



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:58 am GMT

PDB ID : 4V9D  
Title : Structures of the bacterial ribosome in classical and hybrid states of tRNA binding  
Authors : Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.  
Deposited on : 2012-07-31  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.9-1692   |
| EDS                            | : | trunk28620   |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac                         | : | 5.8.0135   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | recalc28972  |

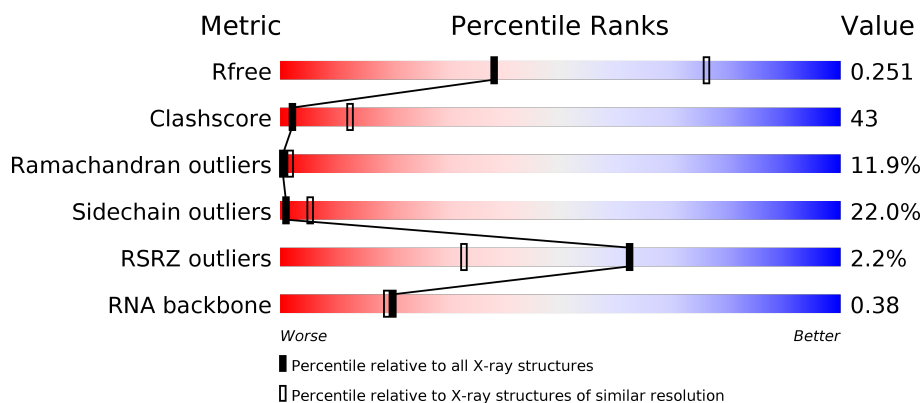
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



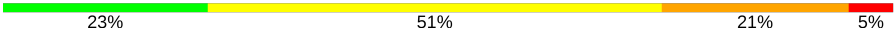

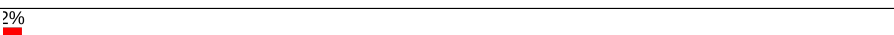
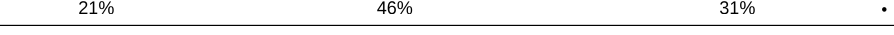
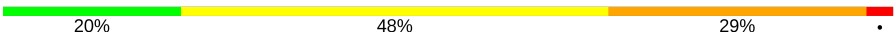

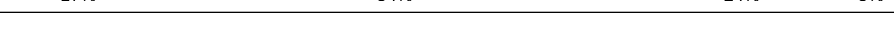



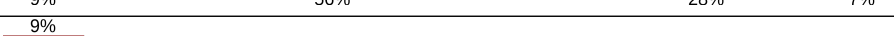
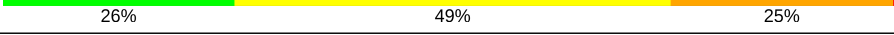

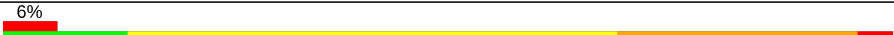


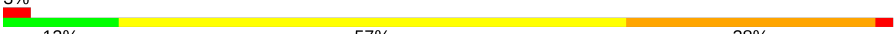

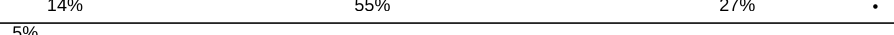


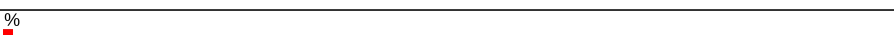
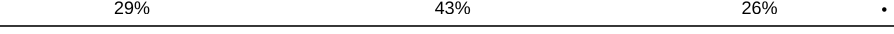
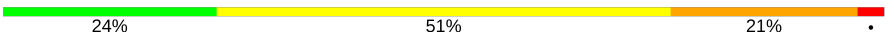

| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1692 (3.00-3.00)                                      |
| Clashscore            | 112137                      | 2037 (3.00-3.00)                                      |
| Ramachandran outliers | 110173                      | 1973 (3.00-3.00)                                      |
| Sidechain outliers    | 110143                      | 1976 (3.00-3.00)                                      |
| RSRZ outliers         | 101464                      | 1716 (3.00-3.00)                                      |
| RNA backbone          | 2435                        | 1007 (3.34-2.66)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | AA    | 1539   | <div> <div>14%</div> <div>55%</div> <div>27%</div> <div>.</div> </div>                |
| 1   | BA    | 1539   | <div> <div>13%</div> <div>56%</div> <div>28%</div> <div>.</div> </div>                |
| 2   | AB    | 218    | <div> <div>6%</div> <div>10%</div> <div>45%</div> <div>36%</div> <div>9%</div> </div> |
| 2   | BB    | 218    | <div> <div>6%</div> <div>15%</div> <div>51%</div> <div>26%</div> <div>8%</div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | AC    | 206    |    |
| 3   | BC    | 206    |    |
| 4   | AD    | 205    |    |
| 4   | BD    | 205    |    |
| 5   | AE    | 150    |    |
| 5   | BE    | 150    |    |
| 6   | AF    | 100    |    |
| 6   | BF    | 100    |    |
| 7   | AG    | 151    |    |
| 7   | BG    | 151    |    |
| 8   | AH    | 129    |    |
| 8   | BH    | 129    |    |
| 9   | AI    | 127    |  |
| 9   | BI    | 127    |  |
| 10  | AJ    | 98     |  |
| 10  | BJ    | 98     |  |
| 11  | AK    | 117    |  |
| 11  | BK    | 117    |  |
| 12  | AL    | 123    |  |
| 12  | BL    | 123    |  |
| 13  | AM    | 114    |  |
| 13  | BM    | 114    |  |
| 14  | AN    | 100    |  |
| 14  | BN    | 100    |  |
| 15  | AO    | 88     |  |



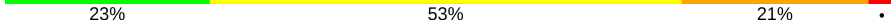

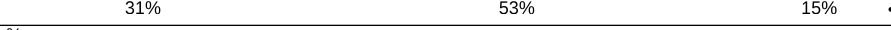
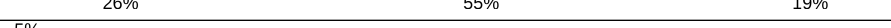
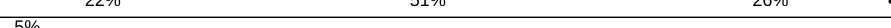
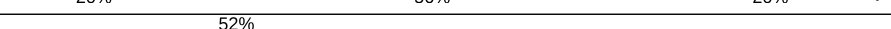
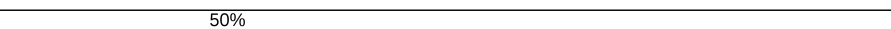
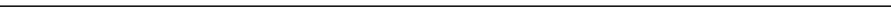





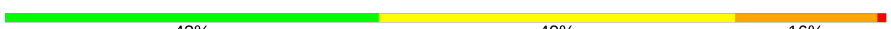


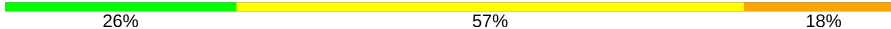

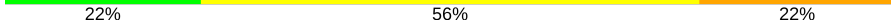




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | BO    | 88     |                  |
| 16  | AP    | 82     |                  |
| 16  | BP    | 82     |                  |
| 17  | AQ    | 80     |                  |
| 17  | BQ    | 80     |                  |
| 18  | AR    | 55     |                  |
| 18  | BR    | 55     |                  |
| 19  | AS    | 79     |                  |
| 19  | BS    | 79     |                  |
| 20  | AT    | 85     |                  |
| 20  | BT    | 85     |                  |
| 21  | AU    | 51     |                  |
| 21  | BU    | 51     |                  |
| 22  | AV    | 76     |                  |
| 22  | BV    | 76     |                  |
| 23  | AX    | 16     |                  |
| 23  | BX    | 16     |                  |
| 24  | AY    | 183    |                  |
| 25  | CA    | 2903   |                  |
| 25  | DA    | 2903   |                  |
| 26  | CB    | 119    |                  |
| 27  | CC    | 271    |                  |
| 27  | DC    | 271    |                  |
| 28  | CD    | 209    |                  |
| 28  | DD    | 209    |                  |

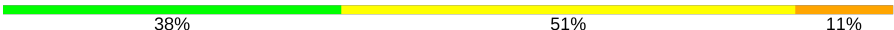

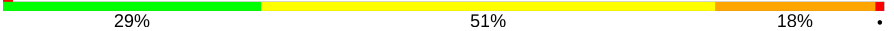





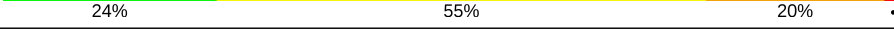





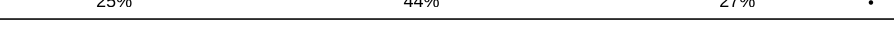

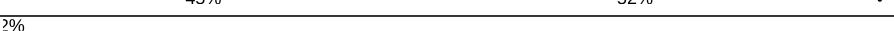

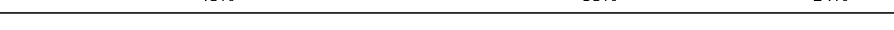
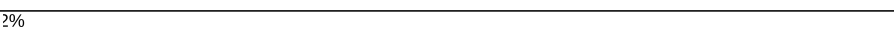
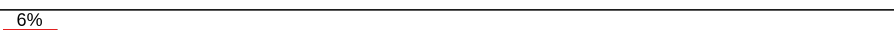
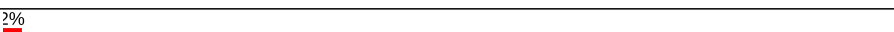
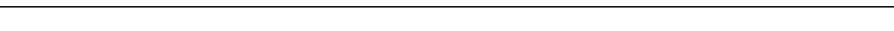
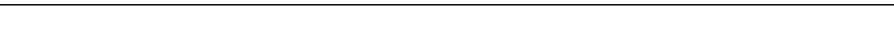

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 29  | CE    | 201    |    |
| 29  | DE    | 201    |    |
| 30  | CF    | 177    |    |
| 30  | DF    | 177    |    |
| 31  | CG    | 176    |    |
| 31  | DG    | 176    |    |
| 32  | CH    | 149    |    |
| 32  | DH    | 149    |    |
| 33  | CI    | 141    |    |
| 33  | DI    | 141    |    |
| 34  | CJ    | 142    |    |
| 34  | DJ    | 142    |   |
| 35  | CK    | 122    |  |
| 35  | DK    | 122    |  |
| 36  | CL    | 143    |  |
| 36  | DL    | 143    |  |
| 37  | CM    | 136    |  |
| 37  | DM    | 136    |  |
| 38  | CN    | 120    |  |
| 38  | DN    | 120    |  |
| 39  | CO    | 116    |  |
| 39  | DO    | 116    |  |
| 40  | CP    | 114    |  |
| 40  | DP    | 114    |  |
| 41  | CQ    | 117    |  |

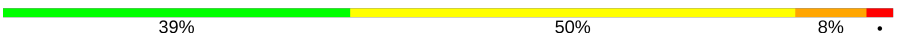
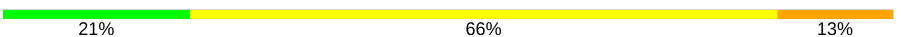
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 41  | DQ    | 117    |    |
| 42  | CR    | 103    |    |
| 42  | DR    | 103    |    |
| 43  | CS    | 110    |    |
| 43  | DS    | 110    |    |
| 44  | CT    | 93     |    |
| 44  | DT    | 93     |    |
| 45  | CU    | 102    |    |
| 45  | DU    | 102    |    |
| 46  | CV    | 94     |    |
| 46  | DV    | 94     |    |
| 47  | CW    | 76     |   |
| 48  | CX    | 77     |  |
| 48  | DX    | 77     |  |
| 49  | CY    | 63     |  |
| 49  | DY    | 63     |  |
| 50  | CZ    | 58     |  |
| 50  | DZ    | 58     |  |
| 51  | C0    | 56     |  |
| 51  | D0    | 56     |  |
| 52  | C1    | 50     |  |
| 52  | D1    | 50     |  |
| 53  | C2    | 46     |  |
| 53  | D2    | 46     |  |
| 54  | C3    | 64     |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 54  | D3    | 64     |  |
| 55  | C4    | 38     |  |
| 55  | D4    | 38     |  |
| 56  | DB    | 118    |  |
| 57  | DW    | 75     |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 58  | MG   | AA    | 1604 | -         | -        | -       | X                |
| 58  | MG   | AA    | 1622 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3066 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3121 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3132 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3147 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3153 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3155 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3159 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3163 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3165 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3175 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3186 | -         | -        | -       | X                |
| 58  | MG   | CA    | 3188 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3108 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3116 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3131 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3139 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3142 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3152 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3154 | -         | -        | -       | X                |
| 58  | MG   | DA    | 3157 | -         | -        | -       | X                |

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |         |       |
| 2   | BB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |
| 3   | BC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 4   | BD    | 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   | BE    | 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   | BF    | 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   | BG    | 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   | BH    | 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   | BI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |
| 15  | BO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 714   | 439 | 144 | 130 | 1 |         |         |       |

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | AV    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |         |       |
| 22  | BV    | 76       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1623  | 723 | 290 | 534 | 76 |         |         |       |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 23  | AX    | 15       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 324   | 145 | 61 | 103 | 15 |         |         |       |
| 23  | BX    | 16       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 346   | 155 | 66 | 109 | 16 |         |         |       |

- Molecule 24 is a protein called ribosome recycling factor.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | AY    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1419  | 871 | 260 | 283 | 5 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| AY    | 2       | GLY      | -      | EXPRESSION TAG | UNP P0A805 |

- Molecule 25 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 25  | CA    | 2897     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62195 | 27745 | 11446 | 20107 | 2897 |         |         |       |
| 25  | DA    | 2896     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62173 | 27735 | 11441 | 20101 | 2896 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 26  | CB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2548  | 1135 | 466 | 829 | 118 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27  | CC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |         |       |
| 27  | DC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | CD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |
| 28  | DD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | CE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |
| 29  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | CF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |         |       |
| 30  | DF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | CG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 31  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | CH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |
| 32  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | CI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |
| 33  | DI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | CJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |
| 34  | DJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | CK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |         |       |
| 35  | DK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | CL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |
| 36  | DL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | CM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |
| 37  | DM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | CN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |         |       |
| 38  | DN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 39  | CO    | 116      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |         |       |
| 39  | DO    | 116      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | CP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 40  | DP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | CQ    | 117      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |         |       |
| 41  | DQ    | 117      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | CR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | DR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | CS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |
| 43  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | CT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |
| 44  | DT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | CU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |   |         |         |       |
| 45  | DU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |   |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | CV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |
| 46  | DV    | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 753   | 479 | 137 | 134 | 3 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | CW    | 76       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 575   | 356 | 117 | 101 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L28.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | CX    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |
| 48  | DX    | 77       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 625   | 388 | 129 | 106 | 2 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49  | CY    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |
| 49  | DY    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 509   | 313 | 99 | 95 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | CZ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |
| 50  | DZ    | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 281 | 87 | 79 | 2 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | C0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |
| 51  | D0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 52  | C1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |         |       |
| 52  | D1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | C2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53  | D2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 54  | C3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 54  | D3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

- Molecule 55 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 55  | C4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |
| 55  | D4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

- Molecule 56 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 56  | DB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2529  | 1126 | 464 | 821 | 118 |         |         |       |

- Molecule 57 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | DW    | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 564   | 350 | 113 | 100 | 1 |         |         |       |

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 58  | BA    | 56       | Total | Mg  | 0       | 0       |
|     |       |          | 56    | 56  |         |         |
| 58  | CA    | 194      | Total | Mg  | 0       | 0       |
|     |       |          | 194   | 194 |         |         |
| 58  | DQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 58  | CB    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 58  | DL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | AA    | 72       | Total<br>72  | Mg<br>72  | 0       | 0       |
| 58  | CQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 58  | DA    | 166      | Total<br>166 | Mg<br>166 | 0       | 0       |
| 58  | DB    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 59  | D4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 59  | C4    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 60 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | AA    | 197      | Total<br>197 | O<br>197 | 0       | 0       |
| 60  | AN    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | AT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | AU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | BA    | 190      | Total<br>190 | O<br>190 | 0       | 0       |
| 60  | BL    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | BN    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | BT    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | BU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | CA    | 625      | Total<br>625 | O<br>625 | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60  | CB    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 60  | CC    | 8        | Total<br>8   | O<br>8   | 0       | 0       |
| 60  | CD    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | CE    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | CF    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | CJ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | CL    | 6        | Total<br>6   | O<br>6   | 0       | 0       |
| 60  | CN    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | CS    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | CV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | C2    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | C3    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | C4    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | DA    | 622      | Total<br>622 | O<br>622 | 0       | 0       |
| 60  | DB    | 14       | Total<br>14  | O<br>14  | 0       | 0       |
| 60  | DC    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | DD    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 60  | DE    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 60  | DJ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 60  | DL    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 60  | DN    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

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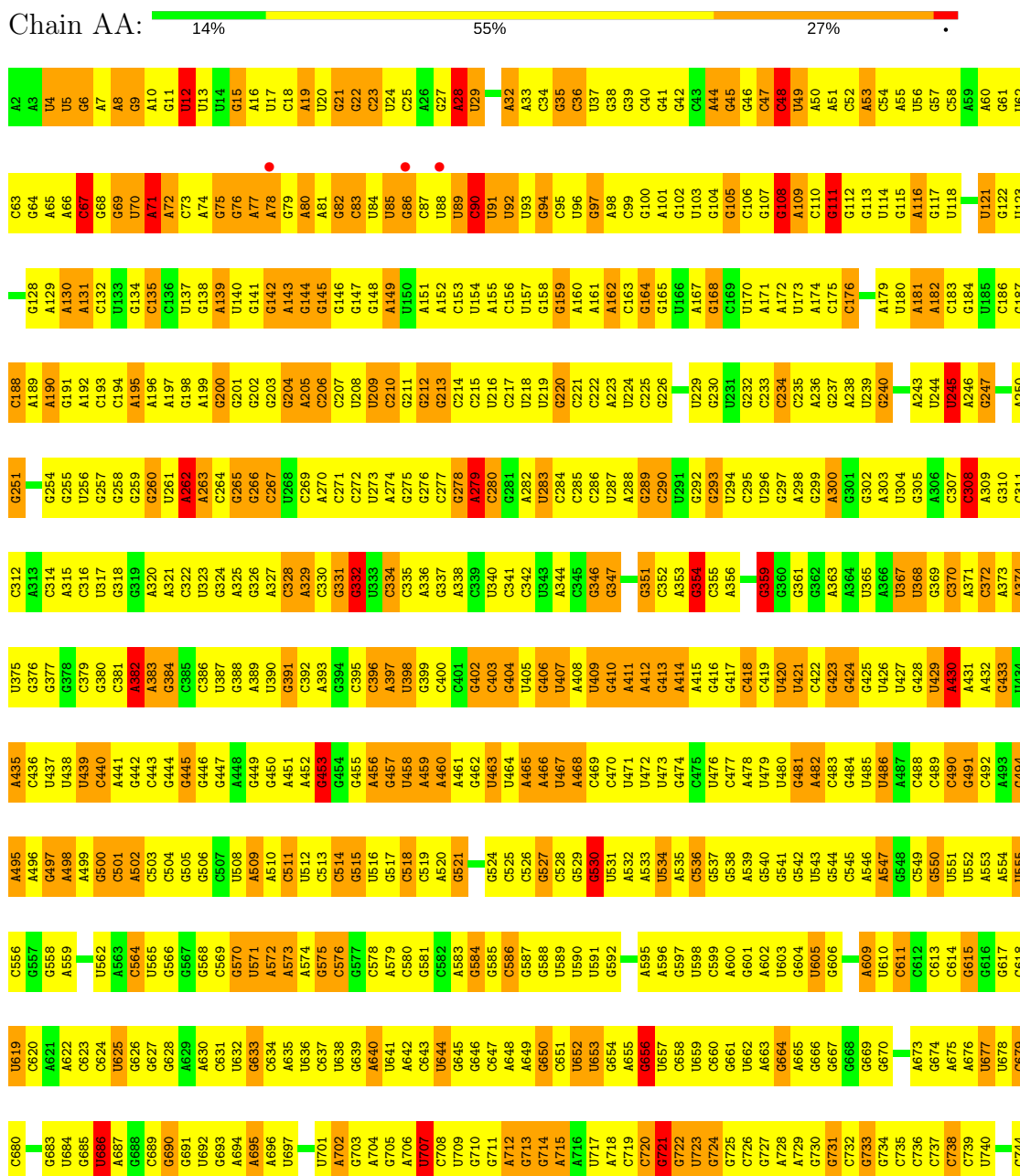
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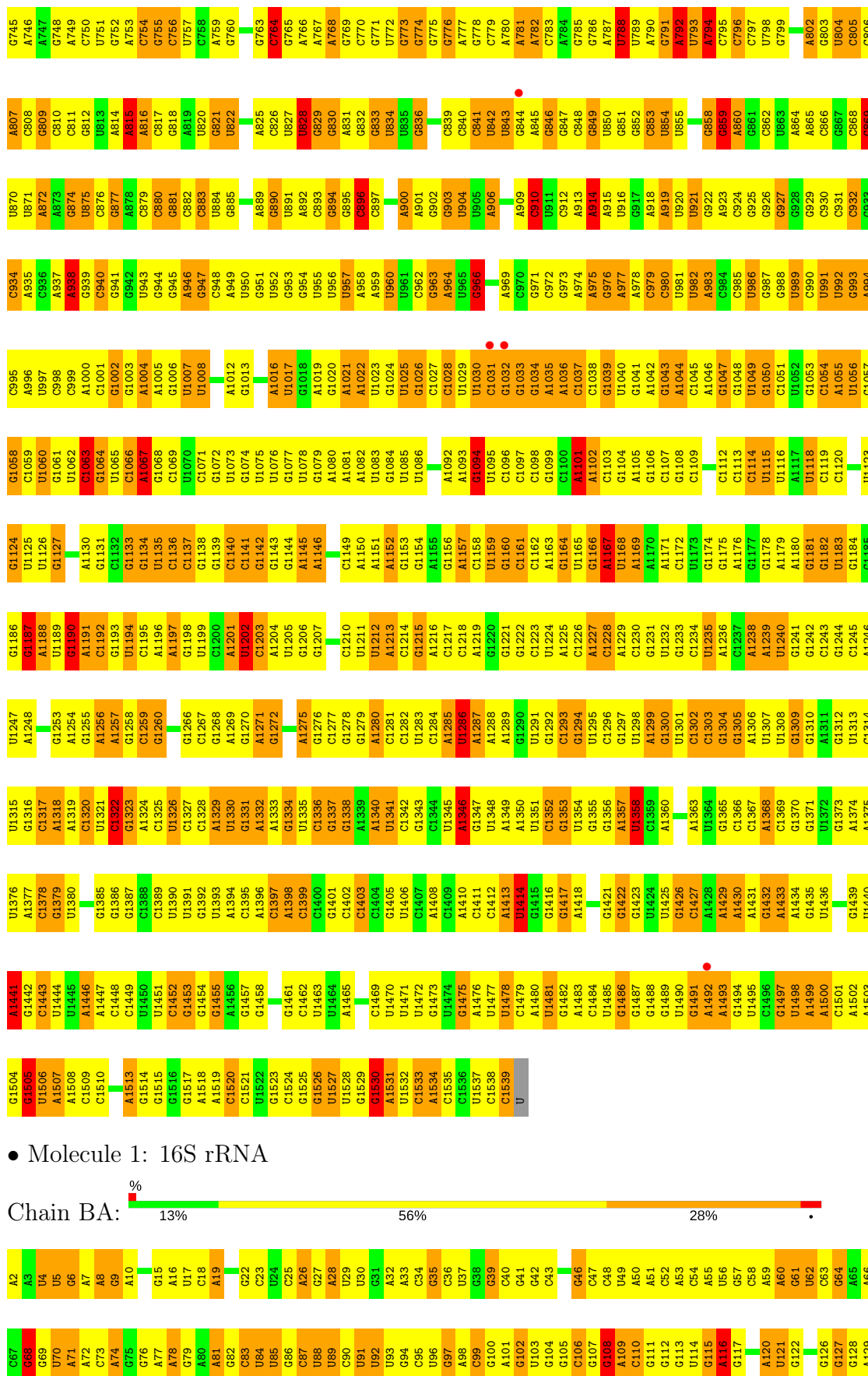
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 60  | DR    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | D2    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 60  | D3    | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 60  | D4    | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots

