 5, 15, 29, 52         | 0     |
| 52  | D4    | 38/38 (100%)      | 2.23   | 18 (47%) 0 0   | 62, 77, 88, 98        | 0     |
| 53  | B5    | 191/228 (83%)     | 6.24   | 186 (97%) 0 0  | 100, 121, 133, 141    | 0     |
| 54  | B6    | 2/8 (25%)         | 0.45   | 0 100 100      | 1, 1, 1, 1            | 0     |
| 54  | D6    | 2/8 (25%)         | -0.02  | 0 100 100      | 46, 46, 46, 51        | 0     |
| All | All   | 20738/20810 (99%) | 0.62   | 2658 (12%) 3 2 | 0, 63, 124, 195       | 0     |

The worst 5 of 2658 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | BI    | 53   | LEU  | 25.2 |
| 53  | B5    | 55   | SER  | 19.9 |
| 22  | BA    | 2101 | A    | 17.4 |
| 22  | BA    | 2184 | A    | 17.4 |
| 53  | B5    | 207  | GLY  | 16.3 |



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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 54  | MHW  | D6    | 1   | 9/10  | 0.87 | 0.20 | 40,52,59,59                | 0     |
| 54  | DBB  | D6    | 3   | 6/7   | 0.91 | 0.30 | 36,38,47,51                | 0     |
| 54  | MHU  | D6    | 5   | 15/16 | 0.92 | 0.32 | 44,54,60,61                | 0     |
| 54  | MHW  | B6    | 1   | 9/10  | 0.94 | 0.18 | 0,0,2,9                    | 0     |
| 54  | MHV  | D6    | 6   | 9/10  | 0.94 | 0.14 | 45,51,58,60                | 0     |
| 54  | 004  | D6    | 7   | 10/11 | 0.94 | 0.21 | 42,47,58,59                | 0     |
| 54  | MHU  | B6    | 5   | 15/16 | 0.96 | 0.20 | 0,0,1,2                    | 0     |
| 54  | DBB  | B6    | 3   | 6/7   | 0.96 | 0.19 | 0,1,1,2                    | 0     |
| 54  | 004  | B6    | 7   | 10/11 | 0.97 | 0.23 | 0,0,2,3                    | 0     |
| 54  | MHV  | B6    | 6   | 9/10  | 0.97 | 0.16 | 0,0,1,1                    | 0     |

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | DA    | 3111 | 1/1   | 0.18 | 0.32 | 107,107,107,107            | 0     |
| 55  | MG   | DA    | 3048 | 1/1   | 0.20 | 0.44 | 127,127,127,127            | 0     |
| 55  | MG   | DA    | 3135 | 1/1   | 0.24 | 0.32 | 101,101,101,101            | 0     |
| 55  | MG   | DA    | 3084 | 1/1   | 0.35 | 0.23 | 105,105,105,105            | 0     |
| 55  | MG   | DA    | 3100 | 1/1   | 0.36 | 0.20 | 77,77,77,77                | 0     |
| 55  | MG   | DA    | 3041 | 1/1   | 0.38 | 0.42 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3017 | 1/1   | 0.38 | 0.25 | 98,98,98,98                | 0     |
| 55  | MG   | DA    | 3026 | 1/1   | 0.43 | 0.48 | 101,101,101,101            | 0     |
| 55  | MG   | DA    | 3093 | 1/1   | 0.46 | 0.11 | 86,86,86,86                | 0     |
| 55  | MG   | BA    | 3134 | 1/1   | 0.46 | 0.42 | 54,54,54,54                | 0     |
| 55  | MG   | CA    | 1630 | 1/1   | 0.48 | 0.36 | 120,120,120,120            | 0     |
| 55  | MG   | AA    | 1619 | 1/1   | 0.50 | 0.31 | 73,73,73,73                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | DA    | 3062 | 1/1   | 0.51 | 0.61 | 82,82,82,82                | 0     |
| 55  | MG   | CA    | 1636 | 1/1   | 0.51 | 0.14 | 126,126,126,126            | 0     |
| 55  | MG   | DA    | 3148 | 1/1   | 0.51 | 0.29 | 65,65,65,65                | 0     |
| 55  | MG   | DA    | 3113 | 1/1   | 0.52 | 0.29 | 66,66,66,66                | 0     |
| 55  | MG   | DA    | 3144 | 1/1   | 0.52 | 0.10 | 68,68,68,68                | 0     |
| 55  | MG   | DA    | 3133 | 1/1   | 0.52 | 0.78 | 100,100,100,100            | 0     |
| 55  | MG   | DA    | 3045 | 1/1   | 0.53 | 0.12 | 94,94,94,94                | 0     |
| 55  | MG   | DA    | 3042 | 1/1   | 0.54 | 0.19 | 87,87,87,87                | 0     |
| 55  | MG   | DA    | 3057 | 1/1   | 0.54 | 0.29 | 95,95,95,95                | 0     |
| 55  | MG   | CA    | 1635 | 1/1   | 0.54 | 0.13 | 124,124,124,124            | 0     |
| 55  | MG   | BA    | 3090 | 1/1   | 0.55 | 0.10 | 19,19,19,19                | 0     |
| 55  | MG   | DA    | 3099 | 1/1   | 0.57 | 0.38 | 86,86,86,86                | 0     |
| 55  | MG   | DA    | 3075 | 1/1   | 0.57 | 0.16 | 91,91,91,91                | 0     |
| 55  | MG   | DA    | 3067 | 1/1   | 0.59 | 0.13 | 58,58,58,58                | 0     |
| 55  | MG   | DA    | 3029 | 1/1   | 0.59 | 0.22 | 73,73,73,73                | 0     |
| 55  | MG   | BA    | 3100 | 1/1   | 0.60 | 0.28 | 52,52,52,52                | 0     |
| 55  | MG   | DA    | 3028 | 1/1   | 0.61 | 0.87 | 103,103,103,103            | 0     |
| 55  | MG   | CA    | 1627 | 1/1   | 0.61 | 0.20 | 89,89,89,89                | 0     |
| 55  | MG   | AA    | 1614 | 1/1   | 0.61 | 0.22 | 69,69,69,69                | 0     |
| 55  | MG   | CA    | 1608 | 1/1   | 0.61 | 0.22 | 84,84,84,84                | 0     |
| 55  | MG   | DA    | 3027 | 1/1   | 0.62 | 0.17 | 91,91,91,91                | 0     |
| 55  | MG   | DA    | 3071 | 1/1   | 0.63 | 0.49 | 92,92,92,92                | 0     |
| 55  | MG   | CA    | 1606 | 1/1   | 0.64 | 0.19 | 89,89,89,89                | 0     |
| 55  | MG   | DA    | 3002 | 1/1   | 0.64 | 0.10 | 78,78,78,78                | 0     |
| 55  | MG   | DA    | 3127 | 1/1   | 0.64 | 0.15 | 71,71,71,71                | 0     |
| 55  | MG   | DA    | 3131 | 1/1   | 0.64 | 1.04 | 99,99,99,99                | 0     |
| 55  | MG   | DA    | 3090 | 1/1   | 0.65 | 0.14 | 90,90,90,90                | 0     |
| 55  | MG   | DA    | 3070 | 1/1   | 0.65 | 0.17 | 108,108,108,108            | 0     |
| 55  | MG   | DA    | 3010 | 1/1   | 0.65 | 0.12 | 80,80,80,80                | 0     |
| 55  | MG   | D2    | 101  | 1/1   | 0.65 | 0.15 | 83,83,83,83                | 0     |
| 55  | MG   | CA    | 1629 | 1/1   | 0.66 | 0.12 | 91,91,91,91                | 0     |
| 55  | MG   | DA    | 3126 | 1/1   | 0.67 | 0.23 | 80,80,80,80                | 0     |
| 55  | MG   | AA    | 1658 | 1/1   | 0.67 | 0.35 | 62,62,62,62                | 0     |
