



## wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 11:54 AM EDT

PDB ID : 9E71 / pdb\_00009e71  
EMDB ID : EMD-47628  
Title : Cryo-EM structure of the Pyrobaculum calidifontis 70S ribosome  
Authors : Nissley, A.J.; Cate, J.H.D.  
Deposited on : 2024-10-31  
Resolution : 2.36 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

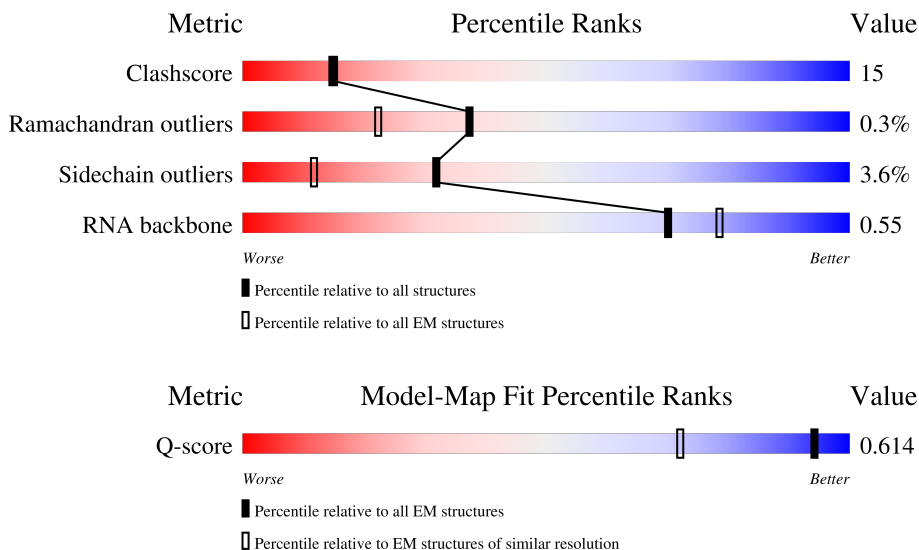
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.36 Å.

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







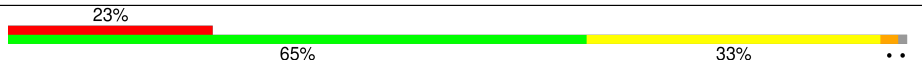

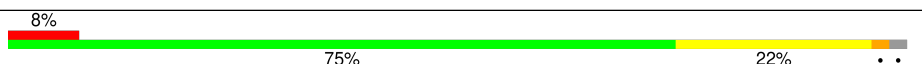
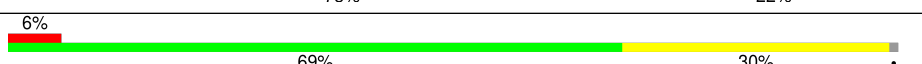
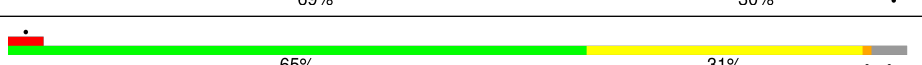

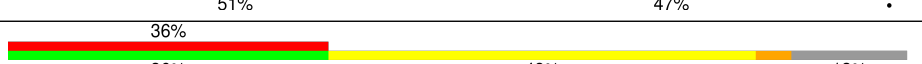
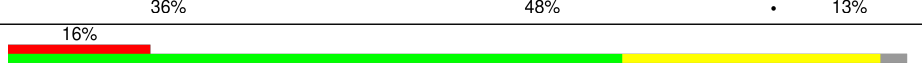

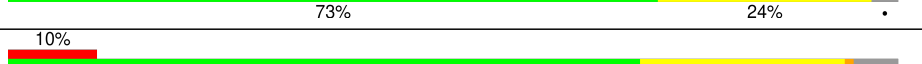





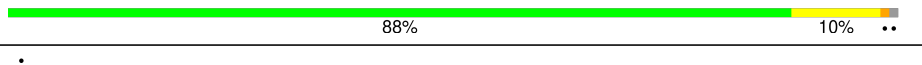
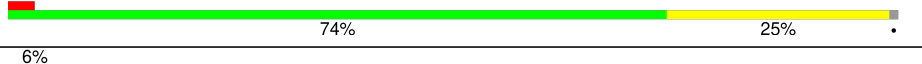


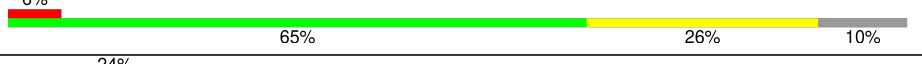
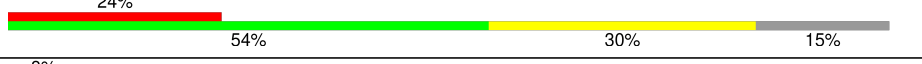
| Metric                | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--------------------------|---|
| Clashscore            | 229148                   | 23984                    | -   |
| Ramachandran outliers | 224038                   | 23583                    | -   |
| Sidechain outliers    | 223484                   | 23102                    | -   |
| RNA backbone          | 8273                     | 3508                     | -   |
| Q-score               | -                        | 25397                    | 4686 ( 1.86 - 2.86 )                                  |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 2     | 129    |                  |
| 2   | 1     | 3024   |                  |
| 3   | 4     | 1498   |                  |


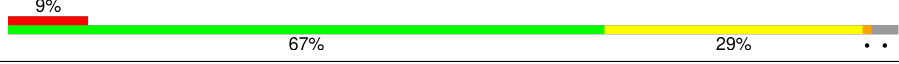
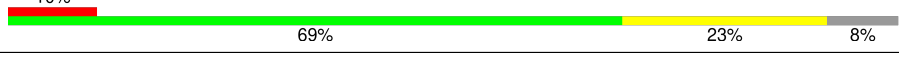



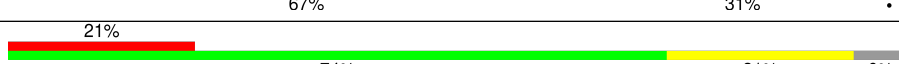
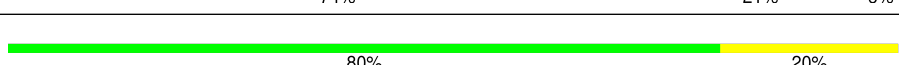
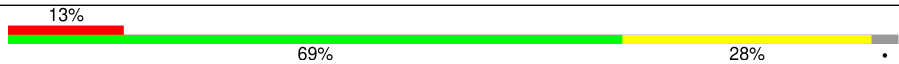


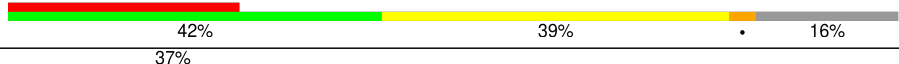
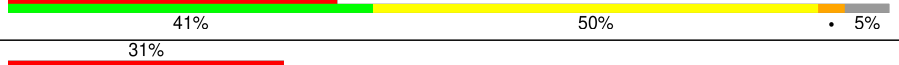

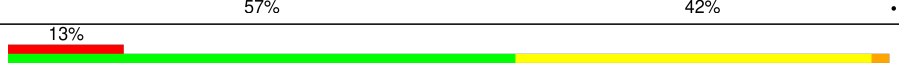
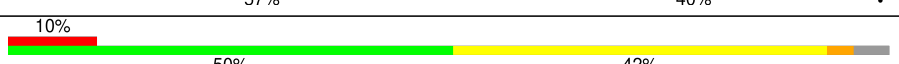
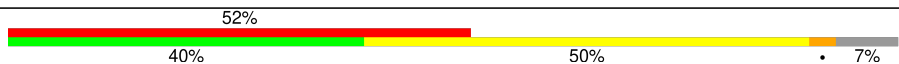








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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | AA    | 244    |    |
| 5   | AB    | 338    |    |
| 6   | AC    | 285    |    |
| 7   | AD    | 178    |    |
| 8   | AE    | 196    |    |
| 9   | AF    | 149    |    |
| 10  | AG    | 186    |    |
| 11  | AH    | 157    |    |
| 12  | AI    | 144    |    |
| 13  | AJ    | 103    |    |
| 13  | AK    | 103    |    |
| 14  | AL    | 156    |    |
| 15  | AM    | 189    |   |
| 16  | AN    | 178    |  |
| 17  | AO    | 205    |  |
| 18  | AP    | 122    |  |
| 19  | AQ    | 147    |  |
| 20  | AR    | 78     |  |
| 21  | AS    | 99     |  |
| 22  | AT    | 184    |  |
| 23  | AU    | 81     |  |
| 24  | AV    | 128    |  |
| 25  | AW    | 62     |  |
| 26  | AX    | 79     |  |
| 27  | AY    | 179    |  |

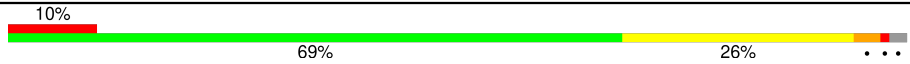

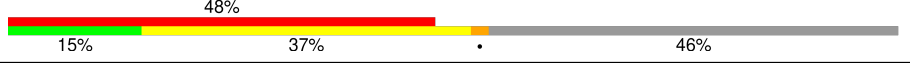
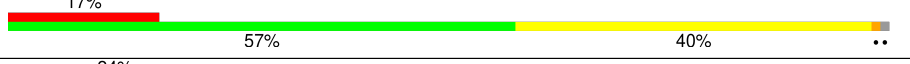


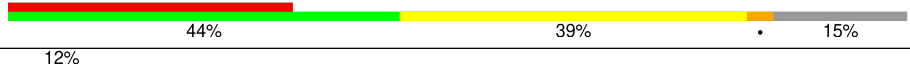

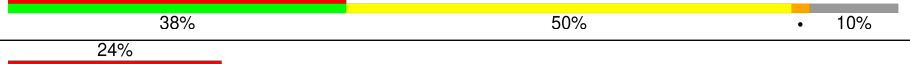
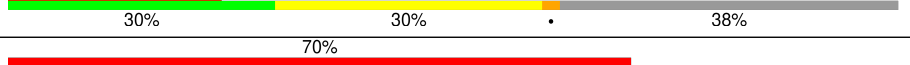

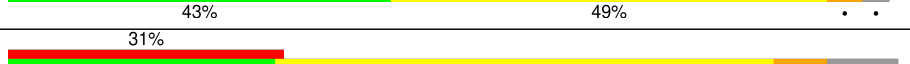
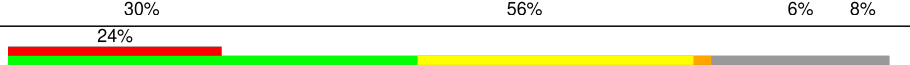

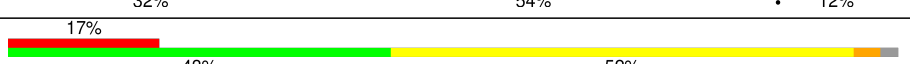
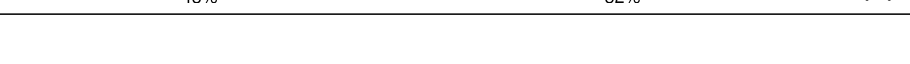
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 28  | AZ    | 101    |    |
| 29  | Aa    | 91     |    |
| 30  | Ab    | 153    |    |
| 31  | Ac    | 84     |    |
| 32  | Ad    | 52     |    |
| 33  | Ae    | 67     |    |
| 34  | Af    | 51     |    |
| 35  | Ag    | 53     |    |
| 36  | Ah    | 91     |    |
| 37  | Ai    | 102    |    |
| 38  | Aj    | 184    |   |
| 39  | Ak    | 93     |  |
| 40  | BA    | 222    |  |
| 41  | BB    | 208    |  |
| 42  | BC    | 216    |  |
| 43  | BD    | 159    |  |
| 44  | BE    | 237    |  |
| 45  | BF    | 202    |  |
| 46  | BG    | 151    |  |
| 47  | BH    | 223    |  |
| 48  | BI    | 130    |  |
| 49  | BJ    | 131    |  |
| 50  | BK    | 142    |  |
| 51  | BL    | 106    |  |
| 52  | BM    | 141    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 53  | BN    | 147    |    |
| 54  | BO    | 153    |    |
| 55  | BP    | 54     |    |
| 56  | BQ    | 151    |    |
| 57  | BR    | 147    |    |
| 58  | BS    | 71     |    |
| 59  | BT    | 158    |    |
| 60  | BU    | 158    |    |
| 61  | BV    | 128    |    |
| 62  | BW    | 110    |    |
| 63  | BX    | 100    |    |
| 64  | BY    | 67     |   |
| 65  | BZ    | 77     |  |
| 66  | Ba    | 54     |  |
| 67  | Bb    | 68     |  |
| 68  | Bc    | 65     |  |

## 2 Entry composition [i](#)

There are 72 unique types of molecules in this entry. The entry contains 171357 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
|     |       |          | Total | C    | N   | O   | P   |         |       |
| 1   | 2     | 129      | 2769  | 1231 | 512 | 897 | 129 | 0       | 0     |

- Molecule 2 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
|     |       |          | Total | C     | N     | O     | P    |         |       |
| 2   | 1     | 2849     | 61386 | 27335 | 11453 | 19749 | 2849 | 0       | 0     |

- Molecule 3 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
|     |       |          | Total | C     | N    | O    | P    |         |       |
| 3   | 4     | 1430     | 30817 | 13730 | 5745 | 9912 | 1430 | 0       | 0     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| 4     | 5       | 4AC      | C      | conflict | GB 343200235 |
| 4     | 1318    | 4AC      | C      | conflict | GB 343200235 |

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 4   | AA    | 239      | 1803  | 1136 | 354 | 308 | 5 | 0       | 0     |

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 5   | AB    | 336      | 2611  | 1681 | 476 | 450 | 4 | 0       | 0     |

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 6   | AC    | 278      | 2178  | 1406 | 395 | 371 | 6 | 0       | 0     |

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 7   | AD    | 178      | 1412  | 894 | 273 | 238 | 7 | 0       | 0     |

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 8   | AE    | 195      | 1520  | 990 | 254 | 272 | 4 | 0       | 0     |

- Molecule 9 is a protein called Large ribosomal subunit protein eL8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 9   | AF    | 145      | 1095  | 705 | 187 | 202 | 1 | 0       | 0     |

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 10  | AG    | 183      | 1510  | 979 | 278 | 246 | 7 | 0       | 0     |

- Molecule 11 is a protein called Large ribosomal subunit protein eL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 11  | AH    | 155      | 1244  | 785 | 249 | 209 | 1 | 0       | 0     |

- Molecule 12 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 12  | AI    | 138      | 1068  | 682 | 202 | 181 | 3 | 0       | 0     |

- Molecule 13 is a protein called Large ribosomal subunit protein eL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | AJ    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 788   | 500 | 143 | 144 | 1 |         |       |
| 13  | AK    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 700   | 441 | 130 | 128 | 1 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | AL    | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 761 | 232 | 202 | 3 |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L15e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AM    | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1558  | 992 | 315 | 245 | 6 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | AN    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1336  | 847 | 254 | 227 | 8 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | AO    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1615  | 1027 | 309 | 278 | 1 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein eL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | AP    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 920   | 583 | 181 | 155 | 1 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein eL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AQ    | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1214  | 759 | 244 | 208 | 3 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein eL20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 20  | AR    | 76       | 603   | 382 | 109 | 109 | 3 | 0       | 0     |

- Molecule 21 is a protein called Large ribosomal subunit protein eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 21  | AS    | 98       | 788   | 503 | 150 | 134 | 1 | 0       | 0     |

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 22  | AT    | 183      | 1496  | 978 | 268 | 247 | 3 | 0       | 0     |

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 23  | AU    | 81       | 651   | 417 | 115 | 117 | 2 | 0       | 0     |

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 24  | AV    | 121      | 976   | 619 | 194 | 161 | 2 | 0       | 0     |

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 25  | AW    | 56       | 449   | 287 | 86 | 70 | 6 | 0       | 0     |

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 26  | AX    | 67       | 554   | 343 | 117 | 92 | 2 | 0       | 0     |

- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 27  | AY    | 172      | 1374  | 888 | 245 | 235 | 6 | 0       | 0     |

- Molecule 28 is a protein called Large ribosomal subunit protein eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 28  | AZ    | 98       | 742   | 481 | 128 | 132 | 1 | 0       | 0     |

- Molecule 29 is a protein called Large ribosomal subunit protein eL31.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 29  | Aa    | 88       | 726   | 460 | 146 | 120 | 0       | 0     |

- Molecule 30 is a protein called Large ribosomal subunit protein eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 30  | Ab    | 140      | 1183  | 757 | 239 | 186 | 1 | 0       | 0     |

- Molecule 31 is a protein called Large ribosomal subunit protein eL34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 31  | Ac    | 83       | 649   | 407 | 138 | 102 | 2 | 0       | 0     |

- Molecule 32 is a protein called Large ribosomal subunit protein eL37.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 32  | Ad    | 52       | 429   | 265 | 93 | 65 | 6 | 0       | 0     |