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

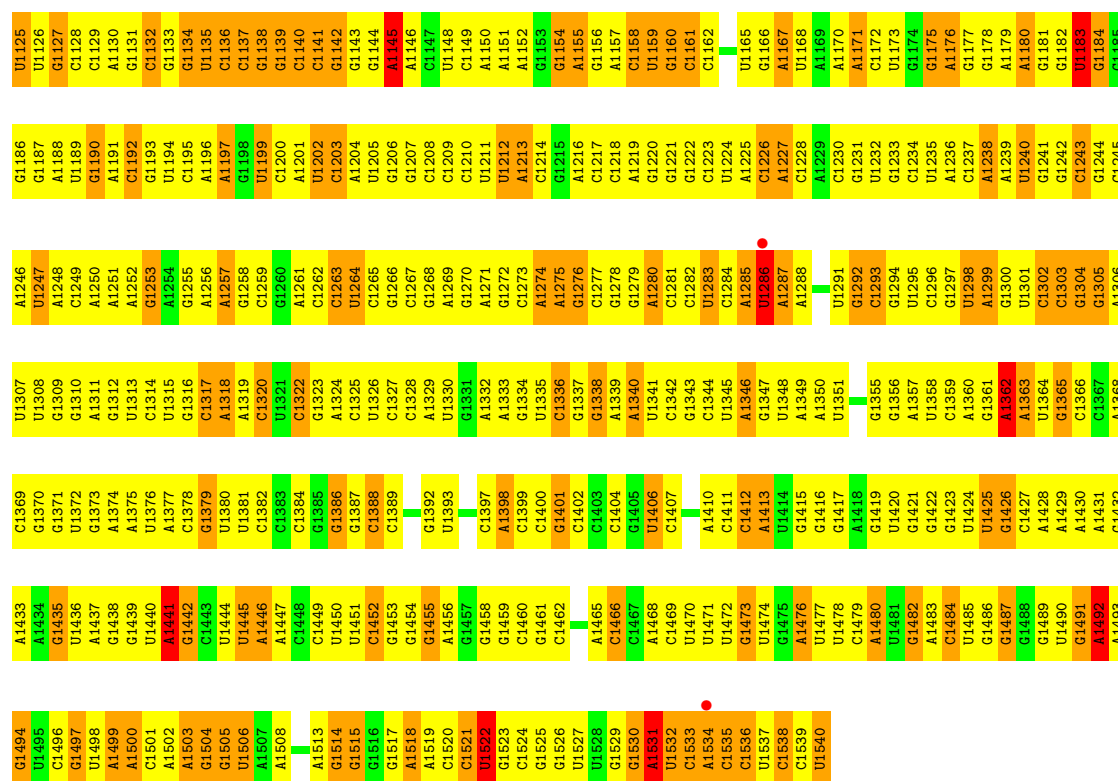
#### • Molecule 1: 16S rRNA



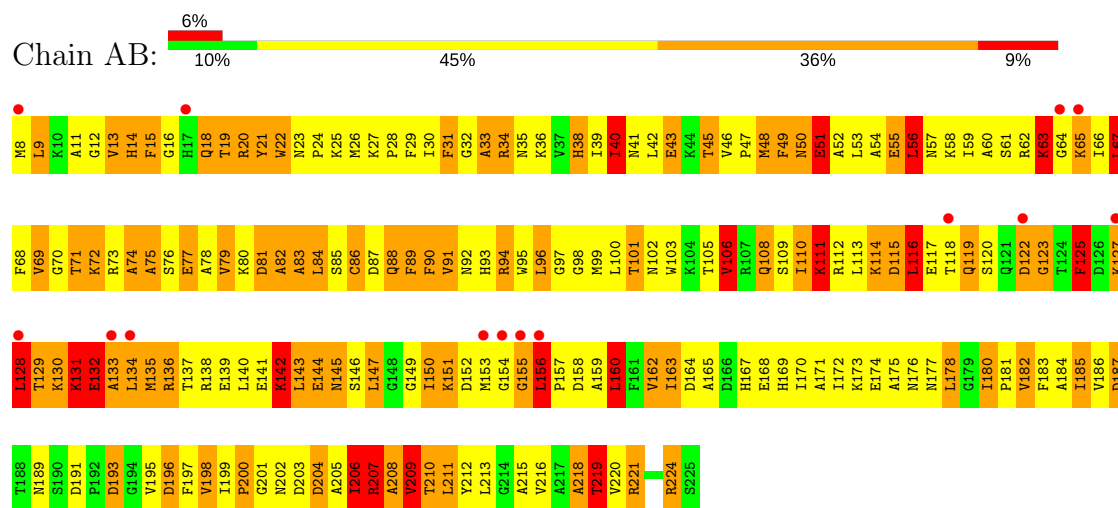


|       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| U1065 | C1066 | A1005 | G939  | G877 | A815 | U751 | C689 | G828 | G566 | A502 | C381 | G319 | G255 | G191 | A130 |
| C1066 | U1007 | G1006 | C940  | A878 | A816 | G752 | G690 | A829 | G567 | C503 | A382 | A320 | U256 | A192 | A131 |
| A1067 | G1068 | U1008 | G941  | C879 | G817 | A753 | G691 | A830 | C589 | G504 | A383 | A321 | G257 | C193 | C132 |
| C1069 | U1009 | G1009 | U943  | G881 | A819 | G755 | G692 | C631 | C588 | G505 | A384 | C322 | G258 | C194 | U133 |
| U1010 | C1011 | U1010 | G944  | C882 | A820 | G756 | A694 | U632 | G570 | G506 | C385 | G325 | G259 | A195 | G134 |
| C1071 | U1070 | C1071 | G945  | C883 | G821 | U757 | A695 | G633 | U571 | C507 | C386 | A325 | G260 | A196 | C135 |
| U1072 | G1073 | A1012 | A949  | U884 | G822 | C758 | G699 | C634 | A572 | A510 | U387 | G326 | U261 | A197 | U136 |
| C1073 | U1013 | G1013 | U950  | G885 | U823 | A759 | C699 | A635 | A573 | C511 | G388 | A327 | U262 | U198 | U137 |
| U1074 | A1014 | G1014 | G951  | G886 | G824 | C760 | G700 | U636 | A574 | G511 | G389 | A328 | C264 | A199 | G141 |
| U1075 | G1015 | U1075 | U952  | A889 | A825 | U762 | U701 | C637 | C575 | A512 | U390 | A329 | G265 | G200 | G145 |
| U1076 | A1016 | G1016 | G953  | G890 | C826 | G763 | U702 | U638 | C576 | C513 | C391 | C330 | G266 | G201 | G146 |
| G1077 | G1077 | U1017 | G954  | U891 | U827 | C764 | A703 | G640 | G577 | U516 | C392 | G331 | C267 | G202 | G147 |
| U1078 | G1018 | G1018 | U955  | A892 | U828 | G765 | A704 | U641 | A579 | G517 | A393 | C332 | U268 | G203 | A143 |
| G1079 | A1019 | U1086 | U956  | C893 | G829 | A766 | A705 | A642 | C580 | C518 | C394 | U333 | C269 | G204 | G144 |
| A1080 | G1020 | U1087 | U957  | G894 | G830 | A767 | U706 | C643 | C581 | C519 | C396 | C335 | A270 | A205 | G145 |
| A1081 | A1021 | U1088 | A958  | G895 | A831 | A768 | U707 | U644 | C582 | G522 | C402 | C342 | C271 | C206 | G146 |
| A1082 | A1022 | G1089 | A959  | C896 | G832 | A769 | C708 | G645 | A583 | C523 | C403 | C343 | C272 | G207 | G147 |
| U1083 | U1023 | U1089 | U960  | C897 | G833 | C770 | U709 | G646 | C584 | A523 | C404 | U343 | C273 | U208 | G148 |
| G1084 | G1024 | U1090 | G963  | C898 | U834 | C771 | G710 | C647 | C585 | G524 | C400 | A338 | A274 | U209 | A149 |
| U1085 | U1025 | C1031 | A964  | C899 | U835 | G775 | G711 | A648 | C586 | C525 | C401 | U340 | G275 | C210 | U150 |
| U1086 | G1026 | G1032 | U965  | A900 | G836 | G776 | A712 | A649 | C587 | C526 | G402 | C342 | G276 | G211 | A151 |
| G1087 | C1027 | U1091 | G966  | A901 | U837 | A777 | G713 | G650 | C588 | G527 | C403 | C343 | C277 | G212 | A152 |
| U1088 | C1028 | C1033 | G967  | G902 | U838 | G778 | G714 | C651 | U589 | G530 | G404 | U344 | A279 | G213 | C153 |
| G1089 | U1029 | U1030 | A968  | G903 | C840 | C779 | A715 | U652 | U590 | U531 | G405 | A344 | C280 | C214 | U154 |
| U1090 | C1031 | G1032 | A969  | U904 | C841 | A780 | A716 | U653 | U591 | A532 | G406 | C345 | G281 | G215 | A155 |
| A1091 | U1032 | A1092 | C970  | U905 | C842 | A781 | A717 | G654 | G592 | A533 | U407 | G346 | A282 | U219 | U157 |
| A1093 | G1033 | G1034 | G971  | A906 | U843 | A782 | A718 | A655 | U593 | A534 | U408 | G347 | U283 | G220 | G158 |
| G1094 | C1034 | U1095 | C972  | A907 | G844 | A783 | C719 | G656 | U594 | U535 | U409 | G348 | G292 | G221 | A160 |
| U1095 | A1035 | C1036 | G973  | A908 | A845 | C783 | C720 | U657 | A595 | C536 | G410 | A349 | C285 | C221 | A161 |
| C1096 | U1036 | A1037 | A974  | A909 | G846 | A784 | G721 | C658 | A596 | U472 | A411 | G350 | C286 | C292 | A162 |
| C1097 | A975  | C1037 | A975  | C910 | G847 | G785 | G722 | U659 | G537 | G331 | A412 | C351 | C287 | A223 | C163 |
| G1098 | U1038 | U1099 | A976  | C911 | G848 | A786 | U723 | C660 | G538 | A414 | G413 | C352 | G289 | G226 | G164 |
| C1099 | G1039 | G1099 | A977  | C912 | G849 | A787 | G724 | G661 | A415 | A339 | A415 | A353 | C290 | G226 | G165 |
| U1100 | U1040 | U1041 | A978  | A914 | G852 | U789 | G725 | A663 | G541 | G542 | G416 | C477 | G292 | U229 | U166 |
| A1101 | G1042 | A1102 | C979  | A915 | C853 | A790 | G727 | G664 | G542 | G541 | G417 | A478 | G293 | U230 | A167 |
| A1102 | G1043 | C1103 | C980  | U916 | U854 | G791 | A728 | A665 | U605 | U543 | C418 | U479 | U294 | U231 | G168 |
| G1103 | A1044 | C1104 | U981  | G917 | U855 | A792 | A729 | A666 | G606 | G544 | C419 | U480 | C295 | G232 | C169 |
| C1104 | C1045 | A1105 | U982  | A918 | C856 | A793 | G730 | G667 | A608 | C545 | U421 | A482 | U296 | C233 | U170 |
| G1106 | U1046 | C1106 | C983  | U920 | G857 | A794 | G731 | U669 | A609 | A547 | C422 | C362 | G297 | C234 | A171 |
| C1107 | G1047 | G1107 | C984  | U921 | G858 | G795 | G732 | G670 | A609 | G548 | G423 | A363 | G299 | A236 | U173 |
| G1108 | U1048 | C1108 | U985  | G922 | G859 | U798 | G733 | G671 | U610 | C549 | G424 | A364 | A300 | G237 | A174 |
| C1109 | U1049 | A1110 | G987  | A923 | A860 | G799 | G734 | U672 | C611 | G550 | G425 | U365 | A303 | G240 | C175 |
| A1110 | G1050 | C1111 | U988  | C924 | G861 | G800 | C735 | A673 | C612 | U551 | U426 | A366 | U304 | G241 | C176 |
| C1112 | U1052 | C1113 | U989  | G925 | C862 | U801 | C736 | G674 | C613 | U552 | U427 | U367 | G305 | G242 | C177 |
| C1113 | G1053 | C1114 | C990  | G926 | U864 | A802 | C737 | A675 | C614 | A553 | G428 | U368 | A306 | A243 | C178 |
| C1114 | U1054 | U1115 | U991  | G927 | A865 | G803 | C738 | U676 | C615 | A554 | U429 | G369 | A306 | G244 | A179 |
| U1115 | A1055 | U1116 | U992  | G928 | C866 | U804 | U740 | U678 | G616 | U555 | A430 | C370 | C307 | U244 | U180 |
| C1116 | U1056 | A1117 | U993  | G929 | G867 | C805 | G741 | C679 | C618 | C556 | A431 | A371 | C308 | U245 | A181 |
| U1118 | G1057 | C1119 | A994  | C930 | C868 | C806 | G742 | C680 | U619 | G557 | A432 | C372 | A309 | A246 | A182 |
| U1119 | U1058 | C1120 | C995  | C931 | G869 | A807 | A743 | A681 | C620 | G558 | A373 | A373 | A309 | G247 | C183 |
| C1120 | G1059 | U1121 | A996  | C932 | U870 | C808 | G744 | G682 | A621 | A559 | U434 | A374 | G310 | G248 | G184 |
| U1121 | U1060 | C1122 | U1000 | G933 | U871 | G809 | G745 | A683 | A622 | A560 | U375 | U375 | C312 | U249 | U185 |
| U1122 | G1061 | U1123 | C1001 | C934 | A872 | C810 | U746 | U684 | C623 | U561 | C436 | G376 | A313 | G250 | C186 |
| G1124 | U1062 | C1124 | C1002 | A935 | A873 | C811 | A747 | G685 | C624 | U562 | U437 | G377 | G316 | G251 | G187 |
|       | U1063 |       | G1003 | C936 | G874 | C812 | G748 | U686 | U625 | A563 | U438 | G378 | U317 | U252 | C188 |
|       |       |       | U1123 | A937 | U875 | U813 | A749 | A687 | A626 | A563 | U439 | C379 | C318 | G254 | A189 |
|       |       |       |       |      | C876 | G688 | C750 |      | G627 | U565 | C440 | G390 |      |      | A190 |

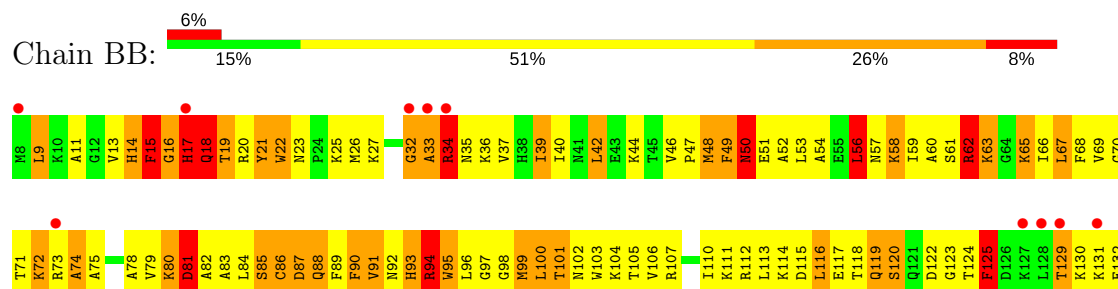


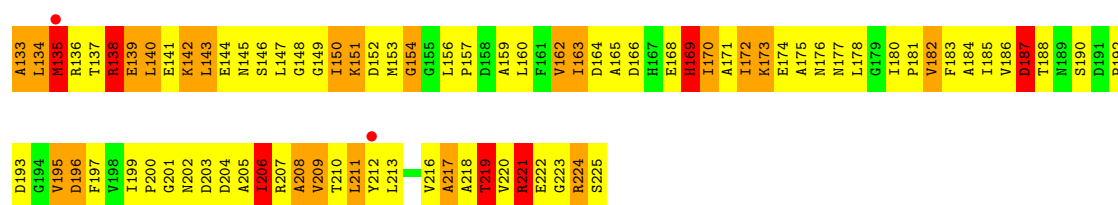


## • Molecule 2: 30S ribosomal protein S2

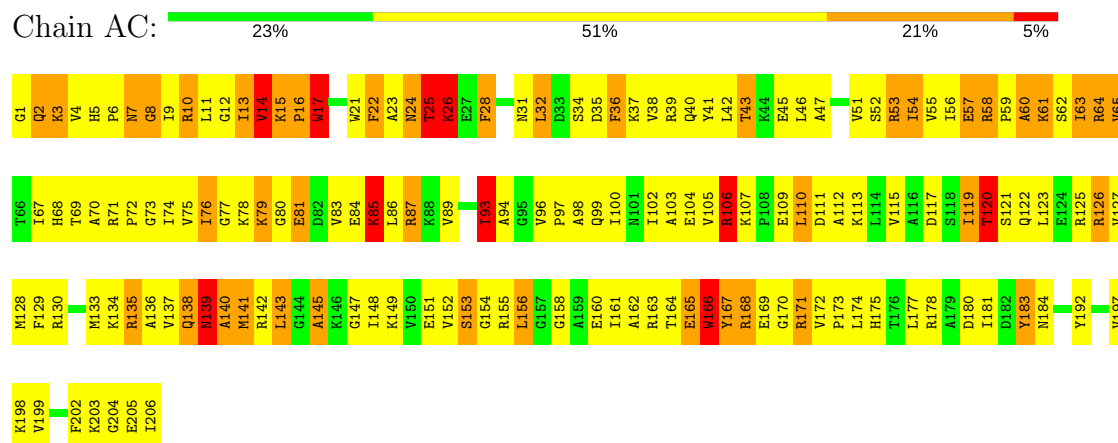


## • Molecule 2: 30S ribosomal protein S2

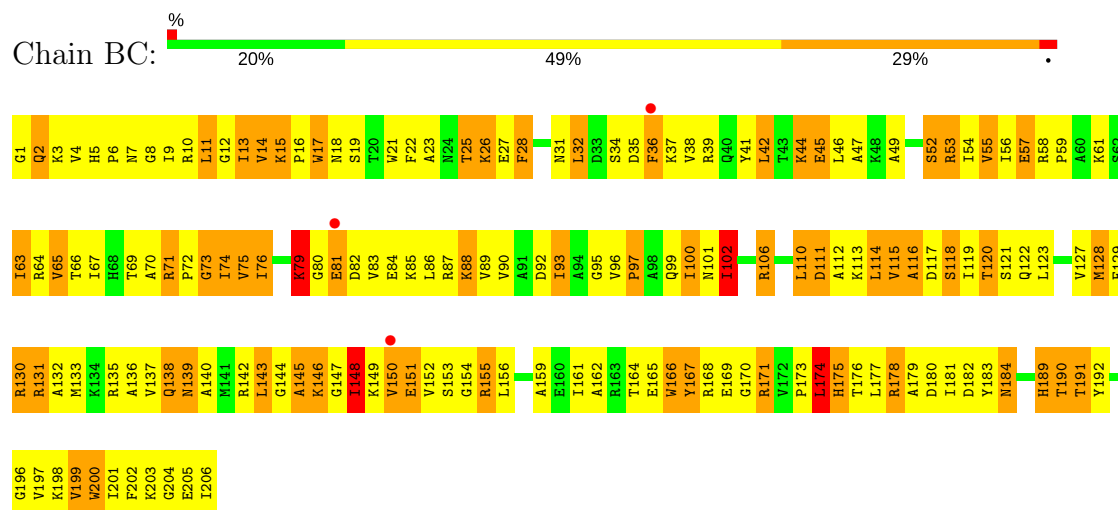




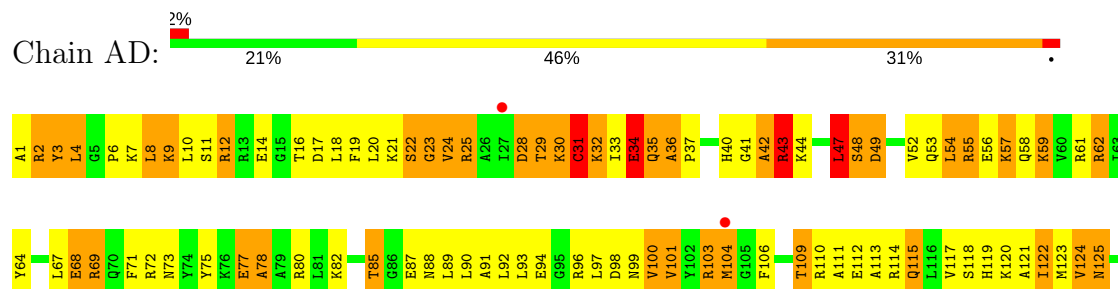
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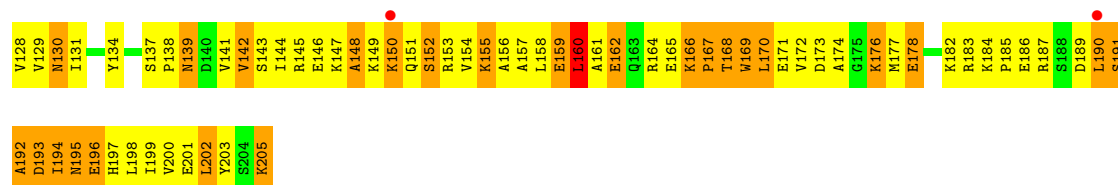


### • Molecule 3: 30S ribosomal protein S3



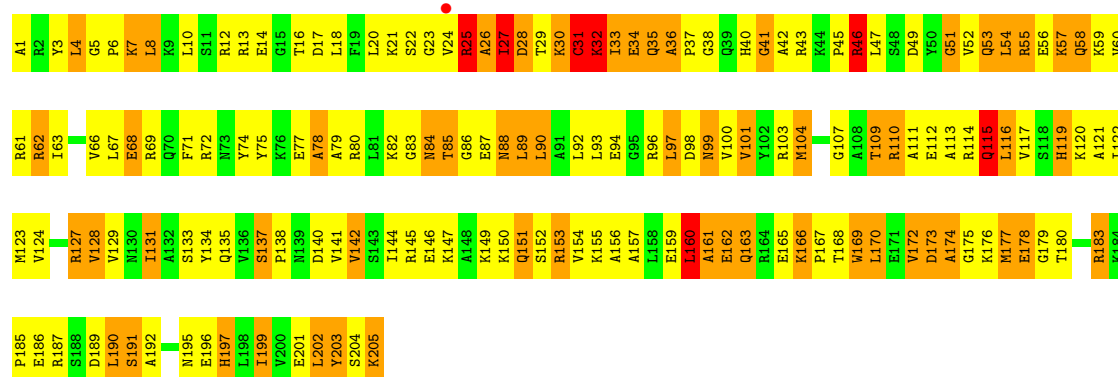
### • Molecule 4: 30S ribosomal protein S4





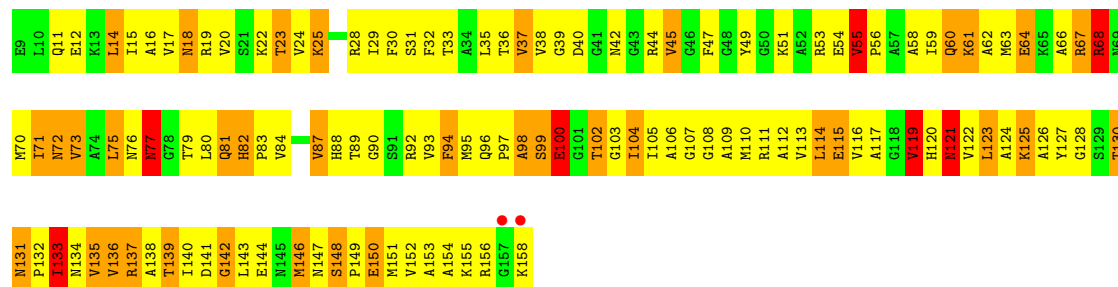
• Molecule 4: 30S ribosomal protein S4

Chain BD: 20% 48% 29%



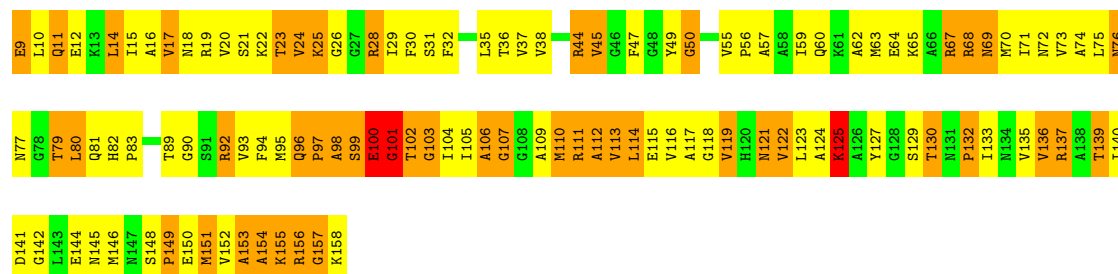
• Molecule 5: 30S ribosomal protein S5

Chain AE: 17% 54% 24% 5%

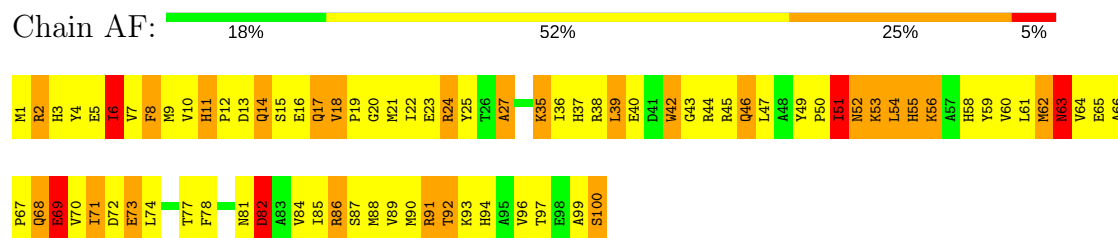


• Molecule 5: 30S ribosomal protein S5

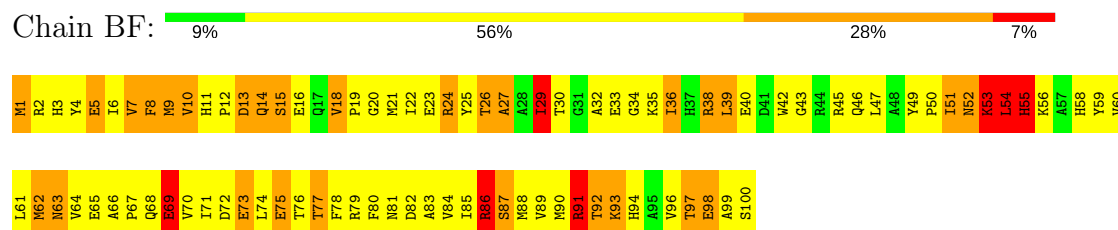
Chain BE: 23% 45% 31%



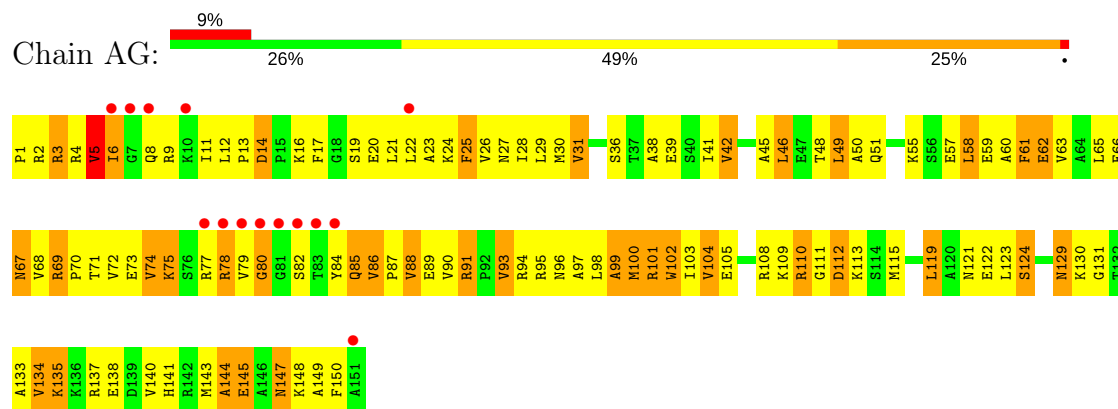
• Molecule 6: 30S ribosomal protein S6



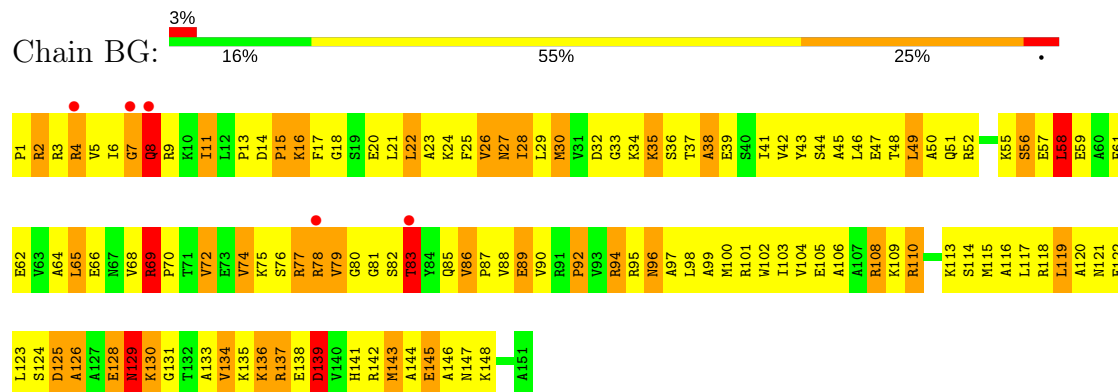
• Molecule 6: 30S ribosomal protein S6



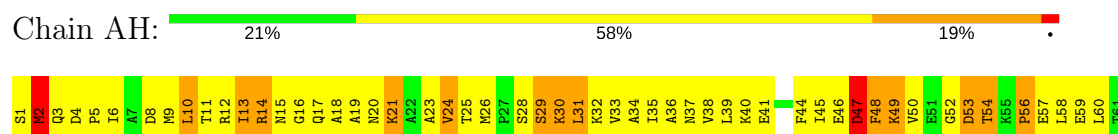
• Molecule 7: 30S ribosomal protein S7

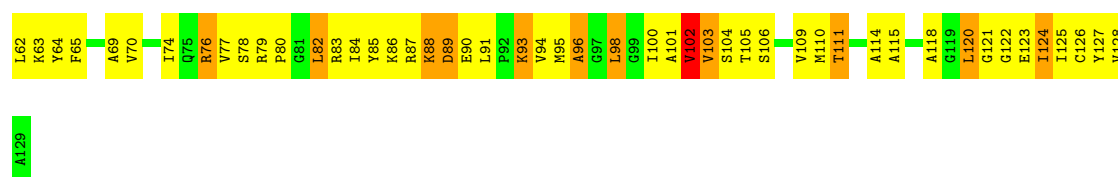


• Molecule 7: 30S ribosomal protein S7

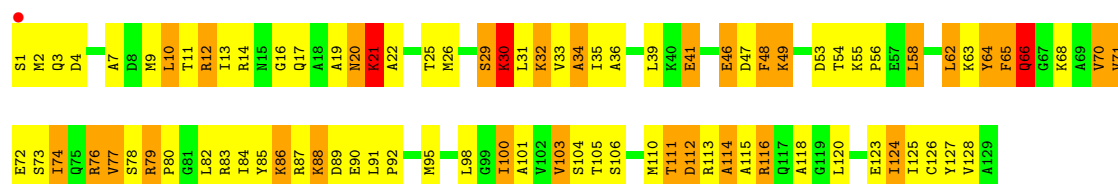


• Molecule 8: 30S ribosomal protein S8

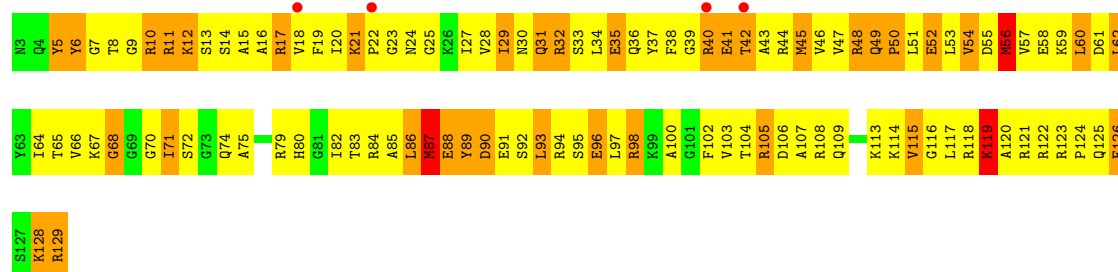
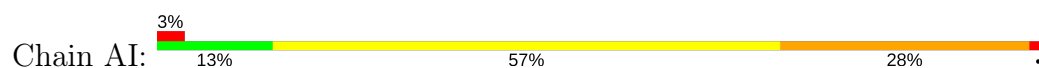




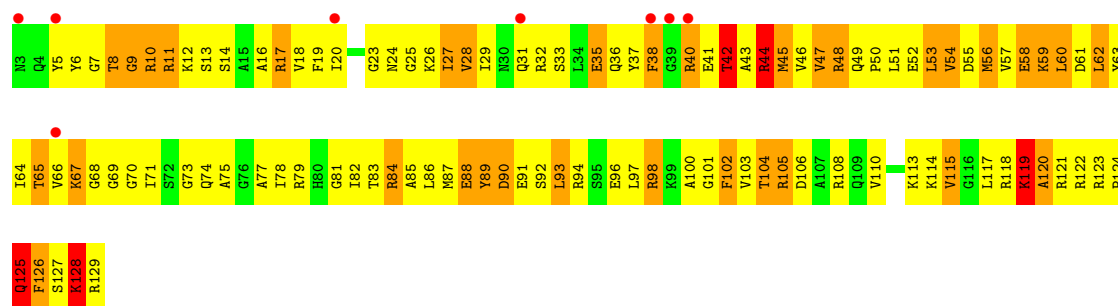
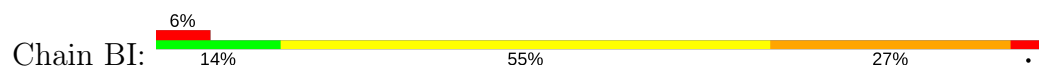
- Molecule 8: 30S ribosomal protein S8



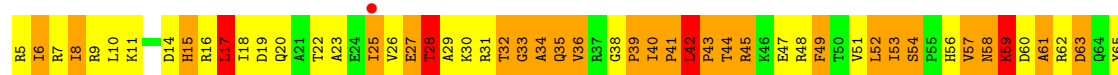
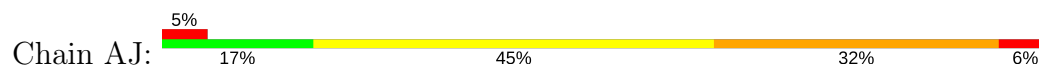
- Molecule 9: 30S ribosomal protein S9

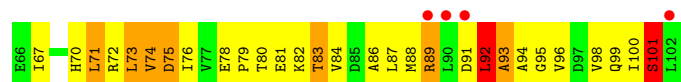


- Molecule 9: 30S ribosomal protein S9

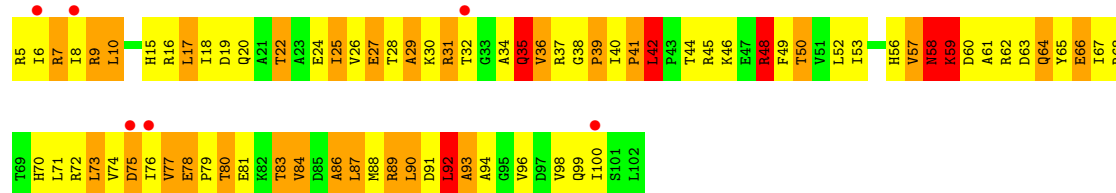
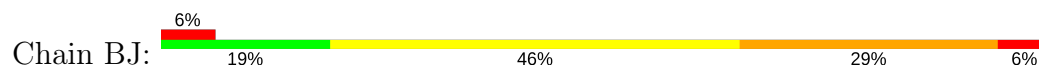


- Molecule 10: 30S ribosomal protein S10

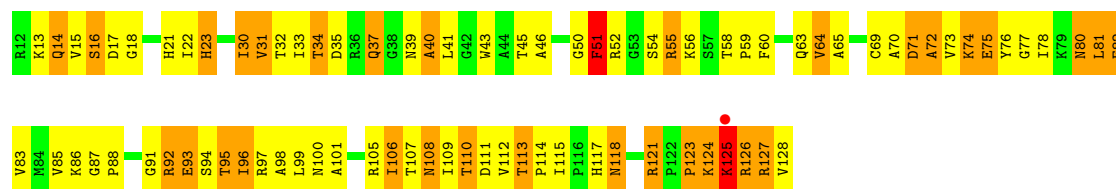




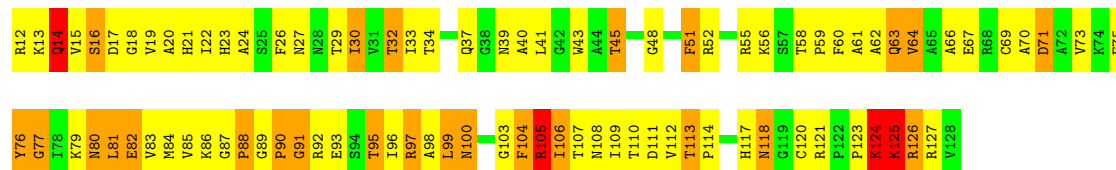
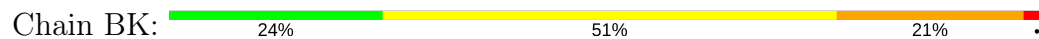
• Molecule 10: 30S ribosomal protein S10



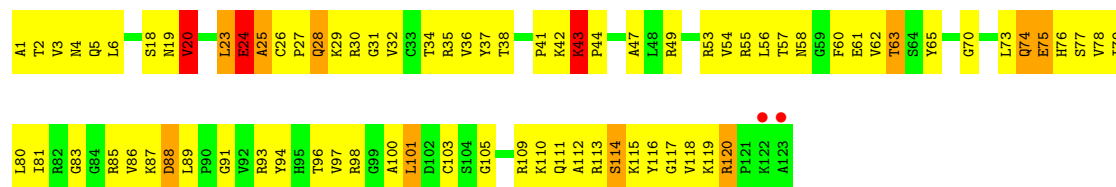
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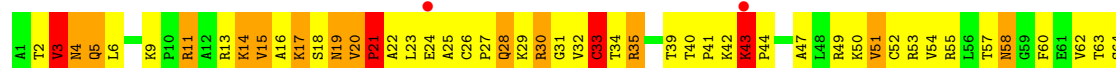
• Molecule 11: 30S ribosomal protein S11