| 55  | MG   | AA    | 1665 | 1/1   | 0.67 | 0.40 | 37,37,37,37                | 0     |
| 55  | MG   | AA    | 1639 | 1/1   | 0.67 | 0.07 | 65,65,65,65                | 0     |
| 55  | MG   | DA    | 3078 | 1/1   | 0.68 | 0.14 | 106,106,106,106            | 0     |
| 55  | MG   | CA    | 1632 | 1/1   | 0.69 | 0.12 | 73,73,73,73                | 0     |
| 55  | MG   | DA    | 3077 | 1/1   | 0.69 | 0.70 | 113,113,113,113            | 0     |
| 55  | MG   | DA    | 3019 | 1/1   | 0.69 | 0.18 | 107,107,107,107            | 0     |
| 55  | MG   | DA    | 3034 | 1/1   | 0.69 | 0.16 | 69,69,69,69                | 0     |
| 55  | MG   | DQ    | 201  | 1/1   | 0.69 | 0.30 | 45,45,45,45                | 0     |
| 55  | MG   | DA    | 3103 | 1/1   | 0.69 | 0.24 | 73,73,73,73                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | DA    | 3044 | 1/1   | 0.70 | 0.40 | 112,112,112,112            | 0     |
| 55  | MG   | DA    | 3155 | 1/1   | 0.71 | 0.45 | 62,62,62,62                | 0     |
| 55  | MG   | CA    | 1602 | 1/1   | 0.72 | 0.11 | 88,88,88,88                | 0     |
| 55  | MG   | DA    | 3088 | 1/1   | 0.72 | 0.10 | 74,74,74,74                | 0     |
| 55  | MG   | DA    | 3060 | 1/1   | 0.72 | 0.31 | 77,77,77,77                | 0     |
| 55  | MG   | DA    | 3012 | 1/1   | 0.72 | 0.10 | 73,73,73,73                | 0     |
| 55  | MG   | DA    | 3098 | 1/1   | 0.72 | 0.16 | 66,66,66,66                | 0     |
| 55  | MG   | AA    | 1620 | 1/1   | 0.73 | 0.12 | 69,69,69,69                | 0     |
| 55  | MG   | DA    | 3134 | 1/1   | 0.73 | 0.14 | 58,58,58,58                | 0     |
| 55  | MG   | DB    | 201  | 1/1   | 0.73 | 0.06 | 116,116,116,116            | 0     |
| 55  | MG   | DA    | 3064 | 1/1   | 0.73 | 0.20 | 48,48,48,48                | 0     |
| 55  | MG   | DA    | 3013 | 1/1   | 0.73 | 0.16 | 44,44,44,44                | 0     |
| 55  | MG   | AA    | 1648 | 1/1   | 0.74 | 0.20 | 47,47,47,47                | 0     |
| 55  | MG   | CA    | 1631 | 1/1   | 0.74 | 0.13 | 95,95,95,95                | 0     |
| 55  | MG   | DA    | 3136 | 1/1   | 0.74 | 0.16 | 91,91,91,91                | 0     |
| 55  | MG   | BA    | 3050 | 1/1   | 0.74 | 0.07 | 27,27,27,27                | 0     |
| 55  | MG   | DA    | 3147 | 1/1   | 0.74 | 0.39 | 54,54,54,54                | 0     |
| 55  | MG   | DA    | 3005 | 1/1   | 0.75 | 0.43 | 102,102,102,102            | 0     |
| 55  | MG   | BA    | 3186 | 1/1   | 0.75 | 0.30 | 29,29,29,29                | 0     |
| 55  | MG   | CA    | 1617 | 1/1   | 0.76 | 0.12 | 39,39,39,39                | 0     |
| 55  | MG   | BA    | 3093 | 1/1   | 0.76 | 0.09 | 58,58,58,58                | 0     |
| 55  | MG   | DA    | 3037 | 1/1   | 0.76 | 0.08 | 93,93,93,93                | 0     |
| 55  | MG   | AA    | 1651 | 1/1   | 0.76 | 0.32 | 61,61,61,61                | 0     |
| 55  | MG   | CA    | 1605 | 1/1   | 0.76 | 0.19 | 86,86,86,86                | 0     |
| 55  | MG   | BA    | 3049 | 1/1   | 0.76 | 0.13 | 44,44,44,44                | 0     |
| 55  | MG   | BA    | 3153 | 1/1   | 0.76 | 0.23 | 31,31,31,31                | 0     |
| 55  | MG   | DA    | 3046 | 1/1   | 0.76 | 0.16 | 62,62,62,62                | 0     |
| 55  | MG   | DA    | 3072 | 1/1   | 0.76 | 0.52 | 90,90,90,90                | 0     |
| 55  | MG   | DA    | 3163 | 1/1   | 0.77 | 0.32 | 54,54,54,54                | 0     |
| 55  | MG   | DA    | 3125 | 1/1   | 0.77 | 0.22 | 62,62,62,62                | 0     |
| 55  | MG   | AA    | 1626 | 1/1   | 0.77 | 0.17 | 23,23,23,23                | 0     |
| 55  | MG   | BA    | 3038 | 1/1   | 0.77 | 0.16 | 42,42,42,42                | 0     |
| 55  | MG   | DA    | 3107 | 1/1   | 0.78 | 0.16 | 75,75,75,75                | 0     |
| 55  | MG   | BA    | 3167 | 1/1   | 0.78 | 0.18 | 25,25,25,25                | 0     |
| 55  | MG   | DA    | 3056 | 1/1   | 0.78 | 0.41 | 93,93,93,93                | 0     |
| 55  | MG   | DB    | 203  | 1/1   | 0.78 | 0.08 | 85,85,85,85                | 0     |
| 55  | MG   | DA    | 3121 | 1/1   | 0.78 | 0.10 | 52,52,52,52                | 0     |
| 55  | MG   | AA    | 1659 | 1/1   | 0.78 | 0.76 | 50,50,50,50                | 0     |
| 55  | MG   | AM    | 201  | 1/1   | 0.79 | 0.86 | 62,62,62,62                | 0     |
| 55  | MG   | AA    | 1652 | 1/1   | 0.79 | 0.19 | 49,49,49,49                | 0     |
| 55  | MG   | AA    | 1635 | 1/1   | 0.79 | 0.17 | 66,66,66,66                | 0     |
| 55  | MG   | AA    | 1667 | 1/1   | 0.79 | 0.19 | 49,49,49,49                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3057 | 1/1   | 0.79 | 0.35 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3058 | 1/1   | 0.79 | 0.29 | 15,15,15,15                 | 0     |
| 55  | MG   | DA    | 3108 | 1/1   | 0.79 | 0.17 | 59,59,59,59                 | 0     |
| 55  | MG   | DA    | 3003 | 1/1   | 0.79 | 0.47 | 99,99,99,99                 | 0     |
| 55  | MG   | BA    | 3077 | 1/1   | 0.79 | 0.17 | 8,8,8,8                     | 0     |
| 55  | MG   | AA    | 1657 | 1/1   | 0.80 | 0.63 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3152 | 1/1   | 0.80 | 0.29 | 52,52,52,52                 | 0     |
| 55  | MG   | CA    | 1621 | 1/1   | 0.80 | 0.09 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3115 | 1/1   | 0.80 | 0.19 | 111,111,111,111             | 0     |
| 55  | MG   | DA    | 3006 | 1/1   | 0.80 | 0.13 | 93,93,93,93                 | 0     |
| 55  | MG   | AA    | 1662 | 1/1   | 0.80 | 0.38 | 57,57,57,57                 | 0     |
| 55  | MG   | BA    | 3059 | 1/1   | 0.80 | 0.25 | 38,38,38,38                 | 0     |
| 55  | MG   | CA    | 1609 | 1/1   | 0.80 | 0.15 | 89,89,89,89                 | 0     |
| 55  | MG   | DA    | 3073 | 1/1   | 0.81 | 0.11 | 60,60,60,60                 | 0     |