- Molecule 33 is a protein called LSU ribosomal protein L38E.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
|     |       |          | Total | C   | N  | O  |         |       |
| 33  | Ae    | 66       | 552   | 363 | 93 | 96 | 0       | 0     |

- Molecule 34 is a protein called Large ribosomal subunit protein eL39.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 34  | Af    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 415   | 260 | 96 | 59 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | Ag    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 417   | 259 | 88 | 66 | 4 |         |       |

- Molecule 36 is a protein called eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Ah    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 739   | 467 | 142 | 123 | 7 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Ai    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 769   | 489 | 148 | 127 | 5 |         |       |

- Molecule 38 is a protein called DJ-1/PfpI domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Aj    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1469  | 954 | 248 | 265 | 2 |         |       |

- Molecule 39 is a protein called PaREP1 domain containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Ak    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 743   | 478 | 127 | 136 | 2 |         |       |

- Molecule 40 is a protein called Small ribosomal subunit protein eS1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | BA    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1487  | 965 | 263 | 256 | 3 |         |       |

- Molecule 41 is a protein called Small ribosomal subunit protein uS2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | BB    | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1600  | 1037 | 277 | 279 | 7 |         |       |

- Molecule 42 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | BC    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 611   | 393 | 110 | 107 | 1 |         |       |

- Molecule 43 is a protein called Small ribosomal subunit protein uS4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | BD    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1284  | 831 | 240 | 209 | 4 |         |       |

- Molecule 44 is a protein called Small ribosomal subunit protein eS4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44  | BE    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1883  | 1223 | 336 | 322 | 2 |         |       |

- Molecule 45 is a protein called Small ribosomal subunit protein uS5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | BF    | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1498  | 951 | 272 | 271 | 4 |         |       |

- Molecule 46 is a protein called Small ribosomal subunit protein eS6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | BG    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 685 | 190 | 188 | 2 |         |       |

- Molecule 47 is a protein called Small ribosomal subunit protein uS7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | BH    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1773  | 1128 | 325 | 313 | 7 |         |       |

- Molecule 48 is a protein called Small ribosomal subunit protein uS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 48  | BI    | 129      | 1036  | 676 | 177 | 180 | 3 | 0       | 0     |

- Molecule 49 is a protein called Small ribosomal subunit protein eS8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 49  | BJ    | 130      | 1007  | 636 | 198 | 172 | 1 | 0       | 0     |

- Molecule 50 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 50  | BK    | 134      | 1058  | 680 | 191 | 182 | 5 | 0       | 0     |

- Molecule 51 is a protein called Small ribosomal subunit protein uS10.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 51  | BL    | 38       | 315   | 201 | 64 | 49 | 1 | 0       | 0     |

- Molecule 52 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 52  | BM    | 127      | 941   | 592 | 182 | 164 | 3 | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BM    | 128     | IAS      | ASP    | conflict | UNP A3MX63 |

- Molecule 53 is a protein called Small ribosomal subunit protein uS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 53  | BN    | 144      | 1133  | 730 | 211 | 189 | 3 | 0       | 0     |

- Molecule 54 is a protein called Small ribosomal subunit protein uS13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | BO    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 700 | 211 | 195 | 2 |         |       |

- Molecule 55 is a protein called Small ribosomal subunit protein uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | BP    | 29       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 241   | 150 | 51 | 36 | 4 |         |       |

- Molecule 56 is a protein called Small ribosomal subunit protein uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | BQ    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1224  | 782 | 233 | 208 | 1 |         |       |

- Molecule 57 is a protein called Small ribosomal subunit protein uS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | BR    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1171  | 756 | 216 | 194 | 5 |         |       |

- Molecule 58 is a protein called Small ribosomal subunit protein eS17.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 58  | BS    | 64       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 517   | 332 | 94 | 91 |         |       |

- Molecule 59 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | BT    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 720 | 203 | 182 | 6 |         |       |

- Molecule 60 is a protein called Small ribosomal subunit protein eS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | BU    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1225  | 789 | 225 | 209 | 2 |         |       |

- Molecule 61 is a protein called Small ribosomal subunit protein eS24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 61  | BV    | 115      | 950   | 597 | 185 | 168 | 0       | 0     |

- Molecule 62 is a protein called SSU ribosomal protein S25E.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 62  | BW    | 68       | 544   | 351 | 96 | 96 | 1 | 0       | 0     |

- Molecule 63 is a protein called SSU ribosomal protein S26E.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 63  | BX    | 95       | 772   | 490 | 150 | 128 | 4 | 0       | 0     |

- Molecule 64 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 64  | BY    | 65       | 501   | 317 | 100 | 79 | 5 | 0       | 0     |

- Molecule 65 is a protein called eS28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
|     |       |          | Total | C   | N   | O  | S |         |       |
| 65  | BZ    | 71       | 552   | 344 | 108 | 99 | 1 | 0       | 0     |

- Molecule 66 is a protein called SSU ribosomal protein S30E.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
|     |       |          | Total | C   | N  | O  |         |       |
| 66  | Ba    | 43       | 357   | 222 | 80 | 55 | 0       | 0     |

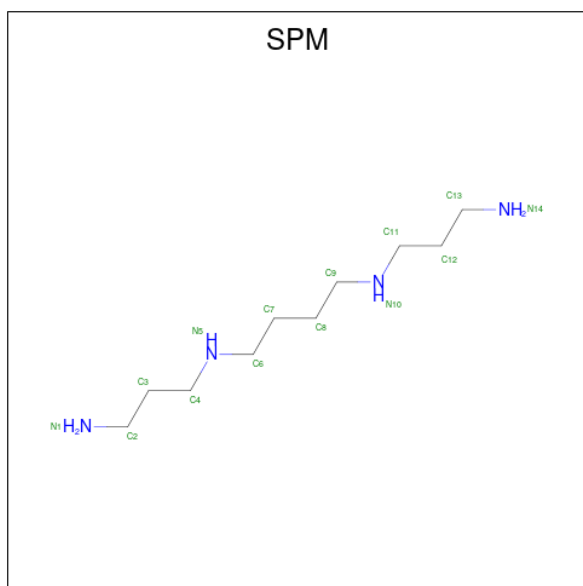
- Molecule 67 is a protein called aS35.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
|     |       |          | Total | C   | N  | O  |         |       |
| 67  | Bb    | 60       | 479   | 301 | 95 | 83 | 0       | 0     |

- Molecule 68 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 68  | Bc    | 64       | 477   | 301 | 90 | 82 | 4 | 0       | 0     |

- Molecule 69 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | C  | N |         |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | C  | N |         |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 1     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |
| 69  | 4     | 1        | 14    | 10 | 4 | 0       |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | 4     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | AL    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 69  | Ah    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

- Molecule 70 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 70  | 1     | 170      | Total | Mg  | 0       |
|     |       |          | 170   | 170 |         |
| 70  | 4     | 78       | Total | Mg  | 0       |
|     |       |          | 78    | 78  |         |
| 70  | AA    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 70  | AL    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 70  | BK    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 71 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 71  | AW    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 71  | Ad    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | Ag    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | Ah    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | Ai    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | BF    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | BP    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | BR    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | BX    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | BY    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 71  | Bc    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 72 is water.

| Mol | Chain | Residues | Atoms         |           | AltConf |
|-----|-------|----------|---------------|-----------|---------|
| 72  | 2     | 181      | Total<br>181  | O<br>181  | 0       |
| 72  | 1     | 5640     | Total<br>5640 | O<br>5640 | 0       |
| 72  | 4     | 1487     | Total<br>1487 | O<br>1487 | 0       |
| 72  | AA    | 12       | Total<br>12   | O<br>12   | 0       |
| 72  | AB    | 1        | Total<br>1    | O<br>1    | 0       |
| 72  | AC    | 6        | Total<br>6    | O<br>6    | 0       |
| 72  | AG    | 2        | Total<br>2    | O<br>2    | 0       |
| 72  | AH    | 3        | Total<br>3    | O<br>3    | 0       |
| 72  | AL    | 10       | Total<br>10   | O<br>10   | 0       |

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| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 72  | AM    | 2        | Total<br>2  | O<br>2  | 0       |
| 72  | AN    | 2        | Total<br>2  | O<br>2  | 0       |
| 72  | AO    | 2        | Total<br>2  | O<br>2  | 0       |
| 72  | AP    | 1        | Total<br>1  | O<br>1  | 0       |
| 72  | AQ    | 1        | Total<br>1  | O<br>1  | 0       |
| 72  | AT    | 2        | Total<br>2  | O<br>2  | 0       |
| 72  | AU    | 1        | Total<br>1  | O<br>1  | 0       |
| 72  | AX    | 22       | Total<br>22 | O<br>22 | 0       |
| 72  | AY    | 2        | Total<br>2  | O<br>2  | 0       |
| 72  | Aa    | 1        | Total<br>1  | O<br>1  | 0       |
| 72  | Ab    | 6        | Total<br>6  | O<br>6  | 0       |
| 72  | Ad    | 3        | Total<br>3  | O<br>3  | 0       |
| 72  | Ah    | 1        | Total<br>1  | O<br>1  | 0       |
| 72  | BA    | 18       | Total<br>18 | O<br>18 | 0       |
| 72  | BB    | 18       | Total<br>18 | O<br>18 | 0       |
| 72  | BC    | 9        | Total<br>9  | O<br>9  | 0       |
| 72  | BD    | 28       | Total<br>28 | O<br>28 | 0       |
| 72  | BE    | 23       | Total<br>23 | O<br>23 | 0       |
| 72  | BF    | 32       | Total<br>32 | O<br>32 | 0       |
| 72  | BG    | 19       | Total<br>19 | O<br>19 | 0       |
| 72  | BH    | 26       | Total<br>26 | O<br>26 | 0       |

*Continued on next page...*

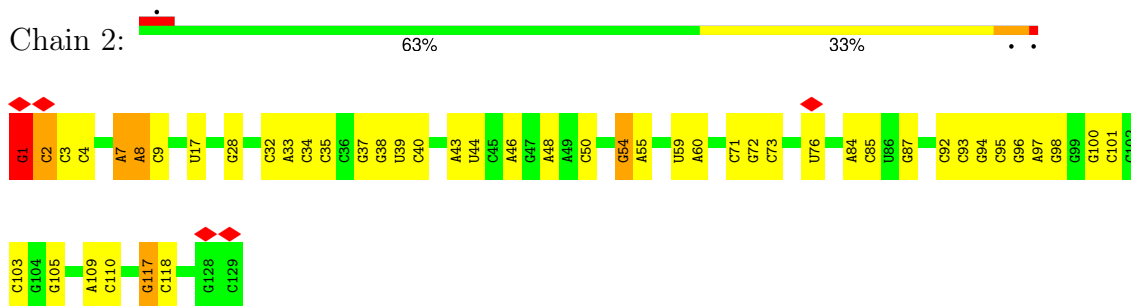
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 72  | BI    | 20       | Total<br>20 | O<br>20 | 0       |
| 72  | BJ    | 13       | Total<br>13 | O<br>13 | 0       |
| 72  | BK    | 12       | Total<br>12 | O<br>12 | 0       |
| 72  | BL    | 7        | Total<br>7  | O<br>7  | 0       |
| 72  | BM    | 9        | Total<br>9  | O<br>9  | 0       |
| 72  | BN    | 12       | Total<br>12 | O<br>12 | 0       |
| 72  | BO    | 26       | Total<br>26 | O<br>26 | 0       |
| 72  | BP    | 8        | Total<br>8  | O<br>8  | 0       |
| 72  | BQ    | 15       | Total<br>15 | O<br>15 | 0       |
| 72  | BR    | 12       | Total<br>12 | O<br>12 | 0       |
| 72  | BS    | 5        | Total<br>5  | O<br>5  | 0       |
| 72  | BT    | 17       | Total<br>17 | O<br>17 | 0       |
| 72  | BU    | 13       | Total<br>13 | O<br>13 | 0       |
| 72  | BV    | 9        | Total<br>9  | O<br>9  | 0       |
| 72  | BW    | 8        | Total<br>8  | O<br>8  | 0       |
| 72  | BX    | 12       | Total<br>12 | O<br>12 | 0       |
| 72  | BY    | 10       | Total<br>10 | O<br>10 | 0       |
| 72  | BZ    | 12       | Total<br>12 | O<br>12 | 0       |
| 72  | Ba    | 8        | Total<br>8  | O<br>8  | 0       |
| 72  | Bb    | 7        | Total<br>7  | O<br>7  | 0       |
| 72  | Bc    | 16       | Total<br>16 | O<br>16 | 0       |

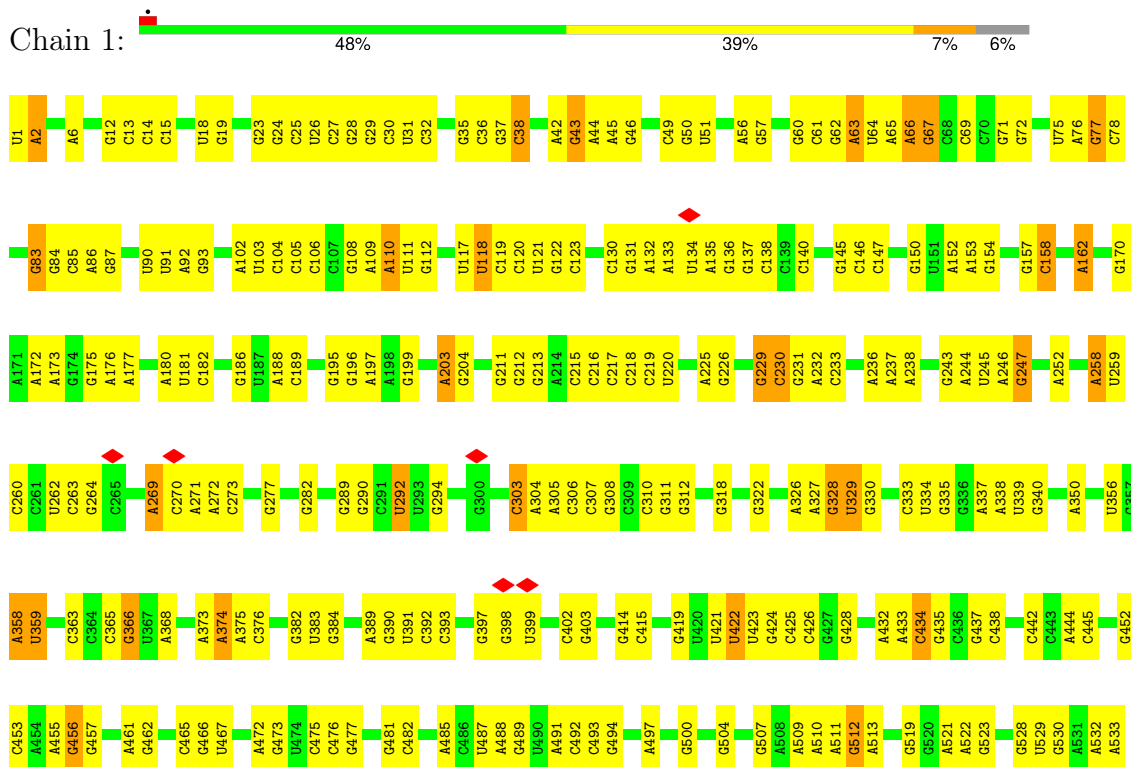
### 3 Residue-property plots [i](#)