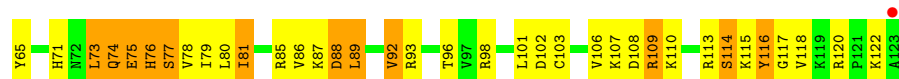


• Molecule 12: 30S ribosomal protein S12

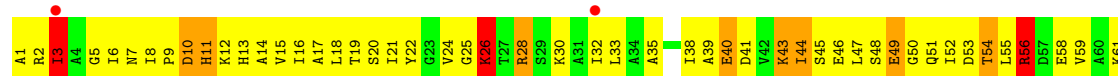


• Molecule 12: 30S ribosomal protein S12

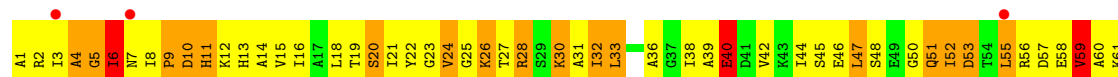
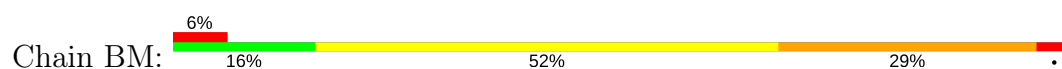




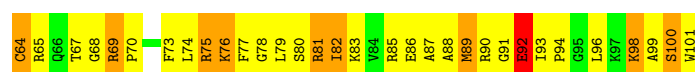
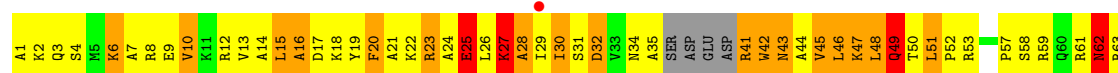
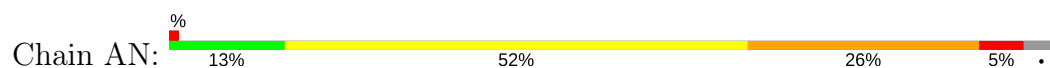
- Molecule 13: 30S ribosomal protein S13



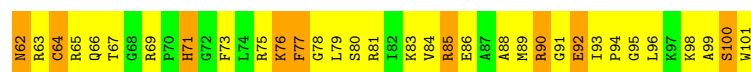
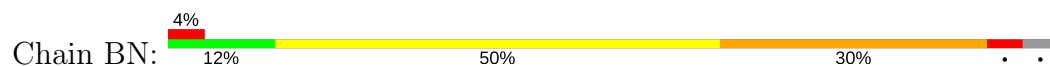
- Molecule 13: 30S ribosomal protein S13



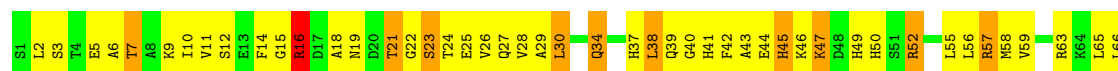
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

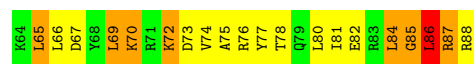


- Molecule 15: 30S ribosomal protein S15

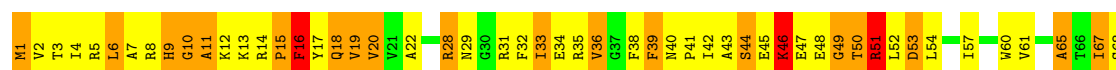
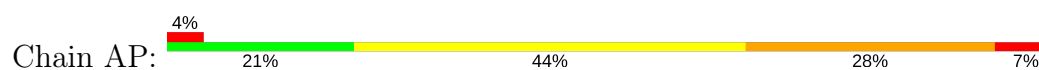




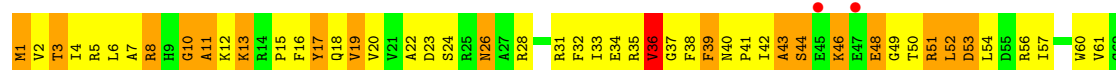
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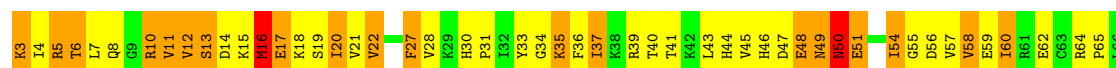
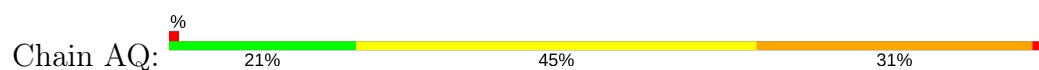
- Molecule 16: 30S ribosomal protein S16



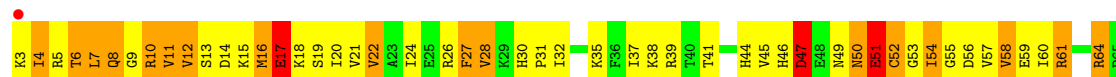
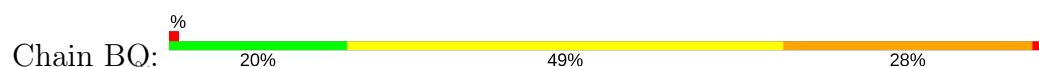
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



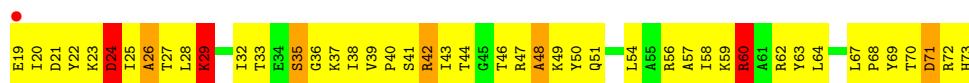
- Molecule 17: 30S ribosomal protein S17



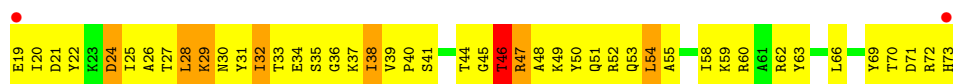




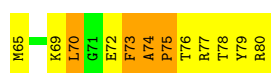
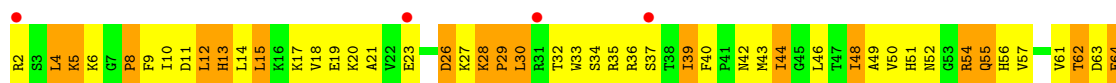
- Molecule 18: 30S ribosomal protein S18



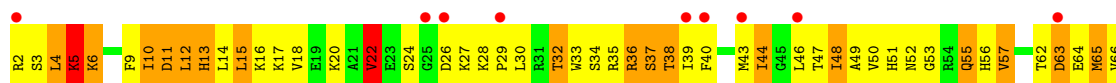
- Molecule 18: 30S ribosomal protein S18



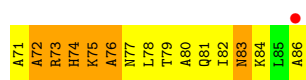
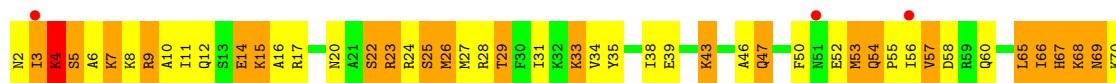
- Molecule 19: 30S ribosomal protein S19



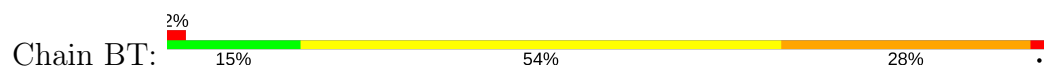
- Molecule 19: 30S ribosomal protein S19

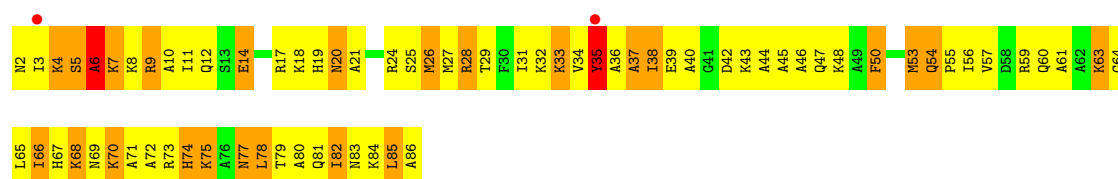


- Molecule 20: 30S ribosomal protein S20

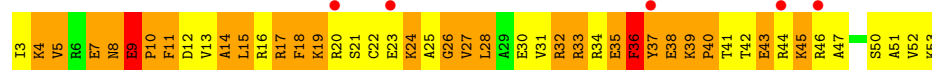


- Molecule 20: 30S ribosomal protein S20

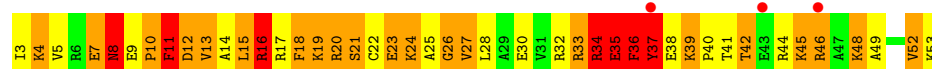




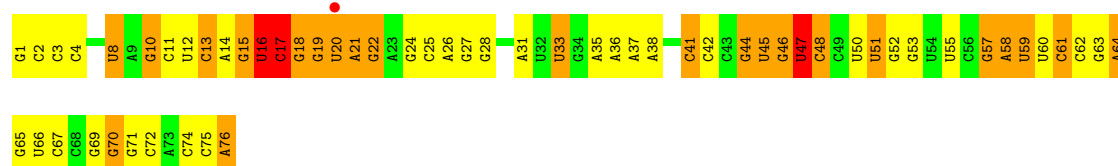
- Molecule 21: 30S ribosomal protein S21



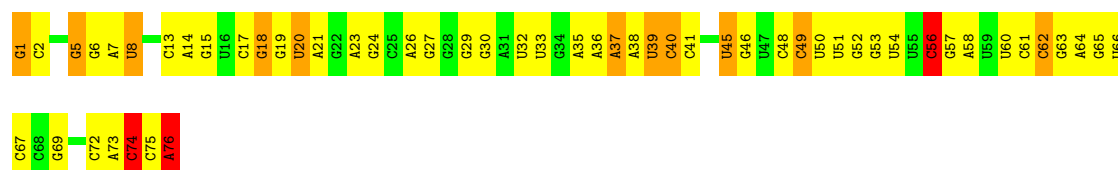
- Molecule 21: 30S ribosomal protein S21



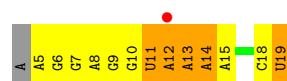
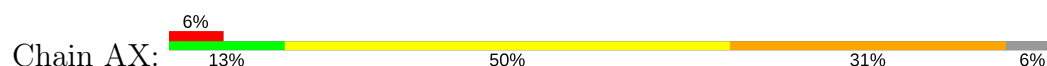
- Molecule 22: phenylalanine specific transfer RNA



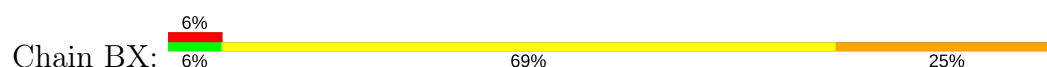
- Molecule 22: phenylalanine specific transfer RNA

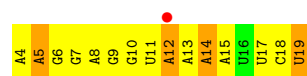


- Molecule 23: messenger RNA

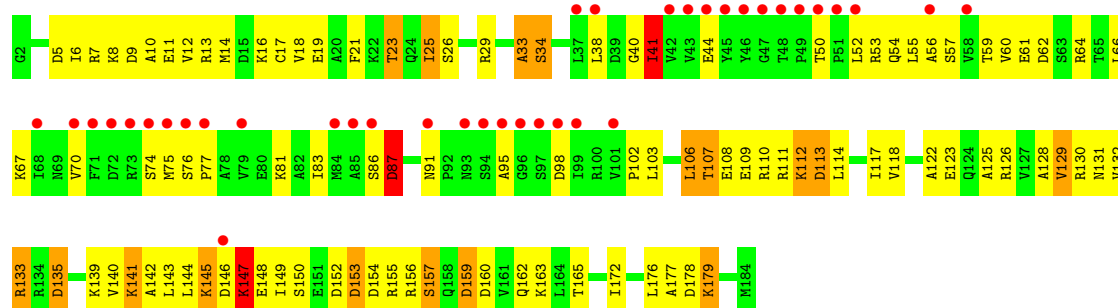


- Molecule 23: messenger RNA

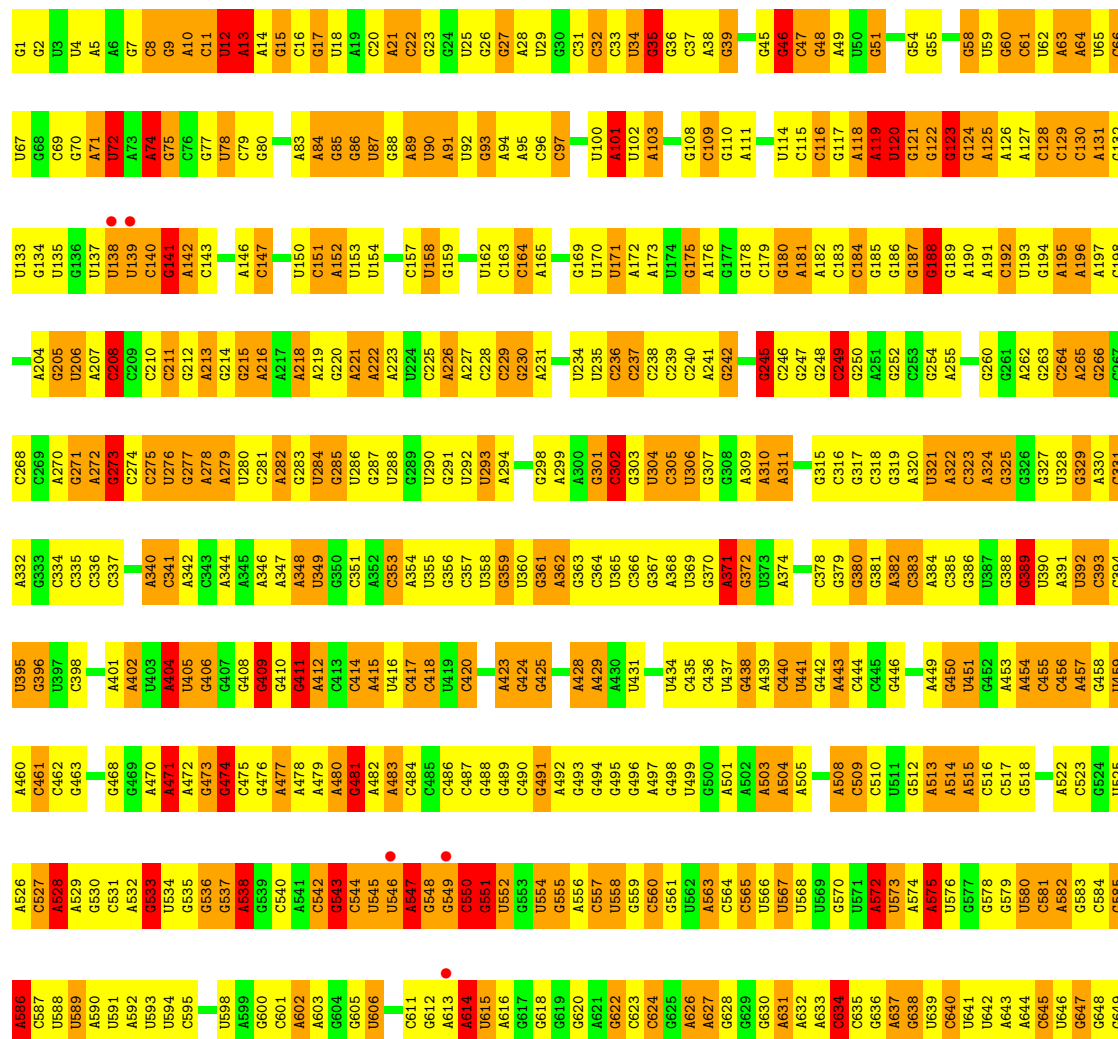
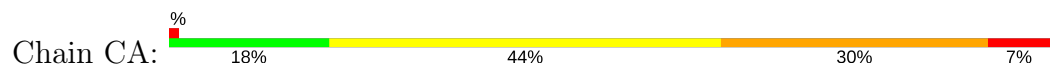




● Molecule 24: ribosome recycling factor

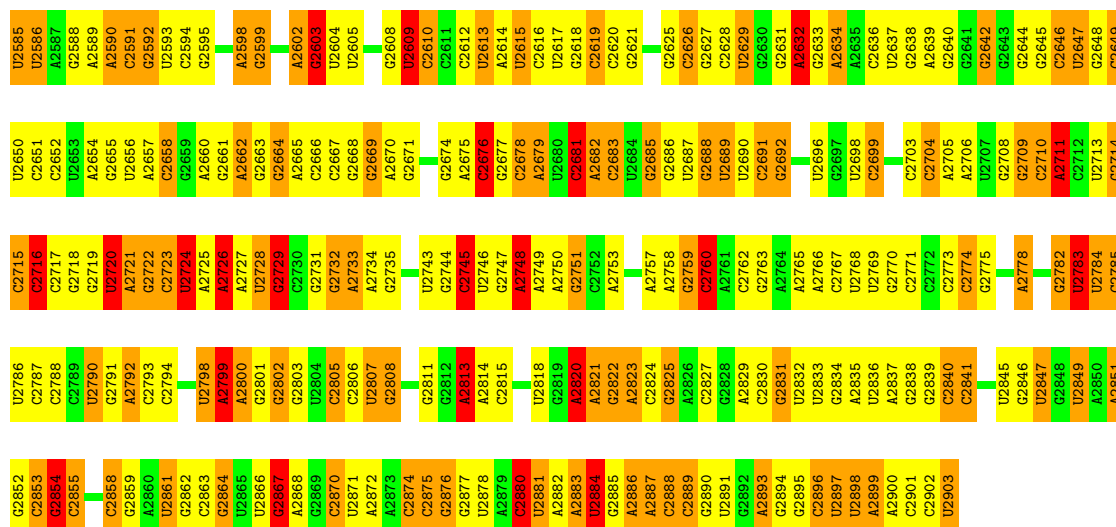


● Molecule 25: 23S rRNA

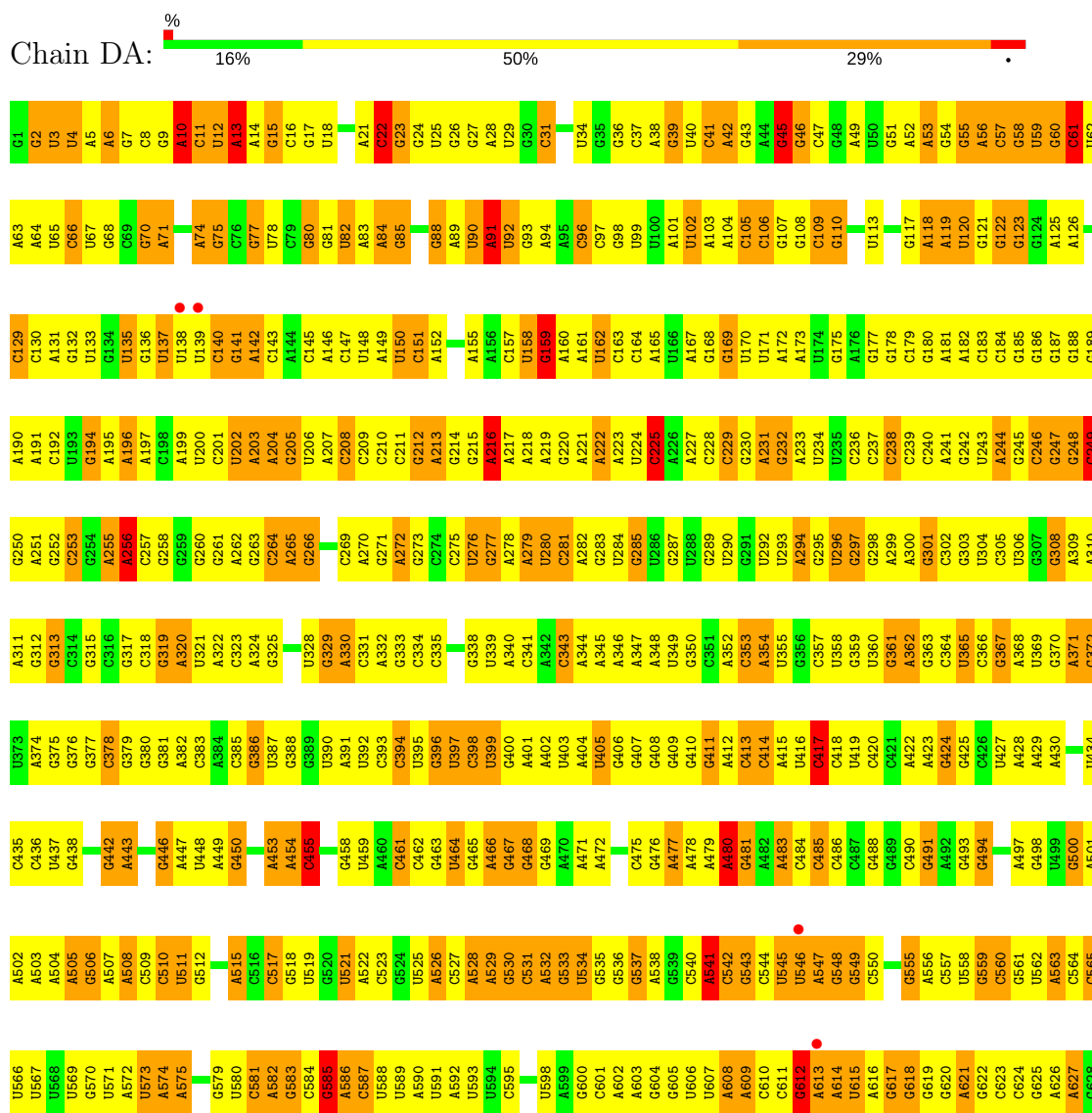


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| C1585 | U1460 | C1396 | C1336 | A1272 | A1143 | U1083 | G1023 | C961  | C997 | C835 | G775 | U714 | U653 |
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| U1632 | U1508 | C1446 | A1384 | C1320 | G1192 | A1129 | A1069 | A1008 | C944 | G883 | A821 | C762 | G701 |
| G1633 | A1509 | U1447 | A1385 | U1258 | U1183 | U1130 | A1070 | A1009 | A945 | U884 | G822 | U763 | U702 |
| A1634 | G1510 | C1448 | C1386 | G1259 | G1195 | G1131 | C1071 | C885  | C946 | C885 | C823 | G763 | U703 |
| C1635 | U1511 | G1449 | A1387 | A1260 | C1196 | U1132 | C1072 | A     | U824 | A    | U824 | A764 | C704 |
| U1636 | C1512 | G1450 | G1388 | C1261 | G1197 | A1133 | A1073 | U     | C948 | U    | A825 | C765 | G705 |
| C1637 | U1513 | G1451 | G1389 | U1325 | U1198 | A1134 | G1074 | C     | G949 | C    | U826 | U766 | A705 |
| U1638 | G1514 | G1452 | U1390 | U1326 | U1199 | C1135 | C1075 | C     | G952 | C    | U827 | U767 | A706 |
| A1639 | U1515 | U1453 | C1391 | A1327 | C1200 | G1136 | C1076 | G1016 | G952 | C    | U828 | G768 | G707 |
| C1640 | C1516 | C1454 | A1392 | A1328 | U1203 | G1137 | A1077 | G1017 | G956 | A892 | A829 | U769 | G708 |
| U1641 | U1517 | A1455 | A1393 | C1329 | U1267 | G1138 | U1078 | U1018 | G957 | A893 | G830 | G770 | U709 |
| G1642 | U1518 | G1456 | A1394 | C1330 | A1268 | G1139 | U1079 | C831  | U958 | U894 | G832 | G771 | U710 |
| C1643 | U1519 | C1457 | A1395 | G1331 | A1269 | C1140 | A1080 | A1020 |      |      |      | C772 | G711 |

|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G2523 | G2524 | G2525 | G2526 | G2527 | G2528 | G2529 | G2530 | A2531 | G2532 | G2533 | A2534 | G2535 | G2538 | G2539 | G2540 | A2541 | G2542 | G2543 | G2544 | G2545 | G2546 | A2547 | G2548 | G2549 | G2550 | G2551 | G2552 | G2553 | G2554 | G2555 | G2556 | G2557 | A2560 | G2561 | G2562 | G2563 | A2564 | A2565 | A2566 | G2567 | G2568 | G2569 | G2570 | G2571 | G2572 | G2573 | G2574 | G2575 | G2576 | G2577 | G2578 | G2579 | G2580 | G2581 | G2582 | G2583 | G2584 |       |       |       |       |       |       |       |       |
| C2461 | C2462 | C2463 | C2464 | C2465 | C2466 | C2467 | C2468 | C2469 | C2470 | C2471 | C2472 | C2473 | C2474 | C2475 | C2476 | C2477 | C2478 | C2479 | C2480 | C2481 | C2482 | C2483 | C2484 | C2485 | C2486 | C2487 | C2488 | C2489 | C2490 | C2491 | C2492 | C2493 | C2494 | C2495 | C2496 | C2497 | C2498 | C2499 | C2500 | C2501 | C2502 | C2503 | C2504 | C2505 | C2506 | C2507 | C2508 | C2509 | C2510 | C2511 | C2512 | C2513 | C2514 | C2515 | C2516 | C2517 | C2518 | C2519 | C2520 | C2521 | C2522 |       |       |       |       |
| G1645 | C1646 | U1647 | U1648 | G1649 | A1650 | G1651 | A1652 | G1653 | A1654 | A1655 | C1656 | U1657 | C1658 | G1659 | G1660 | G1661 | U1662 | G1663 | A1664 | G1665 | G1666 | G1667 | A1668 | C1669 | C1670 | U1671 | G1672 | G1673 | G1674 | C1675 | A1676 | A1677 | A1678 | G1679 | U1680 | G1681 | G1682 | U1683 | G1684 | C1685 | C1686 | G1687 | U1688 | A1689 | A1690 | C1691 | U1692 | U1693 | C1694 | G1695 | G1696 | G1697 | C1698 | G1699 | A1700 | A1701 | G1702 | G1703 | C1704 | C1705 | C1706 |       |       |       |       |
| C1708 | U1709 | A1710 | G1711 | U1712 | A1713 | U1714 | U1715 | U1716 | U1717 | A1718 | G1719 | G1720 | A1721 | A1722 | G1723 | G1724 | U1725 | U1726 | C1727 | G1728 | C1729 | A1730 | G1731 | G1732 | G1733 | G1734 | A1735 | U1736 | G1737 | G1738 | C1739 | A1740 | C1741 | A1742 | G1743 | A1744 | A1745 | A1746 | U1747 | G1748 | A1749 | U1750 | U1751 | C1752 | G1753 | A1754 | U1755 | G1756 | A1757 | U1758 | U1759 | C1760 | G1761 | A1762 | G1763 | G1764 | U1765 | G1766 | C1767 | C1768 |       |       |       |       |       |
| U1769 | G1770 | C1771 | A1772 | A1773 | C1774 | U1775 | U1776 | U1777 | A1778 | U1779 | U1780 | U1781 | U1782 | A1783 | A1784 | U1785 | A1786 | A1787 | C1788 | A1789 | U1790 | A1791 | G1792 | C1793 | A1794 | C1795 | U1796 | G1797 | G1798 | U1799 | A1800 | A1801 | A1802 | A1803 | A1804 | A1805 | G1806 | G1807 | A1808 | A1809 | A1810 | G1811 | C1812 | G1813 | U1814 | U1815 | U1816 | U1817 | U1818 | U1819 | U1820 | U1821 | U1822 | U1823 | U1824 | U1825 | U1826 | U1827 | U1828 | U1829 | U1830 | U1831 | U1832 | U1833 | U1834 |
| G1835 | C1836 | C1837 | C1838 | G1839 | U1840 | U1841 | G1842 | C1843 | C1844 | C1845 | C1846 | A1847 | A1848 | U1849 | A1850 | U1851 | U1852 | U1853 | A1854 | U1855 | U1856 | U1857 | A1858 | U1859 | G1860 | G1861 | G1862 | U1863 | U1864 | U1865 | A1866 | A1867 | C1868 | A1869 | C1870 | A1871 | A1872 | G1873 | C1874 | G1875 | A1876 | A1877 | G1878 | C1879 | U1880 | C1881 | U1882 | U1883 | G1884 | A1885 | U1886 | U1887 | U1888 | U1889 | A1890 | U1891 | A1892 | U1893 | U1894 | U1895 | U1896 | C1897 | C1898 | G1899 |       |
| U1897 | U1898 | A1899 | U1900 | A1901 | G1902 | G1903 | G1904 | U1905 | U1906 | U1907 | C1908 | U1909 | G1910 | U1911 | A1912 | A1913 | U1914 | U1915 | A1916 | U1917 | U1918 | A1919 | C1920 | G1921 | G1922 | U1923 | C1924 | U1925 | U1926 | U1927 | U1928 | G1929 | G1930 | U1931 | A1932 | G1933 | U1934 | A1935 | U1936 | A1937 | U1938 | U1939 | U1940 | C1941 | U1942 | U1943 | U1944 | U1945 | U1946 | C1947 | U1948 | U1949 | U1950 | U1951 | A1952 | A1953 | U1954 | U1955 | U1956 | C1957 | C1958 | U1959 |       |       |       |
| A1960 | C1961 | U1962 | U1963 | U1964 | U1965 | U1966 | U1967 | U1968 | U1969 | U1970 | U1971 | U1972 | U1973 | U1974 | U1975 | U1976 | U1977 | U1978 | U1979 | U1980 | A1981 | U1982 | U1983 | U1984 | C1985 | U1986 | U1987 | U1988 | U1989 | U1990 | U1991 | U1992 | U1993 | C1994 | U1995 | C1996 | U1997 | U1998 | U1999 | C2000 | C2001 | G2002 | A2003 | C2004 | A2005 | C2006 | U2007 | C2008 | A2009 | G2010 | U2011 | G2012 | U2013 | A2014 | A2015 | U2016 | U2017 | U2018 | U2019 | U2020 | C2021 | U2022 | C2023 | G2024 |       |
| C2025 | U2026 | G2027 | U2028 | G2029 | A2030 | A2031 | G2032 | A2033 | U2034 | U2035 | U2036 | G2037 | G2038 | U2039 | G2040 | U2041 | U2042 | C2043 | C2044 | C2045 | G2046 | C2047 | G2048 | G2049 | C2050 | A2051 | A2052 | G2053 | U2054 | C2055 | C2056 | G2057 | U2058 | A2059 | A2060 | G2061 | A2062 | C2063 | C2064 | C2065 | C2066 | G2067 | U2068 | G2069 | A2070 | A2071 | C2072 | U2073 | U2074 | U2075 | U2076 | A2077 | C2078 | U2079 | U2080 | U2081 | A2082 | G2083 | C2084 | U2085 |       |       |       |       |       |
| U2086 | G2087 | A2088 | C2089 | U2090 | C2091 | U2092 | G2093 | A2094 | U2095 | C2096 | A2097 | A2101 | G2102 | C2103 | U2104 | U2105 | U2106 | G2107 | A2108 | U2109 | G2110 | U2111 | G2112 | U2113 | A2114 | U2115 | G2116 | U2117 | U2118 | A2119 | G2120 | U2121 | U2122 | G2123 | G2124 | G2125 | A2126 | G2127 | G2128 | C2129 | U2130 | U2131 | U2132 | G2133 | A2134 | A2135 | G2136 | U2137 | G2138 | U2139 | G2140 | U2141 | U2142 | U2143 | U2144 | U2145 | U2146 | A2147 |       |       |       |       |       |       |       |
| U2148 | U2149 | C2150 | U2151 | C2152 | C2153 | A2154 | U2155 | U2156 | U2157 | U2158 | U2159 | C2160 | C2161 | G2162 | A2163 | C2164 | U2165 | U2166 | U2167 | C2168 | A2169 | G2170 | A2171 | U2172 | A2173 | C2174 | C2175 | A2176 | C2177 | C2178 | C2179 | U2180 | U2181 | U2182 | A2183 | A2184 | U2185 | G2186 | U2187 | U2188 | U2189 | C2190 | A2191 | U2192 | G2193 | U2194 | U2195 | C2196 | U2197 | A2198 | U2199 | U2200 | U2201 | U2202 | U2203 | U2204 | U2205 | U2206 | U2207 | U2208 | U2209 |       |       |       |       |
| U2210 | A2211 | A2212 | U2213 | C2214 | C2215 | G2216 | G2217 | U2218 | U2219 | U2220 | U2221 | C2222 | G2223 | G2224 | A2225 | C2226 | U2227 | A2228 | U2229 | U2230 | U2231 | C2232 | U2233 | G2234 | G2235 | U2236 | A2237 | U2238 | U2239 | C2240 | U2241 | U2242 | U2243 | U2244 | U2245 | G2246 | A2247 | C2248 | U2249 | G2250 | A2251 | C2252 | G2253 | C2254 | G2255 | U2256 | U2257 | C2258 | U2259 | C2260 | C2261 | U2262 | U2263 | U2264 | U2265 | U2266 | U2267 | U2268 | U2269 | U2270 |       |       |       |       |       |
| G2271 | U2272 | A2273 | A2274 | C2275 | G2276 | G2277 | A2278 | U2279 | C2280 | A2281 | U2282 | C2283 | G2284 | C2285 | A2286 | U2287 | C2288 | U2289 | G2290 | U2291 | U2292 | C2293 | G2294 | C2295 | U2296 | A2297 | U2298 | U2299 | C2300 | U2301 | U2302 | G2303 | U2304 | C2305 | C2306 | G2307 | C2308 | A2309 | C2310 | U2311 | U2312 | C2313 | A2314 | G2315 | C2316 | U2317 | C2318 | G2319 | U2320 | U2321 | U2322 | U2323 | U2324 | U2325 | U2326 | U2327 | U2328 | U2329 | U2330 | C2331 | C2332 |       |       |       |       |
| A2333 | U2334 | A2335 | A2336 | C2337 | C2338 | C2339 | A2340 | U2341 | C2342 | U2343 | U2344 | C2345 | A2346 | C2347 | U2348 | C2349 | C2350 | U2351 | A2352 | C2353 | C2354 | G2355 | U2356 | C2357 | A2358 | C2359 | U2360 | C2361 | U2362 | C2363 | C2364 | C2365 | A2366 | C2367 | U2368 | U2369 | U2370 | U2371 | A2372 | C2373 | A2374 | A2375 | A2376 | U2377 | C2378 | C2379 | C2380 | A2381 | C2382 | U2383 | U2384 | C2385 | A2386 | U2387 | U2388 | U2389 | U2390 | C2391 | A2392 | U2393 | C2394 | C2395 | U2396 | C2397 |       |
| G2400 | U2401 | U2402 | C2403 | U2404 | C2405 | A2406 | U2407 | U2408 | U2409 | C2410 | A2411 | A2412 | G2413 | C2414 | G2415 | U2416 | C2417 | U2418 | U2419 | C2420 | G2421 | C2422 | U2423 | C2424 | A2425 | U2426 | C2427 | U2428 | C2429 | A2430 | U2431 | A2432 | A2433 | U2434 | A2435 | G2436 | U2437 | U2438 | C2439 | U2440 | U2441 | C2442 | C2443 | U2444 | G2445 | U2446 | U2447 | U2448 | U2449 | A2450 | U2451 | C2452 | U2453 | U2454 | U2455 | U2456 | U2457 | U2458 | U2459 | U2460 |       |       |       |       |       |
| C2461 | C2462 | C2463 | C2464 | C2465 | C2466 | C2467 | C2468 | C2469 | C2470 | C2471 | C2472 | C2473 | C2474 | C2475 | C2476 | C2477 | C2478 | C2479 | C2480 | C2481 | C2482 | C2483 | C2484 | C2485 | C2486 | C2487 | C2488 | C2489 | C2490 | C2491 | C2492 | C2493 | C2494 | C2495 | C2496 | C2497 | C2498 | C2499 | C2500 | C2501 | C2502 | C2503 | C2504 | C2505 | C2506 | C2507 | C2508 | C2509 | C2510 | C2511 | C2512 | C2513 | C2514 | C2515 | C2516 | C2517 | C2518 | C2519 | C2520 | C2521 | C2522 |       |       |       |       |