| 55  | MG   | DA    | 3097 | 1/1   | 0.81 | 0.25 | 91,91,91,91                 | 0     |
| 55  | MG   | CA    | 1638 | 1/1   | 0.81 | 0.10 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3149 | 1/1   | 0.81 | 0.29 | 35,35,35,35                 | 0     |
| 55  | MG   | DA    | 3009 | 1/1   | 0.81 | 0.37 | 90,90,90,90                 | 0     |
| 55  | MG   | DA    | 3022 | 1/1   | 0.81 | 0.10 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3137 | 1/1   | 0.81 | 0.42 | 49,49,49,49                 | 0     |
| 55  | MG   | BA    | 3103 | 1/1   | 0.81 | 0.17 | 0,0,0,0                     | 0     |
| 55  | MG   | DA    | 3089 | 1/1   | 0.81 | 0.33 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1601 | 1/1   | 0.81 | 0.09 | 58,58,58,58                 | 0     |
| 55  | MG   | DA    | 3092 | 1/1   | 0.81 | 0.58 | 113,113,113,113             | 0     |
| 55  | MG   | BA    | 3075 | 1/1   | 0.82 | 0.16 | 29,29,29,29                 | 0     |
| 55  | MG   | CA    | 1646 | 1/1   | 0.82 | 0.24 | 92,92,92,92                 | 0     |
| 55  | MG   | BA    | 3119 | 1/1   | 0.82 | 0.07 | 20,20,20,20                 | 0     |
| 55  | MG   | BA    | 3180 | 1/1   | 0.82 | 0.19 | 32,32,32,32                 | 0     |
| 55  | MG   | BA    | 3146 | 1/1   | 0.82 | 0.19 | 30,30,30,30                 | 0     |
| 55  | MG   | BA    | 3189 | 1/1   | 0.82 | 0.24 | 45,45,45,45                 | 0     |
| 55  | MG   | DA    | 3120 | 1/1   | 0.82 | 0.11 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3151 | 1/1   | 0.82 | 0.27 | 12,12,12,12                 | 0     |
| 55  | MG   | CA    | 1626 | 1/1   | 0.82 | 0.08 | 48,48,48,48                 | 0     |
| 55  | MG   | DA    | 3033 | 1/1   | 0.83 | 0.10 | 71,71,71,71                 | 0     |
| 55  | MG   | DA    | 3129 | 1/1   | 0.83 | 0.18 | 45,45,45,45                 | 0     |
| 55  | MG   | CA    | 1637 | 1/1   | 0.83 | 0.10 | 64,64,64,64                 | 0     |
| 55  | MG   | DA    | 3114 | 1/1   | 0.83 | 0.14 | 65,65,65,65                 | 0     |
| 55  | MG   | BA    | 3021 | 1/1   | 0.83 | 0.19 | 1,1,1,1                     | 0     |
| 55  | MG   | DA    | 3038 | 1/1   | 0.83 | 0.13 | 63,63,63,63                 | 0     |
| 55  | MG   | DA    | 3091 | 1/1   | 0.83 | 0.09 | 77,77,77,77                 | 0     |
| 55  | MG   | DA    | 3040 | 1/1   | 0.83 | 0.18 | 83,83,83,83                 | 0     |
| 55  | MG   | AA    | 1628 | 1/1   | 0.83 | 0.10 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | BA    | 3054 | 1/1   | 0.84 | 0.09 | 9,9,9,9                    | 0     |
| 55  | MG   | BA    | 3089 | 1/1   | 0.84 | 0.07 | 33,33,33,33                | 0     |
| 55  | MG   | CA    | 1655 | 1/1   | 0.84 | 0.10 | 44,44,44,44                | 0     |
| 55  | MG   | DA    | 3016 | 1/1   | 0.84 | 0.14 | 62,62,62,62                | 0     |
| 55  | MG   | DA    | 3153 | 1/1   | 0.84 | 0.26 | 53,53,53,53                | 0     |
| 55  | MG   | AA    | 1644 | 1/1   | 0.84 | 0.39 | 44,44,44,44                | 0     |
| 55  | MG   | BA    | 3046 | 1/1   | 0.84 | 0.09 | 17,17,17,17                | 0     |
| 55  | MG   | DA    | 3094 | 1/1   | 0.84 | 0.18 | 84,84,84,84                | 0     |
| 55  | MG   | AA    | 1638 | 1/1   | 0.84 | 0.10 | 87,87,87,87                | 0     |
| 55  | MG   | CA    | 1603 | 1/1   | 0.84 | 0.15 | 44,44,44,44                | 0     |
| 55  | MG   | AA    | 1623 | 1/1   | 0.84 | 0.05 | 46,46,46,46                | 0     |
| 55  | MG   | DA    | 3047 | 1/1   | 0.85 | 0.13 | 73,73,73,73                | 0     |
| 55  | MG   | BA    | 3170 | 1/1   | 0.85 | 0.35 | 38,38,38,38                | 0     |
| 55  | MG   | BA    | 3016 | 1/1   | 0.85 | 0.43 | 58,58,58,58                | 0     |
| 55  | MG   | DA    | 3145 | 1/1   | 0.85 | 0.17 | 71,71,71,71                | 0     |
| 55  | MG   | DA    | 3119 | 1/1   | 0.85 | 0.44 | 106,106,106,106            | 0     |
| 55  | MG   | AA    | 1631 | 1/1   | 0.85 | 0.10 | 46,46,46,46                | 0     |
| 55  | MG   | BA    | 3069 | 1/1   | 0.85 | 0.15 | 4,4,4,4                    | 0     |
| 55  | MG   | DA    | 3151 | 1/1   | 0.85 | 0.52 | 59,59,59,59                | 0     |
| 55  | MG   | DA    | 3124 | 1/1   | 0.85 | 0.23 | 89,89,89,89                | 0     |
| 55  | MG   | DA    | 3080 | 1/1   | 0.85 | 0.15 | 95,95,95,95                | 0     |
| 55  | MG   | DA    | 3154 | 1/1   | 0.85 | 0.17 | 40,40,40,40                | 0     |
| 55  | MG   | CA    | 1601 | 1/1   | 0.85 | 0.09 | 39,39,39,39                | 0     |
| 55  | MG   | BA    | 3120 | 1/1   | 0.85 | 0.20 | 37,37,37,37                | 0     |
| 55  | MG   | DA    | 3104 | 1/1   | 0.85 | 0.08 | 79,79,79,79                | 0     |
| 55  | MG   | CA    | 1624 | 1/1   | 0.85 | 0.10 | 45,45,45,45                | 0     |
| 55  | MG   | BA    | 3027 | 1/1   | 0.85 | 0.34 | 46,46,46,46                | 0     |
| 55  | MG   | CA    | 1604 | 1/1   | 0.85 | 0.13 | 95,95,95,95                | 0     |
| 55  | MG   | CA    | 1654 | 1/1   | 0.86 | 0.36 | 56,56,56,56                | 0     |
| 55  | MG   | BA    | 3104 | 1/1   | 0.86 | 0.17 | 17,17,17,17                | 0     |
| 55  | MG   | BA    | 3178 | 1/1   | 0.86 | 0.68 | 30,30,30,30                | 0     |
| 55  | MG   | AA    | 1605 | 1/1   | 0.86 | 0.22 | 23,23,23,23                | 0     |
| 55  | MG   | CA    | 1615 | 1/1   | 0.86 | 0.30 | 58,58,58,58                | 0     |
| 55  | MG   | DA    | 3039 | 1/1   | 0.86 | 0.18 | 57,57,57,57                | 0     |
| 55  | MG   | BA    | 3154 | 1/1   | 0.86 | 0.33 | 25,25,25,25                | 0     |
| 55  | MG   | DA    | 3157 | 1/1   | 0.86 | 0.30 | 58,58,58,58                | 0     |
| 55  | MG   | DA    | 3061 | 1/1   | 0.86 | 1.12 | 96,96,96,96                | 0     |
| 55  | MG   | DA    | 3143 | 1/1   | 0.86 | 0.24 | 60,60,60,60                | 0     |