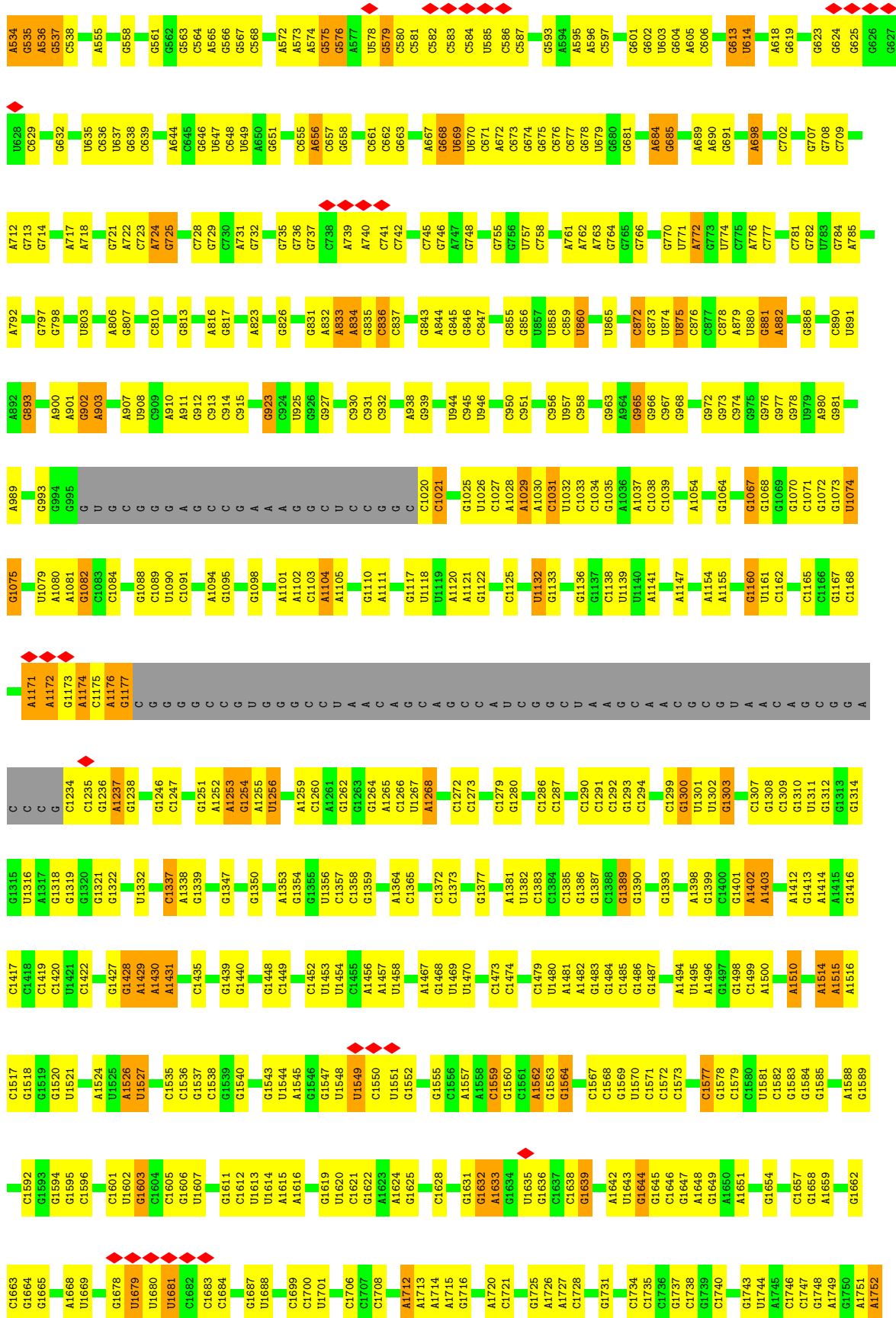
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

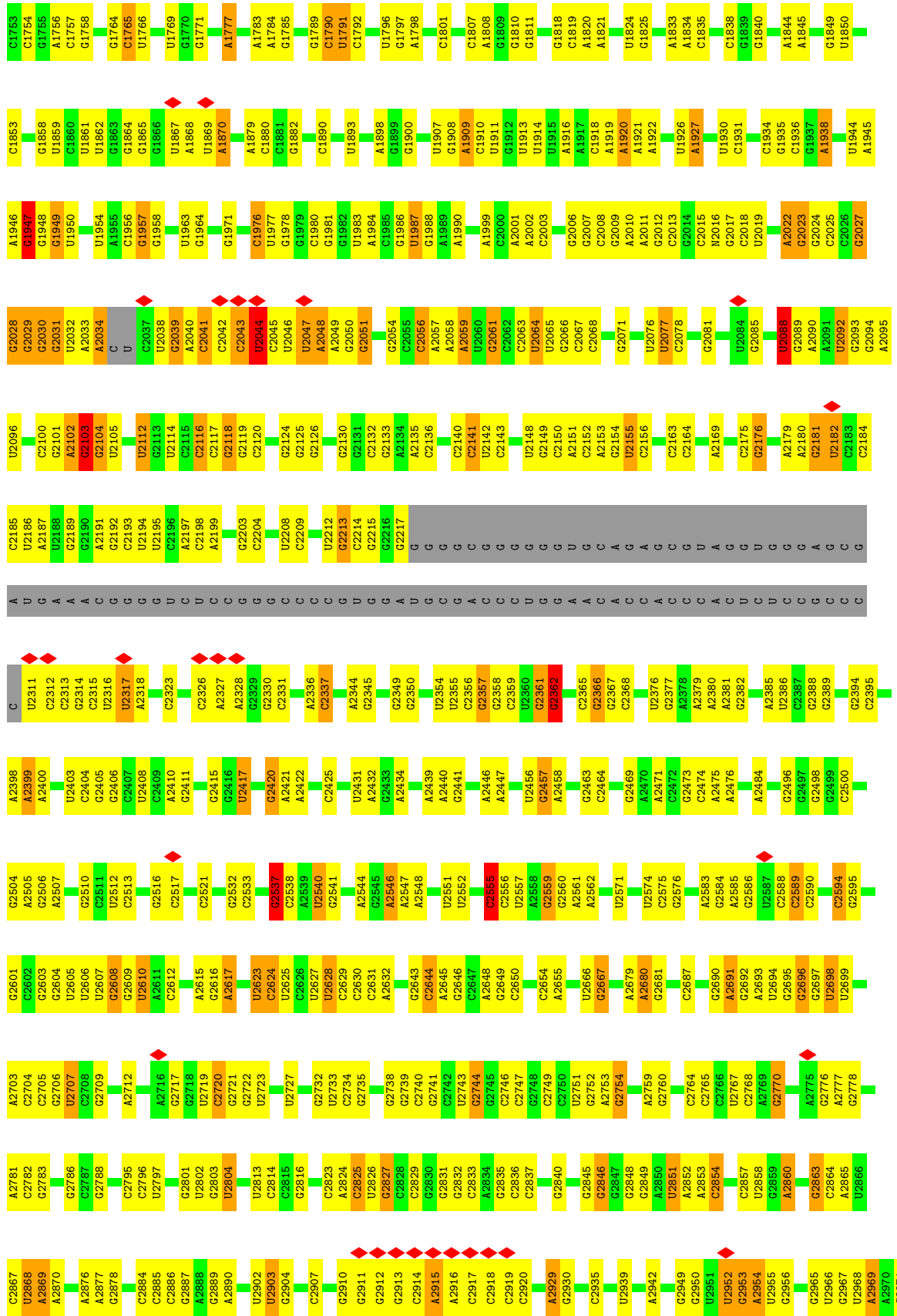
#### • Molecule 1: 5S rRNA

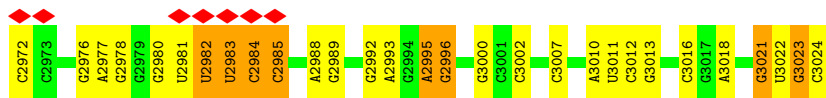


#### • Molecule 2: 23S rRNA

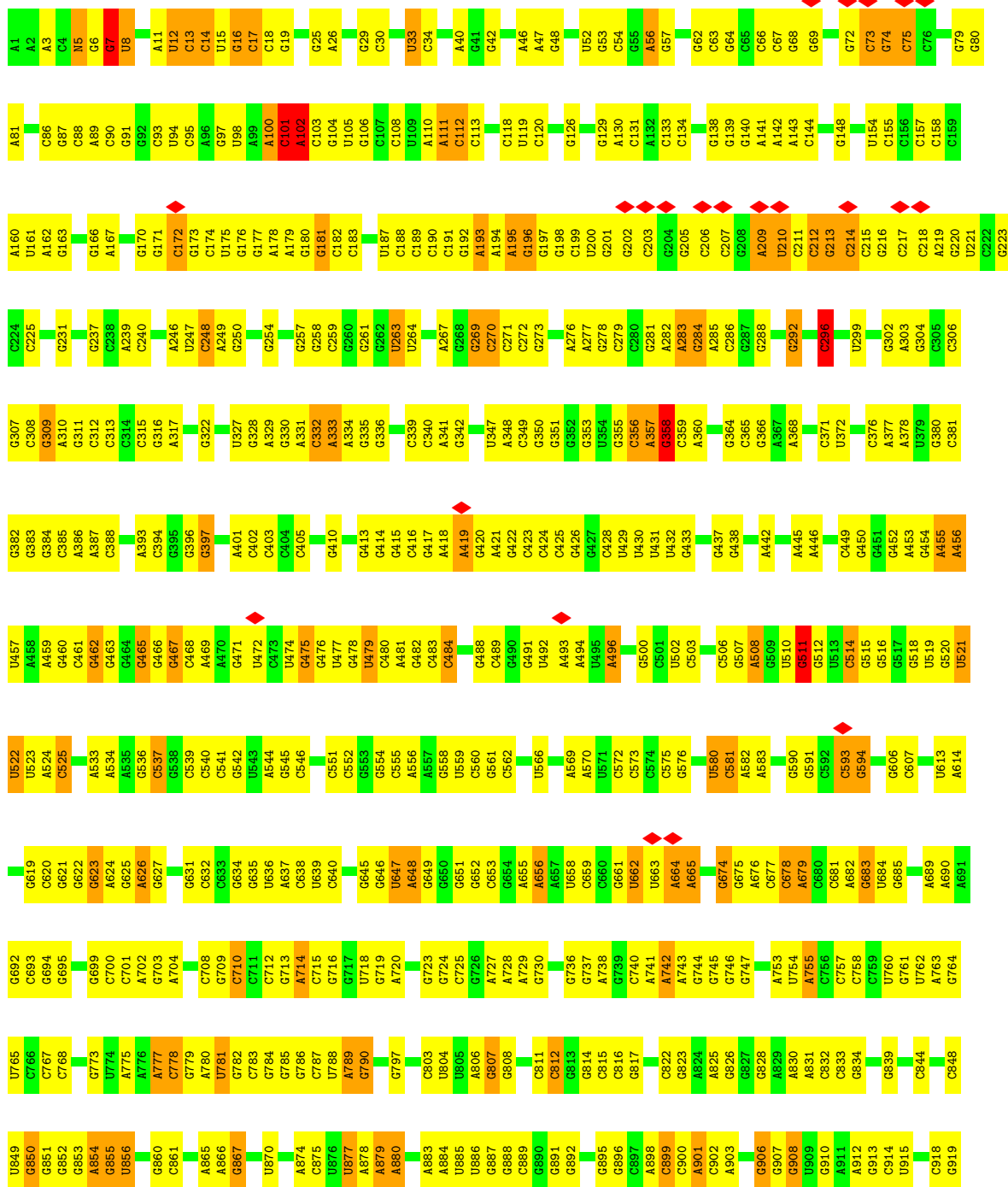


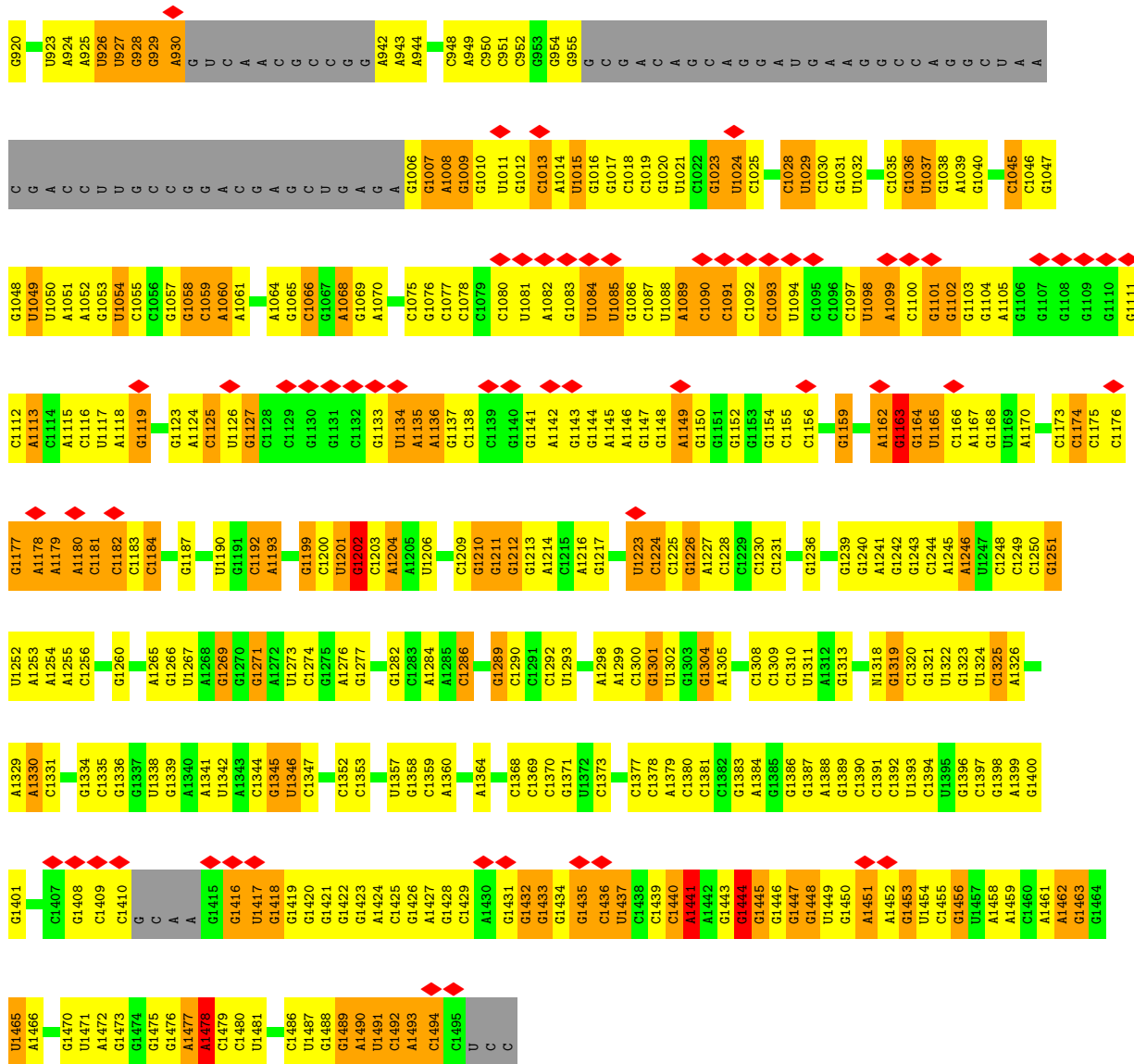




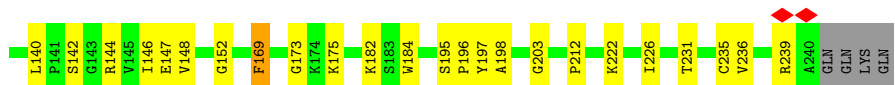
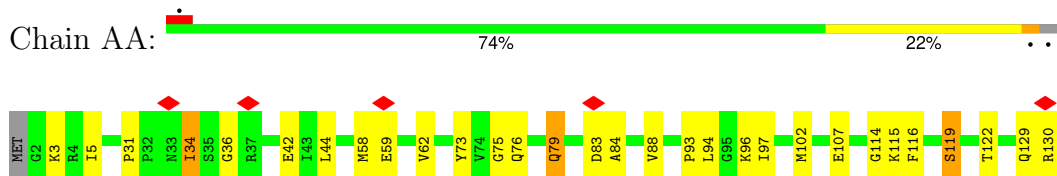