### • Molecule 25: 23S rRNA



|       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|
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| A1569 | A1508 | G1448 | G1388 | A1328 | C1259 | C1196 | C1135 | C1075 | C1013 | C948  | U894 | A821 | C948 | U694 | A631 |
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| A1572 | C1511 | C1451 | U1391 | G1331 | A1262 | U1199 | G1138 | U1078 | G1016 | G954  | A    | U824 | U762 | C634 | C634 |
| G1573 | U1512 | G1452 | A1392 | G1332 | U1263 | C1200 | G1139 | C1079 | G1017 | U955  | U    | A825 | G763 | C635 | C635 |
| C1574 | C1513 | A1453 | A1393 | G1333 | A1264 | U1203 | C1140 | A1080 | U1018 | U956  | C    | U826 | A764 | G636 | G636 |
| G1575 | G1514 | G1454 | U1394 | G1334 | C1265 | U1204 | C1141 | A1081 | U1019 | G956  | C    | U827 | C765 | A637 | A637 |
| U1576 | A1515 | G1455 | A1395 | C1335 | G1266 | A1205 | A143  | U1082 | A1020 | C957  | C    | U828 | G704 | G638 | G638 |
| C1577 | G1516 | G1456 | U1396 | A1336 | U1267 | A1206 | A142  | U1083 | A1021 | U958  | G    | A829 | A705 | U639 | U639 |
| U1578 | C1517 | U1457 | U1397 | G1337 | A1268 | G1207 | A144  | A1084 | G1022 | C961  | A892 | G830 | G770 | C640 | C640 |
| A1579 | U1518 | U1458 | C1398 | G1338 | A1269 | C1208 | C1145 | A1085 | U1023 | G962  | C393 | G831 | G771 | U641 | U641 |
| A1580 | G1519 | G1459 | C1399 | G1339 | C1270 | U1212 | C1146 | A1086 | G1024 | G962  | U894 | U832 | C772 | U642 | U642 |
| G1581 | U1520 | U1460 | U1400 | U1340 | G1271 | G1212 | G1149 | G1087 | G1025 | U963  | U895 | A833 | G773 | A643 | A643 |
| C1582 | G1521 | C1461 | G1401 | A1341 | A1272 | A1213 | C1150 | A1088 | G1026 | C964  | U896 | G834 | G774 | A644 | A644 |
| A1583 | A1522 | A1462 | U1402 | A1342 | U1275 | A1214 | C1151 | A1089 | A1027 | C967  | C397 | G835 | G775 | C645 | C645 |
| U1584 | U1523 | C1463 | A1403 | G1343 | A1276 | G1215 | A1151 | A1090 | A1028 | U967  | C398 | U838 | G776 | U646 | U646 |
| C1585 | G1524 | G1464 | C1404 | U1344 | A1277 | G1216 | C1152 | G1091 | A1029 | C968  | A899 | U839 | G777 | G647 | G647 |
| A1586 | A1525 | G1465 | U1405 | C1345 | C1277 | G1217 | C1153 | C1092 | C1080 | G969  | A900 | U840 | G778 | G648 | G648 |
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| U1588 | G1527 | U1467 | G1407 | A1347 | G1281 | G1218 | A1155 | A1094 | U1032 | A973  | C902 | G842 | G780 | C717 | C650 |
| A1589 | A1528 | U1468 | G1408 | C1348 | U1282 | U1219 | A1156 | A1095 | U1033 | A974  | C903 | G843 | A781 | A718 | A718 |
| U1590 | G1529 | A1469 | U1409 | C1349 | G1283 | G1220 | G1157 | A1096 | G1034 | G974  | A904 | G844 | A782 | C719 | C719 |
| A1591 | G1530 | A1470 | G1410 | C1350 | U1283 | C1221 | C1158 | U1097 | U1035 | A975  | A905 | A844 | A783 | U720 | U720 |
| C1592 | C1531 | G1471 | U1411 | C1351 | U1222 | U1222 | U1159 | A1098 | G1036 | G976  | U906 | A845 | G784 | A721 | A654 |
| A1593 | A1532 | C1472 | A1412 | U1352 | A1286 | G1223 | C1160 | G1099 | G1037 | G977  | G907 | U846 | G785 | G656 | A655 |
| U1594 | C1533 | G1473 | A1413 | A1353 | A1287 | U1224 | G1161 | C1100 | G1038 | G978  | C908 | U847 | C786 | U657 | U657 |
| A1595 | U1534 | U1474 | C1414 | G1354 | G1288 | G1225 | G1162 | U1101 | U1039 | A979  | A909 | U848 | C787 | G659 | G659 |
| C1596 | A1535 | G1475 | U1415 | C1355 | C1289 | A1226 | G1163 | C1102 | G1042 | A980  | A910 | A849 | A788 | G725 | C660 |
| A1597 | G1536 | U1476 | G1416 | G1356 | C1290 | G1227 | C1164 | A1103 | C1043 | A981  | A911 | U850 | A789 | G726 | G661 |
| U1598 | G1537 | A1477 | C1417 | C1357 | C1291 | G1228 | A1165 | C1104 | C1044 | C982  | C912 | C851 | U790 | A727 | A727 |
| A1599 | U1538 | G1478 | G1418 | G1358 | G1292 | C1229 | U1166 | C1105 | C1045 | A983  | U913 | U852 | C791 | G733 | G664 |
| C1600 | U1539 | G1479 | A1419 | A1359 | C1293 | A1230 | C1167 | G1106 | A1046 | A984  | C914 | C853 | A792 | G729 | U665 |
| G1601 | G1540 | C1480 | G1420 | G1360 | U1294 | U1231 | G1168 | G1107 | G1047 | C985  | C915 | C854 | A793 | A730 | A666 |
| U1602 | C1541 | U1481 | G1421 | C1361 | C1295 | G1232 | A1169 | U1108 | A1048 | C986  | G916 | G855 | A794 | C731 | U667 |
| A1603 | U1542 | G1482 | G1422 | C1362 | C1295 | C1233 | C1170 | C1109 | C1049 | C987  | A917 | G856 | C795 | C732 | A668 |
| C1604 | G1543 | G1483 | G1423 | C1363 | C1298 | U1234 | G1171 | G1110 | A1050 | A988  | A918 | G857 | C796 | G733 | G669 |
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| C1607 | G1546 | U1486 | G1426 | A1366 | A1301 | A1237 | U1174 | U1113 | C1053 | C991  | C921 | U860 | G799 | C736 | C672 |
| A1608 | C1547 | U1487 | A1427 | A1367 | A1302 | G1238 | A1175 | C1114 | A1054 | C992  | A861 | U861 | A800 | C737 | C673 |
| U1609 | A1548 | C1488 | G1428 | G1368 | G1303 | G1239 | U1176 | G1115 | G1055 | G993  | A927 | G862 | G801 | G738 | G674 |
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| C1611 | A1551 | A1490 | G1430 | C1370 | G1310 | A1241 | C1178 | C1117 | A1057 | C995  | U929 | G864 | U603 | C740 | A676 |
| G1612 | A1552 | G1491 | A1431 | G1371 | G1311 | U1242 | G1179 | C1118 | U1058 | A996  | U930 | C865 | A904 | U741 | A677 |
| C1613 | U1553 | G1492 | G1432 | U1372 | U1312 | C1243 | U1180 | C1119 | G1059 | G997  | U931 | U872 | U811 | A742 | C678 |
| A1614 | A1554 | C1493 | A1433 | A1373 | U1313 | A1244 | U1181 | G1120 | U1060 | C998  | U932 | G873 | G748 | A743 | C679 |
| C1615 | G1555 | A1494 | A1434 | G1374 | C1314 | G1245 | G1182 | C1121 | U1061 | U999  | A933 | U870 | U607 | U744 | C680 |
| A1616 | C1556 | A1495 | G1435 | U1375 | C1315 | A1246 | U1183 | G1122 | G1062 | A1000 | U934 | G869 | G808 | G745 | G681 |
| C1617 | U1557 | A1496 | G1436 | C1376 | U1316 | A1247 | U1184 | C1123 | G1063 | A1001 | C935 | U871 | G809 | U746 | G682 |
| A1618 | C1558 | U1497 | C1437 | G1377 | G1317 | G1248 | G1185 | G1124 | C1064 | U1002 | A936 | U872 | U810 | U747 | U683 |
| U1621 | U1559 | C1498 | U1438 | A1378 | U1318 | U1249 | G1186 | G1125 | G1065 | G1003 | C939 | U873 | U811 | G749 | A685 |
| G1622 | G1560 | C1499 | A1439 | U1379 | C1319 | G1250 | G1187 | A1126 | U1066 | U1004 | G939 | G874 | C812 | A749 | G686 |
| G1623 | U1561 | G1500 | U1440 | G1380 | C1320 | G1251 | U1188 | A1127 | A1067 | C1005 | G940 | U875 | U613 | A750 | U687 |
| U1624 | U1562 | G1501 | A1321 | G1381 | A1321 | G1252 | A1189 | G1128 | G1068 | C1006 | A941 | C876 | C514 | A751 | C687 |
| C1626 | U1563 | A1502 | U1442 | G1382 | A1322 | A1253 | G1190 | A1129 | A1069 | C1007 | G942 | A877 | C515 | A752 | U688 |
| U1629 | C1564 | A1503 | U1443 | A1383 | C1323 | G1254 | G1191 | U1130 | A1070 | A1008 | A943 | A878 | C516 | A753 | A689 |
| U1630 | G1565 | A1504 | G1324 | G1384 | U1255 | U1255 | C1192 | U1131 | G1071 | A1098 | C944 | G879 | C817 | U754 | G690 |
| U1631 | A1566 | A1505 | G1445 | A1385 | U1325 | G1256 | G1193 | U1132 | C1072 | A1010 | A945 | G880 | G818 | U755 | C691 |

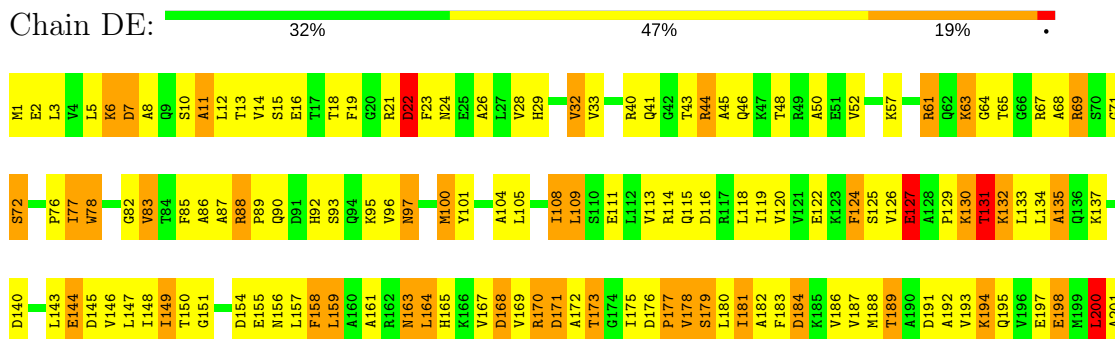




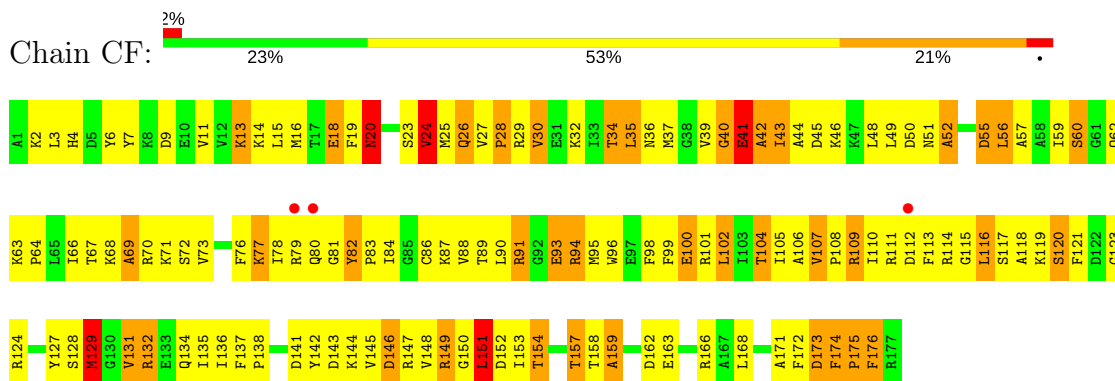




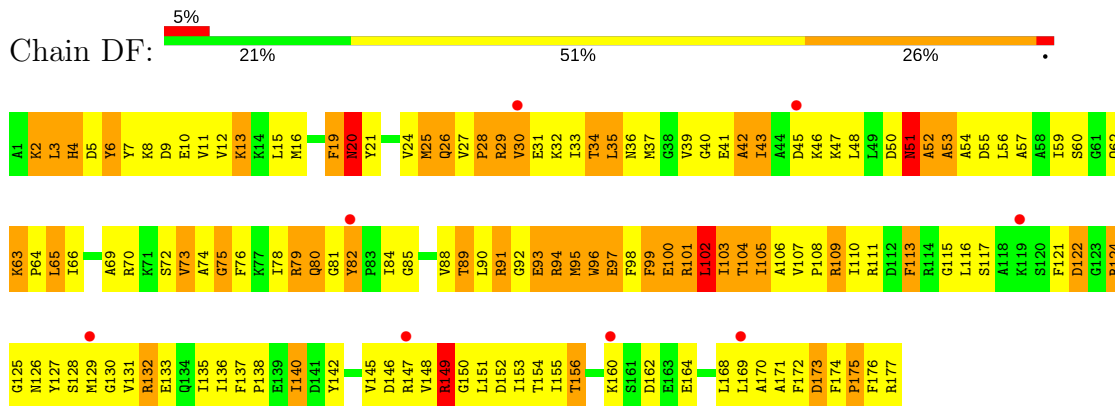
- Molecule 29: 50S ribosomal protein L4



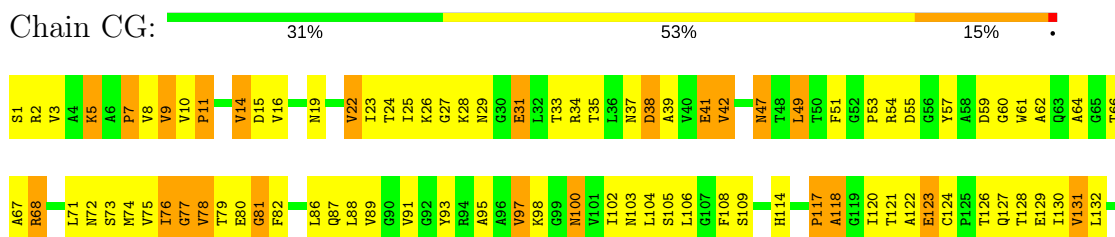
- Molecule 30: 50S ribosomal protein L5



- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6





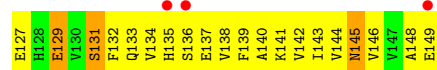
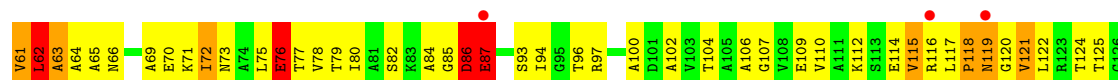
• Molecule 31: 50S ribosomal protein L6



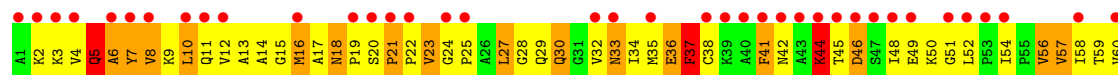
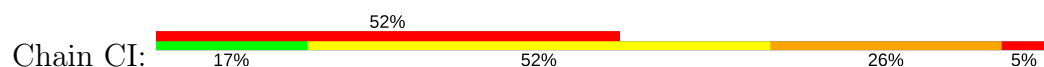
• Molecule 32: 50S ribosomal protein L9

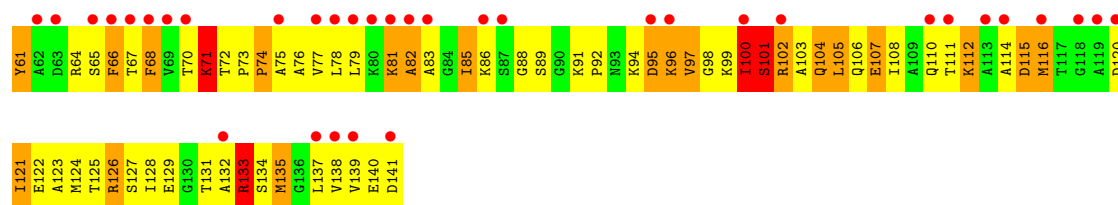


• Molecule 32: 50S ribosomal protein L9

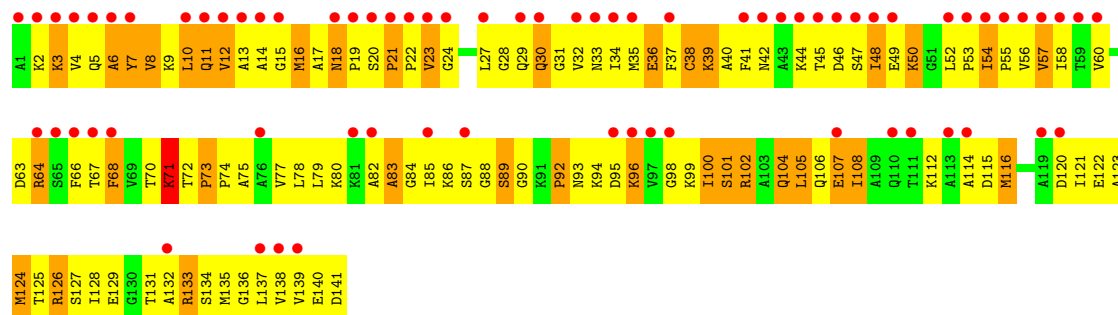
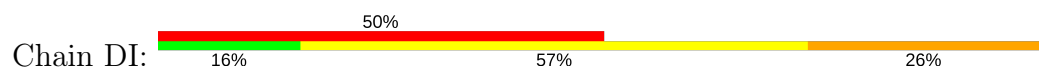


• Molecule 33: 50S ribosomal protein L11

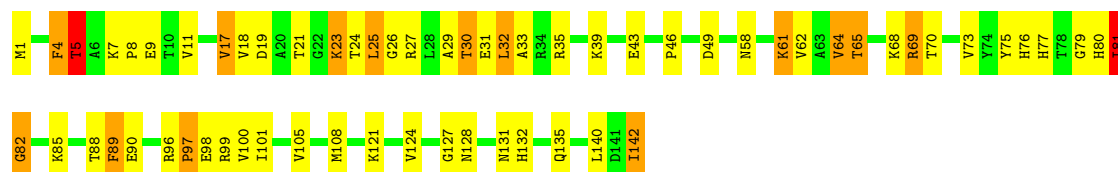




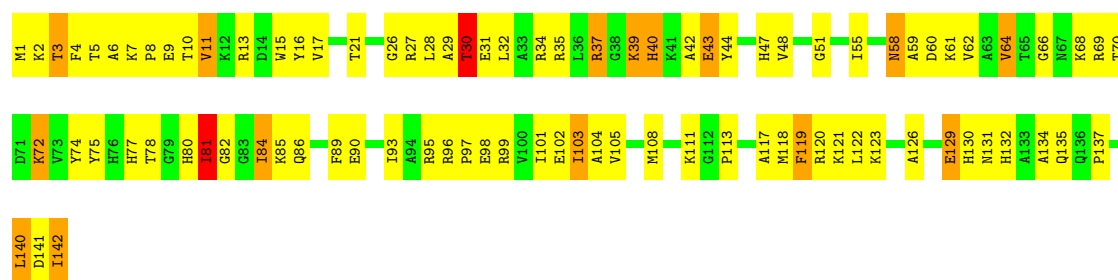
• Molecule 33: 50S ribosomal protein L11



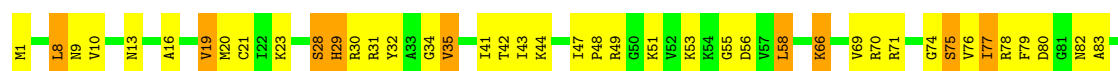
• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13



• Molecule 35: 50S ribosomal protein L14





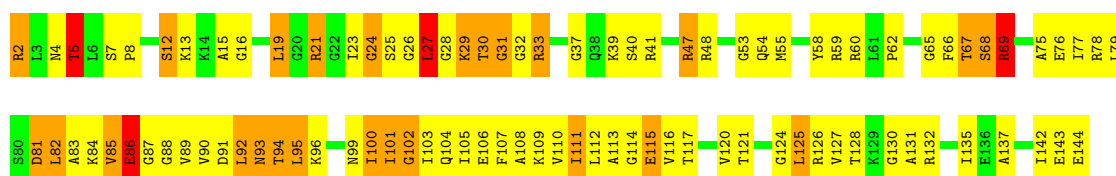
• Molecule 35: 50S ribosomal protein L14

Chain DK: 40% 43% 17%



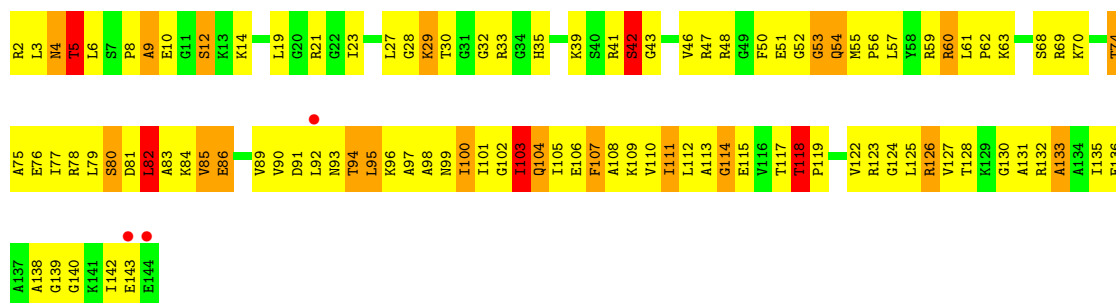
• Molecule 36: 50S ribosomal protein L15

Chain CL: 34% 46% 17%



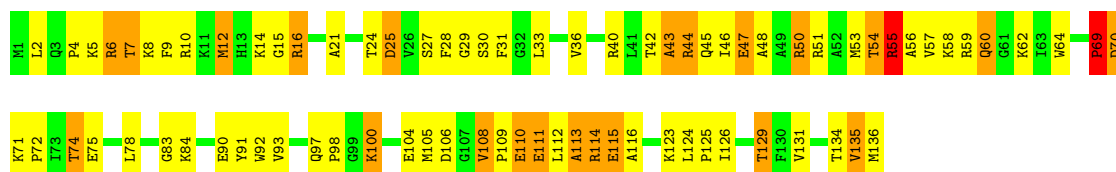
• Molecule 36: 50S ribosomal protein L15

Chain DL: 2% 27% 55% 14%



• Molecule 37: 50S ribosomal protein L16

Chain CM: 42% 40% 16%

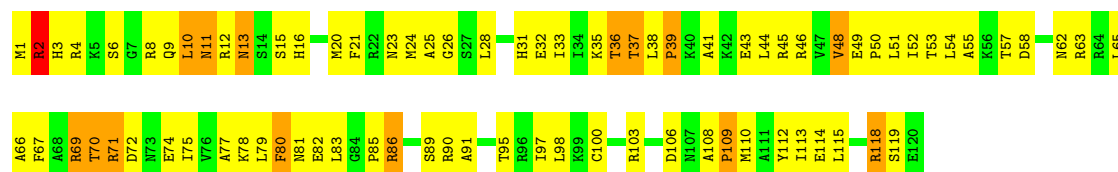


• Molecule 37: 50S ribosomal protein L16

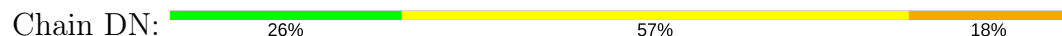
Chain DM: 29% 53% 16%



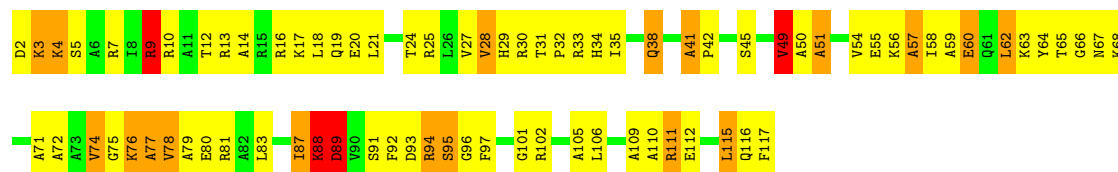
• Molecule 38: 50S ribosomal protein L17



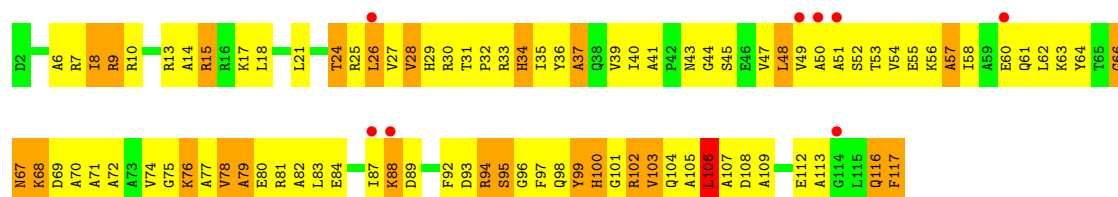
• Molecule 38: 50S ribosomal protein L17



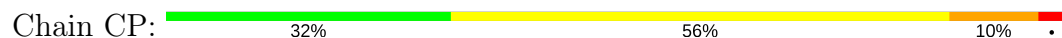
• Molecule 39: 50S ribosomal protein L18