| 55  | MG   | DA    | 3008 | 1/1   | 0.86 | 0.26 | 100,100,100,100            | 0     |
| 55  | MG   | AA    | 1612 | 1/1   | 0.86 | 0.10 | 47,47,47,47                | 0     |
| 55  | MG   | CA    | 1651 | 1/1   | 0.86 | 0.30 | 44,44,44,44                | 0     |
| 55  | MG   | DA    | 3024 | 1/1   | 0.87 | 0.17 | 46,46,46,46                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | DA    | 3025 | 1/1   | 0.87 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | BB    | 202  | 1/1   | 0.87 | 0.10 | 16,16,16,16                 | 0     |
| 55  | MG   | AA    | 1661 | 1/1   | 0.87 | 0.29 | 29,29,29,29                 | 0     |
| 55  | MG   | DA    | 3081 | 1/1   | 0.87 | 0.10 | 60,60,60,60                 | 0     |
| 55  | MG   | CA    | 1656 | 1/1   | 0.87 | 0.37 | 54,54,54,54                 | 0     |
| 55  | MG   | AA    | 1613 | 1/1   | 0.87 | 0.09 | 24,24,24,24                 | 0     |
| 55  | MG   | DA    | 3165 | 1/1   | 0.87 | 0.22 | 42,42,42,42                 | 0     |
| 55  | MG   | CA    | 1628 | 1/1   | 0.87 | 0.18 | 98,98,98,98                 | 0     |
| 55  | MG   | DB    | 202  | 1/1   | 0.87 | 0.11 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3125 | 1/1   | 0.87 | 0.54 | 37,37,37,37                 | 0     |
| 55  | MG   | AA    | 1671 | 1/1   | 0.87 | 0.52 | 59,59,59,59                 | 0     |
| 55  | MG   | AA    | 1664 | 1/1   | 0.87 | 0.14 | 49,49,49,49                 | 0     |
| 55  | MG   | DA    | 3112 | 1/1   | 0.88 | 1.38 | 104,104,104,104             | 0     |
| 55  | MG   | AA    | 1650 | 1/1   | 0.88 | 0.32 | 36,36,36,36                 | 0     |
| 55  | MG   | DA    | 3036 | 1/1   | 0.88 | 0.15 | 62,62,62,62                 | 0     |
| 55  | MG   | AA    | 1670 | 1/1   | 0.88 | 0.29 | 33,33,33,33                 | 0     |
| 55  | MG   | BA    | 3102 | 1/1   | 0.88 | 0.10 | 7,7,7,7                     | 0     |
| 55  | MG   | AA    | 1634 | 1/1   | 0.88 | 0.13 | 35,35,35,35                 | 0     |
| 55  | MG   | AA    | 1643 | 1/1   | 0.88 | 0.14 | 28,28,28,28                 | 0     |
| 55  | MG   | BA    | 3004 | 1/1   | 0.88 | 0.11 | 26,26,26,26                 | 0     |
| 55  | MG   | BA    | 3082 | 1/1   | 0.88 | 0.11 | 6,6,6,6                     | 0     |
| 55  | MG   | BA    | 3179 | 1/1   | 0.88 | 0.33 | 26,26,26,26                 | 0     |
| 55  | MG   | AA    | 1609 | 1/1   | 0.88 | 0.08 | 36,36,36,36                 | 0     |
| 55  | MG   | AA    | 1632 | 1/1   | 0.88 | 0.10 | 55,55,55,55                 | 0     |
| 55  | MG   | DA    | 3160 | 1/1   | 0.88 | 0.24 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3092 | 1/1   | 0.88 | 0.10 | 19,19,19,19                 | 0     |
| 55  | MG   | DA    | 3132 | 1/1   | 0.88 | 0.18 | 54,54,54,54                 | 0     |
| 55  | MG   | DA    | 3031 | 1/1   | 0.88 | 0.08 | 69,69,69,69                 | 0     |
| 55  | MG   | DA    | 3049 | 1/1   | 0.88 | 0.25 | 84,84,84,84                 | 0     |
| 55  | MG   | DA    | 3052 | 1/1   | 0.88 | 0.07 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3141 | 1/1   | 0.88 | 0.15 | 17,17,17,17                 | 0     |
| 55  | MG   | DA    | 3138 | 1/1   | 0.88 | 0.35 | 40,40,40,40                 | 0     |
| 56  | DOL  | DA    | 3001 | 48/48 | 0.88 | 0.26 | 26,45,58,63                 | 0     |
| 55  | MG   | DA    | 3020 | 1/1   | 0.89 | 0.15 | 54,54,54,54                 | 0     |
| 55  | MG   | DA    | 3117 | 1/1   | 0.89 | 0.09 | 67,67,67,67                 | 0     |
| 55  | MG   | AA    | 1630 | 1/1   | 0.89 | 0.18 | 73,73,73,73                 | 0     |
| 55  | MG   | BA    | 3064 | 1/1   | 0.89 | 0.19 | 5,5,5,5                     | 0     |
| 55  | MG   | BA    | 3114 | 1/1   | 0.89 | 0.17 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3157 | 1/1   | 0.89 | 0.19 | 24,24,24,24                 | 0     |
| 55  | MG   | AA    | 1637 | 1/1   | 0.89 | 0.10 | 15,15,15,15                 | 0     |
| 55  | MG   | DA    | 3074 | 1/1   | 0.89 | 0.33 | 77,77,77,77                 | 0     |
| 55  | MG   | BA    | 3191 | 1/1   | 0.89 | 0.23 | 12,12,12,12                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | CA    | 1649 | 1/1   | 0.89 | 0.18 | 52,52,52,52                | 0     |
| 55  | MG   | DA    | 3011 | 1/1   | 0.89 | 0.08 | 75,75,75,75                | 0     |
| 55  | MG   | CA    | 1650 | 1/1   | 0.89 | 0.22 | 35,35,35,35                | 0     |
| 55  | MG   | BA    | 3040 | 1/1   | 0.89 | 0.15 | 0,0,0,0                    | 0     |
| 55  | MG   | DA    | 3110 | 1/1   | 0.89 | 0.23 | 33,33,33,33                | 0     |
| 55  | MG   | DA    | 3014 | 1/1   | 0.89 | 0.14 | 73,73,73,73                | 0     |
| 55  | MG   | BB    | 204  | 1/1   | 0.89 | 0.37 | 16,16,16,16                | 0     |
| 55  | MG   | DA    | 3137 | 1/1   | 0.89 | 0.42 | 47,47,47,47                | 0     |
| 55  | MG   | CA    | 1610 | 1/1   | 0.89 | 0.10 | 63,63,63,63                | 0     |
| 55  | MG   | DA    | 3141 | 1/1   | 0.89 | 0.27 | 40,40,40,40                | 0     |
| 55  | MG   | CA    | 1613 | 1/1   | 0.89 | 0.14 | 19,19,19,19                | 0     |
| 55  | MG   | AA    | 1660 | 1/1   | 0.90 | 0.22 | 51,51,51,51                | 0     |
| 55  | MG   | BA    | 3002 | 1/1   | 0.90 | 0.06 | 18,18,18,18                | 0     |
| 55  | MG   | DA    | 3146 | 1/1   | 0.90 | 0.10 | 43,43,43,43                | 0     |
| 55  | MG   | BA    | 3169 | 1/1   | 0.90 | 0.16 | 35,35,35,35                | 0     |
| 55  | MG   | DA    | 3066 | 1/1   | 0.90 | 0.07 | 47,47,47,47                | 0     |
| 55  | MG   | BA    | 3112 | 1/1   | 0.90 | 0.08 | 20,20,20,20                | 0     |
| 55  | MG   | DA    | 3069 | 1/1   | 0.90 | 0.09 | 79,79,79,79                | 0     |
| 55  | MG   | DA    | 3096 | 1/1   | 0.90 | 0.08 | 57,57,57,57                | 0     |