• Molecule 3: 16S rRNA



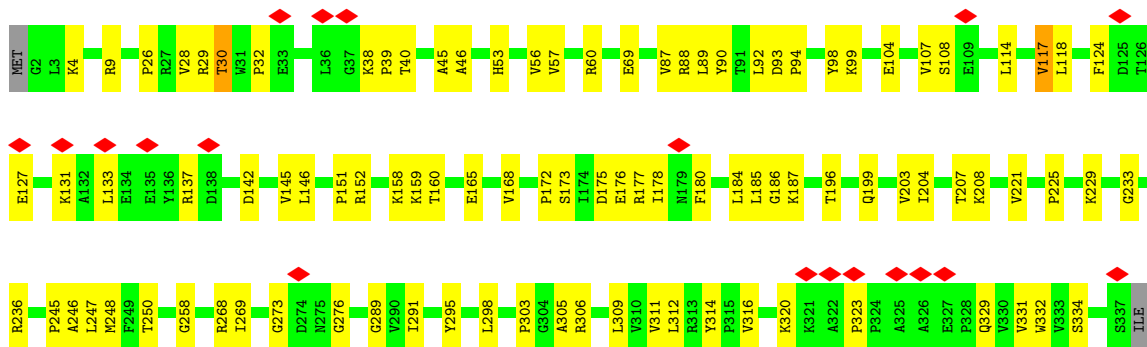


- Molecule 4: Large ribosomal subunit protein uL2

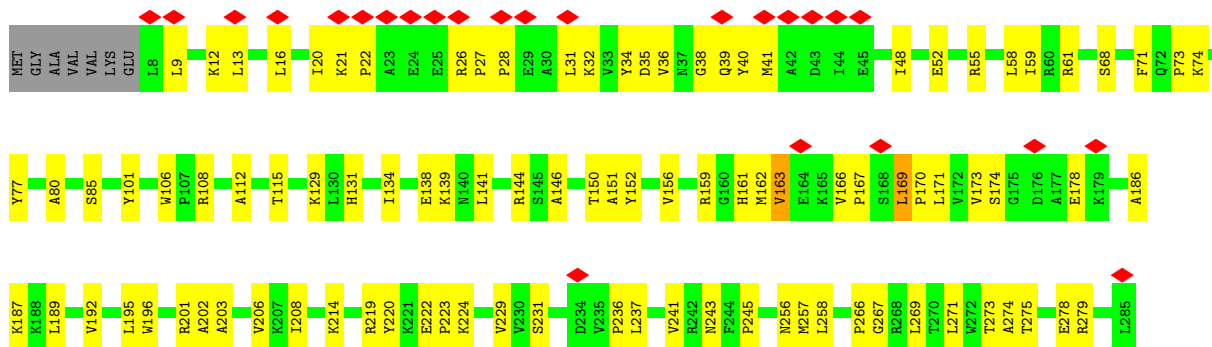


- Molecule 5: Large ribosomal subunit protein uL3

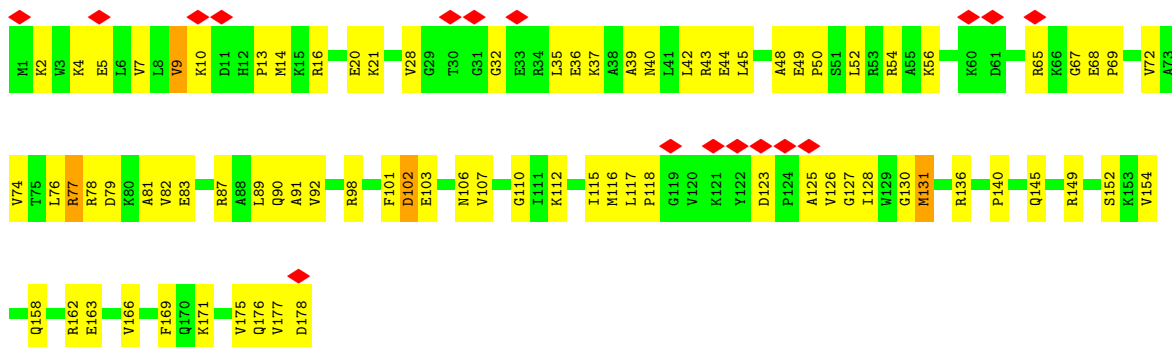




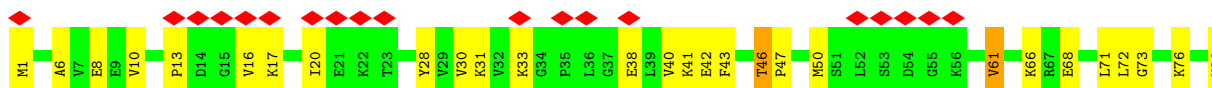
• Molecule 6: Large ribosomal subunit protein uL4

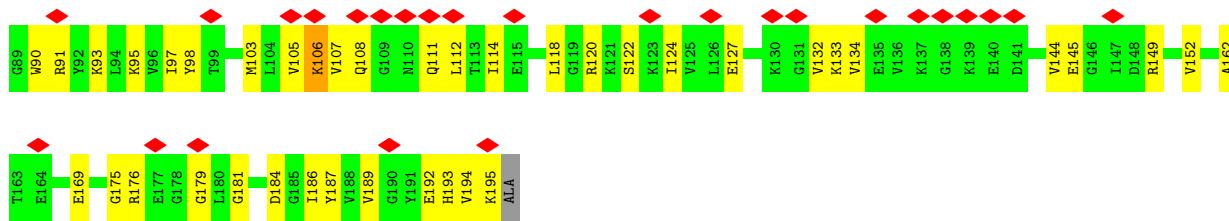


• Molecule 7: Large ribosomal subunit protein uL5

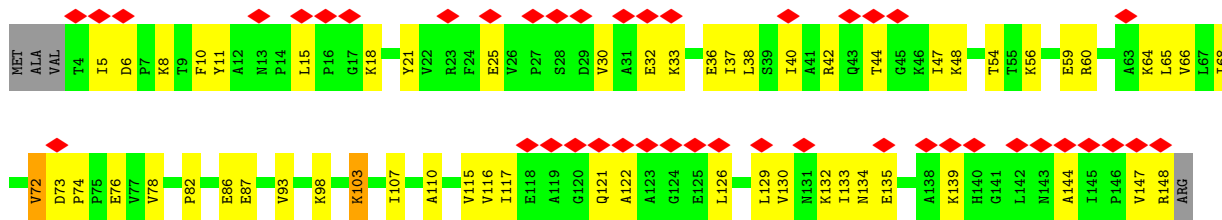


• Molecule 8: Large ribosomal subunit protein uL6

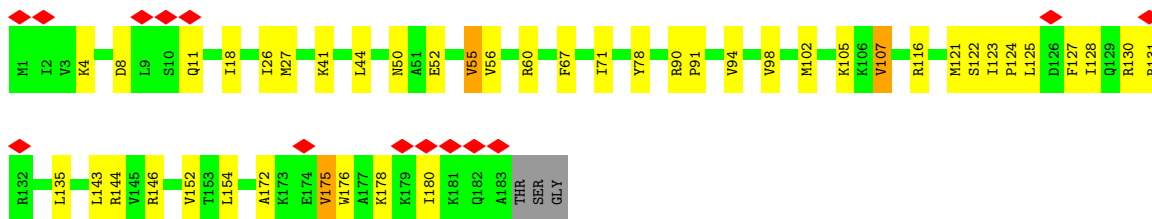
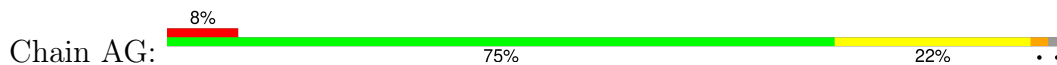




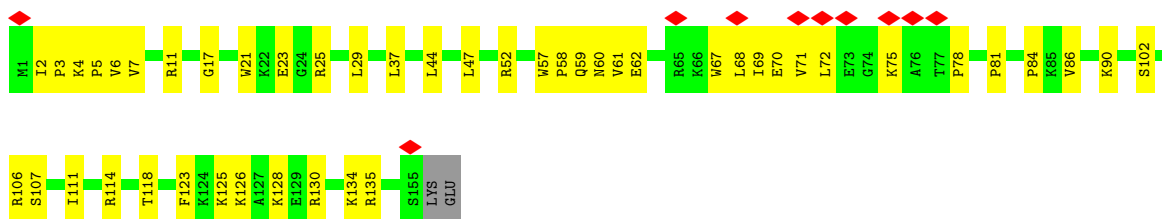
• Molecule 9: Large ribosomal subunit protein eL8



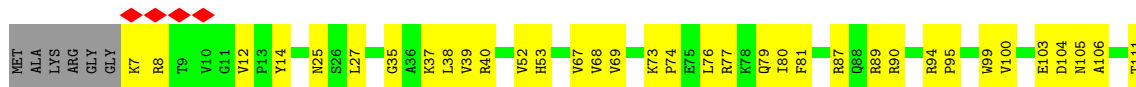
• Molecule 10: Large ribosomal subunit protein uL13



• Molecule 11: Large ribosomal subunit protein eL13

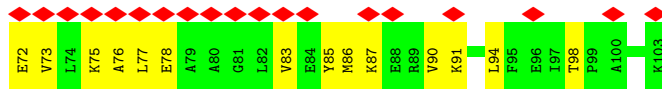
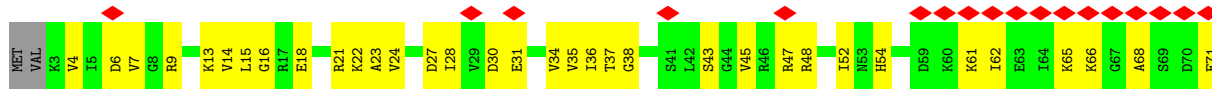


• Molecule 12: Large ribosomal subunit protein uL14

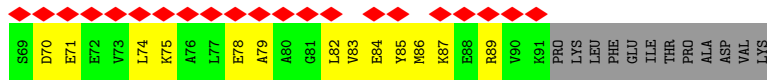
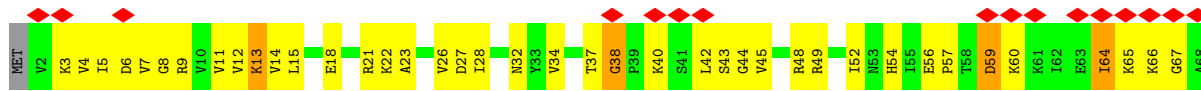




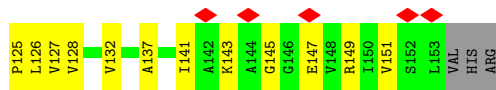
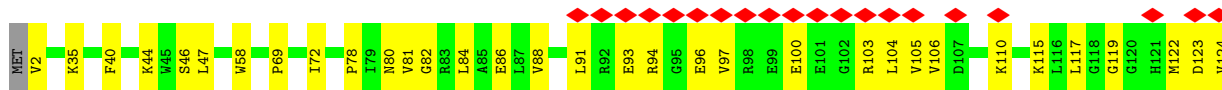
• Molecule 13: Large ribosomal subunit protein eL14



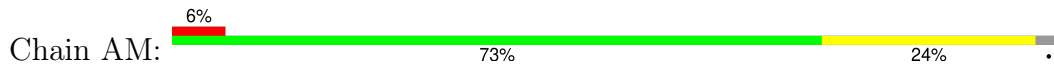
• Molecule 13: Large ribosomal subunit protein eL14



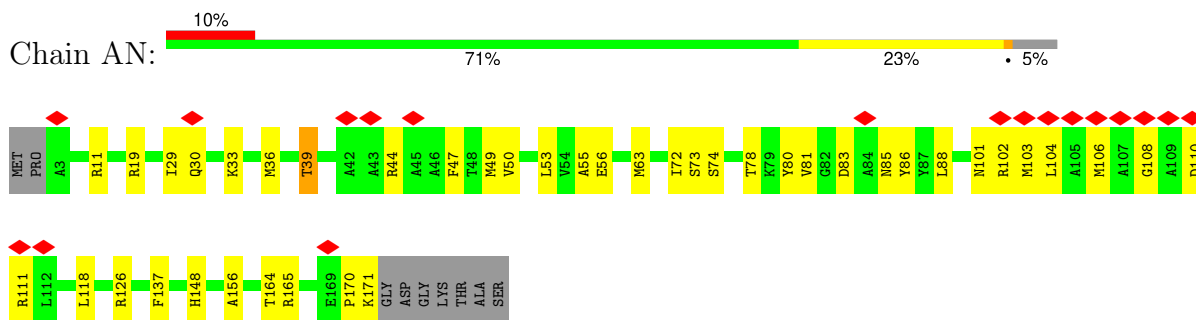
• Molecule 14: Large ribosomal subunit protein uL15



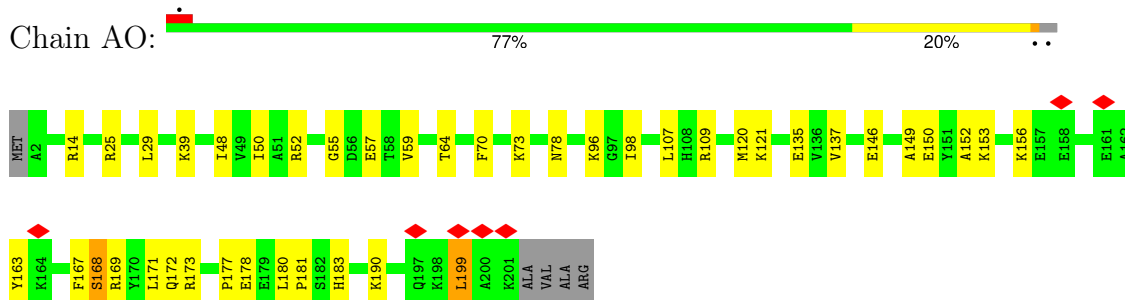
• Molecule 15: 50S ribosomal protein L15e



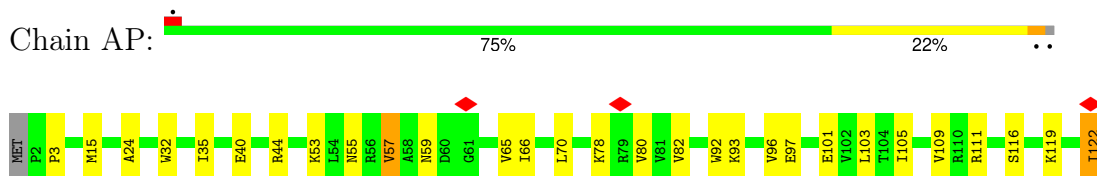
• Molecule 16: Large ribosomal subunit protein uL16



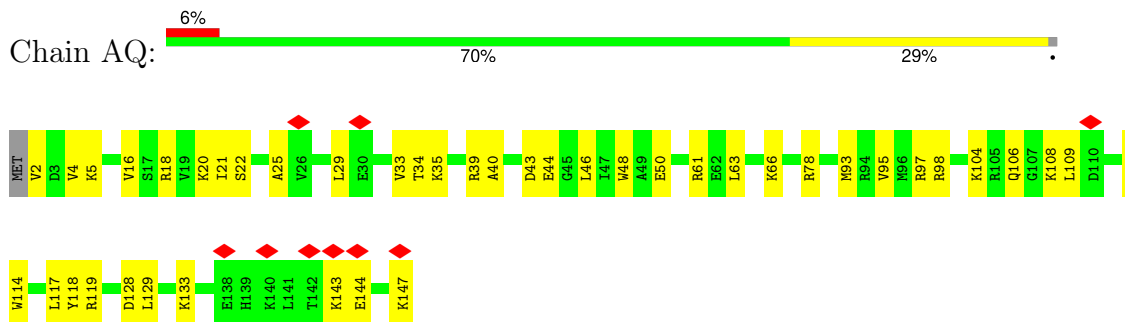
- Molecule 17: Large ribosomal subunit protein uL18



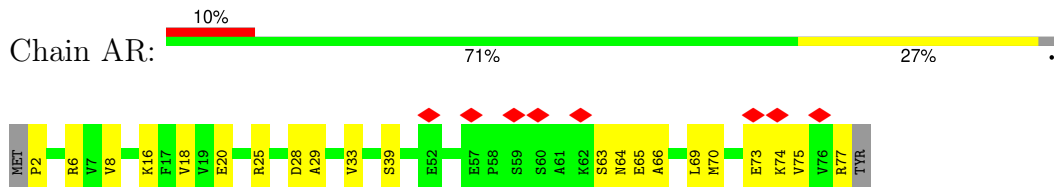
- Molecule 18: Large ribosomal subunit protein eL18



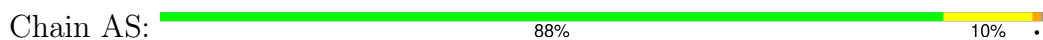
- Molecule 19: Large ribosomal subunit protein eL19



- Molecule 20: Large ribosomal subunit protein eL20

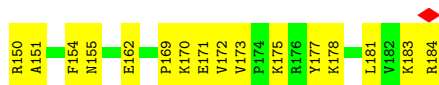
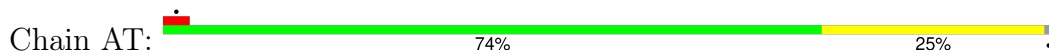


- Molecule 21: Large ribosomal subunit protein eL21





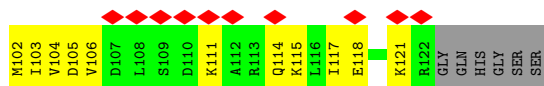
- Molecule 22: Large ribosomal subunit protein uL22



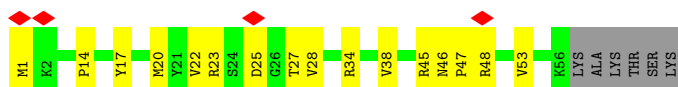
- Molecule 23: Large ribosomal subunit protein uL23



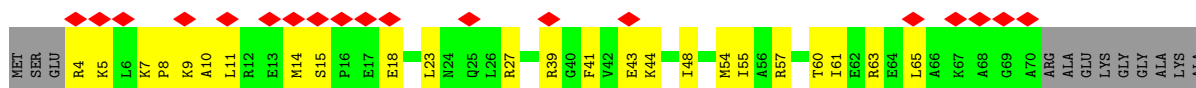
- Molecule 24: Large ribosomal subunit protein uL24



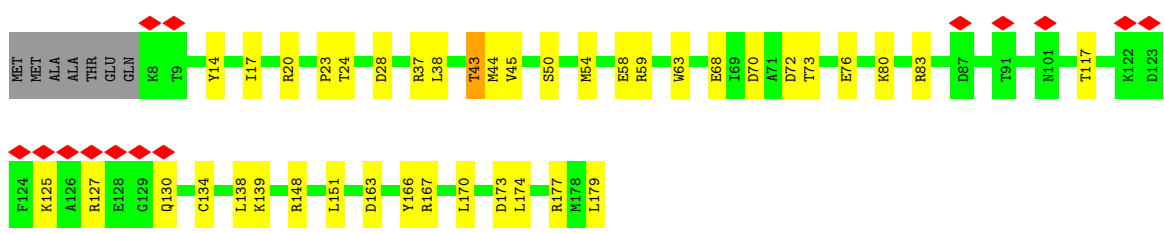
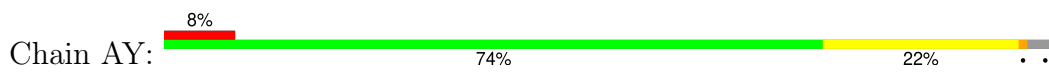
- Molecule 25: Large ribosomal subunit protein eL24