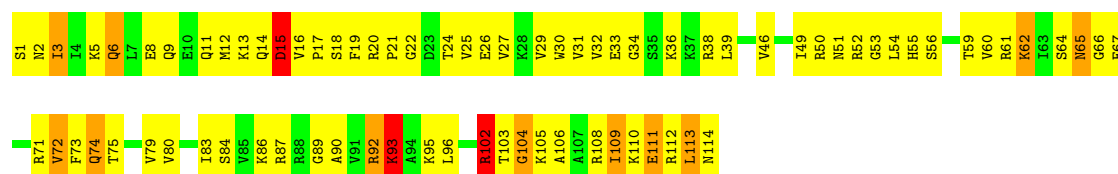


• Molecule 39: 50S ribosomal protein L18

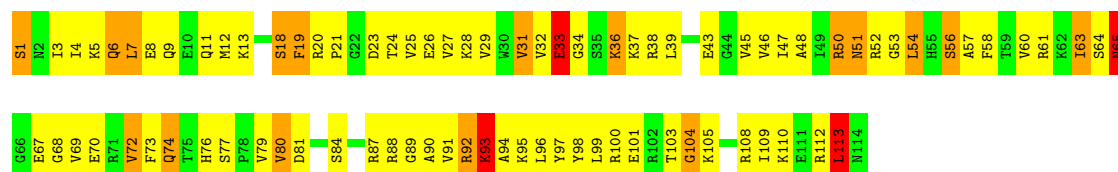


• Molecule 40: 50S ribosomal protein L19

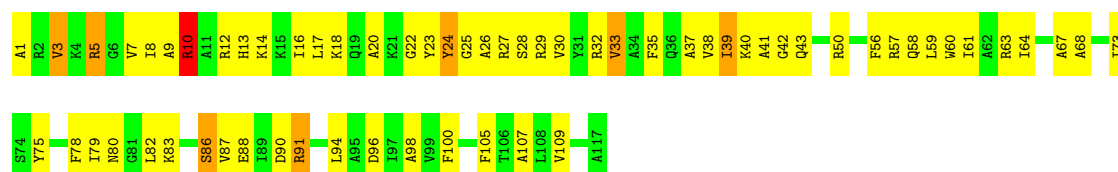




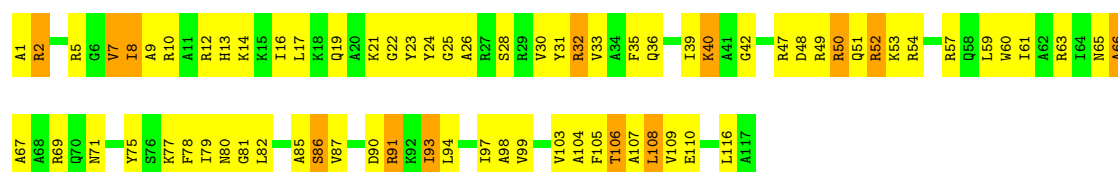
• Molecule 40: 50S ribosomal protein L19



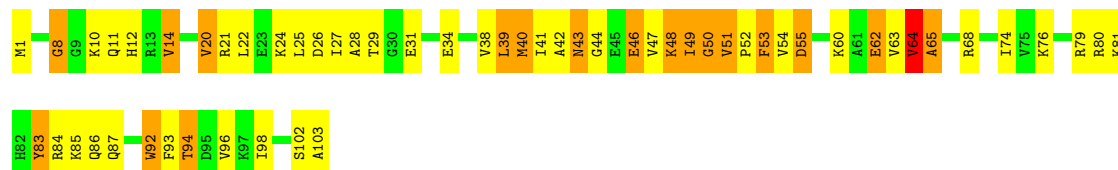
• Molecule 41: 50S ribosomal protein L20



• Molecule 41: 50S ribosomal protein L20



• Molecule 42: 50S ribosomal protein L21



• Molecule 42: 50S ribosomal protein L21



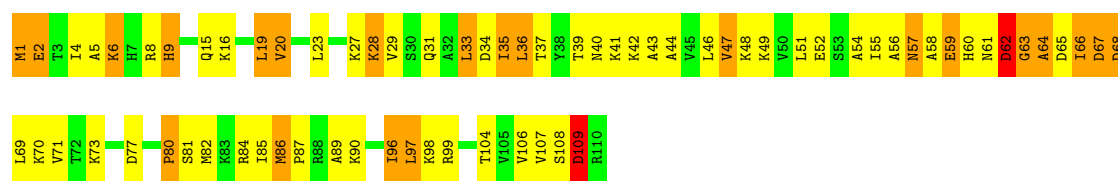




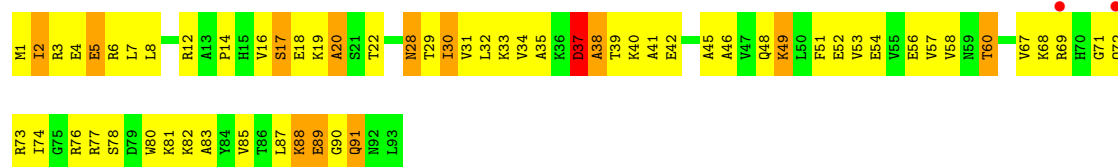
• Molecule 43: 50S ribosomal protein L22



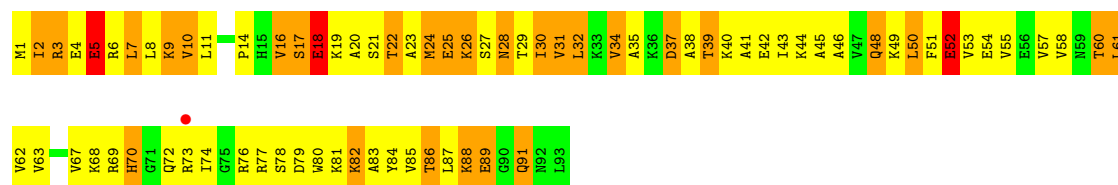
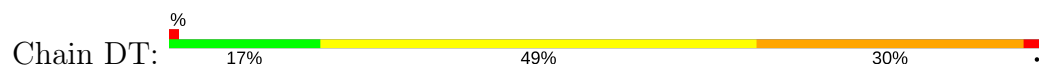
• Molecule 43: 50S ribosomal protein L22



• Molecule 44: 50S ribosomal protein L23

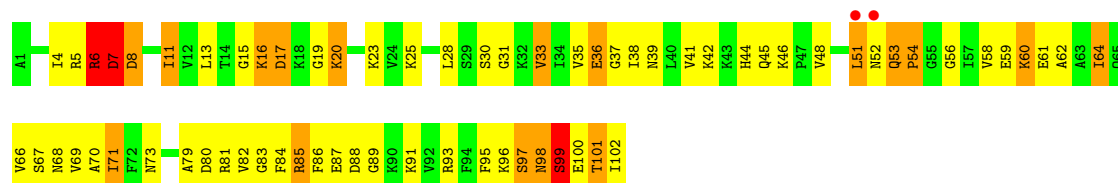


• Molecule 44: 50S ribosomal protein L23

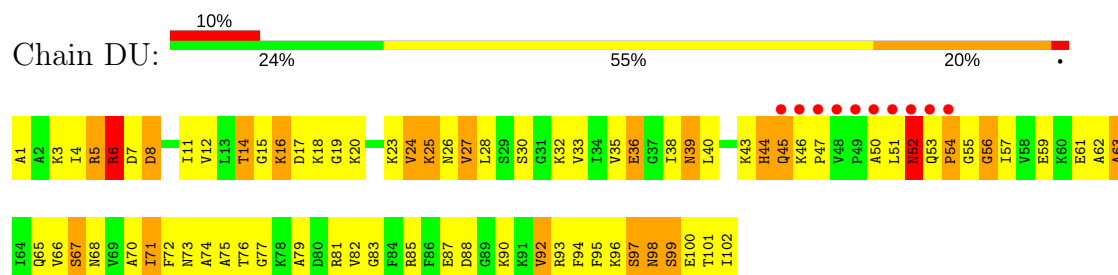


• Molecule 45: 50S ribosomal protein L24

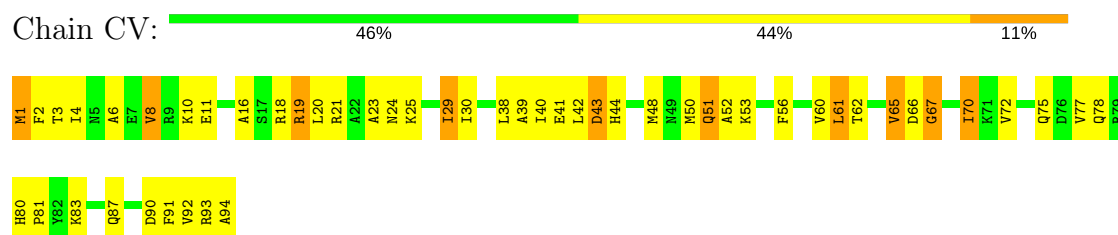




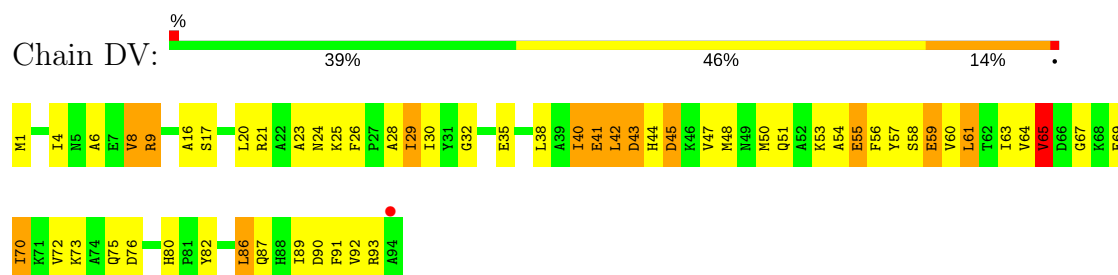
• Molecule 45: 50S ribosomal protein L24



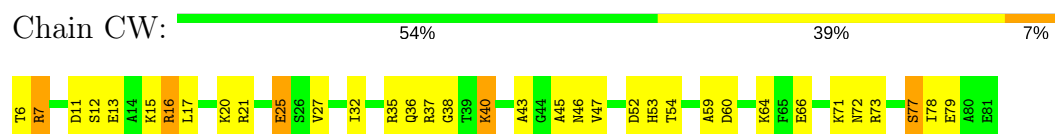
• Molecule 46: 50S ribosomal protein L25



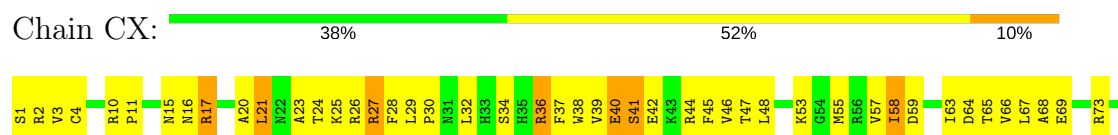
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27



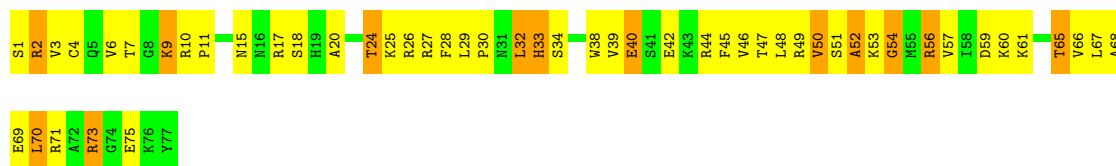
• Molecule 48: 50S ribosomal protein L28





- Molecule 48: 50S ribosomal protein L28

Chain DX: 32% 51% 17%



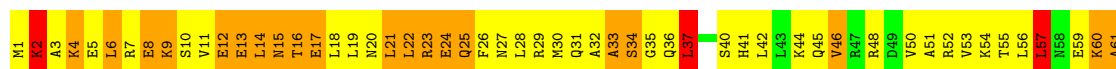
- Molecule 49: 50S ribosomal protein L29

Chain CY: 3% 25% 44% 27%



- Molecule 49: 50S ribosomal protein L29

Chain DY: 13% 51% 32% 5%



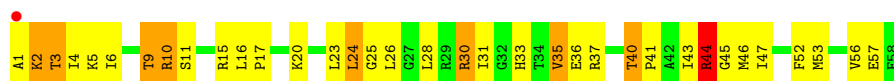
- Molecule 50: 50S ribosomal protein L30

Chain CZ: 45% 52%



- Molecule 50: 50S ribosomal protein L30

Chain DZ: 2% 40% 45% 14%

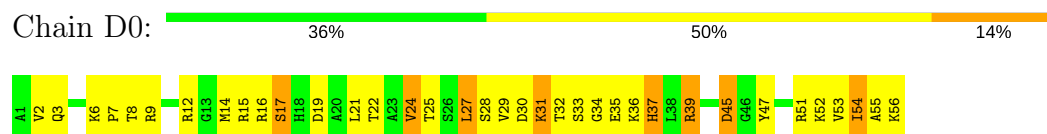


- Molecule 51: 50S ribosomal protein L32

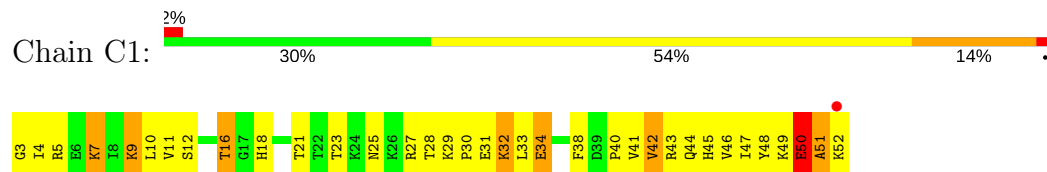
Chain C0: 48% 38% 14%



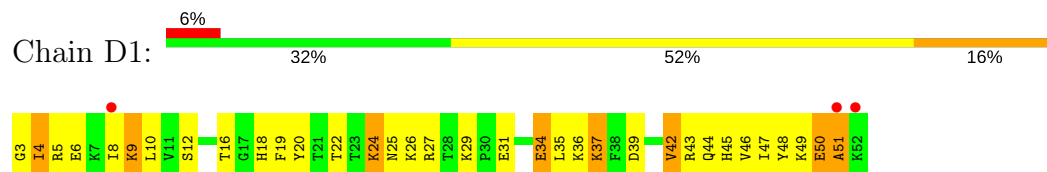
- Molecule 51: 50S ribosomal protein L32



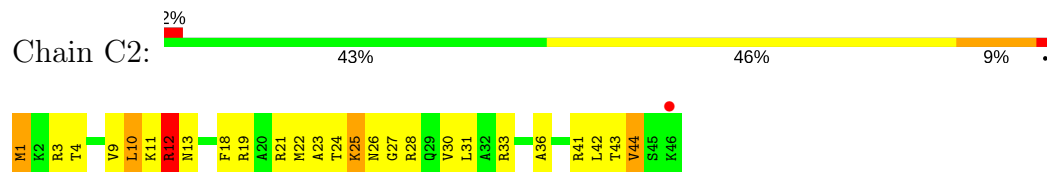
- Molecule 52: 50S ribosomal protein L33



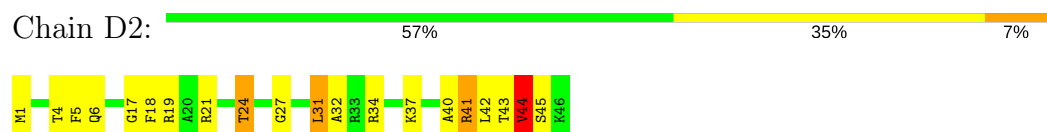
- Molecule 52: 50S ribosomal protein L33



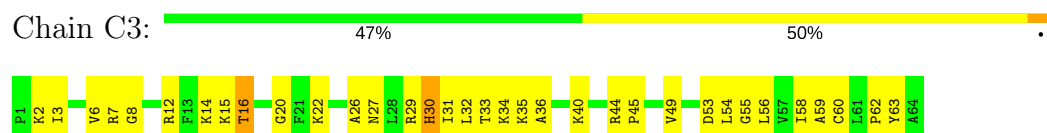
- Molecule 53: 50S ribosomal protein L34



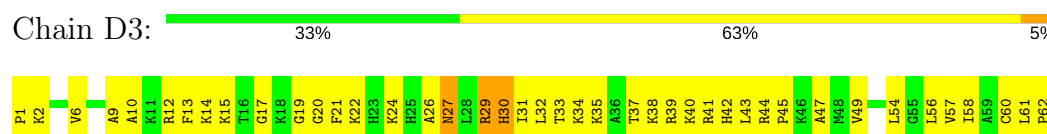
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36

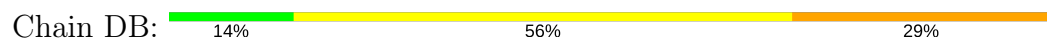




- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 5S rRNA



- Molecule 57: 50S ribosomal protein L27



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.67Å 438.07Å 613.42Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 40.00 – 3.00<br>69.21 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (40.00-3.00)<br>83.5 (69.21-3.00)           | Depositor<br>EDS |
| $R_{merge}$   | 0.19  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.58 (at 3.01Å)   | Xtriage          |
| Refinement program  | PHENIX  | Depositor        |
| R, $R_{free}$   | 0.202 , 0.260<br>0.195 , 0.251                              | Depositor<br>DCC |
| $R_{free}$ test set   | 19047 reflections (2.03%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 44.7  | Xtriage          |
| Anisotropy  | 0.180   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 22.4   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 292354  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 29.0  | wwPDB-VP         |

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

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$      |
| 1   | AA    | 0.87         | 8/36944 (0.0%) | 1.28        | 318/57632 (0.6%) |
| 1   | BA    | 0.86         | 8/36966 (0.0%) | 1.30        | 335/57666 (0.6%) |
| 2   | AB    | 0.60         | 0/1736         | 0.79        | 0/2338           |
| 2   | BB    | 0.54         | 0/1736         | 0.72        | 0/2338           |
| 3   | AC    | 0.56         | 0/1652         | 0.72        | 0/2225           |
| 3   | BC    | 0.51         | 0/1652         | 0.72        | 1/2225 (0.0%)    |
| 4   | AD    | 0.59         | 0/1665         | 0.74        | 1/2227 (0.0%)    |
| 4   | BD    | 0.65         | 0/1665         | 0.80        | 1/2227 (0.0%)    |
| 5   | AE    | 0.62         | 0/1119         | 0.85        | 0/1504           |
| 5   | BE    | 0.62         | 0/1119         | 0.85        | 0/1504           |
| 6   | AF    | 0.65         | 0/836          | 0.82        | 1/1128 (0.1%)    |
| 6   | BF    | 0.55         | 0/836          | 0.80        | 1/1128 (0.1%)    |
| 7   | AG    | 0.50         | 0/1196         | 0.67        | 0/1602           |
| 7   | BG    | 0.48         | 0/1196         | 0.67        | 0/1602           |
| 8   | AH    | 0.60         | 0/989          | 0.77        | 0/1326           |
| 8   | BH    | 0.58         | 0/989          | 0.74        | 0/1326           |
| 9   | AI    | 0.48         | 0/1034         | 0.71        | 0/1375           |
| 9   | BI    | 0.53         | 0/1034         | 0.75        | 0/1375           |
| 10  | AJ    | 0.57         | 0/797          | 0.74        | 0/1077           |
| 10  | BJ    | 0.52         | 0/797          | 0.76        | 1/1077 (0.1%)    |
| 11  | AK    | 0.67         | 0/893          | 0.82        | 0/1205           |
| 11  | BK    | 0.59         | 0/893          | 0.75        | 0/1205           |
| 12  | AL    | 0.61         | 0/969          | 0.81        | 0/1300           |
| 12  | BL    | 0.72         | 0/969          | 0.92        | 0/1300           |
| 13  | AM    | 0.52         | 0/893          | 0.74        | 0/1193           |
| 13  | BM    | 0.50         | 0/893          | 0.71        | 0/1193           |
| 14  | AN    | 0.55         | 0/785          | 0.76        | 0/1043           |
| 14  | BN    | 0.51         | 0/785          | 0.65        | 0/1043           |
| 15  | AO    | 0.55         | 0/722          | 0.73        | 0/964            |
| 15  | BO    | 0.53         | 0/722          | 0.73        | 0/964            |
| 16  | AP    | 0.54         | 0/659          | 0.82        | 1/884 (0.1%)     |
| 16  | BP    | 0.61         | 0/659          | 0.79        | 1/884 (0.1%)     |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5            |
| 17  | AQ    | 0.57         | 0/658            | 0.74        | 0/881              |
| 17  | BQ    | 0.62         | 0/658            | 0.76        | 0/881              |
| 18  | AR    | 0.61         | 0/463            | 0.69        | 0/621              |
| 18  | BR    | 0.54         | 0/463            | 0.68        | 0/621              |
| 19  | AS    | 0.48         | 0/653            | 0.73        | 0/877              |
| 19  | BS    | 0.55         | 0/653            | 0.67        | 0/877              |
| 20  | AT    | 0.54         | 0/671            | 0.69        | 0/888              |
| 20  | BT    | 0.57         | 0/671            | 0.73        | 0/888              |
| 21  | AU    | 0.93         | 0/431            | 0.96        | 0/570              |
| 21  | BU    | 0.78         | 0/431            | 0.85        | 0/570              |
| 22  | AV    | 0.76         | 1/1813 (0.1%)    | 1.22        | 14/2823 (0.5%)     |
| 22  | BV    | 0.74         | 1/1813 (0.1%)    | 1.22        | 10/2823 (0.4%)     |
| 23  | AX    | 0.86         | 0/363            | 1.11        | 0/564              |
| 23  | BX    | 0.73         | 0/388            | 1.09        | 0/603              |
| 24  | AY    | 0.65         | 0/1430           | 0.74        | 0/1924             |
| 25  | CA    | 1.60         | 600/69659 (0.9%) | 1.67        | 2062/108672 (1.9%) |
| 25  | DA    | 1.07         | 82/69633 (0.1%)  | 1.48        | 1284/108629 (1.2%) |
| 26  | CB    | 1.33         | 5/2847 (0.2%)    | 1.58        | 77/4440 (1.7%)     |
| 27  | CC    | 0.80         | 0/2122           | 0.90        | 1/2852 (0.0%)      |
| 27  | DC    | 0.68         | 1/2122 (0.0%)    | 0.86        | 1/2852 (0.0%)      |
| 28  | CD    | 0.96         | 0/1586           | 0.92        | 1/2134 (0.0%)      |
| 28  | DD    | 0.70         | 0/1586           | 0.87        | 2/2134 (0.1%)      |
| 29  | CE    | 0.91         | 0/1571           | 0.89        | 1/2113 (0.0%)      |
| 29  | DE    | 0.67         | 0/1571           | 0.81        | 0/2113             |
| 30  | CF    | 0.64         | 0/1435           | 0.74        | 0/1926             |
| 30  | DF    | 0.51         | 0/1435           | 0.67        | 0/1926             |
| 31  | CG    | 0.75         | 0/1343           | 0.85        | 1/1816 (0.1%)      |
| 31  | DG    | 0.51         | 0/1343           | 0.69        | 0/1816             |
| 32  | CH    | 0.68         | 1/1121 (0.1%)    | 0.77        | 0/1515             |
| 32  | DH    | 0.66         | 1/1121 (0.1%)    | 0.80        | 1/1515 (0.1%)      |
| 33  | CI    | 0.72         | 0/1046           | 0.74        | 0/1410             |
| 33  | DI    | 0.67         | 0/1046           | 0.72        | 0/1410             |
| 34  | CJ    | 1.01         | 0/1152           | 0.84        | 1/1551 (0.1%)      |
| 34  | DJ    | 0.77         | 0/1152           | 0.82        | 0/1551             |
| 35  | CK    | 0.91         | 3/948 (0.3%)     | 0.94        | 1/1268 (0.1%)      |
| 35  | DK    | 0.68         | 0/948            | 0.84        | 0/1268             |
| 36  | CL    | 0.94         | 0/1054           | 1.01        | 0/1403             |
| 36  | DL    | 0.65         | 0/1054           | 0.85        | 0/1403             |
| 37  | CM    | 0.94         | 0/1093           | 0.96        | 0/1460             |
| 37  | DM    | 0.64         | 0/1093           | 0.80        | 0/1460             |
| 38  | CN    | 0.91         | 0/974            | 0.96        | 1/1301 (0.1%)      |
| 38  | DN    | 0.67         | 0/974            | 0.82        | 0/1301             |
| 39  | CO    | 0.76         | 0/902            | 0.87        | 1/1209 (0.1%)      |



| Mol | Chain | Bond lengths |                   | Bond angles |                    |
|-----|-------|--------------|-------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >5           | RMSZ        | # Z  >5            |
| 39  | DO    | 0.50         | 0/902             | 0.66        | 0/1209             |
| 40  | CP    | 0.89         | 0/929             | 0.88        | 1/1242 (0.1%)      |
| 40  | DP    | 0.71         | 0/929             | 0.82        | 0/1242             |
| 41  | CQ    | 1.14         | 0/960             | 0.96        | 1/1278 (0.1%)      |
| 41  | DQ    | 0.80         | 0/960             | 0.79        | 0/1278             |
| 42  | CR    | 1.01         | 1/829 (0.1%)      | 0.98        | 0/1107             |
| 42  | DR    | 0.79         | 0/829             | 0.90        | 1/1107 (0.1%)      |
| 43  | CS    | 1.08         | 1/864 (0.1%)      | 0.97        | 1/1156 (0.1%)      |
| 43  | DS    | 0.71         | 0/864             | 0.89        | 1/1156 (0.1%)      |
| 44  | CT    | 0.82         | 0/745             | 0.86        | 0/994              |
| 44  | DT    | 0.59         | 0/745             | 0.74        | 0/994              |
| 45  | CU    | 0.91         | 0/788             | 0.90        | 0/1051             |
| 45  | DU    | 0.66         | 0/788             | 0.76        | 0/1051             |
| 46  | CV    | 0.79         | 0/766             | 0.81        | 0/1025             |
| 46  | DV    | 0.53         | 0/766             | 0.69        | 0/1025             |
| 47  | CW    | 1.02         | 0/582             | 0.97        | 0/769              |
| 48  | CX    | 0.78         | 0/635             | 0.84        | 0/848              |
| 48  | DX    | 0.61         | 0/635             | 0.77        | 0/848              |
| 49  | CY    | 0.76         | 0/510             | 0.96        | 1/677 (0.1%)       |
| 49  | DY    | 0.56         | 0/510             | 0.77        | 0/677              |
| 50  | CZ    | 1.04         | 0/453             | 0.94        | 0/605              |
| 50  | DZ    | 0.58         | 0/453             | 0.78        | 0/605              |
| 51  | C0    | 0.95         | 0/450             | 0.98        | 2/599 (0.3%)       |
| 51  | D0    | 0.71         | 0/450             | 0.89        | 1/599 (0.2%)       |
| 52  | C1    | 0.74         | 0/417             | 0.76        | 0/554              |
| 52  | D1    | 0.50         | 0/417             | 0.66        | 0/554              |
| 53  | C2    | 1.03         | 0/380             | 0.99        | 2/498 (0.4%)       |
| 53  | D2    | 0.70         | 0/380             | 0.84        | 0/498              |
| 54  | C3    | 0.94         | 0/513             | 0.85        | 0/676              |
| 54  | D3    | 0.60         | 0/513             | 0.78        | 1/676 (0.1%)       |
| 55  | C4    | 0.92         | 0/303             | 0.99        | 0/397              |
| 55  | D4    | 0.68         | 0/303             | 0.76        | 0/397              |
| 56  | DB    | 0.75         | 0/2828            | 1.23        | 18/4410 (0.4%)     |
| 57  | DW    | 0.60         | 0/571             | 0.72        | 0/755              |
| All | All   | 1.08         | 713/315257 (0.2%) | 1.34        | 4150/471496 (0.9%) |

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 |
|-----|-------|---------------------|---------------------|
| 4   | AD    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | BD    | 0                   | 1                   |
| 5   | AE    | 0                   | 1                   |
| 5   | BE    | 0                   | 2                   |
| 6   | BF    | 0                   | 1                   |
| 9   | AI    | 0                   | 1                   |
| 11  | AK    | 0                   | 1                   |
| 11  | BK    | 0                   | 2                   |
| 12  | BL    | 0                   | 2                   |
| 13  | AM    | 0                   | 1                   |
| 14  | AN    | 0                   | 1                   |
| 20  | BT    | 0                   | 1                   |
| 21  | AU    | 0                   | 2                   |
| 21  | BU    | 0                   | 1                   |
| 27  | CC    | 0                   | 1                   |
| 27  | DC    | 0                   | 1                   |
| 28  | CD    | 0                   | 2                   |
| 28  | DD    | 0                   | 1                   |
| 32  | DH    | 0                   | 2                   |
| 33  | CI    | 0                   | 1                   |
| 34  | DJ    | 0                   | 1                   |
| 39  | DO    | 0                   | 1                   |
| 42  | CR    | 0                   | 1                   |
| 45  | CU    | 0                   | 1                   |
| 50  | CZ    | 0                   | 1                   |
| All | All   | 0                   | 31                  |

The worst 5 of 713 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 25  | CA    | 1142 | A    | N9-C4 | -18.22 | 1.26        | 1.37     |
| 25  | CA    | 984  | A    | N9-C4 | -13.29 | 1.29        | 1.37     |
| 25  | DA    | 984  | A    | N9-C4 | -10.51 | 1.31        | 1.37     |
| 25  | CA    | 984  | A    | C5-C6 | -10.44 | 1.31        | 1.41     |
| 25  | CA    | 528  | A    | N7-C5 | -10.29 | 1.33        | 1.39     |

The worst 5 of 4150 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 25  | CA    | 984  | A    | C2-N3-C4 | -18.86 | 101.17      | 110.60   |
| 25  | CA    | 2250 | G    | N3-C4-C5 | 17.23  | 137.22      | 128.60   |
| 25  | CA    | 1638 | C    | N1-C2-O2 | -16.64 | 108.92      | 118.90   |
| 25  | CA    | 1142 | A    | C2-N3-C4 | -16.61 | 102.29      | 110.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 25  | CA    | 1142 | A    | N3-C4-C5 | 16.11 | 138.07      | 126.80   |