| 55  | MG   | BA    | 3171 | 1/1   | 0.90 | 0.20 | 24,24,24,24                | 0     |
| 55  | MG   | BA    | 3076 | 1/1   | 0.90 | 0.07 | 14,14,14,14                | 0     |
| 55  | MG   | DA    | 3007 | 1/1   | 0.90 | 0.44 | 121,121,121,121            | 0     |
| 55  | MG   | CA    | 1640 | 1/1   | 0.90 | 0.14 | 26,26,26,26                | 0     |
| 55  | MG   | BA    | 3051 | 1/1   | 0.90 | 0.17 | 6,6,6,6                    | 0     |
| 55  | MG   | CA    | 1647 | 1/1   | 0.90 | 0.11 | 41,41,41,41                | 0     |
| 55  | MG   | CA    | 1648 | 1/1   | 0.90 | 0.20 | 22,22,22,22                | 0     |
| 55  | MG   | AA    | 1602 | 1/1   | 0.90 | 0.13 | 46,46,46,46                | 0     |
| 55  | MG   | BA    | 3182 | 1/1   | 0.90 | 0.25 | 33,33,33,33                | 0     |
| 55  | MG   | BA    | 3087 | 1/1   | 0.90 | 0.13 | 4,4,4,4                    | 0     |
| 55  | MG   | DA    | 3058 | 1/1   | 0.90 | 1.10 | 109,109,109,109            | 0     |
| 55  | MG   | DA    | 3085 | 1/1   | 0.90 | 0.12 | 67,67,67,67                | 0     |
| 55  | MG   | BA    | 3156 | 1/1   | 0.90 | 0.28 | 19,19,19,19                | 0     |
| 55  | MG   | BA    | 3116 | 1/1   | 0.91 | 0.26 | 34,34,34,34                | 0     |
| 55  | MG   | DA    | 3065 | 1/1   | 0.91 | 0.12 | 36,36,36,36                | 0     |
| 55  | MG   | CA    | 1616 | 1/1   | 0.91 | 0.10 | 37,37,37,37                | 0     |
| 55  | MG   | BA    | 3193 | 1/1   | 0.91 | 0.15 | 38,38,38,38                | 0     |
| 55  | MG   | DA    | 3068 | 1/1   | 0.91 | 0.13 | 65,65,65,65                | 0     |
| 55  | MG   | BA    | 3195 | 1/1   | 0.91 | 0.56 | 23,23,23,23                | 0     |
| 55  | MG   | DA    | 3015 | 1/1   | 0.91 | 0.06 | 55,55,55,55                | 0     |
| 55  | MG   | DA    | 3105 | 1/1   | 0.91 | 0.18 | 80,80,80,80                | 0     |
| 55  | MG   | DA    | 3106 | 1/1   | 0.91 | 0.14 | 52,52,52,52                | 0     |
| 55  | MG   | BA    | 3006 | 1/1   | 0.91 | 0.14 | 50,50,50,50                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | BA    | 3008 | 1/1   | 0.91 | 0.14 | 37,37,37,37                 | 0     |
| 55  | MG   | BA    | 3168 | 1/1   | 0.91 | 0.12 | 35,35,35,35                 | 0     |
| 55  | MG   | BA    | 3015 | 1/1   | 0.91 | 0.07 | 2,2,2,2                     | 0     |
| 55  | MG   | DA    | 3021 | 1/1   | 0.91 | 0.18 | 63,63,63,63                 | 0     |
| 55  | MG   | DA    | 3150 | 1/1   | 0.91 | 0.20 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3132 | 1/1   | 0.91 | 0.09 | 23,23,23,23                 | 0     |
| 55  | MG   | AA    | 1629 | 1/1   | 0.91 | 0.14 | 61,61,61,61                 | 0     |
| 55  | MG   | BA    | 3003 | 1/1   | 0.91 | 0.06 | 17,17,17,17                 | 0     |
| 55  | MG   | AA    | 1641 | 1/1   | 0.91 | 0.15 | 19,19,19,19                 | 0     |
| 55  | MG   | DA    | 3050 | 1/1   | 0.91 | 0.10 | 56,56,56,56                 | 0     |
| 55  | MG   | BA    | 3078 | 1/1   | 0.91 | 0.72 | 79,79,79,79                 | 0     |
| 55  | MG   | DA    | 3159 | 1/1   | 0.91 | 0.30 | 43,43,43,43                 | 0     |
| 55  | MG   | DA    | 3087 | 1/1   | 0.91 | 0.09 | 54,54,54,54                 | 0     |
| 55  | MG   | DA    | 3123 | 1/1   | 0.91 | 0.12 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3164 | 1/1   | 0.91 | 0.18 | 57,57,57,57                 | 0     |
| 55  | MG   | DA    | 3054 | 1/1   | 0.91 | 0.10 | 55,55,55,55                 | 0     |
| 55  | MG   | BA    | 3081 | 1/1   | 0.91 | 0.12 | 24,24,24,24                 | 0     |
| 55  | MG   | BA    | 3033 | 1/1   | 0.91 | 0.12 | 11,11,11,11                 | 0     |
| 55  | MG   | DA    | 3030 | 1/1   | 0.91 | 0.24 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3005 | 1/1   | 0.91 | 0.07 | 34,34,34,34                 | 0     |
| 55  | MG   | DA    | 3032 | 1/1   | 0.91 | 0.26 | 68,68,68,68                 | 0     |
| 55  | MG   | CA    | 1614 | 1/1   | 0.91 | 0.08 | 50,50,50,50                 | 0     |
| 55  | MG   | CA    | 1622 | 1/1   | 0.92 | 0.13 | 51,51,51,51                 | 0     |
| 55  | MG   | DA    | 3004 | 1/1   | 0.92 | 0.11 | 76,76,76,76                 | 0     |
| 55  | MG   | BA    | 3071 | 1/1   | 0.92 | 0.07 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3098 | 1/1   | 0.92 | 0.12 | 2,2,2,2                     | 0     |
| 55  | MG   | AA    | 1654 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 55  | MG   | AA    | 1625 | 1/1   | 0.92 | 0.07 | 47,47,47,47                 | 0     |
| 55  | MG   | BA    | 3152 | 1/1   | 0.92 | 0.19 | 6,6,6,6                     | 0     |
| 55  | MG   | AA    | 1606 | 1/1   | 0.92 | 0.11 | 44,44,44,44                 | 0     |
| 55  | MG   | AA    | 1603 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 55  | MG   | BA    | 3042 | 1/1   | 0.92 | 0.38 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3113 | 1/1   | 0.92 | 0.17 | 22,22,22,22                 | 0     |
| 55  | MG   | AA    | 1666 | 1/1   | 0.92 | 0.19 | 46,46,46,46                 | 0     |
| 55  | MG   | BA    | 3086 | 1/1   | 0.92 | 0.07 | 14,14,14,14                 | 0     |
| 55  | MG   | BA    | 3063 | 1/1   | 0.92 | 0.45 | 31,31,31,31                 | 0     |
| 55  | MG   | CA    | 1639 | 1/1   | 0.92 | 0.10 | 43,43,43,43                 | 0     |
| 55  | MG   | DA    | 3116 | 1/1   | 0.92 | 0.36 | 76,76,76,76                 | 0     |
| 55  | MG   | DA    | 3082 | 1/1   | 0.92 | 0.13 | 60,60,60,60                 | 0     |
| 55  | MG   | CA    | 1607 | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |
| 55  | MG   | BA    | 3047 | 1/1   | 0.92 | 0.10 | 4,4,4,4                     | 0     |