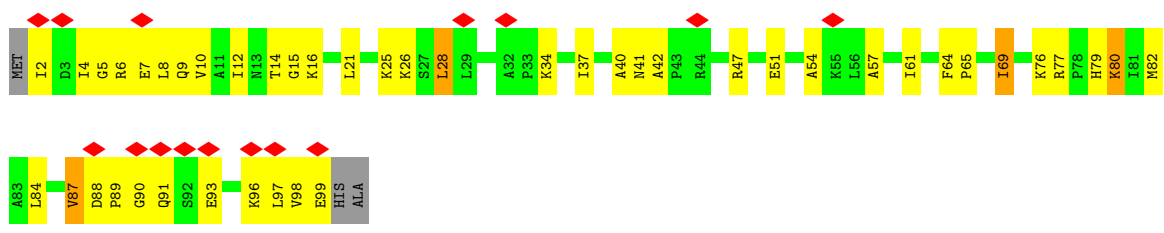
- Molecule 26: Large ribosomal subunit protein uL29



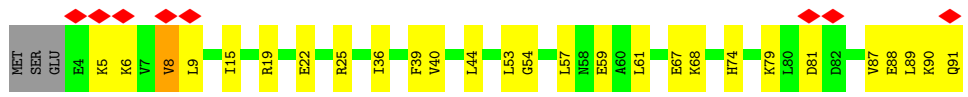
- Molecule 27: Large ribosomal subunit protein uL30



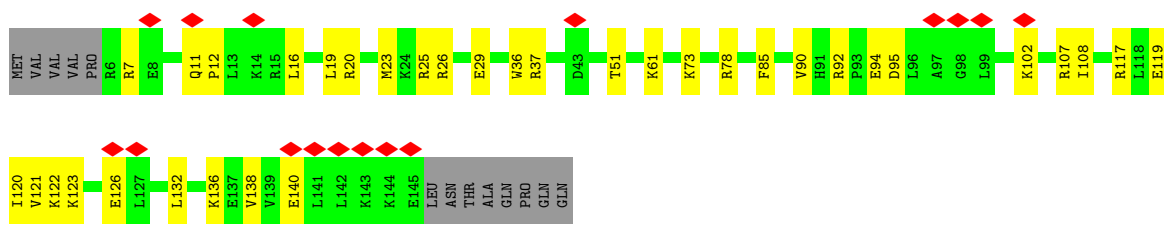
• Molecule 28: Large ribosomal subunit protein eL30



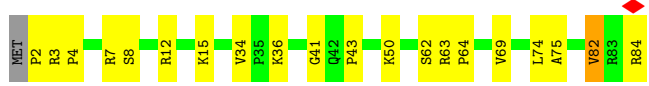
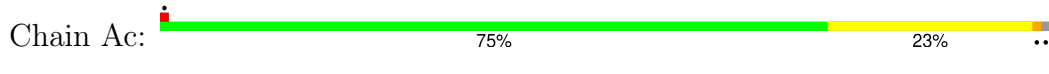
• Molecule 29: Large ribosomal subunit protein eL31



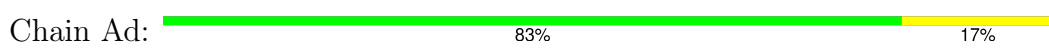
• Molecule 30: Large ribosomal subunit protein eL32



• Molecule 31: Large ribosomal subunit protein eL34



• Molecule 32: Large ribosomal subunit protein eL37





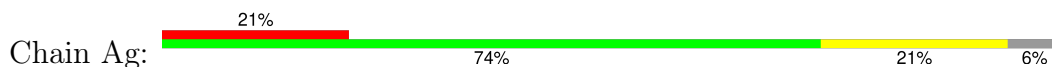
- Molecule 33: LSU ribosomal protein L38E



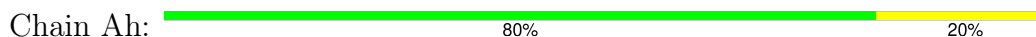
- Molecule 34: Large ribosomal subunit protein eL39



- Molecule 35: Large ribosomal subunit protein eL40



- Molecule 36: eL42

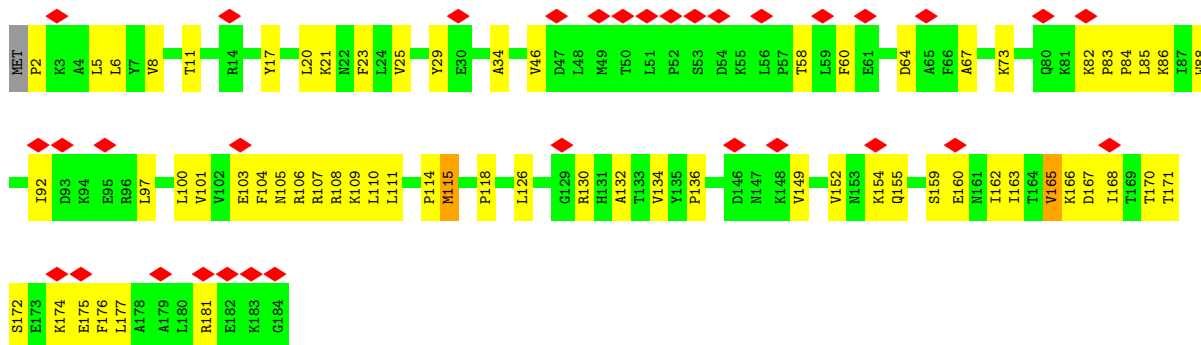


- Molecule 37: Large ribosomal subunit protein eL43

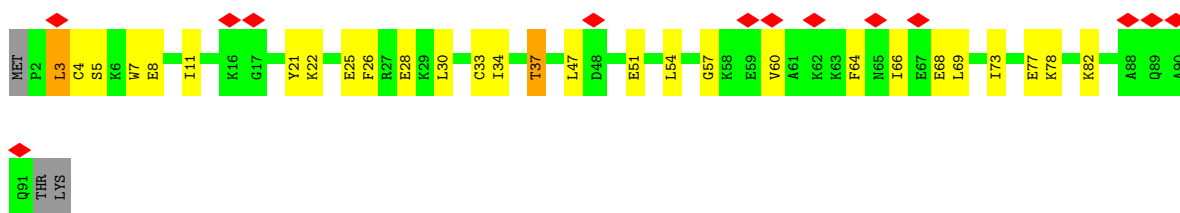


- Molecule 38: DJ-1/PfpI domain-containing protein

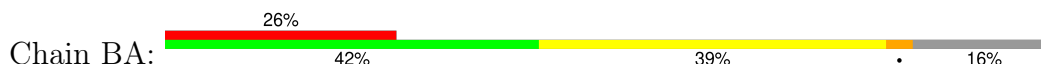




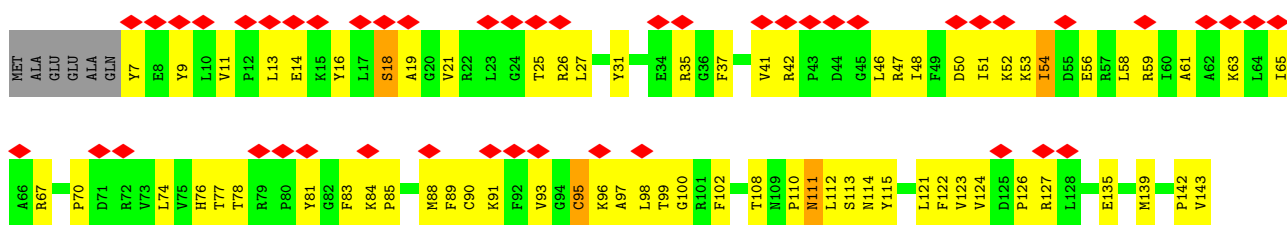
• Molecule 39: PaREP1 domain containing protein



• Molecule 40: Small ribosomal subunit protein eS1



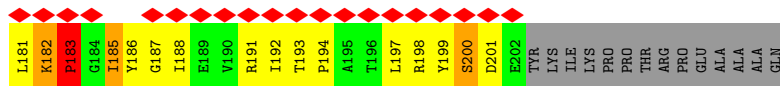
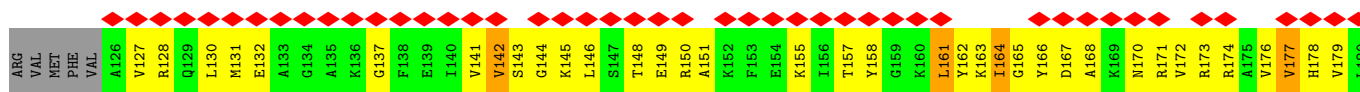
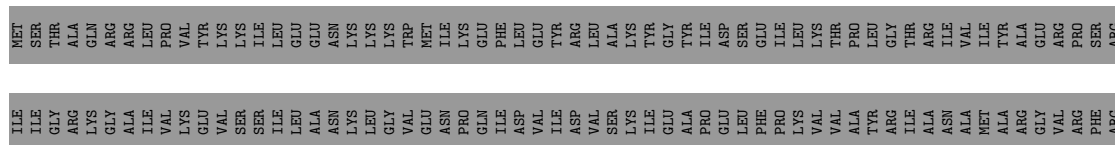
• Molecule 41: Small ribosomal subunit protein uS2



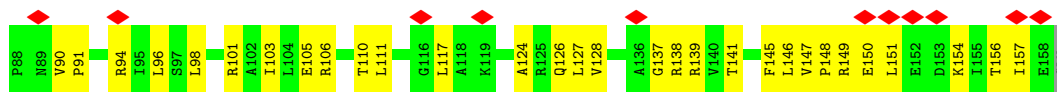
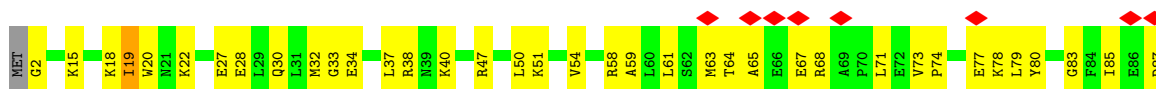


THR

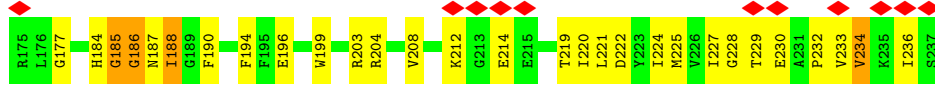
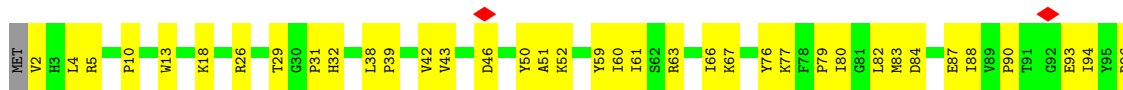
• Molecule 42: Small ribosomal subunit protein uS3



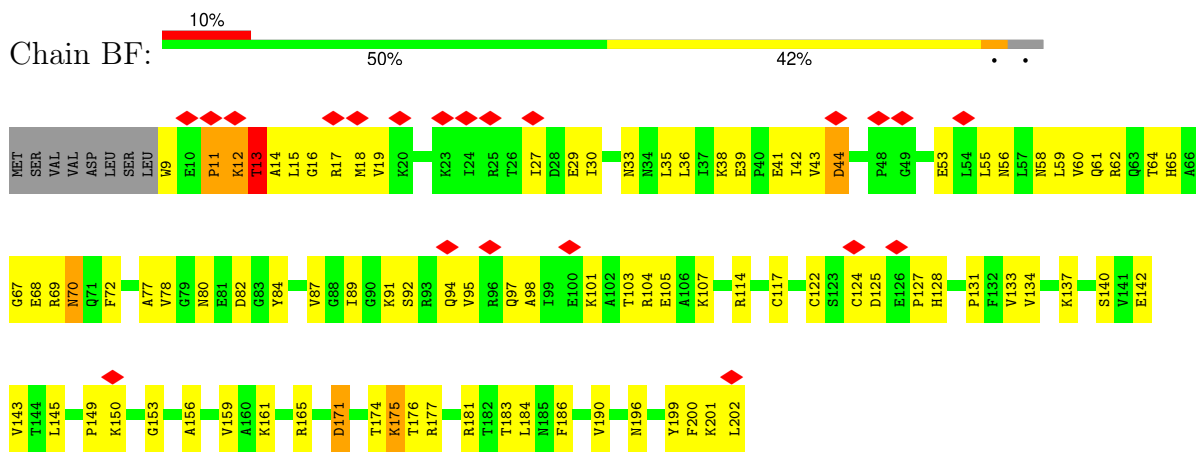
• Molecule 43: Small ribosomal subunit protein uS4



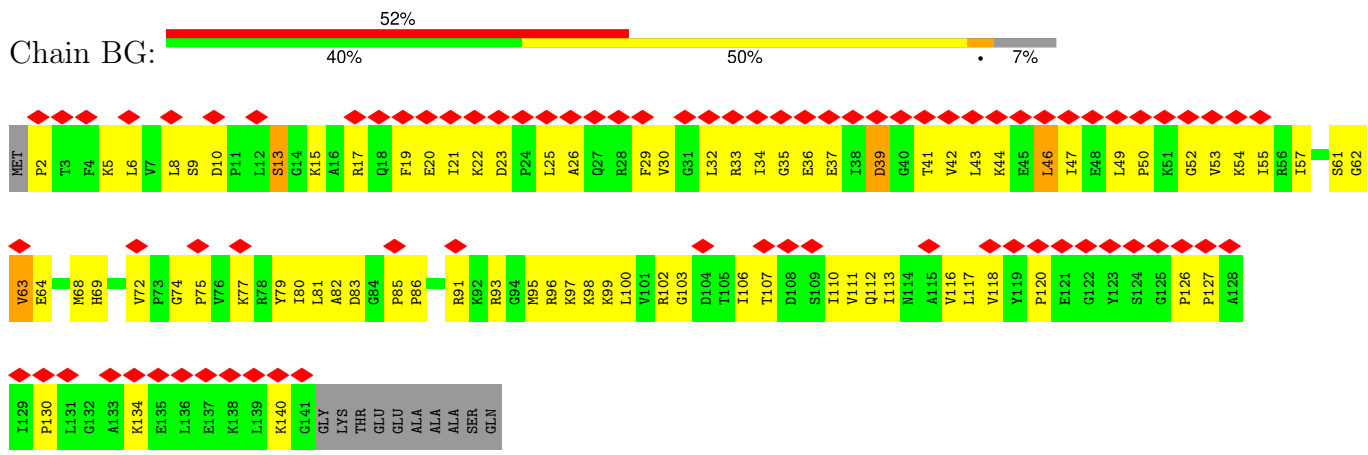
• Molecule 44: Small ribosomal subunit protein eS4



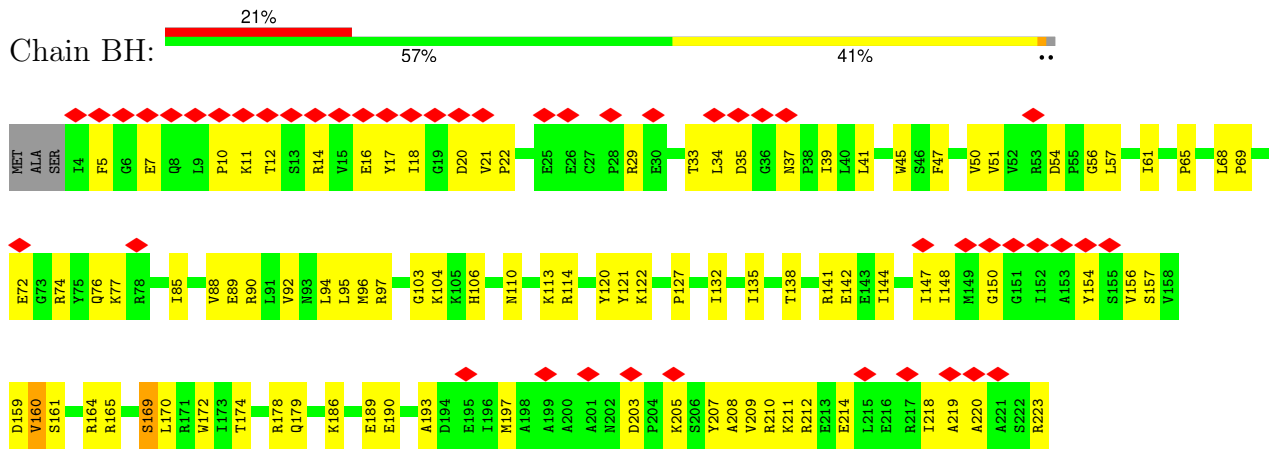
• Molecule 45: Small ribosomal subunit protein uS5