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | AD    | 47  | LEU  | Peptide |
| 5   | AE    | 100 | GLU  | Peptide |
| 9   | AI    | 5   | TYR  | Peptide |
| 11  | AK    | 125 | LYS  | Peptide |
| 13  | AM    | 111 | PRO  | 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    | 2052    | 0            |
| 1   | BA    | 33015 | 0        | 16617    | 2194    | 0            |
| 2   | AB    | 1705  | 0        | 1732     | 374     | 0            |
| 2   | BB    | 1705  | 0        | 1732     | 298     | 0            |
| 3   | AC    | 1625  | 0        | 1699     | 235     | 0            |
| 3   | BC    | 1625  | 0        | 1699     | 237     | 0            |
| 4   | AD    | 1643  | 0        | 1710     | 291     | 0            |
| 4   | BD    | 1643  | 0        | 1710     | 228     | 0            |
| 5   | AE    | 1106  | 0        | 1148     | 214     | 0            |
| 5   | BE    | 1106  | 0        | 1148     | 211     | 0            |
| 6   | AF    | 818   | 0        | 808      | 116     | 0            |
| 6   | BF    | 818   | 0        | 808      | 156     | 0            |
| 7   | AG    | 1182  | 0        | 1240     | 116     | 0            |
| 7   | BG    | 1182  | 0        | 1240     | 166     | 0            |
| 8   | AH    | 979   | 0        | 1034     | 161     | 0            |
| 8   | BH    | 979   | 0        | 1034     | 119     | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 189     | 0            |
| 9   | BI    | 1022  | 0        | 1070     | 186     | 0            |
| 10  | AJ    | 787   | 0        | 828      | 178     | 0            |
| 10  | BJ    | 787   | 0        | 828      | 142     | 0            |
| 11  | AK    | 877   | 0        | 887      | 160     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | BK    | 877   | 0        | 887      | 136     | 0            |
| 12  | AL    | 955   | 0        | 1019     | 94      | 0            |
| 12  | BL    | 955   | 0        | 1019     | 118     | 0            |
| 13  | AM    | 884   | 0        | 944      | 163     | 0            |
| 13  | BM    | 884   | 0        | 944      | 144     | 0            |
| 14  | AN    | 774   | 0        | 827      | 130     | 0            |
| 14  | BN    | 774   | 0        | 827      | 131     | 0            |
| 15  | AO    | 714   | 0        | 737      | 61      | 0            |
| 15  | BO    | 714   | 0        | 737      | 87      | 0            |
| 16  | AP    | 649   | 0        | 666      | 106     | 0            |
| 16  | BP    | 649   | 0        | 666      | 87      | 0            |
| 17  | AQ    | 649   | 0        | 691      | 118     | 0            |
| 17  | BQ    | 649   | 0        | 691      | 103     | 0            |
| 18  | AR    | 456   | 0        | 478      | 46      | 0            |
| 18  | BR    | 456   | 0        | 478      | 57      | 0            |
| 19  | AS    | 638   | 0        | 665      | 88      | 0            |
| 19  | BS    | 638   | 0        | 665      | 96      | 0            |
| 20  | AT    | 665   | 0        | 714      | 84      | 0            |
| 20  | BT    | 665   | 0        | 714      | 129     | 0            |
| 21  | AU    | 426   | 0        | 449      | 139     | 0            |
| 21  | BU    | 426   | 0        | 449      | 119     | 0            |
| 22  | AV    | 1623  | 0        | 821      | 88      | 0            |
| 22  | BV    | 1623  | 0        | 821      | 47      | 0            |
| 23  | AX    | 324   | 0        | 162      | 19      | 0            |
| 23  | BX    | 346   | 0        | 173      | 24      | 0            |
| 24  | AY    | 1419  | 0        | 1467     | 97      | 0            |
| 25  | CA    | 62195 | 0        | 31271    | 2445    | 0            |
| 25  | DA    | 62173 | 0        | 31270    | 3398    | 0            |
| 26  | CB    | 2548  | 0        | 1292     | 98      | 0            |
| 27  | CC    | 2083  | 0        | 2157     | 227     | 0            |
| 27  | DC    | 2083  | 0        | 2157     | 213     | 0            |
| 28  | CD    | 1565  | 0        | 1616     | 129     | 0            |
| 28  | DD    | 1565  | 0        | 1616     | 114     | 0            |
| 29  | CE    | 1552  | 0        | 1619     | 143     | 0            |
| 29  | DE    | 1552  | 0        | 1619     | 163     | 0            |
| 30  | CF    | 1411  | 0        | 1447     | 202     | 0            |
| 30  | DF    | 1411  | 0        | 1447     | 197     | 0            |
| 31  | CG    | 1323  | 0        | 1374     | 146     | 0            |
| 31  | DG    | 1323  | 0        | 1374     | 177     | 0            |
| 32  | CH    | 1110  | 0        | 1148     | 145     | 0            |
| 32  | DH    | 1110  | 0        | 1148     | 210     | 0            |
| 33  | CI    | 1032  | 0        | 1088     | 246     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | DI    | 1032  | 0        | 1088     | 180     | 0            |
| 34  | CJ    | 1129  | 0        | 1162     | 57      | 0            |
| 34  | DJ    | 1129  | 0        | 1162     | 96      | 0            |
| 35  | CK    | 939   | 0        | 1012     | 75      | 0            |
| 35  | DK    | 939   | 0        | 1012     | 79      | 0            |
| 36  | CL    | 1045  | 0        | 1117     | 130     | 0            |
| 36  | DL    | 1045  | 0        | 1117     | 168     | 0            |
| 37  | CM    | 1074  | 0        | 1157     | 96      | 0            |
| 37  | DM    | 1074  | 0        | 1157     | 127     | 0            |
| 38  | CN    | 961   | 0        | 1000     | 94      | 0            |
| 38  | DN    | 961   | 0        | 1000     | 124     | 0            |
| 39  | CO    | 892   | 0        | 923      | 84      | 0            |
| 39  | DO    | 892   | 0        | 923      | 141     | 0            |
| 40  | CP    | 917   | 0        | 965      | 93      | 0            |
| 40  | DP    | 917   | 0        | 965      | 107     | 0            |
| 41  | CQ    | 947   | 0        | 1022     | 63      | 0            |
| 41  | DQ    | 947   | 0        | 1022     | 83      | 0            |
| 42  | CR    | 816   | 0        | 839      | 84      | 0            |
| 42  | DR    | 816   | 0        | 839      | 99      | 0            |
| 43  | CS    | 857   | 0        | 922      | 42      | 0            |
| 43  | DS    | 857   | 0        | 922      | 82      | 0            |
| 44  | CT    | 739   | 0        | 807      | 71      | 0            |
| 44  | DT    | 739   | 0        | 807      | 114     | 0            |
| 45  | CU    | 780   | 0        | 834      | 66      | 0            |
| 45  | DU    | 780   | 0        | 834      | 111     | 0            |
| 46  | CV    | 753   | 0        | 780      | 59      | 0            |
| 46  | DV    | 753   | 0        | 780      | 71      | 0            |
| 47  | CW    | 575   | 0        | 589      | 27      | 0            |
| 48  | CX    | 625   | 0        | 655      | 41      | 0            |
| 48  | DX    | 625   | 0        | 655      | 58      | 0            |
| 49  | CY    | 509   | 0        | 543      | 88      | 0            |
| 49  | DY    | 509   | 0        | 543      | 109     | 0            |
| 50  | CZ    | 449   | 0        | 491      | 26      | 0            |
| 50  | DZ    | 449   | 0        | 491      | 47      | 0            |
| 51  | C0    | 444   | 0        | 461      | 35      | 0            |
| 51  | D0    | 444   | 0        | 461      | 41      | 0            |
| 52  | C1    | 410   | 0        | 440      | 37      | 0            |
| 52  | D1    | 410   | 0        | 440      | 45      | 0            |
| 53  | C2    | 377   | 0        | 418      | 26      | 0            |
| 53  | D2    | 377   | 0        | 418      | 18      | 0            |
| 54  | C3    | 504   | 0        | 574      | 40      | 0            |
| 54  | D3    | 504   | 0        | 574      | 42      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 55  | C4    | 302   | 0        | 340      | 23      | 0            |
| 55  | D4    | 302   | 0        | 340      | 34      | 0            |
| 56  | DB    | 2529  | 0        | 1281     | 163     | 0            |
| 57  | DW    | 564   | 0        | 576      | 36      | 0            |
| 58  | AA    | 72    | 0        | 0        | 0       | 0            |
| 58  | BA    | 56    | 0        | 0        | 0       | 0            |
| 58  | CA    | 194   | 0        | 0        | 0       | 0            |
| 58  | CB    | 4     | 0        | 0        | 0       | 0            |
| 58  | CQ    | 1     | 0        | 0        | 0       | 0            |
| 58  | DA    | 166   | 0        | 0        | 0       | 0            |
| 58  | DB    | 3     | 0        | 0        | 0       | 0            |
| 58  | DL    | 1     | 0        | 0        | 0       | 0            |
| 58  | DQ    | 1     | 0        | 0        | 0       | 0            |
| 59  | C4    | 1     | 0        | 0        | 0       | 0            |
| 59  | D4    | 1     | 0        | 0        | 0       | 0            |
| 60  | AA    | 197   | 0        | 0        | 11      | 0            |
| 60  | AN    | 4     | 0        | 0        | 0       | 0            |
| 60  | AT    | 1     | 0        | 0        | 0       | 0            |
| 60  | AU    | 1     | 0        | 0        | 0       | 0            |
| 60  | BA    | 190   | 0        | 0        | 12      | 0            |
| 60  | BL    | 1     | 0        | 0        | 0       | 0            |
| 60  | BN    | 5     | 0        | 0        | 1       | 0            |
| 60  | BT    | 1     | 0        | 0        | 0       | 0            |
| 60  | BU    | 1     | 0        | 0        | 0       | 0            |
| 60  | C2    | 1     | 0        | 0        | 0       | 0            |
| 60  | C3    | 1     | 0        | 0        | 0       | 0            |
| 60  | C4    | 2     | 0        | 0        | 0       | 0            |
| 60  | CA    | 625   | 0        | 0        | 62      | 0            |
| 60  | CB    | 13    | 0        | 0        | 0       | 0            |
| 60  | CC    | 8     | 0        | 0        | 0       | 0            |
| 60  | CD    | 2     | 0        | 0        | 0       | 0            |
| 60  | CE    | 2     | 0        | 0        | 0       | 0            |
| 60  | CF    | 1     | 0        | 0        | 0       | 0            |
| 60  | CJ    | 1     | 0        | 0        | 0       | 0            |
| 60  | CL    | 6     | 0        | 0        | 2       | 0            |
| 60  | CN    | 4     | 0        | 0        | 0       | 0            |
| 60  | CS    | 1     | 0        | 0        | 0       | 0            |
| 60  | CV    | 1     | 0        | 0        | 0       | 0            |
| 60  | D2    | 1     | 0        | 0        | 0       | 0            |
| 60  | D3    | 2     | 0        | 0        | 0       | 0            |
| 60  | D4    | 1     | 0        | 0        | 0       | 0            |
| 60  | DA    | 622   | 0        | 0        | 70      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 60  | DB    | 14     | 0        | 0        | 0       | 0            |
| 60  | DC    | 4      | 0        | 0        | 0       | 0            |
| 60  | DD    | 5      | 0        | 0        | 2       | 0            |
| 60  | DE    | 2      | 0        | 0        | 0       | 0            |
| 60  | DJ    | 1      | 0        | 0        | 0       | 0            |
| 60  | DL    | 4      | 0        | 0        | 1       | 0            |
| 60  | DN    | 1      | 0        | 0        | 0       | 0            |
| 60  | DR    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 292354 | 0        | 195461   | 20868   | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

The worst 5 of 20868 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) |
|------------------|--------------------|--------------------------|-------------------|
| 32:DH:93:SER:OG  | 32:DH:121:VAL:HG12 | 1.46                     | 1.15              |
| 1:BA:1053:G:H4'  | 1:BA:1054:C:H5'    | 1.29                     | 1.11              |
| 32:DH:93:SER:OG  | 32:DH:121:VAL:CG1  | 2.03                     | 1.06              |
| 25:DA:1153:C:OP2 | 60:DA:3363:HOH:O   | 1.78                     | 1.01              |
| 12:BL:33:CYS:HA  | 12:BL:54:VAL:HA    | 1.44                     | 0.99              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles       |
|-----|-------|---------------|-----------|----------|----------|-------------------|
| 2   | AB    | 216/218 (99%) | 109 (50%) | 49 (23%) | 58 (27%) | <b>0</b> <b>0</b> |
| 2   | BB    | 216/218 (99%) | 112 (52%) | 49 (23%) | 55 (26%) | <b>0</b> <b>0</b> |
| 3   | AC    | 204/206 (99%) | 125 (61%) | 49 (24%) | 30 (15%) | <b>0</b> <b>1</b> |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | BC    | 204/206 (99%) | 126 (62%) | 47 (23%) | 31 (15%) | 0           | 1  |
| 4   | AD    | 203/205 (99%) | 123 (61%) | 41 (20%) | 39 (19%) | 0           | 0  |
| 4   | BD    | 203/205 (99%) | 136 (67%) | 36 (18%) | 31 (15%) | 0           | 1  |
| 5   | AE    | 148/150 (99%) | 87 (59%)  | 38 (26%) | 23 (16%) | 0           | 1  |
| 5   | BE    | 148/150 (99%) | 90 (61%)  | 31 (21%) | 27 (18%) | 0           | 0  |
| 6   | AF    | 98/100 (98%)  | 62 (63%)  | 21 (21%) | 15 (15%) | 0           | 1  |
| 6   | BF    | 98/100 (98%)  | 54 (55%)  | 23 (24%) | 21 (21%) | 0           | 0  |
| 7   | AG    | 149/151 (99%) | 86 (58%)  | 41 (28%) | 22 (15%) | 0           | 1  |
| 7   | BG    | 149/151 (99%) | 79 (53%)  | 46 (31%) | 24 (16%) | 0           | 1  |
| 8   | AH    | 127/129 (98%) | 79 (62%)  | 37 (29%) | 11 (9%)  | 1           | 4  |
| 8   | BH    | 127/129 (98%) | 82 (65%)  | 32 (25%) | 13 (10%) | 1           | 3  |
| 9   | AI    | 125/127 (98%) | 76 (61%)  | 34 (27%) | 15 (12%) | 0           | 2  |
| 9   | BI    | 125/127 (98%) | 77 (62%)  | 33 (26%) | 15 (12%) | 0           | 2  |
| 10  | AJ    | 96/98 (98%)   | 60 (62%)  | 14 (15%) | 22 (23%) | 0           | 0  |
| 10  | BJ    | 96/98 (98%)   | 64 (67%)  | 14 (15%) | 18 (19%) | 0           | 0  |
| 11  | AK    | 115/117 (98%) | 84 (73%)  | 17 (15%) | 14 (12%) | 0           | 1  |
| 11  | BK    | 115/117 (98%) | 81 (70%)  | 19 (16%) | 15 (13%) | 0           | 1  |
| 12  | AL    | 121/123 (98%) | 85 (70%)  | 29 (24%) | 7 (6%)   | 2           | 11 |
| 12  | BL    | 121/123 (98%) | 91 (75%)  | 16 (13%) | 14 (12%) | 0           | 2  |
| 13  | AM    | 112/114 (98%) | 78 (70%)  | 22 (20%) | 12 (11%) | 0           | 2  |
| 13  | BM    | 112/114 (98%) | 65 (58%)  | 24 (21%) | 23 (20%) | 0           | 0  |
| 14  | AN    | 92/100 (92%)  | 47 (51%)  | 27 (29%) | 18 (20%) | 0           | 0  |
| 14  | BN    | 92/100 (92%)  | 39 (42%)  | 30 (33%) | 23 (25%) | 0           | 0  |
| 15  | AO    | 86/88 (98%)   | 57 (66%)  | 22 (26%) | 7 (8%)   | 1           | 5  |
| 15  | BO    | 86/88 (98%)   | 52 (60%)  | 17 (20%) | 17 (20%) | 0           | 0  |
| 16  | AP    | 80/82 (98%)   | 48 (60%)  | 11 (14%) | 21 (26%) | 0           | 0  |
| 16  | BP    | 80/82 (98%)   | 47 (59%)  | 22 (28%) | 11 (14%) | 0           | 1  |
| 17  | AQ    | 78/80 (98%)   | 47 (60%)  | 18 (23%) | 13 (17%) | 0           | 1  |
| 17  | BQ    | 78/80 (98%)   | 48 (62%)  | 18 (23%) | 12 (15%) | 0           | 1  |
| 18  | AR    | 53/55 (96%)   | 34 (64%)  | 13 (24%) | 6 (11%)  | 0           | 2  |
| 18  | BR    | 53/55 (96%)   | 31 (58%)  | 19 (36%) | 3 (6%)   | 2           | 12 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 19  | AS    | 77/79 (98%)   | 36 (47%)  | 29 (38%) | 12 (16%) | 0           | 1  |
| 19  | BS    | 77/79 (98%)   | 56 (73%)  | 14 (18%) | 7 (9%)   | 1           | 4  |
| 20  | AT    | 83/85 (98%)   | 37 (45%)  | 31 (37%) | 15 (18%) | 0           | 0  |
| 20  | BT    | 83/85 (98%)   | 46 (55%)  | 23 (28%) | 14 (17%) | 0           | 1  |
| 21  | AU    | 49/51 (96%)   | 20 (41%)  | 15 (31%) | 14 (29%) | 0           | 0  |
| 21  | BU    | 49/51 (96%)   | 22 (45%)  | 10 (20%) | 17 (35%) | 0           | 0  |
| 24  | AY    | 181/183 (99%) | 135 (75%) | 35 (19%) | 11 (6%)  | 2           | 10 |
| 27  | CC    | 269/271 (99%) | 216 (80%) | 32 (12%) | 21 (8%)  | 1           | 5  |
| 27  | DC    | 269/271 (99%) | 198 (74%) | 43 (16%) | 28 (10%) | 0           | 3  |
| 28  | CD    | 207/209 (99%) | 166 (80%) | 30 (14%) | 11 (5%)  | 2           | 13 |
| 28  | DD    | 207/209 (99%) | 162 (78%) | 35 (17%) | 10 (5%)  | 2           | 16 |
| 29  | CE    | 199/201 (99%) | 158 (79%) | 32 (16%) | 9 (4%)   | 3           | 17 |
| 29  | DE    | 199/201 (99%) | 142 (71%) | 38 (19%) | 19 (10%) | 1           | 3  |
| 30  | CF    | 175/177 (99%) | 118 (67%) | 38 (22%) | 19 (11%) | 0           | 2  |
| 30  | DF    | 175/177 (99%) | 113 (65%) | 34 (19%) | 28 (16%) | 0           | 1  |
| 31  | CG    | 174/176 (99%) | 129 (74%) | 30 (17%) | 15 (9%)  | 1           | 4  |
| 31  | DG    | 174/176 (99%) | 106 (61%) | 43 (25%) | 25 (14%) | 0           | 1  |
| 32  | CH    | 147/149 (99%) | 95 (65%)  | 29 (20%) | 23 (16%) | 0           | 1  |
| 32  | DH    | 147/149 (99%) | 95 (65%)  | 27 (18%) | 25 (17%) | 0           | 1  |
| 33  | CI    | 139/141 (99%) | 65 (47%)  | 47 (34%) | 27 (19%) | 0           | 0  |
| 33  | DI    | 139/141 (99%) | 71 (51%)  | 46 (33%) | 22 (16%) | 0           | 1  |
| 34  | CJ    | 140/142 (99%) | 123 (88%) | 11 (8%)  | 6 (4%)   | 3           | 18 |
| 34  | DJ    | 140/142 (99%) | 112 (80%) | 24 (17%) | 4 (3%)   | 5           | 28 |
| 35  | CK    | 120/122 (98%) | 88 (73%)  | 24 (20%) | 8 (7%)   | 1           | 7  |
| 35  | DK    | 120/122 (98%) | 87 (72%)  | 21 (18%) | 12 (10%) | 1           | 3  |
| 36  | CL    | 141/143 (99%) | 99 (70%)  | 21 (15%) | 21 (15%) | 0           | 1  |
| 36  | DL    | 141/143 (99%) | 88 (62%)  | 36 (26%) | 17 (12%) | 0           | 2  |
| 37  | CM    | 134/136 (98%) | 110 (82%) | 15 (11%) | 9 (7%)   | 1           | 7  |
| 37  | DM    | 134/136 (98%) | 97 (72%)  | 23 (17%) | 14 (10%) | 0           | 3  |
| 38  | CN    | 118/120 (98%) | 91 (77%)  | 21 (18%) | 6 (5%)   | 2           | 14 |
| 38  | DN    | 118/120 (98%) | 82 (70%)  | 28 (24%) | 8 (7%)   | 1           | 7  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 39  | CO    | 114/116 (98%) | 83 (73%)  | 17 (15%) | 14 (12%) | 0           | 1   |
| 39  | DO    | 114/116 (98%) | 77 (68%)  | 25 (22%) | 12 (10%) | 0           | 2   |
| 40  | CP    | 112/114 (98%) | 96 (86%)  | 12 (11%) | 4 (4%)   | 4           | 22  |
| 40  | DP    | 112/114 (98%) | 86 (77%)  | 19 (17%) | 7 (6%)   | 1           | 9   |
| 41  | CQ    | 115/117 (98%) | 100 (87%) | 13 (11%) | 2 (2%)   | 11          | 44  |
| 41  | DQ    | 115/117 (98%) | 95 (83%)  | 18 (16%) | 2 (2%)   | 11          | 44  |
| 42  | CR    | 101/103 (98%) | 84 (83%)  | 9 (9%)   | 8 (8%)   | 1           | 5   |
| 42  | DR    | 101/103 (98%) | 78 (77%)  | 14 (14%) | 9 (9%)   | 1           | 4   |
| 43  | CS    | 108/110 (98%) | 90 (83%)  | 12 (11%) | 6 (6%)   | 2           | 12  |
| 43  | DS    | 108/110 (98%) | 78 (72%)  | 19 (18%) | 11 (10%) | 1           | 3   |
| 44  | CT    | 91/93 (98%)   | 67 (74%)  | 13 (14%) | 11 (12%) | 0           | 2   |
| 44  | DT    | 91/93 (98%)   | 59 (65%)  | 20 (22%) | 12 (13%) | 0           | 1   |
| 45  | CU    | 100/102 (98%) | 74 (74%)  | 14 (14%) | 12 (12%) | 0           | 2   |
| 45  | DU    | 100/102 (98%) | 73 (73%)  | 14 (14%) | 13 (13%) | 0           | 1   |
| 46  | CV    | 92/94 (98%)   | 78 (85%)  | 12 (13%) | 2 (2%)   | 8           | 36  |
| 46  | DV    | 92/94 (98%)   | 71 (77%)  | 15 (16%) | 6 (6%)   | 1           | 8   |
| 47  | CW    | 74/76 (97%)   | 68 (92%)  | 4 (5%)   | 2 (3%)   | 6           | 30  |
| 48  | CX    | 75/77 (97%)   | 64 (85%)  | 9 (12%)  | 2 (3%)   | 6           | 30  |
| 48  | DX    | 75/77 (97%)   | 54 (72%)  | 15 (20%) | 6 (8%)   | 1           | 5   |
| 49  | CY    | 61/63 (97%)   | 34 (56%)  | 13 (21%) | 14 (23%) | 0           | 0   |
| 49  | DY    | 61/63 (97%)   | 28 (46%)  | 16 (26%) | 17 (28%) | 0           | 0   |
| 50  | CZ    | 56/58 (97%)   | 50 (89%)  | 6 (11%)  | 0        | 100         | 100 |
| 50  | DZ    | 56/58 (97%)   | 50 (89%)  | 4 (7%)   | 2 (4%)   | 4           | 22  |
| 51  | C0    | 54/56 (96%)   | 44 (82%)  | 8 (15%)  | 2 (4%)   | 4           | 22  |
| 51  | D0    | 54/56 (96%)   | 39 (72%)  | 10 (18%) | 5 (9%)   | 1           | 4   |
| 52  | C1    | 48/50 (96%)   | 32 (67%)  | 12 (25%) | 4 (8%)   | 1           | 4   |
| 52  | D1    | 48/50 (96%)   | 36 (75%)  | 10 (21%) | 2 (4%)   | 3           | 18  |
| 53  | C2    | 44/46 (96%)   | 37 (84%)  | 6 (14%)  | 1 (2%)   | 7           | 35  |
| 53  | D2    | 44/46 (96%)   | 31 (70%)  | 8 (18%)  | 5 (11%)  | 0           | 2   |
| 54  | C3    | 62/64 (97%)   | 56 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 54  | D3    | 62/64 (97%)   | 49 (79%)  | 11 (18%) | 2 (3%)   | 5           | 26  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers   | Percentiles |    |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 55  | C4    | 36/38 (95%)       | 31 (86%)   | 4 (11%)    | 1 (3%)     | 6           | 29 |
| 55  | D4    | 36/38 (95%)       | 31 (86%)   | 4 (11%)    | 1 (3%)     | 6           | 29 |
| 57  | DW    | 73/75 (97%)       | 57 (78%)   | 12 (16%)   | 4 (6%)     | 2           | 12 |
| All | All   | 11416/11626 (98%) | 7804 (68%) | 2248 (20%) | 1364 (12%) | 0           | 2  |

5 of 1364 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 15  | PHE  |
| 2   | AB    | 21  | TYR  |
| 2   | AB    | 33  | ALA  |
| 2   | AB    | 63  | LYS  |
| 2   | AB    | 67  | LEU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 2   | AB    | 180/180 (100%) | 114 (63%) | 66 (37%) | 0           | 1 |
| 2   | BB    | 180/180 (100%) | 131 (73%) | 49 (27%) | 0           | 2 |
| 3   | AC    | 170/170 (100%) | 127 (75%) | 43 (25%) | 0           | 3 |
| 3   | BC    | 170/170 (100%) | 123 (72%) | 47 (28%) | 0           | 2 |
| 4   | AD    | 172/172 (100%) | 132 (77%) | 40 (23%) | 1           | 4 |
| 4   | BD    | 172/172 (100%) | 123 (72%) | 49 (28%) | 0           | 2 |
| 5   | AE    | 113/113 (100%) | 80 (71%)  | 33 (29%) | 0           | 2 |
| 5   | BE    | 113/113 (100%) | 87 (77%)  | 26 (23%) | 1           | 4 |
| 6   | AF    | 87/87 (100%)   | 60 (69%)  | 27 (31%) | 0           | 1 |
| 6   | BF    | 87/87 (100%)   | 61 (70%)  | 26 (30%) | 0           | 2 |
| 7   | AG    | 124/124 (100%) | 90 (73%)  | 34 (27%) | 0           | 2 |
| 7   | BG    | 124/124 (100%) | 85 (68%)  | 39 (32%) | 0           | 1 |
| 8   | AH    | 104/104 (100%) | 78 (75%)  | 26 (25%) | 1           | 3 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 8   | BH    | 104/104 (100%) | 78 (75%)  | 26 (25%) | 1           | 3  |
| 9   | AI    | 105/105 (100%) | 74 (70%)  | 31 (30%) | 0           | 2  |
| 9   | BI    | 105/105 (100%) | 67 (64%)  | 38 (36%) | 0           | 1  |
| 10  | AJ    | 86/86 (100%)   | 63 (73%)  | 23 (27%) | 0           | 3  |
| 10  | BJ    | 86/86 (100%)   | 61 (71%)  | 25 (29%) | 0           | 2  |
| 11  | AK    | 90/90 (100%)   | 66 (73%)  | 24 (27%) | 0           | 3  |
| 11  | BK    | 90/90 (100%)   | 67 (74%)  | 23 (26%) | 0           | 3  |
| 12  | AL    | 103/103 (100%) | 86 (84%)  | 17 (16%) | 2           | 13 |
| 12  | BL    | 103/103 (100%) | 75 (73%)  | 28 (27%) | 0           | 2  |
| 13  | AM    | 92/92 (100%)   | 73 (79%)  | 19 (21%) | 1           | 6  |
| 13  | BM    | 92/92 (100%)   | 71 (77%)  | 21 (23%) | 1           | 5  |
| 14  | AN    | 79/83 (95%)    | 56 (71%)  | 23 (29%) | 0           | 2  |
| 14  | BN    | 79/83 (95%)    | 60 (76%)  | 19 (24%) | 1           | 4  |
| 15  | AO    | 76/76 (100%)   | 61 (80%)  | 15 (20%) | 1           | 8  |
| 15  | BO    | 76/76 (100%)   | 60 (79%)  | 16 (21%) | 1           | 6  |
| 16  | AP    | 65/65 (100%)   | 45 (69%)  | 20 (31%) | 0           | 1  |
| 16  | BP    | 65/65 (100%)   | 48 (74%)  | 17 (26%) | 0           | 3  |
| 17  | AQ    | 74/74 (100%)   | 54 (73%)  | 20 (27%) | 0           | 2  |
| 17  | BQ    | 74/74 (100%)   | 47 (64%)  | 27 (36%) | 0           | 1  |
| 18  | AR    | 48/48 (100%)   | 40 (83%)  | 8 (17%)  | 2           | 13 |
| 18  | BR    | 48/48 (100%)   | 40 (83%)  | 8 (17%)  | 2           | 13 |
| 19  | AS    | 70/70 (100%)   | 56 (80%)  | 14 (20%) | 1           | 8  |
| 19  | BS    | 70/70 (100%)   | 53 (76%)  | 17 (24%) | 1           | 4  |
| 20  | AT    | 65/65 (100%)   | 45 (69%)  | 20 (31%) | 0           | 1  |
| 20  | BT    | 65/65 (100%)   | 47 (72%)  | 18 (28%) | 0           | 2  |
| 21  | AU    | 44/44 (100%)   | 23 (52%)  | 21 (48%) | 0           | 0  |
| 21  | BU    | 44/44 (100%)   | 26 (59%)  | 18 (41%) | 0           | 0  |
| 24  | AY    | 157/157 (100%) | 139 (88%) | 18 (12%) | 6           | 27 |
| 27  | CC    | 216/216 (100%) | 182 (84%) | 34 (16%) | 3           | 14 |
| 27  | DC    | 216/216 (100%) | 173 (80%) | 43 (20%) | 1           | 8  |
| 28  | CD    | 164/164 (100%) | 143 (87%) | 21 (13%) | 5           | 22 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 28  | DD    | 164/164 (100%) | 135 (82%) | 29 (18%) | 2           | 11 |
| 29  | CE    | 165/165 (100%) | 143 (87%) | 22 (13%) | 4           | 20 |
| 29  | DE    | 165/165 (100%) | 126 (76%) | 39 (24%) | 1           | 4  |
| 30  | CF    | 148/148 (100%) | 112 (76%) | 36 (24%) | 1           | 4  |
| 30  | DF    | 148/148 (100%) | 114 (77%) | 34 (23%) | 1           | 4  |
| 31  | CG    | 137/137 (100%) | 114 (83%) | 23 (17%) | 2           | 12 |
| 31  | DG    | 137/137 (100%) | 119 (87%) | 18 (13%) | 5           | 21 |
| 32  | CH    | 114/114 (100%) | 89 (78%)  | 25 (22%) | 1           | 5  |
| 32  | DH    | 114/114 (100%) | 92 (81%)  | 22 (19%) | 1           | 9  |
| 33  | CI    | 109/109 (100%) | 78 (72%)  | 31 (28%) | 0           | 2  |
| 33  | DI    | 109/109 (100%) | 83 (76%)  | 26 (24%) | 1           | 4  |
| 34  | CJ    | 116/116 (100%) | 97 (84%)  | 19 (16%) | 2           | 13 |
| 34  | DJ    | 116/116 (100%) | 95 (82%)  | 21 (18%) | 2           | 10 |
| 35  | CK    | 103/103 (100%) | 85 (82%)  | 18 (18%) | 2           | 11 |
| 35  | DK    | 103/103 (100%) | 85 (82%)  | 18 (18%) | 2           | 11 |
| 36  | CL    | 102/102 (100%) | 81 (79%)  | 21 (21%) | 1           | 7  |
| 36  | DL    | 102/102 (100%) | 81 (79%)  | 21 (21%) | 1           | 7  |
| 37  | CM    | 109/109 (100%) | 87 (80%)  | 22 (20%) | 1           | 7  |
| 37  | DM    | 109/109 (100%) | 87 (80%)  | 22 (20%) | 1           | 7  |
| 38  | CN    | 100/100 (100%) | 83 (83%)  | 17 (17%) | 2           | 12 |
| 38  | DN    | 100/100 (100%) | 80 (80%)  | 20 (20%) | 1           | 8  |
| 39  | CO    | 86/86 (100%)   | 68 (79%)  | 18 (21%) | 1           | 6  |
| 39  | DO    | 86/86 (100%)   | 66 (77%)  | 20 (23%) | 1           | 4  |
| 40  | CP    | 99/99 (100%)   | 78 (79%)  | 21 (21%) | 1           | 6  |
| 40  | DP    | 99/99 (100%)   | 76 (77%)  | 23 (23%) | 1           | 4  |
| 41  | CQ    | 89/89 (100%)   | 76 (85%)  | 13 (15%) | 3           | 17 |
| 41  | DQ    | 89/89 (100%)   | 74 (83%)  | 15 (17%) | 2           | 12 |
| 42  | CR    | 84/84 (100%)   | 70 (83%)  | 14 (17%) | 2           | 13 |
| 42  | DR    | 84/84 (100%)   | 66 (79%)  | 18 (21%) | 1           | 6  |
| 43  | CS    | 93/93 (100%)   | 83 (89%)  | 10 (11%) | 7           | 29 |
| 43  | DS    | 93/93 (100%)   | 71 (76%)  | 22 (24%) | 1           | 4  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 44  | CT    | 80/80 (100%)     | 69 (86%)   | 11 (14%)   | 4           | 19 |
| 44  | DT    | 80/80 (100%)     | 57 (71%)   | 23 (29%)   | 0           | 2  |
| 45  | CU    | 83/83 (100%)     | 64 (77%)   | 19 (23%)   | 1           | 5  |
| 45  | DU    | 83/83 (100%)     | 63 (76%)   | 20 (24%)   | 1           | 4  |
| 46  | CV    | 78/78 (100%)     | 63 (81%)   | 15 (19%)   | 1           | 9  |
| 46  | DV    | 78/78 (100%)     | 63 (81%)   | 15 (19%)   | 1           | 9  |
| 47  | CW    | 56/58 (97%)      | 50 (89%)   | 6 (11%)    | 8           | 29 |
| 48  | CX    | 67/67 (100%)     | 56 (84%)   | 11 (16%)   | 2           | 13 |
| 48  | DX    | 67/67 (100%)     | 56 (84%)   | 11 (16%)   | 2           | 13 |
| 49  | CY    | 55/55 (100%)     | 46 (84%)   | 9 (16%)    | 2           | 13 |
| 49  | DY    | 55/55 (100%)     | 43 (78%)   | 12 (22%)   | 1           | 6  |
| 50  | CZ    | 48/48 (100%)     | 40 (83%)   | 8 (17%)    | 2           | 13 |
| 50  | DZ    | 48/48 (100%)     | 38 (79%)   | 10 (21%)   | 1           | 6  |
| 51  | C0    | 47/47 (100%)     | 41 (87%)   | 6 (13%)    | 5           | 22 |
| 51  | D0    | 47/47 (100%)     | 41 (87%)   | 6 (13%)    | 5           | 22 |
| 52  | C1    | 45/45 (100%)     | 38 (84%)   | 7 (16%)    | 3           | 15 |
| 52  | D1    | 45/45 (100%)     | 37 (82%)   | 8 (18%)    | 2           | 11 |
| 53  | C2    | 38/38 (100%)     | 32 (84%)   | 6 (16%)    | 3           | 14 |
| 53  | D2    | 38/38 (100%)     | 33 (87%)   | 5 (13%)    | 5           | 20 |
| 54  | C3    | 51/51 (100%)     | 48 (94%)   | 3 (6%)     | 23          | 60 |
| 54  | D3    | 51/51 (100%)     | 48 (94%)   | 3 (6%)     | 23          | 60 |
| 55  | C4    | 34/34 (100%)     | 28 (82%)   | 6 (18%)    | 2           | 11 |
| 55  | D4    | 34/34 (100%)     | 27 (79%)   | 7 (21%)    | 1           | 7  |
| 57  | DW    | 55/57 (96%)      | 47 (86%)   | 8 (14%)    | 4           | 17 |
| All | All   | 9482/9494 (100%) | 7392 (78%) | 2090 (22%) | 1           | 5  |