| 55  | MG   | DA    | 3158 | 1/1   | 0.92 | 0.19 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | BA    | 3066 | 1/1   | 0.92 | 0.15 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3174 | 1/1   | 0.92 | 0.12 | 12,12,12,12                | 0     |
| 55  | MG   | DA    | 3023 | 1/1   | 0.92 | 0.05 | 69,69,69,69                | 0     |
| 55  | MG   | BA    | 3127 | 1/1   | 0.92 | 0.12 | 9,9,9,9                    | 0     |
| 55  | MG   | BA    | 3131 | 1/1   | 0.92 | 0.18 | 1,1,1,1                    | 0     |
| 55  | MG   | BA    | 3091 | 1/1   | 0.92 | 0.09 | 3,3,3,3                    | 0     |
| 55  | MG   | BA    | 3133 | 1/1   | 0.92 | 0.10 | 32,32,32,32                | 0     |
| 55  | MG   | AA    | 1646 | 1/1   | 0.92 | 0.20 | 49,49,49,49                | 0     |
| 55  | MG   | DA    | 3095 | 1/1   | 0.92 | 0.41 | 91,91,91,91                | 0     |
| 55  | MG   | CA    | 1620 | 1/1   | 0.92 | 0.06 | 61,61,61,61                | 0     |
| 55  | MG   | BA    | 3187 | 1/1   | 0.92 | 0.06 | 33,33,33,33                | 0     |
| 55  | MG   | DA    | 3101 | 1/1   | 0.93 | 0.09 | 57,57,57,57                | 0     |
| 55  | MG   | BA    | 3155 | 1/1   | 0.93 | 0.21 | 20,20,20,20                | 0     |
| 55  | MG   | AA    | 1669 | 1/1   | 0.93 | 0.42 | 51,51,51,51                | 0     |
| 55  | MG   | DA    | 3140 | 1/1   | 0.93 | 0.43 | 43,43,43,43                | 0     |
| 55  | MG   | BA    | 3121 | 1/1   | 0.93 | 0.12 | 3,3,3,3                    | 0     |
| 55  | MG   | DA    | 3142 | 1/1   | 0.93 | 0.26 | 33,33,33,33                | 0     |
| 55  | MG   | BA    | 3166 | 1/1   | 0.93 | 0.17 | 19,19,19,19                | 0     |
| 55  | MG   | CA    | 1633 | 1/1   | 0.93 | 0.32 | 64,64,64,64                | 0     |
| 55  | MG   | AA    | 1663 | 1/1   | 0.93 | 0.22 | 48,48,48,48                | 0     |
| 55  | MG   | BA    | 3126 | 1/1   | 0.93 | 0.12 | 6,6,6,6                    | 0     |
| 55  | MG   | BA    | 3030 | 1/1   | 0.93 | 0.14 | 9,9,9,9                    | 0     |
| 55  | MG   | BA    | 3031 | 1/1   | 0.93 | 0.07 | 14,14,14,14                | 0     |
| 55  | MG   | AA    | 1610 | 1/1   | 0.93 | 0.23 | 65,65,65,65                | 0     |
| 55  | MG   | BA    | 3173 | 1/1   | 0.93 | 0.14 | 27,27,27,27                | 0     |
| 55  | MG   | CA    | 1643 | 1/1   | 0.93 | 0.24 | 50,50,50,50                | 0     |
| 55  | MG   | BA    | 3056 | 1/1   | 0.93 | 0.08 | 5,5,5,5                    | 0     |
| 55  | MG   | BA    | 3034 | 1/1   | 0.93 | 0.10 | 6,6,6,6                    | 0     |
| 55  | MG   | BA    | 3136 | 1/1   | 0.93 | 0.12 | 21,21,21,21                | 0     |
| 55  | MG   | DA    | 3053 | 1/1   | 0.93 | 0.11 | 40,40,40,40                | 0     |
| 55  | MG   | BA    | 3079 | 1/1   | 0.93 | 0.09 | 22,22,22,22                | 0     |
| 55  | MG   | BA    | 3181 | 1/1   | 0.93 | 0.20 | 24,24,24,24                | 0     |
| 55  | MG   | AA    | 1617 | 1/1   | 0.93 | 0.12 | 52,52,52,52                | 0     |
| 55  | MG   | CA    | 1652 | 1/1   | 0.93 | 0.11 | 83,83,83,83                | 0     |
| 55  | MG   | DA    | 3161 | 1/1   | 0.93 | 0.11 | 57,57,57,57                | 0     |
| 55  | MG   | BA    | 3185 | 1/1   | 0.93 | 0.30 | 16,16,16,16                | 0     |
| 55  | MG   | BA    | 3013 | 1/1   | 0.93 | 0.21 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3149 | 1/1   | 0.93 | 0.12 | 38,38,38,38                | 0     |
| 55  | MG   | DA    | 3130 | 1/1   | 0.93 | 0.10 | 81,81,81,81                | 0     |
| 55  | MG   | BA    | 3085 | 1/1   | 0.93 | 0.22 | 27,27,27,27                | 0     |
| 55  | MG   | BA    | 3190 | 1/1   | 0.93 | 0.10 | 31,31,31,31                | 0     |
| 55  | MG   | AA    | 1627 | 1/1   | 0.93 | 0.09 | 37,37,37,37                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1618 | 1/1   | 0.93 | 0.08 | 37,37,37,37                 | 0     |
| 55  | MG   | BA    | 3065 | 1/1   | 0.93 | 0.14 | 0,0,0,0                     | 0     |
| 55  | MG   | AA    | 1616 | 1/1   | 0.94 | 0.12 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3140 | 1/1   | 0.94 | 0.39 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3043 | 1/1   | 0.94 | 0.13 | 16,16,16,16                 | 0     |
| 55  | MG   | DA    | 3079 | 1/1   | 0.94 | 0.13 | 96,96,96,96                 | 0     |
| 55  | MG   | BA    | 3084 | 1/1   | 0.94 | 0.05 | 6,6,6,6                     | 0     |
| 55  | MG   | CA    | 1625 | 1/1   | 0.94 | 0.15 | 22,22,22,22                 | 0     |
| 55  | MG   | AA    | 1607 | 1/1   | 0.94 | 0.09 | 44,44,44,44                 | 0     |
| 55  | MG   | CA    | 1653 | 1/1   | 0.94 | 0.09 | 52,52,52,52                 | 0     |
| 55  | MG   | BA    | 3150 | 1/1   | 0.94 | 0.20 | 37,37,37,37                 | 0     |
| 55  | MG   | BA    | 3025 | 1/1   | 0.94 | 0.10 | 2,2,2,2                     | 0     |
| 55  | MG   | DA    | 3055 | 1/1   | 0.94 | 0.13 | 72,72,72,72                 | 0     |
| 55  | MG   | AA    | 1649 | 1/1   | 0.94 | 0.14 | 32,32,32,32                 | 0     |
| 55  | MG   | BA    | 3130 | 1/1   | 0.94 | 0.12 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3039 | 1/1   | 0.94 | 0.27 | 0,0,0,0                     | 0     |
| 55  | MG   | AA    | 1668 | 1/1   | 0.94 | 0.13 | 29,29,29,29                 | 0     |
| 55  | MG   | BA    | 3053 | 1/1   | 0.94 | 0.14 | 2,2,2,2                     | 0     |
| 55  | MG   | BA    | 3115 | 1/1   | 0.94 | 0.12 | 20,20,20,20                 | 0     |
| 55  | MG   | BA    | 3159 | 1/1   | 0.94 | 0.22 | 14,14,14,14                 | 0     |
| 55  | MG   | BA    | 3160 | 1/1   | 0.94 | 0.10 | 10,10,10,10                 | 0     |
| 55  | MG   | DA    | 3035 | 1/1   | 0.94 | 0.09 | 79,79,79,79                 | 0     |
| 55  | MG   | BA    | 3164 | 1/1   | 0.94 | 0.14 | 4,4,4,4                     | 0     |
| 55  | MG   | BA    | 3165 | 1/1   | 0.94 | 0.30 | 43,43,43,43                 | 0     |