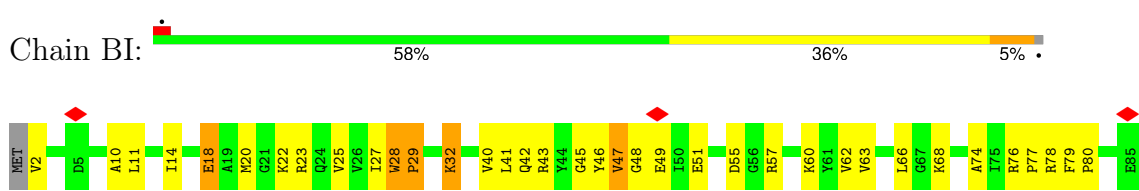
• Molecule 46: Small ribosomal subunit protein eS6



• Molecule 47: Small ribosomal subunit protein uS7

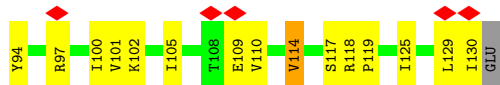
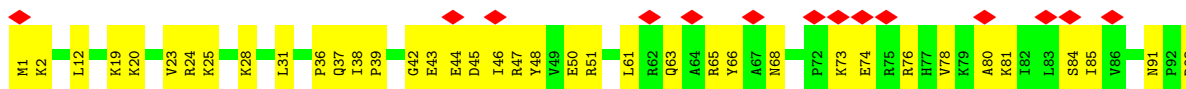


• Molecule 48: Small ribosomal subunit protein uS8

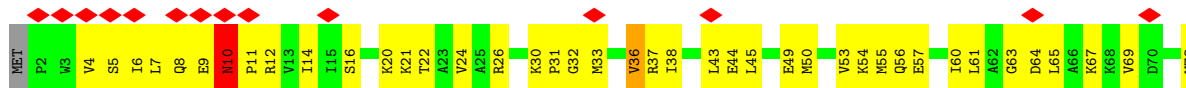




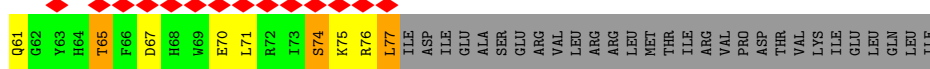
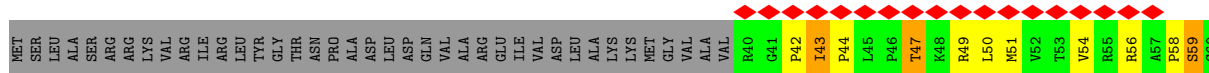
• Molecule 49: Small ribosomal subunit protein eS8



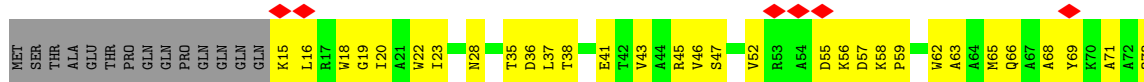
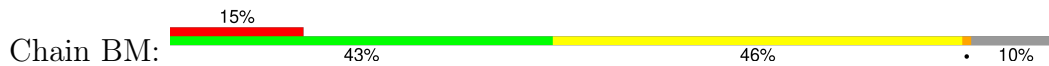
• Molecule 50: Small ribosomal subunit protein uS9



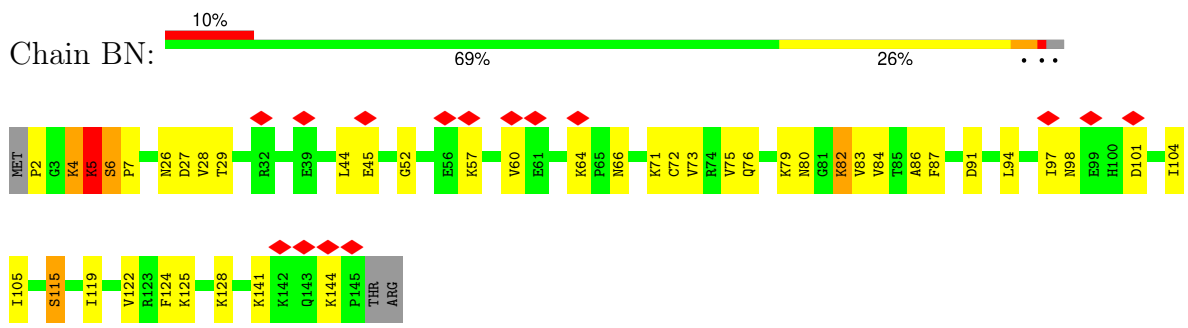
• Molecule 51: Small ribosomal subunit protein uS10



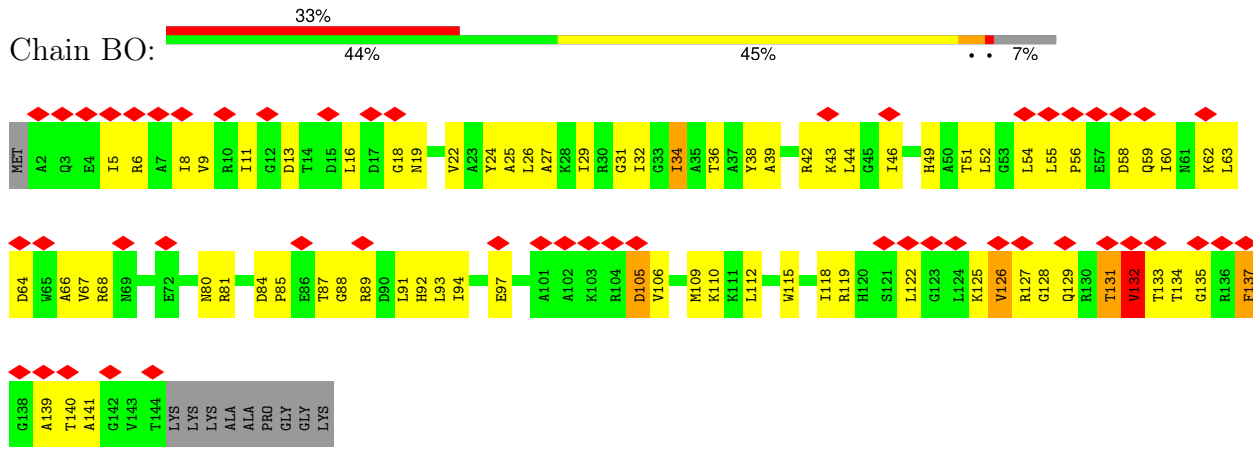
• Molecule 52: Small ribosomal subunit protein uS11



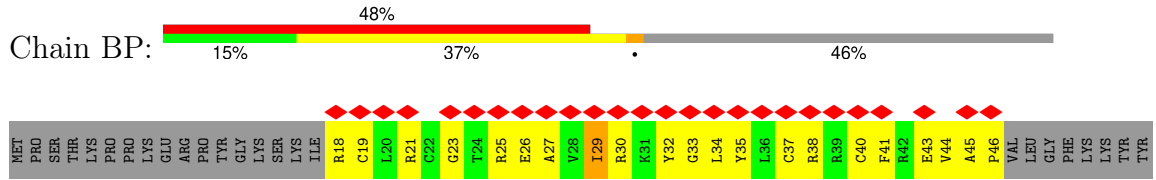
• Molecule 53: Small ribosomal subunit protein uS12



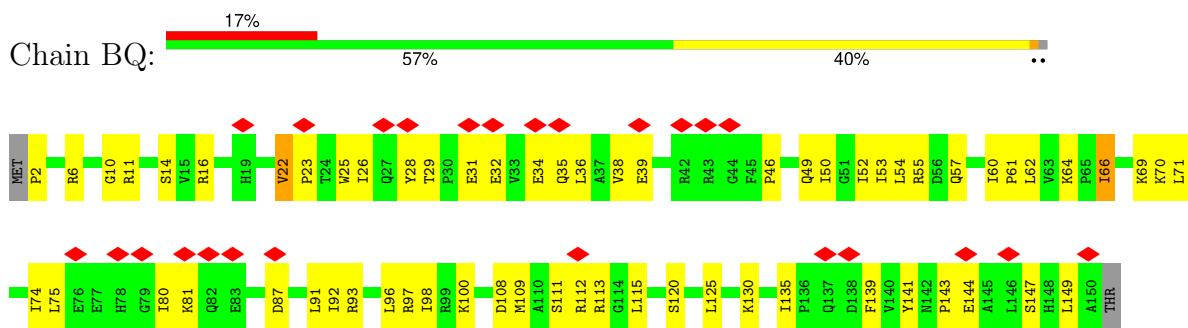
• Molecule 54: Small ribosomal subunit protein uS13



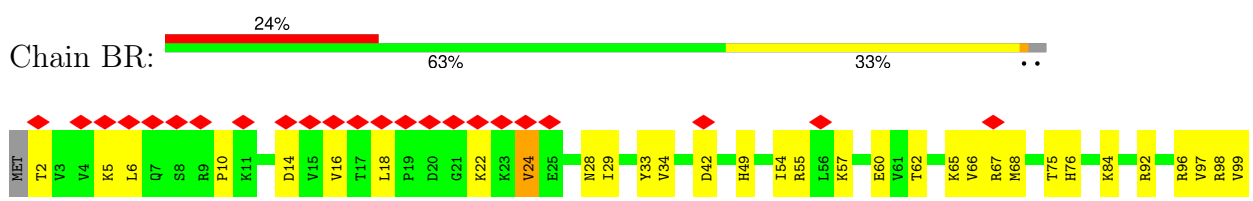
• Molecule 55: Small ribosomal subunit protein uS14



• Molecule 56: Small ribosomal subunit protein uS15

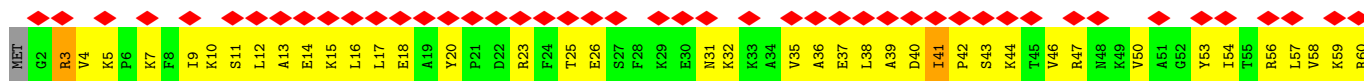
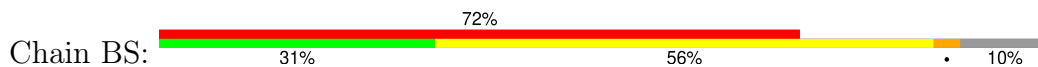


• Molecule 57: Small ribosomal subunit protein uS17

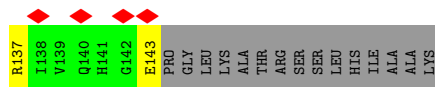
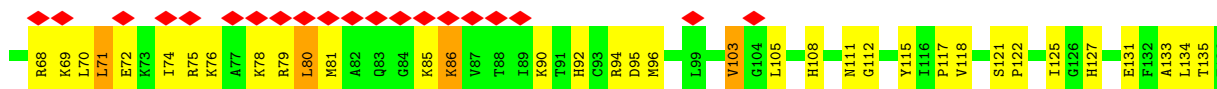
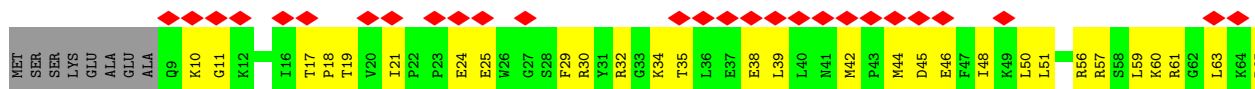




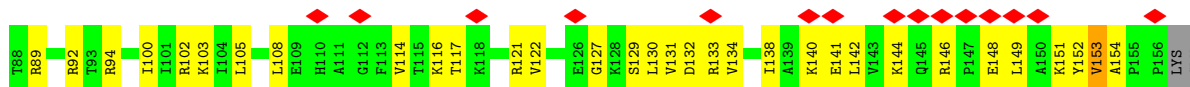
• Molecule 58: Small ribosomal subunit protein eS17



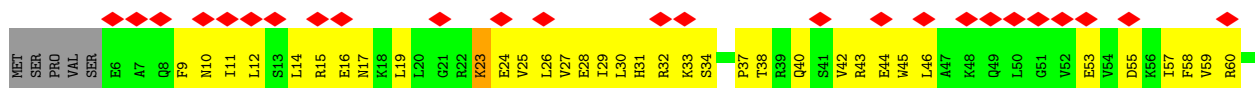
• Molecule 59: Small ribosomal subunit protein uS19



• Molecule 60: Small ribosomal subunit protein eS19

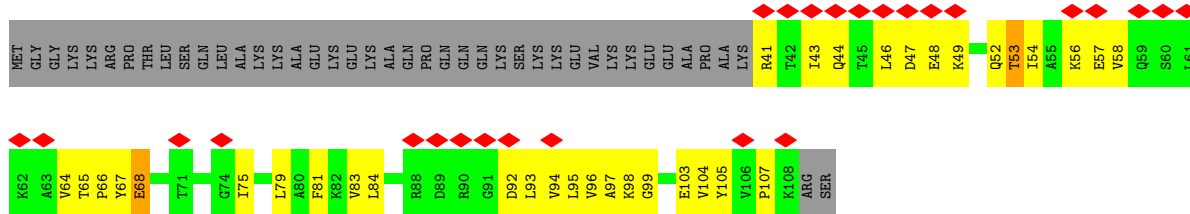
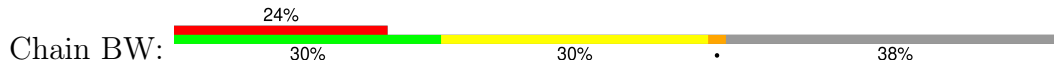


• Molecule 61: Small ribosomal subunit protein eS24

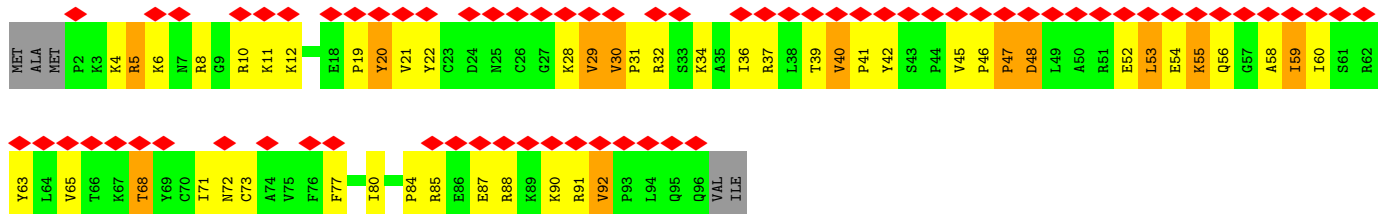




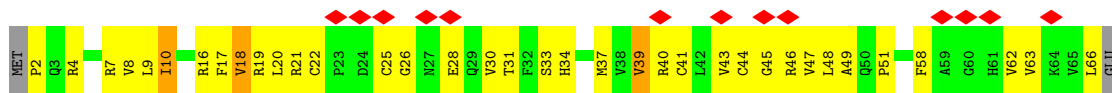
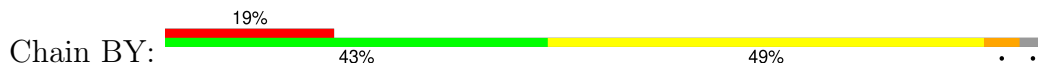
• Molecule 62: SSU ribosomal protein S25E



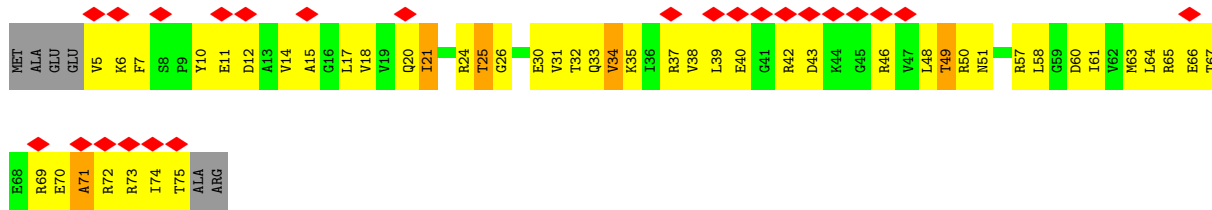
• Molecule 63: SSU ribosomal protein S26E