5 of 2090 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | BN    | 25  | GLU  |
| 30  | CF    | 55  | ASP  |
| 42  | DR    | 48  | LYS  |
| 15  | BO    | 87  | ARG  |
| 21  | BU    | 4   | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | CC    | 116 | GLN  |
| 34  | CJ    | 58  | ASN  |
| 45  | DU    | 26  | ASN  |
| 28  | CD    | 67  | HIS  |
| 30  | CF    | 62  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1537/1539 (99%) | 441 (28%)         | 0               |
| 1   | BA    | 1538/1539 (99%) | 445 (28%)         | 0               |
| 22  | AV    | 75/76 (98%)     | 29 (38%)          | 0               |
| 22  | BV    | 75/76 (98%)     | 15 (20%)          | 0               |
| 23  | AX    | 14/16 (87%)     | 5 (35%)           | 0               |
| 23  | BX    | 15/16 (93%)     | 4 (26%)           | 0               |
| 25  | CA    | 2895/2903 (99%) | 747 (25%)         | 0               |
| 25  | DA    | 2893/2903 (99%) | 764 (26%)         | 0               |
| 26  | CB    | 118/119 (99%)   | 24 (20%)          | 0               |
| 56  | DB    | 117/118 (99%)   | 34 (29%)          | 0               |
| All | All   | 9277/9305 (99%) | 2508 (27%)        | 0               |

5 of 2508 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 5   | U    |
| 1   | AA    | 6   | G    |
| 1   | AA    | 7   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 12  | U    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1538/1539 (99%)  | -0.64  | 7 (0%) 90 74  | 0, 31, 105, 170       | 0     |
| 1   | BA    | 1539/1539 (100%) | -0.58  | 10 (0%) 89 71 | 0, 33, 101, 147       | 0     |
| 2   | AB    | 218/218 (100%)   | 0.58   | 14 (6%) 20 7  | 12, 52, 84, 115       | 0     |
| 2   | BB    | 218/218 (100%)   | 0.41   | 12 (5%) 26 10 | 19, 59, 88, 113       | 0     |
| 3   | AC    | 206/206 (100%)   | -0.32  | 0 100 100     | 0, 35, 69, 93         | 0     |
| 3   | BC    | 206/206 (100%)   | 0.23   | 3 (1%) 74 47  | 9, 46, 75, 92         | 0     |
| 4   | AD    | 205/205 (100%)   | 0.08   | 4 (1%) 65 36  | 14, 42, 73, 98        | 0     |
| 4   | BD    | 205/205 (100%)   | -0.26  | 1 (0%) 90 74  | 0, 24, 64, 82         | 0     |
| 5   | AE    | 150/150 (100%)   | -0.15  | 2 (1%) 77 51  | 0, 32, 68, 105        | 0     |
| 5   | BE    | 150/150 (100%)   | -0.38  | 0 100 100     | 0, 31, 68, 98         | 0     |
| 6   | AF    | 100/100 (100%)   | -0.37  | 0 100 100     | 0, 33, 68, 86         | 0     |
| 6   | BF    | 100/100 (100%)   | -0.01  | 0 100 100     | 17, 54, 80, 93        | 0     |
| 7   | AG    | 151/151 (100%)   | 0.50   | 14 (9%) 9 3   | 12, 56, 86, 111       | 0     |
| 7   | BG    | 151/151 (100%)   | 0.01   | 5 (3%) 47 21  | 20, 54, 81, 94        | 0     |
| 8   | AH    | 129/129 (100%)   | -0.48  | 0 100 100     | 0, 32, 60, 71         | 0     |
| 8   | BH    | 129/129 (100%)   | -0.25  | 1 (0%) 86 64  | 4, 34, 58, 82         | 0     |
| 9   | AI    | 127/127 (100%)   | 0.17   | 4 (3%) 49 22  | 6, 54, 79, 108        | 0     |
| 9   | BI    | 127/127 (100%)   | 0.37   | 8 (6%) 21 7   | 20, 55, 85, 117       | 0     |
| 10  | AJ    | 98/98 (100%)     | 0.42   | 5 (5%) 29 12  | 8, 55, 89, 104        | 0     |
| 10  | BJ    | 98/98 (100%)     | 0.38   | 6 (6%) 22 8   | 25, 58, 82, 113       | 0     |
| 11  | AK    | 117/117 (100%)   | -0.37  | 1 (0%) 84 61  | 0, 19, 50, 87         | 0     |
| 11  | BK    | 117/117 (100%)   | -0.24  | 0 100 100     | 0, 32, 66, 79         | 0     |
| 12  | AL    | 123/123 (100%)   | -0.32  | 2 (1%) 72 44  | 0, 22, 67, 93         | 0     |
| 12  | BL    | 123/123 (100%)   | -0.27  | 3 (2%) 59 30  | 0, 17, 58, 93         | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | AM    | 114/114 (100%)  | 0.08   | 4 (3%) 44 19  | 9, 53, 87, 100        | 0     |
| 13  | BM    | 114/114 (100%)  | 0.73   | 7 (6%) 22 8   | 26, 63, 87, 97        | 0     |
| 14  | AN    | 96/100 (96%)    | -0.03  | 1 (1%) 82 58  | 12, 45, 84, 107       | 0     |
| 14  | BN    | 96/100 (96%)    | 0.26   | 4 (4%) 37 15  | 10, 56, 84, 98        | 0     |
| 15  | AO    | 88/88 (100%)    | -0.40  | 1 (1%) 80 55  | 0, 28, 55, 93         | 0     |
| 15  | BO    | 88/88 (100%)    | -0.07  | 1 (1%) 80 55  | 1, 33, 66, 89         | 0     |
| 16  | AP    | 82/82 (100%)    | 0.12   | 3 (3%) 42 18  | 5, 30, 73, 86         | 0     |
| 16  | BP    | 82/82 (100%)    | -0.12  | 4 (4%) 30 12  | 0, 24, 67, 91         | 0     |
| 17  | AQ    | 80/80 (100%)    | 0.03   | 1 (1%) 77 51  | 8, 42, 75, 96         | 0     |
| 17  | BQ    | 80/80 (100%)    | -0.11  | 1 (1%) 77 51  | 7, 44, 79, 94         | 0     |
| 18  | AR    | 55/55 (100%)    | -0.37  | 1 (1%) 69 40  | 0, 25, 59, 93         | 0     |
| 18  | BR    | 55/55 (100%)    | -0.11  | 2 (3%) 43 18  | 5, 38, 80, 101        | 0     |
| 19  | AS    | 79/79 (100%)    | 0.51   | 4 (5%) 29 12  | 21, 52, 83, 98        | 0     |
| 19  | BS    | 79/79 (100%)    | 0.78   | 9 (11%) 6 2   | 37, 65, 83, 95        | 0     |
| 20  | AT    | 85/85 (100%)    | 0.19   | 4 (4%) 32 13  | 7, 37, 67, 80         | 0     |
| 20  | BT    | 85/85 (100%)    | 0.20   | 2 (2%) 59 30  | 8, 38, 69, 96         | 0     |
| 21  | AU    | 51/51 (100%)    | 0.20   | 5 (9%) 8 3    | 7, 39, 74, 77         | 0     |
| 21  | BU    | 51/51 (100%)    | 0.27   | 3 (5%) 23 9   | 8, 47, 74, 80         | 0     |
| 22  | AV    | 76/76 (100%)    | -0.22  | 1 (1%) 77 51  | 0, 70, 127, 154       | 0     |
| 22  | BV    | 76/76 (100%)    | -0.33  | 0 100 100     | 22, 43, 72, 119       | 0     |
| 23  | AX    | 15/16 (93%)     | 0.40   | 1 (6%) 19 7   | 6, 76, 115, 133       | 0     |
| 23  | BX    | 16/16 (100%)    | 0.19   | 1 (6%) 21 7   | 16, 77, 102, 124      | 0     |
| 24  | AY    | 183/183 (100%)  | 0.71   | 38 (20%) 1 1  | 0, 50, 96, 117        | 0     |
| 25  | CA    | 2897/2903 (99%) | -0.52  | 33 (1%) 80 55 | 0, 0, 103, 162        | 0     |
| 25  | DA    | 2896/2903 (99%) | -0.60  | 25 (0%) 84 61 | 0, 15, 109, 162       | 0     |
| 26  | CB    | 119/119 (100%)  | -0.84  | 0 100 100     | 0, 7, 32, 85          | 0     |
| 27  | CC    | 271/271 (100%)  | -0.62  | 0 100 100     | 0, 1, 29, 56          | 0     |
| 27  | DC    | 271/271 (100%)  | -0.53  | 0 100 100     | 0, 19, 47, 77         | 0     |
| 28  | CD    | 209/209 (100%)  | -0.63  | 0 100 100     | 0, 0, 19, 61          | 0     |
| 28  | DD    | 209/209 (100%)  | -0.55  | 1 (0%) 90 74  | 0, 10, 52, 66         | 0     |
| 29  | CE    | 201/201 (100%)  | -0.53  | 0 100 100     | 0, 0, 39, 84          | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 29  | DE    | 201/201 (100%) | -0.38  | 0 100 100    | 0, 21, 60, 89         | 0     |
| 30  | CF    | 177/177 (100%) | 0.07   | 3 (1%) 70 42 | 0, 35, 82, 91         | 0     |
| 30  | DF    | 177/177 (100%) | 0.41   | 8 (4%) 34 13 | 12, 58, 84, 95        | 0     |
| 31  | CG    | 176/176 (100%) | -0.37  | 0 100 100    | 0, 15, 48, 88         | 0     |
| 31  | DG    | 176/176 (100%) | 0.20   | 2 (1%) 80 55 | 15, 48, 73, 93        | 0     |
| 32  | CH    | 149/149 (100%) | 0.10   | 7 (4%) 32 13 | 0, 52, 87, 100        | 0     |
| 32  | DH    | 149/149 (100%) | 0.60   | 7 (4%) 32 13 | 8, 58, 92, 107        | 0     |
| 33  | CI    | 141/141 (100%) | 2.32   | 73 (51%) 0 0 | 44, 79, 102, 124      | 0     |
| 33  | DI    | 141/141 (100%) | 2.44   | 71 (50%) 0 0 | 54, 82, 104, 118      | 0     |
| 34  | CJ    | 142/142 (100%) | -0.61  | 0 100 100    | 0, 0, 21, 56          | 0     |
| 34  | DJ    | 142/142 (100%) | -0.45  | 0 100 100    | 0, 8, 37, 65          | 0     |
| 35  | CK    | 122/122 (100%) | -0.64  | 0 100 100    | 0, 0, 27, 73          | 0     |
| 35  | DK    | 122/122 (100%) | -0.45  | 0 100 100    | 0, 15, 50, 71         | 0     |
| 36  | CL    | 143/143 (100%) | -0.54  | 0 100 100    | 0, 0, 27, 68          | 0     |
| 36  | DL    | 143/143 (100%) | -0.30  | 3 (2%) 64 34 | 0, 18, 56, 82         | 0     |
| 37  | CM    | 136/136 (100%) | -0.61  | 0 100 100    | 0, 0, 21, 83          | 0     |
| 37  | DM    | 136/136 (100%) | -0.17  | 1 (0%) 87 67 | 0, 21, 55, 88         | 0     |
| 38  | CN    | 120/120 (100%) | -0.57  | 0 100 100    | 0, 0, 14, 68          | 0     |
| 38  | DN    | 120/120 (100%) | -0.50  | 0 100 100    | 0, 12, 44, 78         | 0     |
| 39  | CO    | 116/116 (100%) | -0.55  | 0 100 100    | 0, 11, 39, 49         | 0     |
| 39  | DO    | 116/116 (100%) | 0.33   | 8 (6%) 18 6  | 5, 49, 78, 98         | 0     |
| 40  | CP    | 114/114 (100%) | -0.61  | 0 100 100    | 0, 0, 47, 70          | 0     |
| 40  | DP    | 114/114 (100%) | -0.46  | 0 100 100    | 0, 21, 51, 81         | 0     |
| 41  | CQ    | 117/117 (100%) | -0.60  | 0 100 100    | 0, 0, 7, 63           | 0     |
| 41  | DQ    | 117/117 (100%) | -0.70  | 0 100 100    | 0, 2, 27, 45          | 0     |
| 42  | CR    | 103/103 (100%) | -0.57  | 0 100 100    | 0, 0, 35, 57          | 0     |
| 42  | DR    | 103/103 (100%) | -0.61  | 1 (0%) 82 58 | 0, 10, 46, 78         | 0     |
| 43  | CS    | 110/110 (100%) | -0.46  | 1 (0%) 84 61 | 0, 0, 22, 98          | 0     |
| 43  | DS    | 110/110 (100%) | -0.63  | 0 100 100    | 0, 8, 40, 77          | 0     |
| 44  | CT    | 93/93 (100%)   | -0.27  | 2 (2%) 62 33 | 0, 6, 68, 78          | 0     |
| 44  | DT    | 93/93 (100%)   | 0.13   | 1 (1%) 80 55 | 0, 35, 71, 96         | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 45  | CU    | 102/102 (100%)    | -0.50  | 2 (1%) 65 36   | 0, 5, 42, 79          | 0     |
| 45  | DU    | 102/102 (100%)    | 0.35   | 10 (9%) 8 3    | 0, 34, 74, 100        | 0     |
| 46  | CV    | 94/94 (100%)      | -0.55  | 0 100 100      | 0, 6, 42, 62          | 0     |
| 46  | DV    | 94/94 (100%)      | -0.10  | 1 (1%) 80 55   | 11, 43, 68, 82        | 0     |
| 47  | CW    | 76/76 (100%)      | -0.54  | 0 100 100      | 0, 1, 31, 69          | 0     |
| 48  | CX    | 77/77 (100%)      | -0.47  | 0 100 100      | 0, 1, 47, 74          | 0     |
| 48  | DX    | 77/77 (100%)      | -0.42  | 0 100 100      | 0, 23, 55, 67         | 0     |
| 49  | CY    | 63/63 (100%)      | -0.32  | 2 (3%) 48 21   | 0, 14, 56, 97         | 0     |
| 49  | DY    | 63/63 (100%)      | -0.18  | 0 100 100      | 8, 43, 70, 111        | 0     |
| 50  | CZ    | 58/58 (100%)      | -0.53  | 0 100 100      | 0, 0, 13, 50          | 0     |
| 50  | DZ    | 58/58 (100%)      | -0.39  | 1 (1%) 70 42   | 0, 20, 52, 72         | 0     |
| 51  | C0    | 56/56 (100%)      | -0.60  | 0 100 100      | 0, 0, 25, 69          | 0     |
| 51  | D0    | 56/56 (100%)      | -0.54  | 0 100 100      | 0, 10, 53, 94         | 0     |
| 52  | C1    | 50/50 (100%)      | -0.03  | 1 (2%) 65 36   | 0, 8, 51, 93          | 0     |
| 52  | D1    | 50/50 (100%)      | 0.48   | 3 (6%) 23 9    | 21, 38, 70, 88        | 0     |
| 53  | C2    | 46/46 (100%)      | -0.50  | 1 (2%) 62 33   | 0, 0, 15, 101         | 0     |
| 53  | D2    | 46/46 (100%)      | -0.64  | 0 100 100      | 0, 10, 26, 94         | 0     |
| 54  | C3    | 64/64 (100%)      | -0.61  | 0 100 100      | 0, 0, 11, 38          | 0     |
| 54  | D3    | 64/64 (100%)      | -0.42  | 0 100 100      | 0, 15, 35, 52         | 0     |
| 55  | C4    | 38/38 (100%)      | -0.38  | 0 100 100      | 0, 1, 32, 72          | 0     |
| 55  | D4    | 38/38 (100%)      | -0.12  | 0 100 100      | 3, 26, 59, 65         | 0     |
| 56  | DB    | 118/118 (100%)    | -0.71  | 0 100 100      | 6, 58, 86, 106        | 0     |
| 57  | DW    | 75/75 (100%)      | -0.16  | 0 100 100      | 0, 27, 54, 94         | 0     |
| All | All   | 20908/20931 (99%) | -0.31  | 468 (2%) 62 33 | 0, 23, 86, 170        | 0     |