| 55  | MG   | BA    | 3080 | 1/1   | 0.94 | 0.07 | 39,39,39,39                 | 0     |
| 55  | MG   | DA    | 3167 | 1/1   | 0.94 | 0.29 | 100,100,100,100             | 0     |
| 55  | MG   | CA    | 1641 | 1/1   | 0.94 | 0.68 | 73,73,73,73                 | 0     |
| 55  | MG   | DA    | 3102 | 1/1   | 0.94 | 0.22 | 62,62,62,62                 | 0     |
| 55  | MG   | CA    | 1642 | 1/1   | 0.94 | 0.25 | 25,25,25,25                 | 0     |
| 55  | MG   | BA    | 3192 | 1/1   | 0.94 | 0.21 | 22,22,22,22                 | 0     |
| 55  | MG   | CA    | 1645 | 1/1   | 0.94 | 0.20 | 32,32,32,32                 | 0     |
| 55  | MG   | CA    | 1619 | 1/1   | 0.94 | 0.10 | 33,33,33,33                 | 0     |
| 55  | MG   | AA    | 1608 | 1/1   | 0.95 | 0.14 | 17,17,17,17                 | 0     |
| 55  | MG   | AA    | 1653 | 1/1   | 0.95 | 0.17 | 28,28,28,28                 | 0     |
| 55  | MG   | AA    | 1640 | 1/1   | 0.95 | 0.09 | 36,36,36,36                 | 0     |
| 55  | MG   | BA    | 3094 | 1/1   | 0.95 | 0.05 | 31,31,31,31                 | 0     |
| 55  | MG   | BA    | 3045 | 1/1   | 0.95 | 0.08 | 9,9,9,9                     | 0     |
| 55  | MG   | BA    | 3061 | 1/1   | 0.95 | 0.35 | 30,30,30,30                 | 0     |
| 55  | MG   | DA    | 3118 | 1/1   | 0.95 | 0.08 | 60,60,60,60                 | 0     |
| 55  | MG   | CA    | 1611 | 1/1   | 0.95 | 0.29 | 90,90,90,90                 | 0     |
| 55  | MG   | BA    | 3062 | 1/1   | 0.95 | 0.36 | 50,50,50,50                 | 0     |
| 55  | MG   | AA    | 1655 | 1/1   | 0.95 | 0.11 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1624 | 1/1   | 0.95 | 0.04 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3188 | 1/1   | 0.95 | 0.14 | 10,10,10,10                 | 0     |
| 55  | MG   | BA    | 3017 | 1/1   | 0.95 | 0.06 | 2,2,2,2                     | 0     |
| 55  | MG   | BA    | 3161 | 1/1   | 0.95 | 0.17 | 31,31,31,31                 | 0     |
| 55  | MG   | BA    | 3035 | 1/1   | 0.95 | 0.18 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3036 | 1/1   | 0.95 | 0.12 | 11,11,11,11                 | 0     |
| 55  | MG   | DA    | 3043 | 1/1   | 0.95 | 0.13 | 66,66,66,66                 | 0     |
| 55  | MG   | BA    | 3138 | 1/1   | 0.95 | 0.45 | 1,1,1,1                     | 0     |
| 55  | MG   | BA    | 3088 | 1/1   | 0.95 | 0.23 | 2,2,2,2                     | 0     |
| 55  | MG   | BA    | 3020 | 1/1   | 0.95 | 0.09 | 22,22,22,22                 | 0     |
| 55  | MG   | BB    | 203  | 1/1   | 0.95 | 0.06 | 7,7,7,7                     | 0     |
| 55  | MG   | DA    | 3166 | 1/1   | 0.95 | 0.09 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3145 | 1/1   | 0.95 | 0.29 | 28,28,28,28                 | 0     |
| 55  | MG   | BA    | 3118 | 1/1   | 0.95 | 0.12 | 1,1,1,1                     | 0     |
| 55  | MG   | BA    | 3148 | 1/1   | 0.95 | 0.12 | 29,29,29,29                 | 0     |
| 55  | MG   | DA    | 3051 | 1/1   | 0.95 | 0.09 | 28,28,28,28                 | 0     |
| 55  | MG   | DA    | 3109 | 1/1   | 0.95 | 0.22 | 42,42,42,42                 | 0     |
| 55  | MG   | BA    | 3172 | 1/1   | 0.95 | 0.17 | 31,31,31,31                 | 0     |
| 55  | MG   | AA    | 1647 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 55  | MG   | CA    | 1612 | 1/1   | 0.96 | 0.05 | 40,40,40,40                 | 0     |
| 55  | MG   | BA    | 3135 | 1/1   | 0.96 | 0.14 | 2,2,2,2                     | 0     |
| 55  | MG   | BA    | 3023 | 1/1   | 0.96 | 0.14 | 1,1,1,1                     | 0     |
| 55  | MG   | BA    | 3024 | 1/1   | 0.96 | 0.17 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3012 | 1/1   | 0.96 | 0.05 | 14,14,14,14                 | 0     |
| 55  | MG   | CA    | 1644 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 55  | MG   | DA    | 3018 | 1/1   | 0.96 | 0.12 | 60,60,60,60                 | 0     |
| 55  | MG   | BA    | 3026 | 1/1   | 0.96 | 0.15 | 3,3,3,3                     | 0     |
| 55  | MG   | CA    | 1618 | 1/1   | 0.96 | 0.11 | 37,37,37,37                 | 0     |
| 55  | MG   | AA    | 1633 | 1/1   | 0.96 | 0.12 | 30,30,30,30                 | 0     |
| 55  | MG   | DA    | 3083 | 1/1   | 0.96 | 0.10 | 69,69,69,69                 | 0     |
| 55  | MG   | BA    | 3029 | 1/1   | 0.96 | 0.08 | 21,21,21,21                 | 0     |
| 55  | MG   | BA    | 3095 | 1/1   | 0.96 | 0.09 | 21,21,21,21                 | 0     |
| 55  | MG   | BB    | 201  | 1/1   | 0.96 | 0.10 | 20,20,20,20                 | 0     |
| 55  | MG   | CA    | 1623 | 1/1   | 0.96 | 0.16 | 50,50,50,50                 | 0     |
| 55  | MG   | BA    | 3147 | 1/1   | 0.96 | 0.31 | 9,9,9,9                     | 0     |
| 55  | MG   | BA    | 3014 | 1/1   | 0.96 | 0.18 | 0,0,0,0                     | 0     |
| 55  | MG   | DA    | 3122 | 1/1   | 0.96 | 0.15 | 41,41,41,41                 | 0     |
| 55  | MG   | BA    | 3122 | 1/1   | 0.96 | 0.04 | 18,18,18,18                 | 0     |
| 55  | MG   | BA    | 3124 | 1/1   | 0.96 | 0.09 | 11,11,11,11                 | 0     |
| 55  | MG   | DA    | 3059 | 1/1   | 0.96 | 0.10 | 51,51,51,51                 | 0     |
| 55  | MG   | BA    | 3009 | 1/1   | 0.96 | 0.09 | 4,4,4,4                     | 0     |
| 55  | MG   | BA    | 3175 | 1/1   | 0.96 | 0.11 | 27,27,27,27                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 55  | MG   | DA    | 3128 | 1/1   | 0.96 | 0.08 | 80,80,80,80                | 0     |
| 55  | MG   | BA    | 3176 | 1/1   | 0.96 | 0.10 | 20,20,20,20                | 0     |
| 55  | MG   | BA    | 3101 | 1/1   | 0.96 | 0.07 | 1,1,1,1                    | 0     |
| 55  | MG   | BA    | 3070 | 1/1   | 0.96 | 0.21 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3044 | 1/1   | 0.96 | 0.14 | 3,3,3,3                    | 0     |