• Molecule 64: Small ribosomal subunit protein eS27

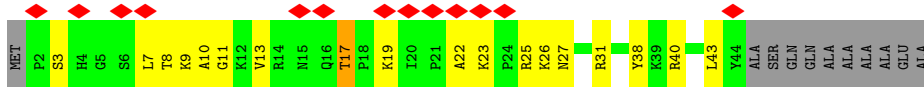


• Molecule 65: eS28

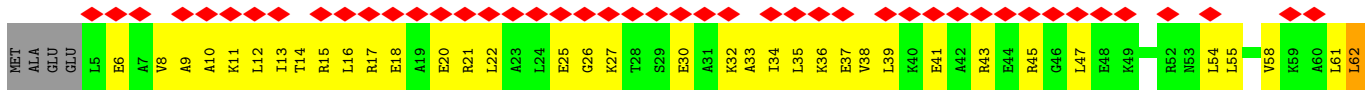


• Molecule 66: SSU ribosomal protein S30E

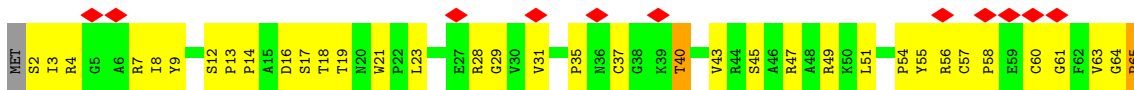




• Molecule 67: aS35



• Molecule 68: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 129829                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.526                                   | Depositor |
| Minimum map value                    | -0.618                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.049                                   | Depositor |
| Recommended contour level            | 0.215                                   | Depositor |
| Map size (Å)                         | 504.2144, 504.2144, 504.2144            | wwPDB     |
| Map dimensions                       | 608, 608, 608                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.8293, 0.8293, 0.8293                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, UR3, MG, M7A, MA6, OMU, 6MZ, B8T, OMC, G7M, PSU, OMG, SPM, 4AC, IAS, A2M, 5MC

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   | 2     | 0.35         | 0/3096         | 0.36        | 1/4830 (0.0%)   |
| 2   | 1     | 0.30         | 3/67134 (0.0%) | 0.34        | 8/104802 (0.0%) |
| 3   | 4     | 0.27         | 3/33464 (0.0%) | 0.39        | 21/52215 (0.0%) |
| 4   | AA    | 0.26         | 0/1847         | 0.44        | 0/2489          |
| 5   | AB    | 0.24         | 0/2678         | 0.38        | 0/3643          |
| 6   | AC    | 0.24         | 0/2234         | 0.43        | 0/3024          |
| 7   | AD    | 0.29         | 0/1431         | 0.43        | 0/1913          |
| 8   | AE    | 0.22         | 0/1548         | 0.40        | 0/2087          |
| 9   | AF    | 0.23         | 0/1114         | 0.46        | 0/1513          |
| 10  | AG    | 0.22         | 0/1542         | 0.34        | 0/2076          |
| 11  | AH    | 0.21         | 0/1265         | 0.37        | 0/1692          |
| 12  | AI    | 0.25         | 0/1093         | 0.44        | 0/1487          |
| 13  | AJ    | 0.24         | 0/795          | 0.52        | 0/1068          |
| 13  | AK    | 0.20         | 0/704          | 0.39        | 0/944           |
| 14  | AL    | 0.25         | 0/1225         | 0.39        | 0/1639          |
| 15  | AM    | 0.22         | 0/1594         | 0.33        | 0/2138          |
| 16  | AN    | 0.25         | 0/1365         | 0.42        | 0/1841          |
| 17  | AO    | 0.29         | 0/1647         | 0.39        | 0/2212          |
| 18  | AP    | 0.22         | 0/933          | 0.40        | 0/1263          |
| 19  | AQ    | 0.23         | 0/1233         | 0.43        | 0/1645          |
| 20  | AR    | 0.24         | 0/610          | 0.49        | 0/817           |
| 21  | AS    | 0.33         | 0/805          | 0.41        | 0/1081          |
| 22  | AT    | 0.22         | 0/1536         | 0.39        | 0/2075          |
| 23  | AU    | 0.21         | 0/655          | 0.39        | 0/877           |
| 24  | AV    | 0.23         | 0/990          | 0.42        | 0/1325          |
| 25  | AW    | 0.24         | 0/460          | 0.34        | 0/613           |
| 26  | AX    | 0.26         | 0/557          | 0.47        | 0/738           |
| 27  | AY    | 0.30         | 0/1407         | 0.47        | 0/1905          |
| 28  | AZ    | 0.26         | 0/754          | 0.49        | 0/1021          |
| 29  | Aa    | 0.23         | 0/735          | 0.38        | 0/986           |
| 30  | Ab    | 0.23         | 0/1209         | 0.42        | 0/1621          |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 31  | Ac    | 0.21         | 0/663           | 0.31        | 0/889            |
| 32  | Ad    | 0.24         | 0/442           | 0.35        | 0/587            |
| 33  | Ae    | 0.22         | 0/562           | 0.37        | 0/753            |
| 34  | Af    | 0.25         | 0/423           | 0.40        | 0/566            |
| 35  | Ag    | 0.20         | 0/424           | 0.38        | 0/564            |
| 36  | Ah    | 0.29         | 0/753           | 0.42        | 0/1001           |
| 37  | Ai    | 0.24         | 0/788           | 0.47        | 0/1057           |
| 38  | Aj    | 0.23         | 0/1497          | 0.46        | 1/2029 (0.0%)    |
| 39  | Ak    | 0.24         | 0/754           | 0.40        | 0/1005           |
| 40  | BA    | 0.25         | 0/1515          | 0.57        | 4/2043 (0.2%)    |
| 41  | BB    | 0.28         | 0/1638          | 0.53        | 2/2221 (0.1%)    |
| 42  | BC    | 0.33         | 0/620           | 0.71        | 1/831 (0.1%)     |
| 43  | BD    | 0.21         | 0/1308          | 0.41        | 0/1755           |
| 44  | BE    | 0.26         | 0/1929          | 0.53        | 0/2621           |
| 45  | BF    | 0.28         | 0/1522          | 0.60        | 4/2059 (0.2%)    |
| 46  | BG    | 0.22         | 0/1087          | 0.51        | 0/1465           |
| 47  | BH    | 0.22         | 0/1809          | 0.43        | 0/2444           |
| 48  | BI    | 0.30         | 0/1055          | 0.48        | 0/1425           |
| 49  | BJ    | 0.24         | 0/1023          | 0.38        | 0/1370           |
| 50  | BK    | 0.25         | 0/1079          | 0.50        | 0/1452           |
| 51  | BL    | 0.21         | 0/324           | 0.55        | 0/437            |
| 52  | BM    | 0.23         | 0/951           | 0.46        | 0/1288           |
| 53  | BN    | 0.29         | 0/1157          | 0.48        | 0/1551           |
| 54  | BO    | 0.22         | 0/1125          | 0.54        | 2/1518 (0.1%)    |
| 55  | BP    | 0.32         | 0/244           | 0.56        | 0/324            |
| 56  | BQ    | 0.22         | 0/1254          | 0.36        | 0/1692           |
| 57  | BR    | 0.23         | 0/1200          | 0.37        | 0/1629           |
| 58  | BS    | 0.23         | 0/524           | 0.49        | 0/698            |
| 59  | BT    | 0.22         | 0/1139          | 0.47        | 0/1533           |
| 60  | BU    | 0.22         | 0/1253          | 0.41        | 0/1695           |
| 61  | BV    | 0.21         | 0/960           | 0.42        | 0/1280           |
| 62  | BW    | 0.25         | 0/551           | 0.53        | 0/741            |
| 63  | BX    | 0.25         | 0/787           | 0.65        | 0/1054           |
| 64  | BY    | 0.23         | 0/511           | 0.50        | 1/689 (0.1%)     |
| 65  | BZ    | 0.27         | 0/555           | 0.65        | 1/745 (0.1%)     |
| 66  | Ba    | 0.18         | 0/364           | 0.31        | 0/486            |
| 67  | Bb    | 0.23         | 0/478           | 0.56        | 0/634            |
| 68  | Bc    | 0.27         | 0/491           | 0.53        | 0/670            |
| All | All   | 0.27         | 6/172419 (0.0%) | 0.39        | 46/254381 (0.0%) |

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

sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | AD    | 0                   | 2                   |
| 13  | AK    | 0                   | 1                   |
| 48  | BI    | 0                   | 3                   |
| 50  | BK    | 0                   | 1                   |
| All | All   | 0                   | 7                   |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | 4     | 880  | A2M  | O3'-P | 5.16 | 1.61        | 1.56     |
| 2   | 1     | 2059 | A2M  | O3'-P | 5.10 | 1.61        | 1.56     |
| 2   | 1     | 1990 | A2M  | O3'-P | 5.09 | 1.61        | 1.56     |
| 3   | 4     | 496  | A2M  | O3'-P | 5.05 | 1.61        | 1.56     |
| 2   | 1     | 2691 | A2M  | O3'-P | 5.02 | 1.61        | 1.56     |

The worst 5 of 46 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3   | 4     | 812 | C    | OP1-P-O3' | -11.30 | 74.10       | 108.00   |
| 3   | 4     | 101 | C    | OP1-P-O3' | -11.29 | 74.14       | 108.00   |
| 45  | BF    | 13  | THR  | CA-C-N    | 9.78   | 134.66      | 120.38   |
| 45  | BF    | 13  | THR  | C-N-CA    | 9.78   | 134.66      | 120.38   |
| 3   | 4     | 812 | C    | OP2-P-O3' | -9.44  | 79.69       | 108.00   |

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | AD    | 77  | ARG  | Sidechain |
| 7   | AD    | 78  | ARG  | Sidechain |
| 13  | AK    | 38  | GLY  | Peptide   |
| 48  | BI    | 28  | TRP  | Peptide   |
| 48  | BI    | 76  | ARG  | Sidechain |

## 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   | 2     | 2769  | 0        | 1405     | 34      | 0            |
| 2   | 1     | 61386 | 0        | 31065    | 1009    | 0            |
| 3   | 4     | 30817 | 0        | 15598    | 832     | 0            |
| 4   | AA    | 1803  | 0        | 1849     | 49      | 0            |
| 5   | AB    | 2611  | 0        | 2737     | 75      | 0            |
| 6   | AC    | 2178  | 0        | 2263     | 66      | 0            |
| 7   | AD    | 1412  | 0        | 1511     | 54      | 0            |
| 8   | AE    | 1520  | 0        | 1607     | 48      | 0            |
| 9   | AF    | 1095  | 0        | 1156     | 44      | 0            |
| 10  | AG    | 1510  | 0        | 1627     | 32      | 0            |
| 11  | AH    | 1244  | 0        | 1346     | 39      | 0            |
| 12  | AI    | 1068  | 0        | 1110     | 36      | 0            |
| 13  | AJ    | 788   | 0        | 853      | 51      | 0            |
| 13  | AK    | 700   | 0        | 760      | 49      | 0            |
| 14  | AL    | 1198  | 0        | 1233     | 41      | 0            |
| 15  | AM    | 1558  | 0        | 1641     | 37      | 0            |
| 16  | AN    | 1336  | 0        | 1378     | 30      | 0            |
| 17  | AO    | 1615  | 0        | 1688     | 32      | 0            |
| 18  | AP    | 920   | 0        | 1010     | 21      | 0            |
| 19  | AQ    | 1214  | 0        | 1272     | 30      | 0            |
| 20  | AR    | 603   | 0        | 647      | 14      | 0            |
| 21  | AS    | 788   | 0        | 832      | 9       | 0            |
| 22  | AT    | 1496  | 0        | 1575     | 31      | 0            |
| 23  | AU    | 651   | 0        | 720      | 22      | 0            |
| 24  | AV    | 976   | 0        | 1073     | 37      | 0            |
| 25  | AW    | 449   | 0        | 465      | 14      | 0            |
| 26  | AX    | 554   | 0        | 613      | 21      | 0            |
| 27  | AY    | 1374  | 0        | 1422     | 30      | 0            |
| 28  | AZ    | 742   | 0        | 796      | 39      | 0            |
| 29  | Aa    | 726   | 0        | 794      | 18      | 0            |
| 30  | Ab    | 1183  | 0        | 1270     | 29      | 0            |
| 31  | Ac    | 649   | 0        | 698      | 23      | 0            |
| 32  | Ad    | 429   | 0        | 430      | 7       | 0            |
| 33  | Ae    | 552   | 0        | 592      | 22      | 0            |
| 34  | Af    | 415   | 0        | 464      | 12      | 0            |
| 35  | Ag    | 417   | 0        | 440      | 9       | 0            |
| 36  | Ah    | 739   | 0        | 782      | 14      | 0            |
| 37  | Ai    | 769   | 0        | 792      | 27      | 0            |
| 38  | Aj    | 1469  | 0        | 1535     | 50      | 0            |
| 39  | Ak    | 743   | 0        | 775      | 20      | 0            |
| 40  | BA    | 1487  | 0        | 1589     | 78      | 0            |
| 41  | BB    | 1600  | 0        | 1645     | 104     | 0            |
| 42  | BC    | 611   | 0        | 648      | 55      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | BD    | 1284  | 0        | 1391     | 64      | 0            |
| 44  | BE    | 1883  | 0        | 1968     | 81      | 0            |
| 45  | BF    | 1498  | 0        | 1557     | 96      | 0            |
| 46  | BG    | 1065  | 0        | 1139     | 92      | 0            |
| 47  | BH    | 1773  | 0        | 1828     | 85      | 0            |
| 48  | BI    | 1036  | 0        | 1090     | 46      | 0            |
| 49  | BJ    | 1007  | 0        | 1086     | 44      | 0            |
| 50  | BK    | 1058  | 0        | 1123     | 66      | 0            |
| 51  | BL    | 315   | 0        | 329      | 30      | 0            |
| 52  | BM    | 941   | 0        | 984      | 68      | 0            |
| 53  | BN    | 1133  | 0        | 1203     | 44      | 0            |
| 54  | BO    | 1108  | 0        | 1163     | 75      | 0            |
| 55  | BP    | 241   | 0        | 251      | 26      | 0            |
| 56  | BQ    | 1224  | 0        | 1287     | 57      | 0            |
| 57  | BR    | 1171  | 0        | 1244     | 50      | 0            |
| 58  | BS    | 517   | 0        | 560      | 50      | 0            |
| 59  | BT    | 1111  | 0        | 1170     | 68      | 0            |
| 60  | BU    | 1225  | 0        | 1301     | 60      | 0            |
| 61  | BV    | 950   | 0        | 1013     | 63      | 0            |
| 62  | BW    | 544   | 0        | 587      | 27      | 0            |
| 63  | BX    | 772   | 0        | 827      | 70      | 0            |
| 64  | BY    | 501   | 0        | 524      | 30      | 0            |
| 65  | BZ    | 552   | 0        | 594      | 54      | 0            |
| 66  | Ba    | 357   | 0        | 394      | 16      | 0            |
| 67  | Bb    | 479   | 0        | 545      | 52      | 0            |
| 68  | Bc    | 477   | 0        | 479      | 47      | 0            |
| 69  | 1     | 616   | 0        | 1144     | 23      | 0            |
| 69  | 4     | 252   | 0        | 468      | 13      | 0            |
| 69  | AL    | 14    | 0        | 26       | 0       | 0            |
| 69  | Ah    | 14    | 0        | 26       | 0       | 0            |
| 70  | 1     | 170   | 0        | 0        | 0       | 0            |
| 70  | 4     | 78    | 0        | 0        | 0       | 0            |
| 70  | AA    | 1     | 0        | 0        | 0       | 0            |
| 70  | AL    | 2     | 0        | 0        | 0       | 0            |
| 70  | BK    | 1     | 0        | 0        | 0       | 0            |
| 71  | AW    | 1     | 0        | 0        | 0       | 0            |
| 71  | Ad    | 1     | 0        | 0        | 0       | 0            |
| 71  | Ag    | 1     | 0        | 0        | 0       | 0            |
| 71  | Ah    | 1     | 0        | 0        | 0       | 0            |
| 71  | Ai    | 1     | 0        | 0        | 0       | 0            |
| 71  | BF    | 1     | 0        | 0        | 0       | 0            |
| 71  | BP    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 71  | BR    | 1     | 0        | 0        | 0       | 0            |
| 71  | BX    | 1     | 0        | 0        | 0       | 0            |
| 71  | BY    | 1     | 0        | 0        | 0       | 0            |
| 71  | Bc    | 1     | 0        | 0        | 0       | 0            |
| 72  | 1     | 5640  | 0        | 0        | 140     | 0            |
| 72  | 2     | 181   | 0        | 0        | 1       | 0            |
| 72  | 4     | 1487  | 0        | 0        | 83      | 0            |
| 72  | AA    | 12    | 0        | 0        | 0       | 0            |
| 72  | AB    | 1     | 0        | 0        | 0       | 0            |
| 72  | AC    | 6     | 0        | 0        | 0       | 0            |
| 72  | AG    | 2     | 0        | 0        | 0       | 0            |
| 72  | AH    | 3     | 0        | 0        | 0       | 0            |
| 72  | AL    | 10    | 0        | 0        | 0       | 0            |
| 72  | AM    | 2     | 0        | 0        | 0       | 0            |
| 72  | AN    | 2     | 0        | 0        | 0       | 0            |
| 72  | AO    | 2     | 0        | 0        | 0       | 0            |
| 72  | AP    | 1     | 0        | 0        | 1       | 0            |
| 72  | AQ    | 1     | 0        | 0        | 0       | 0            |
| 72  | AT    | 2     | 0        | 0        | 0       | 0            |
| 72  | AU    | 1     | 0        | 0        | 0       | 0            |
| 72  | AX    | 22    | 0        | 0        | 4       | 0            |
| 72  | AY    | 2     | 0        | 0        | 0       | 0            |
| 72  | Aa    | 1     | 0        | 0        | 0       | 0            |
| 72  | Ab    | 6     | 0        | 0        | 0       | 0            |
| 72  | Ad    | 3     | 0        | 0        | 0       | 0            |
| 72  | Ah    | 1     | 0        | 0        | 0       | 0            |
| 72  | BA    | 18    | 0        | 0        | 6       | 0            |
| 72  | BB    | 18    | 0        | 0        | 3       | 0            |
| 72  | BC    | 9     | 0        | 0        | 6       | 0            |
| 72  | BD    | 28    | 0        | 0        | 6       | 0            |
| 72  | BE    | 23    | 0        | 0        | 2       | 0            |
| 72  | BF    | 32    | 0        | 0        | 10      | 0            |
| 72  | BG    | 19    | 0        | 0        | 2       | 0            |
| 72  | BH    | 26    | 0        | 0        | 3       | 0            |
| 72  | BI    | 20    | 0        | 0        | 3       | 0            |
| 72  | BJ    | 13    | 0        | 0        | 0       | 0            |
| 72  | BK    | 12    | 0        | 0        | 0       | 0            |
| 72  | BL    | 7     | 0        | 0        | 0       | 0            |
| 72  | BM    | 9     | 0        | 0        | 3       | 0            |
| 72  | BN    | 12    | 0        | 0        | 3       | 0            |
| 72  | BO    | 26    | 0        | 0        | 5       | 0            |
| 72  | BP    | 8     | 0        | 0        | 6       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 72  | BQ    | 15     | 0        | 0        | 0       | 0            |
| 72  | BR    | 12     | 0        | 0        | 0       | 0            |
| 72  | BS    | 5      | 0        | 0        | 1       | 0            |
| 72  | BT    | 17     | 0        | 0        | 10      | 0            |
| 72  | BU    | 13     | 0        | 0        | 2       | 0            |
| 72  | BV    | 9      | 0        | 0        | 4       | 0            |
| 72  | BW    | 8      | 0        | 0        | 2       | 0            |
| 72  | BX    | 12     | 0        | 0        | 9       | 0            |
| 72  | BY    | 10     | 0        | 0        | 2       | 0            |
| 72  | BZ    | 12     | 0        | 0        | 8       | 0            |
| 72  | Ba    | 8      | 0        | 0        | 0       | 0            |
| 72  | Bb    | 7      | 0        | 0        | 4       | 0            |
| 72  | Bc    | 16     | 0        | 0        | 4       | 0            |
| All | All   | 171357 | 0        | 121007   | 4232    | 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 15.