The worst 5 of 468 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 33  | CI    | 52  | LEU  | 10.7 |
| 33  | DI    | 2   | LYS  | 9.5  |
| 33  | DI    | 59  | THR  | 9.0  |
| 33  | DI    | 4   | VAL  | 8.8  |
| 33  | CI    | 48  | ILE  | 8.7  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 58  | MG   | DA    | 3131 | 1/1   | 0.90 | 0.58 | 38.79 | 55,55,55,55                | 0     |
| 58  | MG   | CA    | 3132 | 1/1   | 0.93 | 0.40 | 20.73 | 24,24,24,24                | 0     |
| 58  | MG   | DA    | 3139 | 1/1   | 0.96 | 0.28 | 13.40 | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3147 | 1/1   | 0.98 | 0.26 | 12.45 | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3159 | 1/1   | 0.98 | 0.26 | 10.17 | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3186 | 1/1   | 0.98 | 0.27 | 8.84  | 0,0,0,0                    | 0     |
| 58  | MG   | DA    | 3154 | 1/1   | 0.96 | 0.17 | 8.45  | 0,0,0,0                    | 0     |
| 58  | MG   | AA    | 1604 | 1/1   | 0.91 | 0.18 | 8.36  | 22,22,22,22                | 0     |
| 58  | MG   | DA    | 3157 | 1/1   | 0.97 | 0.22 | 6.86  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3121 | 1/1   | 0.95 | 0.19 | 4.89  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3175 | 1/1   | 0.95 | 0.17 | 4.39  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3153 | 1/1   | 0.95 | 0.29 | 4.38  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3066 | 1/1   | 0.98 | 0.22 | 4.27  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3155 | 1/1   | 0.96 | 0.37 | 4.23  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3188 | 1/1   | 0.96 | 0.15 | 4.06  | 2,2,2,2                    | 0     |
| 58  | MG   | CA    | 3165 | 1/1   | 0.96 | 0.19 | 3.98  | 0,0,0,0                    | 0     |
| 58  | MG   | CA    | 3163 | 1/1   | 0.97 | 0.20 | 3.49  | 0,0,0,0                    | 0     |
| 58  | MG   | DA    | 3152 | 1/1   | 0.92 | 0.17 | 3.47  | 6,6,6,6                    | 0     |
| 58  | MG   | DA    | 3142 | 1/1   | 0.98 | 0.16 | 2.94  | 0,0,0,0                    | 0     |
| 58  | MG   | AA    | 1622 | 1/1   | 0.96 | 0.17 | 2.47  | 0,0,0,0                    | 0     |
| 58  | MG   | DA    | 3108 | 1/1   | 0.99 | 0.17 | 2.09  | 0,0,0,0                    | 0     |
| 58  | MG   | DA    | 3116 | 1/1   | 0.85 | 0.14 | 2.09  | 13,13,13,13                | 0     |
| 58  | MG   | CA    | 3161 | 1/1   | 0.98 | 0.19 | 1.97  | 0,0,0,0                    | 0     |
| 58  | MG   | BA    | 1640 | 1/1   | 0.98 | 0.14 | 1.48  | 0,0,0,0                    | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58  | MG   | CA    | 3110 | 1/1   | 0.97 | 0.17 | 1.14  | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3064 | 1/1   | 0.98 | 0.18 | 0.72  | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3025 | 1/1   | 0.93 | 0.17 | 0.64  | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3152 | 1/1   | 0.98 | 0.18 | 0.55  | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1656 | 1/1   | 0.96 | 0.13 | 0.52  | 14,14,14,14                 | 0     |
| 58  | MG   | DA    | 3063 | 1/1   | 0.92 | 0.15 | 0.51  | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3012 | 1/1   | 0.98 | 0.18 | 0.50  | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3084 | 1/1   | 0.78 | 0.11 | 0.38  | 22,22,22,22                 | 0     |
| 58  | MG   | CA    | 3106 | 1/1   | 0.84 | 0.18 | 0.37  | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1646 | 1/1   | 0.95 | 0.14 | 0.15  | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3050 | 1/1   | 1.00 | 0.16 | 0.13  | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3040 | 1/1   | 0.96 | 0.14 | 0.10  | 5,5,5,5                     | 0     |
| 58  | MG   | CA    | 3130 | 1/1   | 0.98 | 0.18 | 0.06  | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3145 | 1/1   | 0.95 | 0.11 | -0.02 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3151 | 1/1   | 0.99 | 0.15 | -0.05 | 11,11,11,11                 | 0     |
| 58  | MG   | DA    | 3057 | 1/1   | 0.89 | 0.14 | -0.07 | 14,14,14,14                 | 0     |
| 58  | MG   | DA    | 3013 | 1/1   | 0.96 | 0.14 | -0.12 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3109 | 1/1   | 0.94 | 0.13 | -0.21 | 2,2,2,2                     | 0     |
| 58  | MG   | CA    | 3131 | 1/1   | 0.98 | 0.15 | -0.23 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3017 | 1/1   | 0.98 | 0.16 | -0.48 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3105 | 1/1   | 0.84 | 0.16 | -0.59 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3145 | 1/1   | 0.97 | 0.13 | -0.73 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3017 | 1/1   | 0.98 | 0.13 | -0.78 | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1636 | 1/1   | 0.92 | 0.08 | -0.79 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3136 | 1/1   | 0.85 | 0.11 | -0.81 | 28,28,28,28                 | 0     |
| 58  | MG   | CA    | 3041 | 1/1   | 0.95 | 0.16 | -0.88 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3109 | 1/1   | 0.95 | 0.15 | -0.94 | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1607 | 1/1   | 0.94 | 0.08 | -0.94 | 10,10,10,10                 | 0     |
| 58  | MG   | DA    | 3101 | 1/1   | 0.87 | 0.12 | -1.01 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1631 | 1/1   | 0.78 | 0.13 | -1.03 | 35,35,35,35                 | 0     |
| 58  | MG   | DA    | 3120 | 1/1   | 0.94 | 0.11 | -1.08 | 8,8,8,8                     | 0     |
| 58  | MG   | DA    | 3005 | 1/1   | 0.87 | 0.10 | -1.16 | 25,25,25,25                 | 0     |
| 58  | MG   | CA    | 3013 | 1/1   | 0.97 | 0.15 | -1.18 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1616 | 1/1   | 0.95 | 0.11 | -1.19 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1614 | 1/1   | 0.90 | 0.07 | -1.27 | 19,19,19,19                 | 0     |
| 58  | MG   | AA    | 1616 | 1/1   | 0.94 | 0.09 | -1.28 | 11,11,11,11                 | 0     |
| 58  | MG   | AA    | 1632 | 1/1   | 0.92 | 0.07 | -1.29 | 15,15,15,15                 | 0     |
| 58  | MG   | DA    | 3153 | 1/1   | 0.99 | 0.10 | -1.32 | 11,11,11,11                 | 0     |
| 58  | MG   | DA    | 3077 | 1/1   | 0.94 | 0.05 | -1.35 | 12,12,12,12                 | 0     |
| 58  | MG   | CA    | 3074 | 1/1   | 0.97 | 0.15 | -1.40 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3054 | 1/1   | 0.98 | 0.14 | -1.44 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3008 | 1/1   | 0.98 | 0.10 | -1.55 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58  | MG   | CA    | 3117 | 1/1   | 0.89 | 0.14 | -1.60 | 5,5,5,5                     | 0     |
| 58  | MG   | DA    | 3038 | 1/1   | 0.93 | 0.12 | -1.68 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3097 | 1/1   | 0.97 | 0.08 | -1.68 | 13,13,13,13                 | 0     |
| 58  | MG   | DA    | 3036 | 1/1   | 0.90 | 0.08 | -1.73 | 21,21,21,21                 | 0     |
| 58  | MG   | CA    | 3113 | 1/1   | 0.97 | 0.12 | -1.86 | 0,0,0,0                     | 0     |
| 59  | ZN   | C4    | 101  | 1/1   | 0.99 | 0.07 | -1.90 | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1617 | 1/1   | 0.88 | 0.05 | -1.94 | 21,21,21,21                 | 0     |
| 58  | MG   | DA    | 3078 | 1/1   | 0.82 | 0.09 | -1.96 | 15,15,15,15                 | 0     |
| 59  | ZN   | D4    | 101  | 1/1   | 0.99 | 0.06 | -1.96 | 41,41,41,41                 | 0     |
| 58  | MG   | BA    | 1603 | 1/1   | 0.93 | 0.09 | -1.96 | 13,13,13,13                 | 0     |
| 58  | MG   | CA    | 3033 | 1/1   | 0.98 | 0.14 | -2.22 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1601 | 1/1   | 0.98 | 0.08 | -2.30 | 2,2,2,2                     | 0     |
| 58  | MG   | CA    | 3137 | 1/1   | 0.96 | 0.09 | -2.30 | 4,4,4,4                     | 0     |
| 58  | MG   | CA    | 3023 | 1/1   | 0.97 | 0.13 | -2.34 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3098 | 1/1   | 0.95 | 0.14 | -2.37 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3073 | 1/1   | 0.97 | 0.11 | -2.49 | 6,6,6,6                     | 0     |
| 58  | MG   | DA    | 3012 | 1/1   | 0.96 | 0.11 | -2.53 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3018 | 1/1   | 0.96 | 0.07 | -2.53 | 6,6,6,6                     | 0     |
| 58  | MG   | DA    | 3105 | 1/1   | 0.96 | 0.11 | -2.54 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3107 | 1/1   | 0.98 | 0.09 | -2.56 | 9,9,9,9                     | 0     |
| 58  | MG   | CA    | 3102 | 1/1   | 0.92 | 0.15 | -2.59 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3133 | 1/1   | 0.99 | 0.05 | -2.60 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3071 | 1/1   | 0.92 | 0.08 | -2.60 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3112 | 1/1   | 0.94 | 0.09 | -2.67 | 5,5,5,5                     | 0     |
| 58  | MG   | DA    | 3070 | 1/1   | 0.92 | 0.08 | -2.69 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3069 | 1/1   | 0.98 | 0.14 | -2.69 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3027 | 1/1   | 0.95 | 0.10 | -2.75 | 14,14,14,14                 | 0     |
| 58  | MG   | DA    | 3132 | 1/1   | 0.96 | 0.05 | -2.77 | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3097 | 1/1   | 0.98 | 0.12 | -2.89 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1630 | 1/1   | 0.81 | 0.07 | -2.92 | 41,41,41,41                 | 0     |
| 58  | MG   | DA    | 3028 | 1/1   | 0.95 | 0.11 | -2.93 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3051 | 1/1   | 0.95 | 0.09 | -3.07 | 3,3,3,3                     | 0     |
| 58  | MG   | CA    | 3024 | 1/1   | 0.93 | 0.11 | -3.10 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3134 | 1/1   | 0.99 | 0.07 | -3.20 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3059 | 1/1   | 0.95 | 0.07 | -3.30 | 4,4,4,4                     | 0     |
| 58  | MG   | CA    | 3022 | 1/1   | 0.99 | 0.14 | -3.34 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3029 | 1/1   | 0.98 | 0.13 | -3.43 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3108 | 1/1   | 0.97 | 0.10 | -3.50 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3021 | 1/1   | 0.95 | 0.08 | -3.55 | 3,3,3,3                     | 0     |
| 58  | MG   | DA    | 3114 | 1/1   | 0.94 | 0.08 | -3.62 | 14,14,14,14                 | 0     |
| 58  | MG   | AA    | 1629 | 1/1   | 0.99 | 0.07 | -3.65 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3063 | 1/1   | 0.95 | 0.12 | -3.80 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 58  | MG   | DA    | 3129 | 1/1   | 0.99 | 0.08 | -3.85 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3024 | 1/1   | 0.98 | 0.07 | -3.88 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1619 | 1/1   | 0.98 | 0.08 | -3.98 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3053 | 1/1   | 0.99 | 0.06 | -4.02 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3028 | 1/1   | 0.92 | 0.14 | -4.11 | 21,21,21,21                 | 0     |
| 58  | MG   | AA    | 1618 | 1/1   | 0.96 | 0.07 | -4.12 | 21,21,21,21                 | 0     |
| 58  | MG   | AA    | 1630 | 1/1   | 0.92 | 0.09 | -4.14 | 16,16,16,16                 | 0     |
| 58  | MG   | DA    | 3079 | 1/1   | 0.92 | 0.08 | -4.24 | 27,27,27,27                 | 0     |
| 58  | MG   | DA    | 3023 | 1/1   | 0.97 | 0.06 | -4.35 | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1642 | 1/1   | 0.98 | 0.06 | -4.36 | 1,1,1,1                     | 0     |
| 58  | MG   | DA    | 3068 | 1/1   | 0.97 | 0.06 | -4.36 | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3008 | 1/1   | 0.97 | 0.09 | -4.40 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3104 | 1/1   | 0.97 | 0.09 | -4.47 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3056 | 1/1   | 0.94 | 0.08 | -4.49 | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3125 | 1/1   | 0.96 | 0.09 | -4.55 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3124 | 1/1   | 0.94 | 0.05 | -4.59 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3170 | 1/1   | 0.97 | 0.07 | -4.63 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3046 | 1/1   | 0.96 | 0.07 | -4.67 | 1,1,1,1                     | 0     |
| 58  | MG   | BA    | 1635 | 1/1   | 0.92 | 0.08 | -4.78 | 21,21,21,21                 | 0     |
| 58  | MG   | DA    | 3096 | 1/1   | 0.95 | 0.06 | -4.99 | 13,13,13,13                 | 0     |
| 58  | MG   | AA    | 1613 | 1/1   | 0.92 | 0.06 | -5.01 | 2,2,2,2                     | 0     |
| 58  | MG   | AA    | 1641 | 1/1   | 0.93 | 0.09 | -5.04 | 0,0,0,0                     | 0     |
| 58  | MG   | CB    | 201  | 1/1   | 0.94 | 0.05 | -5.10 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1617 | 1/1   | 0.94 | 0.06 | -5.28 | 13,13,13,13                 | 0     |
| 58  | MG   | DA    | 3110 | 1/1   | 0.94 | 0.05 | -5.33 | 18,18,18,18                 | 0     |
| 58  | MG   | BA    | 1607 | 1/1   | 0.97 | 0.06 | -5.37 | 1,1,1,1                     | 0     |
| 58  | MG   | CA    | 3135 | 1/1   | 0.94 | 0.12 | -5.43 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3080 | 1/1   | 0.93 | 0.06 | -5.51 | 1,1,1,1                     | 0     |
| 58  | MG   | CA    | 3043 | 1/1   | 0.98 | 0.07 | -5.55 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3071 | 1/1   | 0.96 | 0.07 | -5.65 | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3058 | 1/1   | 0.98 | 0.07 | -5.69 | 6,6,6,6                     | 0     |
| 58  | MG   | BA    | 1632 | 1/1   | 0.94 | 0.04 | -5.86 | 18,18,18,18                 | 0     |
| 58  | MG   | BA    | 1634 | 1/1   | 0.93 | 0.05 | -6.08 | 10,10,10,10                 | 0     |
| 58  | MG   | DA    | 3050 | 1/1   | 0.89 | 0.06 | -6.31 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3072 | 1/1   | 0.98 | 0.07 | -6.53 | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1625 | 1/1   | 0.94 | 0.07 | -6.90 | 6,6,6,6                     | 0     |
| 58  | MG   | DA    | 3065 | 1/1   | 0.93 | 0.08 | -7.02 | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1612 | 1/1   | 0.94 | 0.05 | -7.13 | 18,18,18,18                 | 0     |
| 58  | MG   | BA    | 1626 | 1/1   | 0.94 | 0.06 | -7.13 | 14,14,14,14                 | 0     |
| 58  | MG   | DA    | 3002 | 1/1   | 0.97 | 0.05 | -7.26 | 1,1,1,1                     | 0     |
| 58  | MG   | BA    | 1610 | 1/1   | 0.97 | 0.03 | -7.56 | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1609 | 1/1   | 0.98 | 0.05 | -7.63 | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF   | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 58  | MG   | DA    | 3049 | 1/1   | 0.98 | 0.05 | -8.10  | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1621 | 1/1   | 0.98 | 0.05 | -8.76  | 12,12,12,12                 | 0     |
| 58  | MG   | CA    | 3111 | 1/1   | 0.96 | 0.04 | -9.79  | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3035 | 1/1   | 0.94 | 0.07 | -10.50 | 1,1,1,1                     | 0     |
| 58  | MG   | CA    | 3009 | 1/1   | 0.95 | 0.11 | -10.56 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3002 | 1/1   | 0.93 | 0.07 | -10.61 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3119 | 1/1   | 0.99 | 0.02 | -13.00 | 8,8,8,8                     | 0     |
| 58  | MG   | DA    | 3022 | 1/1   | 0.98 | 0.07 | -14.11 | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3037 | 1/1   | 0.97 | 0.06 | -15.97 | 11,11,11,11                 | 0     |
| 58  | MG   | CA    | 3127 | 1/1   | 0.95 | 0.12 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3103 | 1/1   | 0.97 | 0.09 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3168 | 1/1   | 0.95 | 0.20 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CB    | 202  | 1/1   | 0.96 | 0.10 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3173 | 1/1   | 0.95 | 0.25 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3091 | 1/1   | 0.92 | 0.08 | -      | 3,3,3,3                     | 0     |
| 58  | MG   | BA    | 1637 | 1/1   | 0.95 | 0.16 | -      | 19,19,19,19                 | 0     |
| 58  | MG   | DA    | 3166 | 1/1   | 0.96 | 0.20 | -      | 9,9,9,9                     | 0     |
| 58  | MG   | AA    | 1605 | 1/1   | 0.99 | 0.07 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3055 | 1/1   | 0.98 | 0.10 | -      | 6,6,6,6                     | 0     |
| 58  | MG   | DA    | 3130 | 1/1   | 0.99 | 0.11 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3093 | 1/1   | 0.96 | 0.12 | -      | 11,11,11,11                 | 0     |
| 58  | MG   | AA    | 1650 | 1/1   | 0.97 | 0.11 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3156 | 1/1   | 0.98 | 0.29 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3035 | 1/1   | 0.98 | 0.10 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3136 | 1/1   | 0.96 | 0.09 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3085 | 1/1   | 0.95 | 0.21 | -      | 12,12,12,12                 | 0     |
| 58  | MG   | DA    | 3081 | 1/1   | 0.97 | 0.06 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3038 | 1/1   | 0.99 | 0.20 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3058 | 1/1   | 0.95 | 0.10 | -      | 10,10,10,10                 | 0     |
| 58  | MG   | DA    | 3121 | 1/1   | 0.96 | 0.07 | -      | 7,7,7,7                     | 0     |
| 58  | MG   | AA    | 1637 | 1/1   | 0.91 | 0.09 | -      | 1,1,1,1                     | 0     |
| 58  | MG   | BA    | 1609 | 1/1   | 0.90 | 0.09 | -      | 26,26,26,26                 | 0     |
| 58  | MG   | CA    | 3011 | 1/1   | 0.97 | 0.20 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3062 | 1/1   | 0.93 | 0.09 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3149 | 1/1   | 0.98 | 0.32 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1639 | 1/1   | 0.95 | 0.06 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3085 | 1/1   | 0.94 | 0.20 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3118 | 1/1   | 0.98 | 0.07 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3048 | 1/1   | 0.91 | 0.09 | -      | 13,13,13,13                 | 0     |
| 58  | MG   | CA    | 3193 | 1/1   | 0.96 | 0.25 | -      | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3025 | 1/1   | 0.88 | 0.20 | -      | 16,16,16,16                 | 0     |
| 58  | MG   | BA    | 1618 | 1/1   | 0.87 | 0.19 | -      | 4,4,4,4                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | BA    | 1656 | 1/1   | 0.96 | 0.19 | -    | 9,9,9,9                     | 0     |
| 58  | MG   | DA    | 3044 | 1/1   | 0.94 | 0.05 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | AA    | 1639 | 1/1   | 0.86 | 0.10 | -    | 22,22,22,22                 | 0     |
| 58  | MG   | BA    | 1602 | 1/1   | 0.82 | 0.08 | -    | 21,21,21,21                 | 0     |
| 58  | MG   | DA    | 3161 | 1/1   | 0.93 | 0.09 | -    | 15,15,15,15                 | 0     |
| 58  | MG   | DA    | 3014 | 1/1   | 0.93 | 0.11 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | CA    | 3166 | 1/1   | 0.96 | 0.14 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1627 | 1/1   | 0.89 | 0.12 | -    | 35,35,35,35                 | 0     |
| 58  | MG   | CA    | 3010 | 1/1   | 0.98 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1640 | 1/1   | 0.74 | 0.19 | -    | 34,34,34,34                 | 0     |
| 58  | MG   | DA    | 3033 | 1/1   | 0.94 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3056 | 1/1   | 0.97 | 0.05 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | CA    | 3099 | 1/1   | 0.88 | 0.85 | -    | 53,53,53,53                 | 0     |
| 58  | MG   | CA    | 3021 | 1/1   | 0.96 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1620 | 1/1   | 0.83 | 0.07 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | DA    | 3140 | 1/1   | 0.97 | 0.28 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1664 | 1/1   | 0.98 | 0.11 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | CA    | 3178 | 1/1   | 0.94 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1654 | 1/1   | 0.93 | 0.16 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | AA    | 1612 | 1/1   | 0.96 | 0.05 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3020 | 1/1   | 0.98 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3046 | 1/1   | 0.95 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3080 | 1/1   | 0.85 | 0.09 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | CA    | 3177 | 1/1   | 0.96 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1665 | 1/1   | 0.95 | 0.08 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3128 | 1/1   | 0.98 | 0.14 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3143 | 1/1   | 0.99 | 0.28 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1648 | 1/1   | 0.96 | 0.17 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3143 | 1/1   | 0.98 | 0.21 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3119 | 1/1   | 0.94 | 0.15 | -    | 44,44,44,44                 | 0     |
| 58  | MG   | DA    | 3162 | 1/1   | 0.94 | 0.20 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | DA    | 3037 | 1/1   | 0.95 | 0.18 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3098 | 1/1   | 0.65 | 0.54 | -    | 49,49,49,49                 | 0     |
| 58  | MG   | BA    | 1628 | 1/1   | 0.99 | 0.08 | -    | 25,25,25,25                 | 0     |
| 58  | MG   | AA    | 1651 | 1/1   | 0.97 | 0.24 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1649 | 1/1   | 0.96 | 0.23 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1622 | 1/1   | 0.94 | 0.05 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | DA    | 3059 | 1/1   | 0.94 | 0.11 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | AA    | 1671 | 1/1   | 0.94 | 0.17 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | AA    | 1610 | 1/1   | 0.97 | 0.07 | -    | 32,32,32,32                 | 0     |
| 58  | MG   | DA    | 3011 | 1/1   | 0.98 | 0.08 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1655 | 1/1   | 0.92 | 0.15 | -    | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | AA    | 1626 | 1/1   | 0.85 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3073 | 1/1   | 0.98 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3003 | 1/1   | 0.94 | 0.07 | -    | 8,8,8,8                     | 0     |
| 58  | MG   | DA    | 3084 | 1/1   | 0.87 | 0.12 | -    | 32,32,32,32                 | 0     |
| 58  | MG   | AA    | 1669 | 1/1   | 0.90 | 0.14 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3164 | 1/1   | 0.92 | 0.24 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3087 | 1/1   | 0.90 | 0.05 | -    | 20,20,20,20                 | 0     |
| 58  | MG   | CA    | 3092 | 1/1   | 0.90 | 0.09 | -    | 16,16,16,16                 | 0     |
| 58  | MG   | DA    | 3115 | 1/1   | 0.60 | 0.18 | -    | 27,27,27,27                 | 0     |
| 58  | MG   | DA    | 3102 | 1/1   | 0.90 | 0.09 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | CA    | 3057 | 1/1   | 0.98 | 0.04 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3189 | 1/1   | 0.98 | 0.14 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3154 | 1/1   | 0.94 | 0.29 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3122 | 1/1   | 1.00 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3031 | 1/1   | 0.97 | 0.22 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3118 | 1/1   | 0.95 | 0.10 | -    | 7,7,7,7                     | 0     |
| 58  | MG   | CA    | 3150 | 1/1   | 0.96 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3095 | 1/1   | 0.92 | 0.11 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | DA    | 3010 | 1/1   | 0.94 | 0.09 | -    | 7,7,7,7                     | 0     |
| 58  | MG   | DA    | 3026 | 1/1   | 0.94 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3006 | 1/1   | 0.94 | 0.07 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | DL    | 201  | 1/1   | 0.93 | 0.05 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3174 | 1/1   | 0.98 | 0.31 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3115 | 1/1   | 0.97 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3006 | 1/1   | 0.91 | 0.05 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | BA    | 1652 | 1/1   | 0.95 | 0.10 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | DB    | 201  | 1/1   | 0.95 | 0.05 | -    | 24,24,24,24                 | 0     |
| 58  | MG   | CA    | 3034 | 1/1   | 0.95 | 0.20 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1624 | 1/1   | 0.96 | 0.06 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3001 | 1/1   | 0.95 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3094 | 1/1   | 0.96 | 0.08 | -    | 43,43,43,43                 | 0     |
| 58  | MG   | DA    | 3034 | 1/1   | 0.94 | 0.06 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | AA    | 1638 | 1/1   | 0.98 | 0.06 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | DA    | 3041 | 1/1   | 0.98 | 0.04 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | AA    | 1661 | 1/1   | 0.97 | 0.15 | -    | 15,15,15,15                 | 0     |
| 58  | MG   | BA    | 1620 | 1/1   | 0.96 | 0.07 | -    | 19,19,19,19                 | 0     |
| 58  | MG   | AA    | 1615 | 1/1   | 0.97 | 0.08 | -    | 9,9,9,9                     | 0     |
| 58  | MG   | DA    | 3004 | 1/1   | 0.93 | 0.10 | -    | 30,30,30,30                 | 0     |
| 58  | MG   | AA    | 1643 | 1/1   | 0.96 | 0.27 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1613 | 1/1   | 0.95 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3160 | 1/1   | 0.94 | 0.32 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3117 | 1/1   | 0.95 | 0.05 | -    | 5,5,5,5                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | BA    | 1615 | 1/1   | 0.94 | 0.18 | -    | 9,9,9,9                     | 0     |
| 58  | MG   | DA    | 3127 | 1/1   | 0.98 | 0.05 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3049 | 1/1   | 0.97 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3147 | 1/1   | 0.97 | 0.18 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3162 | 1/1   | 0.98 | 0.28 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3111 | 1/1   | 0.95 | 0.08 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | CA    | 3191 | 1/1   | 0.94 | 0.20 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1648 | 1/1   | 0.96 | 0.12 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | DA    | 3076 | 1/1   | 0.95 | 0.09 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | DA    | 3007 | 1/1   | 0.99 | 0.19 | -    | 26,26,26,26                 | 0     |
| 58  | MG   | CA    | 3040 | 1/1   | 0.94 | 0.16 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3015 | 1/1   | 0.79 | 0.25 | -    | 36,36,36,36                 | 0     |
| 58  | MG   | BA    | 1624 | 1/1   | 0.89 | 0.07 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | AA    | 1621 | 1/1   | 0.97 | 0.03 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3060 | 1/1   | 0.97 | 0.04 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | CA    | 3134 | 1/1   | 0.89 | 0.32 | -    | 14,14,14,14                 | 0     |
| 58  | MG   | DA    | 3159 | 1/1   | 0.98 | 0.26 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | CA    | 3018 | 1/1   | 0.99 | 0.18 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1659 | 1/1   | 0.92 | 0.08 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | AA    | 1603 | 1/1   | 0.85 | 0.08 | -    | 28,28,28,28                 | 0     |
| 58  | MG   | CA    | 3053 | 1/1   | 0.97 | 0.08 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3100 | 1/1   | 0.93 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3141 | 1/1   | 0.98 | 0.27 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1601 | 1/1   | 0.82 | 0.10 | -    | 44,44,44,44                 | 0     |
| 58  | MG   | DA    | 3165 | 1/1   | 0.87 | 0.23 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3030 | 1/1   | 0.92 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3078 | 1/1   | 0.98 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1657 | 1/1   | 0.96 | 0.18 | -    | 2,2,2,2                     | 0     |
| 58  | MG   | CA    | 3081 | 1/1   | 0.95 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3171 | 1/1   | 0.95 | 0.14 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3185 | 1/1   | 0.93 | 0.28 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1608 | 1/1   | 0.92 | 0.15 | -    | 18,18,18,18                 | 0     |
| 58  | MG   | DA    | 3061 | 1/1   | 0.81 | 0.19 | -    | 24,24,24,24                 | 0     |
| 58  | MG   | CA    | 3179 | 1/1   | 0.96 | 0.15 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1614 | 1/1   | 0.96 | 0.05 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | AA    | 1634 | 1/1   | 0.90 | 0.05 | -    | 2,2,2,2                     | 0     |
| 58  | MG   | CA    | 3086 | 1/1   | 0.96 | 0.16 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3142 | 1/1   | 0.99 | 0.41 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3065 | 1/1   | 0.97 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3007 | 1/1   | 0.96 | 0.04 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3060 | 1/1   | 0.95 | 0.13 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | DA    | 3067 | 1/1   | 0.97 | 0.07 | -    | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | CA    | 3088 | 1/1   | 0.98 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3031 | 1/1   | 0.97 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3158 | 1/1   | 0.99 | 0.14 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3083 | 1/1   | 0.98 | 0.04 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3032 | 1/1   | 0.95 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1642 | 1/1   | 0.96 | 0.23 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3079 | 1/1   | 0.97 | 0.05 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | CA    | 3181 | 1/1   | 0.96 | 0.15 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3069 | 1/1   | 0.97 | 0.09 | -    | 41,41,41,41                 | 0     |
| 58  | MG   | CA    | 3144 | 1/1   | 0.98 | 0.33 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3055 | 1/1   | 0.71 | 0.13 | -    | 28,28,28,28                 | 0     |
| 58  | MG   | CA    | 3075 | 1/1   | 0.96 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3082 | 1/1   | 0.95 | 0.05 | -    | 7,7,7,7                     | 0     |
| 58  | MG   | CA    | 3169 | 1/1   | 0.95 | 0.22 | -    | 7,7,7,7                     | 0     |
| 58  | MG   | AA    | 1619 | 1/1   | 0.94 | 0.16 | -    | 32,32,32,32                 | 0     |
| 58  | MG   | BA    | 1623 | 1/1   | 0.97 | 0.08 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | DA    | 3045 | 1/1   | 0.95 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1658 | 1/1   | 0.87 | 0.19 | -    | 16,16,16,16                 | 0     |
| 58  | MG   | CA    | 3045 | 1/1   | 0.95 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3113 | 1/1   | 0.95 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3094 | 1/1   | 0.96 | 0.05 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | CA    | 3112 | 1/1   | 0.93 | 0.10 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | DA    | 3048 | 1/1   | 0.98 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3047 | 1/1   | 0.99 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1660 | 1/1   | 0.91 | 0.12 | -    | 15,15,15,15                 | 0     |
| 58  | MG   | AA    | 1635 | 1/1   | 0.91 | 0.09 | -    | 18,18,18,18                 | 0     |
| 58  | MG   | DA    | 3123 | 1/1   | 0.98 | 0.05 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3076 | 1/1   | 0.93 | 0.15 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1667 | 1/1   | 0.92 | 0.26 | -    | 13,13,13,13                 | 0     |
| 58  | MG   | CA    | 3014 | 1/1   | 0.88 | 0.14 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | DB    | 203  | 1/1   | 0.88 | 0.06 | -    | 16,16,16,16                 | 0     |
| 58  | MG   | AA    | 1645 | 1/1   | 0.88 | 0.24 | -    | 8,8,8,8                     | 0     |
| 58  | MG   | AA    | 1662 | 1/1   | 0.87 | 0.10 | -    | 8,8,8,8                     | 0     |
| 58  | MG   | CA    | 3052 | 1/1   | 0.97 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CB    | 204  | 1/1   | 0.98 | 0.39 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3158 | 1/1   | 0.97 | 0.34 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3149 | 1/1   | 0.95 | 0.18 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3009 | 1/1   | 0.94 | 0.09 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | CB    | 203  | 1/1   | 0.98 | 0.04 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | DA    | 3083 | 1/1   | 0.65 | 0.22 | -    | 31,31,31,31                 | 0     |
| 58  | MG   | BA    | 1641 | 1/1   | 0.88 | 0.09 | -    | 20,20,20,20                 | 0     |
| 58  | MG   | DA    | 3099 | 1/1   | 0.95 | 0.07 | -    | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | DA    | 3100 | 1/1   | 0.96 | 0.06 | -    | 4,4,4,4                     | 0     |
| 58  | MG   | DA    | 3043 | 1/1   | 0.97 | 0.05 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | DA    | 3039 | 1/1   | 0.98 | 0.09 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | DA    | 3148 | 1/1   | 0.99 | 0.27 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3128 | 1/1   | 0.97 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3044 | 1/1   | 0.95 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3137 | 1/1   | 0.97 | 0.46 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3163 | 1/1   | 0.98 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3090 | 1/1   | 0.86 | 0.08 | -    | 15,15,15,15                 | 0     |
| 58  | MG   | DA    | 3015 | 1/1   | 0.88 | 0.18 | -    | 23,23,23,23                 | 0     |
| 58  | MG   | CA    | 3116 | 1/1   | 0.93 | 0.22 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | CA    | 3039 | 1/1   | 0.98 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3104 | 1/1   | 0.97 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3093 | 1/1   | 0.96 | 0.08 | -    | 2,2,2,2                     | 0     |
| 58  | MG   | DA    | 3106 | 1/1   | 0.98 | 0.17 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3082 | 1/1   | 0.86 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3088 | 1/1   | 0.74 | 0.10 | -    | 12,12,12,12                 | 0     |
| 58  | MG   | DA    | 3160 | 1/1   | 0.91 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3124 | 1/1   | 0.96 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1654 | 1/1   | 0.96 | 0.09 | -    | 22,22,22,22                 | 0     |
| 58  | MG   | CA    | 3187 | 1/1   | 0.93 | 0.16 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1623 | 1/1   | 0.87 | 0.07 | -    | 24,24,24,24                 | 0     |
| 58  | MG   | CA    | 3062 | 1/1   | 0.80 | 0.46 | -    | 46,46,46,46                 | 0     |
| 58  | MG   | CA    | 3114 | 1/1   | 0.91 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3089 | 1/1   | 0.98 | 0.08 | -    | 24,24,24,24                 | 0     |
| 58  | MG   | CA    | 3020 | 1/1   | 0.98 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3126 | 1/1   | 0.94 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3070 | 1/1   | 0.96 | 0.12 | -    | 25,25,25,25                 | 0     |
| 58  | MG   | DA    | 3042 | 1/1   | 0.97 | 0.06 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | DA    | 3074 | 1/1   | 0.99 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1611 | 1/1   | 0.92 | 0.11 | -    | 13,13,13,13                 | 0     |
| 58  | MG   | CA    | 3068 | 1/1   | 0.99 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1605 | 1/1   | 0.92 | 0.06 | -    | 21,21,21,21                 | 0     |
| 58  | MG   | CA    | 3026 | 1/1   | 0.91 | 0.33 | -    | 30,30,30,30                 | 0     |
| 58  | MG   | DA    | 3064 | 1/1   | 0.88 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3052 | 1/1   | 0.98 | 0.05 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3092 | 1/1   | 0.92 | 0.25 | -    | 34,34,34,34                 | 0     |
| 58  | MG   | CA    | 3042 | 1/1   | 0.97 | 0.10 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3016 | 1/1   | 0.93 | 0.08 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | DA    | 3103 | 1/1   | 0.90 | 0.08 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1608 | 1/1   | 0.95 | 0.20 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3164 | 1/1   | 0.97 | 0.15 | -    | 0,0,0,0                     | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | BA    | 1644 | 1/1   | 0.97 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1604 | 1/1   | 0.97 | 0.07 | -    | 13,13,13,13                 | 0     |
| 58  | MG   | BA    | 1651 | 1/1   | 0.97 | 0.14 | -    | 7,7,7,7                     | 0     |
| 58  | MG   | BA    | 1633 | 1/1   | 0.94 | 0.12 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | AA    | 1663 | 1/1   | 0.95 | 0.10 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3077 | 1/1   | 0.98 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3190 | 1/1   | 0.99 | 0.23 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3146 | 1/1   | 0.97 | 0.18 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3067 | 1/1   | 0.96 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3032 | 1/1   | 0.98 | 0.08 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3148 | 1/1   | 0.98 | 0.47 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3183 | 1/1   | 0.97 | 0.18 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1606 | 1/1   | 0.91 | 0.06 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3182 | 1/1   | 0.99 | 0.30 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3061 | 1/1   | 0.95 | 0.12 | -    | 9,9,9,9                     | 0     |
| 58  | MG   | DA    | 3001 | 1/1   | 0.96 | 0.05 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3135 | 1/1   | 0.94 | 0.08 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | DA    | 3072 | 1/1   | 0.97 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3139 | 1/1   | 0.99 | 0.42 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1643 | 1/1   | 0.96 | 0.14 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | DA    | 3150 | 1/1   | 0.96 | 0.15 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3151 | 1/1   | 0.99 | 0.32 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1646 | 1/1   | 0.96 | 0.17 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3027 | 1/1   | 0.95 | 0.14 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3172 | 1/1   | 0.96 | 0.17 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1672 | 1/1   | 0.96 | 0.21 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | CA    | 3176 | 1/1   | 0.97 | 0.14 | -    | 10,10,10,10                 | 0     |
| 58  | MG   | AA    | 1647 | 1/1   | 0.96 | 0.23 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | AA    | 1628 | 1/1   | 0.98 | 0.04 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | DA    | 3091 | 1/1   | 0.71 | 0.26 | -    | 50,50,50,50                 | 0     |
| 58  | MG   | BA    | 1647 | 1/1   | 0.98 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3125 | 1/1   | 0.98 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1631 | 1/1   | 0.82 | 0.17 | -    | 35,35,35,35                 | 0     |
| 58  | MG   | CA    | 3129 | 1/1   | 0.93 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1644 | 1/1   | 0.84 | 0.19 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | CA    | 3140 | 1/1   | 0.96 | 0.52 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DB    | 202  | 1/1   | 0.96 | 0.04 | -    | 9,9,9,9                     | 0     |
| 58  | MG   | CQ    | 201  | 1/1   | 0.97 | 0.31 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DQ    | 801  | 1/1   | 0.97 | 0.26 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3003 | 1/1   | 0.96 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3138 | 1/1   | 0.92 | 0.43 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3095 | 1/1   | 0.98 | 0.16 | -    | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | AA    | 1633 | 1/1   | 0.96 | 0.04 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | DA    | 3047 | 1/1   | 0.91 | 0.05 | -    | 28,28,28,28                 | 0     |
| 58  | MG   | CA    | 3180 | 1/1   | 0.95 | 0.19 | -    | 6,6,6,6                     | 0     |
| 58  | MG   | CA    | 3030 | 1/1   | 0.94 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3019 | 1/1   | 0.92 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3107 | 1/1   | 0.98 | 0.17 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1653 | 1/1   | 0.95 | 0.15 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | BA    | 1625 | 1/1   | 0.93 | 0.06 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3019 | 1/1   | 0.89 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3156 | 1/1   | 0.94 | 0.23 | -    | 3,3,3,3                     | 0     |
| 58  | MG   | AA    | 1668 | 1/1   | 0.97 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3029 | 1/1   | 0.99 | 0.05 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3004 | 1/1   | 0.97 | 0.05 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | BA    | 1649 | 1/1   | 0.92 | 0.15 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | CA    | 3192 | 1/1   | 0.98 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1627 | 1/1   | 0.94 | 0.14 | -    | 19,19,19,19                 | 0     |
| 58  | MG   | CA    | 3157 | 1/1   | 0.97 | 0.21 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1650 | 1/1   | 0.98 | 0.21 | -    | 5,5,5,5                     | 0     |
| 58  | MG   | AA    | 1602 | 1/1   | 0.95 | 0.11 | -    | 17,17,17,17                 | 0     |
| 58  | MG   | CA    | 3090 | 1/1   | 0.96 | 0.08 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | BA    | 1655 | 1/1   | 0.91 | 0.11 | -    | 9,9,9,9                     | 0     |
| 58  | MG   | CA    | 3123 | 1/1   | 0.98 | 0.20 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3087 | 1/1   | 0.99 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3133 | 1/1   | 0.91 | 0.17 | -    | 16,16,16,16                 | 0     |
| 58  | MG   | CA    | 3005 | 1/1   | 0.99 | 0.05 | -    | 14,14,14,14                 | 0     |
| 58  | MG   | CA    | 3167 | 1/1   | 0.97 | 0.30 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1636 | 1/1   | 0.86 | 0.10 | -    | 42,42,42,42                 | 0     |
| 58  | MG   | DA    | 3144 | 1/1   | 0.97 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1638 | 1/1   | 0.96 | 0.09 | -    | 27,27,27,27                 | 0     |
| 58  | MG   | AA    | 1670 | 1/1   | 0.92 | 0.27 | -    | 11,11,11,11                 | 0     |
| 58  | MG   | CA    | 3016 | 1/1   | 0.99 | 0.12 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1653 | 1/1   | 0.91 | 0.09 | -    | 7,7,7,7                     | 0     |
| 58  | MG   | CA    | 3120 | 1/1   | 0.94 | 0.12 | -    | 2,2,2,2                     | 0     |
| 58  | MG   | CA    | 3126 | 1/1   | 0.95 | 0.13 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3075 | 1/1   | 0.93 | 0.12 | -    | 8,8,8,8                     | 0     |
| 58  | MG   | CA    | 3101 | 1/1   | 0.95 | 0.11 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3089 | 1/1   | 0.90 | 0.08 | -    | 19,19,19,19                 | 0     |
| 58  | MG   | CA    | 3184 | 1/1   | 0.97 | 0.22 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1611 | 1/1   | 0.85 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1652 | 1/1   | 0.98 | 0.12 | -    | 13,13,13,13                 | 0     |
| 58  | MG   | DA    | 3138 | 1/1   | 0.92 | 0.45 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1629 | 1/1   | 0.92 | 0.06 | -    | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 58  | MG   | BA    | 1645 | 1/1   | 0.93 | 0.08 | -    | 8,8,8,8                     | 0     |
| 58  | MG   | DA    | 3054 | 1/1   | 0.98 | 0.09 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3122 | 1/1   | 0.95 | 0.15 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3051 | 1/1   | 0.97 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3194 | 1/1   | 0.94 | 0.19 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3086 | 1/1   | 0.98 | 0.15 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3066 | 1/1   | 0.95 | 0.05 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | CA    | 3036 | 1/1   | 0.98 | 0.16 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3141 | 1/1   | 0.99 | 0.23 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | DA    | 3155 | 1/1   | 0.98 | 0.18 | -    | 1,1,1,1                     | 0     |
| 58  | MG   | CA    | 3096 | 1/1   | 0.98 | 0.07 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | AA    | 1666 | 1/1   | 0.90 | 0.16 | -    | 13,13,13,13                 | 0     |
| 58  | MG   | CA    | 3146 | 1/1   | 0.96 | 0.33 | -    | 0,0,0,0                     | 0     |
| 58  | MG   | BA    | 1606 | 1/1   | 0.97 | 0.12 | -    | 24,24,24,24                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.