| 55  | MG   | CA    | 1634 | 1/1   | 0.96 | 0.13 | 49,49,49,49                | 0     |
| 55  | MG   | BA    | 3074 | 1/1   | 0.96 | 0.18 | 1,1,1,1                    | 0     |
| 55  | MG   | BA    | 3108 | 1/1   | 0.96 | 0.24 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3110 | 1/1   | 0.96 | 0.20 | 3,3,3,3                    | 0     |
| 56  | DOL  | BA    | 3001 | 48/48 | 0.96 | 0.21 | 0,3,25,36                  | 0     |
| 55  | MG   | BA    | 3022 | 1/1   | 0.96 | 0.08 | 2,2,2,2                    | 0     |
| 55  | MG   | BA    | 3111 | 1/1   | 0.97 | 0.20 | 6,6,6,6                    | 0     |
| 55  | MG   | DA    | 3086 | 1/1   | 0.97 | 0.10 | 76,76,76,76                | 0     |
| 55  | MG   | BA    | 3072 | 1/1   | 0.97 | 0.08 | 3,3,3,3                    | 0     |
| 55  | MG   | BA    | 3183 | 1/1   | 0.97 | 0.21 | 12,12,12,12                | 0     |
| 55  | MG   | BA    | 3184 | 1/1   | 0.97 | 0.20 | 6,6,6,6                    | 0     |
| 55  | MG   | BA    | 3158 | 1/1   | 0.97 | 0.12 | 19,19,19,19                | 0     |
| 55  | MG   | BA    | 3073 | 1/1   | 0.97 | 0.07 | 7,7,7,7                    | 0     |
| 55  | MG   | DA    | 3063 | 1/1   | 0.97 | 0.22 | 54,54,54,54                | 0     |
| 55  | MG   | BA    | 3037 | 1/1   | 0.97 | 0.17 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3060 | 1/1   | 0.97 | 0.06 | 15,15,15,15                | 0     |
| 55  | MG   | BA    | 3163 | 1/1   | 0.97 | 0.33 | 15,15,15,15                | 0     |
| 55  | MG   | AA    | 1615 | 1/1   | 0.97 | 0.06 | 47,47,47,47                | 0     |
| 55  | MG   | DA    | 3156 | 1/1   | 0.97 | 0.19 | 41,41,41,41                | 0     |
| 55  | MG   | BA    | 3117 | 1/1   | 0.97 | 0.17 | 1,1,1,1                    | 0     |
| 55  | MG   | BA    | 3007 | 1/1   | 0.97 | 0.09 | 22,22,22,22                | 0     |
| 55  | MG   | AA    | 1611 | 1/1   | 0.97 | 0.09 | 21,21,21,21                | 0     |
| 55  | MG   | BA    | 3142 | 1/1   | 0.97 | 0.43 | 2,2,2,2                    | 0     |
| 55  | MG   | BA    | 3052 | 1/1   | 0.97 | 0.06 | 11,11,11,11                | 0     |
| 55  | MG   | BA    | 3032 | 1/1   | 0.97 | 0.16 | 4,4,4,4                    | 0     |
| 55  | MG   | AA    | 1604 | 1/1   | 0.97 | 0.06 | 48,48,48,48                | 0     |
| 55  | MG   | BA    | 3123 | 1/1   | 0.97 | 0.16 | 0,0,0,0                    | 0     |
| 55  | MG   | DA    | 3076 | 1/1   | 0.97 | 0.12 | 69,69,69,69                | 0     |
| 55  | MG   | BQ    | 201  | 1/1   | 0.97 | 0.20 | 3,3,3,3                    | 0     |
| 55  | MG   | BA    | 3067 | 1/1   | 0.97 | 0.17 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3083 | 1/1   | 0.97 | 0.17 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3068 | 1/1   | 0.97 | 0.17 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3010 | 1/1   | 0.97 | 0.11 | 0,0,0,0                    | 0     |
| 55  | MG   | BA    | 3129 | 1/1   | 0.97 | 0.19 | 4,4,4,4                    | 0     |
| 55  | MG   | BA    | 3018 | 1/1   | 0.97 | 0.20 | 0,0,0,0                    | 0     |
| 55  | MG   | AA    | 1642 | 1/1   | 0.97 | 0.15 | 23,23,23,23                | 0     |
| 55  | MG   | BA    | 3109 | 1/1   | 0.98 | 0.19 | 12,12,12,12                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | AA    | 1636 | 1/1   | 0.98 | 0.08 | 27,27,27,27                 | 0     |
| 55  | MG   | BA    | 3041 | 1/1   | 0.98 | 0.18 | 6,6,6,6                     | 0     |
| 55  | MG   | BA    | 3128 | 1/1   | 0.98 | 0.10 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3096 | 1/1   | 0.98 | 0.07 | 11,11,11,11                 | 0     |
| 55  | MG   | BA    | 3097 | 1/1   | 0.98 | 0.07 | 4,4,4,4                     | 0     |
| 55  | MG   | AA    | 1622 | 1/1   | 0.98 | 0.20 | 16,16,16,16                 | 0     |
| 55  | MG   | BA    | 3099 | 1/1   | 0.98 | 0.12 | 4,4,4,4                     | 0     |
| 55  | MG   | BA    | 3194 | 1/1   | 0.98 | 0.07 | 8,8,8,8                     | 0     |
| 55  | MG   | BA    | 3028 | 1/1   | 0.98 | 0.08 | 5,5,5,5                     | 0     |
| 55  | MG   | DA    | 3162 | 1/1   | 0.98 | 0.21 | 38,38,38,38                 | 0     |
| 55  | MG   | AA    | 1656 | 1/1   | 0.98 | 0.15 | 43,43,43,43                 | 0     |
| 55  | MG   | AA    | 1621 | 1/1   | 0.98 | 0.08 | 39,39,39,39                 | 0     |
| 55  | MG   | BA    | 3055 | 1/1   | 0.98 | 0.17 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3177 | 1/1   | 0.98 | 0.17 | 17,17,17,17                 | 0     |
| 55  | MG   | AA    | 1645 | 1/1   | 0.98 | 0.12 | 42,42,42,42                 | 0     |
| 55  | MG   | BA    | 3105 | 1/1   | 0.98 | 0.10 | 4,4,4,4                     | 0     |
| 55  | MG   | BA    | 3139 | 1/1   | 0.98 | 0.37 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3106 | 1/1   | 0.98 | 0.20 | 16,16,16,16                 | 0     |
| 55  | MG   | BA    | 3107 | 1/1   | 0.98 | 0.19 | 0,0,0,0                     | 0     |
| 55  | MG   | BA    | 3162 | 1/1   | 0.98 | 0.07 | 36,36,36,36                 | 0     |
| 55  | MG   | BA    | 3019 | 1/1   | 0.98 | 0.12 | 11,11,11,11                 | 0     |
| 55  | MG   | BA    | 3144 | 1/1   | 0.98 | 0.26 | 15,15,15,15                 | 0     |
| 57  | ZN   | B4    | 101  | 1/1   | 0.98 | 0.10 | 33,33,33,33                 | 0     |
| 57  | ZN   | D4    | 101  | 1/1   | 0.98 | 0.10 | 87,87,87,87                 | 0     |
| 55  | MG   | BA    | 3143 | 1/1   | 0.99 | 0.36 | 12,12,12,12                 | 0     |
| 55  | MG   | BA    | 3011 | 1/1   | 0.99 | 0.15 | 1,1,1,1                     | 0     |
| 55  | MG   | DA    | 3139 | 1/1   | 0.99 | 0.33 | 30,30,30,30                 | 0     |
| 55  | MG   | BA    | 3048 | 1/1   | 0.99 | 0.15 | 8,8,8,8                     | 0     |

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.