The worst 5 of 4232 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) |
|-------------------|------------------|--------------------------|-------------------|
| 43:BD:150:GLU:HG2 | 72:BD:204:HOH:O  | 1.37                     | 1.23              |
| 72:4:3318:HOH:O   | 57:BR:98:ARG:HD2 | 1.43                     | 1.14              |
| 59:BT:10:LYS:HD3  | 72:BT:204:HOH:O  | 1.46                     | 1.14              |
| 42:BC:191:ARG:HG3 | 72:BC:303:HOH:O  | 1.50                     | 1.11              |
| 40:BA:24:LEU:HD23 | 72:BA:308:HOH:O  | 1.50                     | 1.10              |

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 PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 4   | AA    | 237/244 (97%) | 228 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 5   | AB    | 334/338 (99%) | 326 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 6   | AC    | 276/285 (97%) | 271 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 7   | AD    | 176/178 (99%) | 169 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 8   | AE    | 193/196 (98%) | 189 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 9   | AF    | 143/149 (96%) | 141 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 10  | AG    | 181/186 (97%) | 177 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 11  | AH    | 153/157 (98%) | 151 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 12  | AI    | 136/144 (94%) | 134 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 13  | AJ    | 99/103 (96%)  | 95 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 13  | AK    | 88/103 (85%)  | 83 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 14  | AL    | 150/156 (96%) | 144 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 15  | AM    | 182/189 (96%) | 178 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 16  | AN    | 167/178 (94%) | 162 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 17  | AO    | 198/205 (97%) | 198 (100%) | 0       | 0        | 100         | 100 |
| 18  | AP    | 119/122 (98%) | 118 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 19  | AQ    | 144/147 (98%) | 143 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 20  | AR    | 74/78 (95%)   | 74 (100%)  | 0       | 0        | 100         | 100 |
| 21  | AS    | 96/99 (97%)   | 89 (93%)   | 7 (7%)  | 0        | 100         | 100 |
| 22  | AT    | 181/184 (98%) | 180 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 23  | AU    | 79/81 (98%)   | 76 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 24  | AV    | 119/128 (93%) | 117 (98%)  | 1 (1%)  | 1 (1%)   | 16          | 17  |
| 25  | AW    | 54/62 (87%)   | 53 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 26  | AX    | 65/79 (82%)   | 65 (100%)  | 0       | 0        | 100         | 100 |
| 27  | AY    | 170/179 (95%) | 161 (95%)  | 8 (5%)  | 1 (1%)   | 21          | 24  |
| 28  | AZ    | 96/101 (95%)  | 93 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 29  | Aa    | 86/91 (94%)   | 85 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 30  | Ab    | 138/153 (90%) | 137 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 31  | Ac    | 81/84 (96%)   | 80 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 32  | Ad    | 50/52 (96%)   | 48 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 33  | Ae    | 64/67 (96%)   | 63 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 34  | Af    | 48/51 (94%)   | 45 (94%)   | 3 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 35  | Ag    | 48/53 (91%)   | 48 (100%) | 0        | 0        | 100         | 100 |
| 36  | Ah    | 89/91 (98%)   | 89 (100%) | 0        | 0        | 100         | 100 |
| 37  | Ai    | 97/102 (95%)  | 89 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 38  | Aj    | 181/184 (98%) | 172 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 39  | Ak    | 88/93 (95%)   | 87 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 40  | BA    | 185/222 (83%) | 180 (97%) | 4 (2%)   | 1 (0%)   | 24          | 27  |
| 41  | BB    | 196/208 (94%) | 187 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 42  | BC    | 75/216 (35%)  | 58 (77%)  | 16 (21%) | 1 (1%)   | 9           | 8   |
| 43  | BD    | 155/159 (98%) | 153 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 44  | BE    | 234/237 (99%) | 219 (94%) | 13 (6%)  | 2 (1%)   | 14          | 14  |
| 45  | BF    | 192/202 (95%) | 180 (94%) | 11 (6%)  | 1 (0%)   | 24          | 27  |
| 46  | BG    | 138/151 (91%) | 130 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 47  | BH    | 218/223 (98%) | 206 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 48  | BI    | 127/130 (98%) | 121 (95%) | 5 (4%)   | 1 (1%)   | 16          | 17  |
| 49  | BJ    | 128/131 (98%) | 124 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 50  | BK    | 132/142 (93%) | 119 (90%) | 11 (8%)  | 2 (2%)   | 8           | 7   |
| 51  | BL    | 36/106 (34%)  | 30 (83%)  | 5 (14%)  | 1 (3%)   | 4           | 2   |
| 52  | BM    | 123/141 (87%) | 116 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 53  | BN    | 142/147 (97%) | 130 (92%) | 10 (7%)  | 2 (1%)   | 9           | 7   |
| 54  | BO    | 141/153 (92%) | 129 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 55  | BP    | 27/54 (50%)   | 21 (78%)  | 5 (18%)  | 1 (4%)   | 2           | 1   |
| 56  | BQ    | 147/151 (97%) | 146 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 57  | BR    | 142/147 (97%) | 139 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 58  | BS    | 62/71 (87%)   | 57 (92%)  | 5 (8%)   | 0        | 100         | 100 |
| 59  | BT    | 133/158 (84%) | 128 (96%) | 4 (3%)   | 1 (1%)   | 16          | 17  |
| 60  | BU    | 153/158 (97%) | 146 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 61  | BV    | 113/128 (88%) | 111 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 62  | BW    | 66/110 (60%)  | 64 (97%)  | 1 (2%)   | 1 (2%)   | 8           | 7   |
| 63  | BX    | 93/100 (93%)  | 69 (74%)  | 18 (19%) | 6 (6%)   | 1           | 0   |
| 64  | BY    | 63/67 (94%)   | 57 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 65  | BZ    | 69/77 (90%)   | 63 (91%)  | 6 (9%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 66  | Ba    | 41/54 (76%)     | 41 (100%)  | 0        | 0        | 100         | 100 |
| 67  | Bb    | 58/68 (85%)     | 57 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 68  | Bc    | 62/65 (95%)     | 59 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| All | All   | 8331/9068 (92%) | 7998 (96%) | 311 (4%) | 22 (0%)  | 37          | 43  |

5 of 22 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | BE    | 185 | GLY  |
| 44  | BE    | 186 | GLY  |
| 50  | BK    | 10  | ASN  |
| 53  | BN    | 5   | LYS  |
| 53  | BN    | 6   | SER  |

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4   | AA    | 181/186 (97%)  | 177 (98%) | 4 (2%)   | 45          | 59  |
| 5   | AB    | 280/282 (99%)  | 275 (98%) | 5 (2%)   | 51          | 66  |
| 6   | AC    | 226/231 (98%)  | 222 (98%) | 4 (2%)   | 51          | 66  |
| 7   | AD    | 149/149 (100%) | 140 (94%) | 9 (6%)   | 17          | 21  |
| 8   | AE    | 165/165 (100%) | 161 (98%) | 4 (2%)   | 43          | 57  |
| 9   | AF    | 115/118 (98%)  | 113 (98%) | 2 (2%)   | 53          | 68  |
| 10  | AG    | 163/165 (99%)  | 160 (98%) | 3 (2%)   | 51          | 66  |
| 11  | AH    | 133/135 (98%)  | 129 (97%) | 4 (3%)   | 36          | 48  |
| 12  | AI    | 115/118 (98%)  | 114 (99%) | 1 (1%)   | 70          | 82  |
| 13  | AJ    | 87/89 (98%)    | 87 (100%) | 0        | 100         | 100 |
| 13  | AK    | 77/89 (86%)    | 73 (95%)  | 4 (5%)   | 21          | 25  |
| 14  | AL    | 121/125 (97%)  | 116 (96%) | 5 (4%)   | 27          | 36  |
| 15  | AM    | 161/165 (98%)  | 158 (98%) | 3 (2%)   | 50          | 65  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 16  | AN    | 134/140 (96%)  | 132 (98%) | 2 (2%)   | 57          | 72  |
| 17  | AO    | 166/169 (98%)  | 163 (98%) | 3 (2%)   | 51          | 66  |
| 18  | AP    | 99/100 (99%)   | 95 (96%)  | 4 (4%)   | 28          | 37  |
| 19  | AQ    | 127/128 (99%)  | 123 (97%) | 4 (3%)   | 35          | 47  |
| 20  | AR    | 69/71 (97%)    | 67 (97%)  | 2 (3%)   | 37          | 49  |
| 21  | AS    | 84/85 (99%)    | 83 (99%)  | 1 (1%)   | 63          | 77  |
| 22  | AT    | 157/158 (99%)  | 154 (98%) | 3 (2%)   | 50          | 65  |
| 23  | AU    | 71/71 (100%)   | 71 (100%) | 0        | 100         | 100 |
| 24  | AV    | 107/112 (96%)  | 104 (97%) | 3 (3%)   | 38          | 51  |
| 25  | AW    | 48/53 (91%)    | 48 (100%) | 0        | 100         | 100 |
| 26  | AX    | 58/65 (89%)    | 57 (98%)  | 1 (2%)   | 53          | 68  |
| 27  | AY    | 147/152 (97%)  | 145 (99%) | 2 (1%)   | 59          | 73  |
| 28  | AZ    | 77/79 (98%)    | 71 (92%)  | 6 (8%)   | 11          | 12  |
| 29  | Aa    | 78/81 (96%)    | 76 (97%)  | 2 (3%)   | 40          | 54  |
| 30  | Ab    | 125/137 (91%)  | 124 (99%) | 1 (1%)   | 73          | 84  |
| 31  | Ac    | 67/68 (98%)    | 66 (98%)  | 1 (2%)   | 57          | 72  |
| 32  | Ad    | 44/44 (100%)   | 44 (100%) | 0        | 100         | 100 |
| 33  | Ae    | 60/61 (98%)    | 59 (98%)  | 1 (2%)   | 53          | 68  |
| 34  | Af    | 42/43 (98%)    | 41 (98%)  | 1 (2%)   | 43          | 57  |
| 35  | Ag    | 46/49 (94%)    | 46 (100%) | 0        | 100         | 100 |
| 36  | Ah    | 82/82 (100%)   | 81 (99%)  | 1 (1%)   | 63          | 77  |
| 37  | Ai    | 77/80 (96%)    | 76 (99%)  | 1 (1%)   | 61          | 76  |
| 38  | Aj    | 161/162 (99%)  | 158 (98%) | 3 (2%)   | 50          | 65  |
| 39  | Ak    | 79/82 (96%)    | 76 (96%)  | 3 (4%)   | 29          | 39  |
| 40  | BA    | 157/181 (87%)  | 147 (94%) | 10 (6%)  | 16          | 18  |
| 41  | BB    | 174/182 (96%)  | 165 (95%) | 9 (5%)   | 21          | 25  |
| 42  | BC    | 63/183 (34%)   | 53 (84%)  | 10 (16%) | 2           | 2   |
| 43  | BD    | 136/138 (99%)  | 131 (96%) | 5 (4%)   | 30          | 40  |
| 44  | BE    | 203/204 (100%) | 194 (96%) | 9 (4%)   | 25          | 33  |
| 45  | BF    | 161/169 (95%)  | 151 (94%) | 10 (6%)  | 16          | 19  |
| 46  | BG    | 114/121 (94%)  | 110 (96%) | 4 (4%)   | 32          | 42  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 47  | BH    | 191/193 (99%)   | 185 (97%)  | 6 (3%)   | 35          | 47  |
| 48  | BI    | 109/110 (99%)   | 102 (94%)  | 7 (6%)   | 16          | 18  |
| 49  | BJ    | 105/106 (99%)   | 104 (99%)  | 1 (1%)   | 68          | 81  |
| 50  | BK    | 110/117 (94%)   | 104 (94%)  | 6 (6%)   | 19          | 24  |
| 51  | BL    | 34/94 (36%)     | 29 (85%)   | 5 (15%)  | 3           | 2   |
| 52  | BM    | 93/106 (88%)    | 90 (97%)   | 3 (3%)   | 34          | 46  |
| 53  | BN    | 117/120 (98%)   | 113 (97%)  | 4 (3%)   | 32          | 43  |
| 54  | BO    | 113/119 (95%)   | 104 (92%)  | 9 (8%)   | 11          | 12  |
| 55  | BP    | 25/48 (52%)     | 25 (100%)  | 0        | 100         | 100 |
| 56  | BQ    | 135/137 (98%)   | 129 (96%)  | 6 (4%)   | 25          | 33  |
| 57  | BR    | 131/134 (98%)   | 122 (93%)  | 9 (7%)   | 14          | 16  |
| 58  | BS    | 55/59 (93%)     | 51 (93%)   | 4 (7%)   | 13          | 14  |
| 59  | BT    | 120/137 (88%)   | 115 (96%)  | 5 (4%)   | 26          | 35  |
| 60  | BU    | 127/130 (98%)   | 120 (94%)  | 7 (6%)   | 19          | 24  |
| 61  | BV    | 101/111 (91%)   | 97 (96%)   | 4 (4%)   | 28          | 37  |
| 62  | BW    | 59/94 (63%)     | 54 (92%)   | 5 (8%)   | 10          | 11  |
| 63  | BX    | 85/89 (96%)     | 78 (92%)   | 7 (8%)   | 10          | 11  |
| 64  | BY    | 55/57 (96%)     | 51 (93%)   | 4 (7%)   | 13          | 14  |
| 65  | BZ    | 59/63 (94%)     | 52 (88%)   | 7 (12%)  | 5           | 4   |
| 66  | Ba    | 39/44 (89%)     | 35 (90%)   | 4 (10%)  | 7           | 6   |
| 67  | Bb    | 49/56 (88%)     | 48 (98%)   | 1 (2%)   | 48          | 63  |
| 68  | Bc    | 51/52 (98%)     | 48 (94%)   | 3 (6%)   | 18          | 22  |
| All | All   | 7149/7643 (94%) | 6892 (96%) | 257 (4%) | 32          | 41  |

5 of 257 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | BX    | 30  | VAL  |
| 64  | BY    | 18  | VAL  |
| 40  | BA    | 89  | THR  |
| 40  | BA    | 29  | SER  |
| 65  | BZ    | 25  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | BB    | 29  | ASN  |
| 62  | BW    | 52  | GLN  |
| 45  | BF    | 33  | ASN  |
| 54  | BO    | 19  | ASN  |
| 43  | BD    | 39  | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 2     | 129/129 (100%)  | 10 (7%)           | 2 (1%)          |
| 2   | 1     | 2844/3024 (94%) | 341 (11%)         | 28 (0%)         |
| 3   | 4     | 1426/1498 (95%) | 260 (18%)         | 38 (2%)         |
| All | All   | 4399/4651 (94%) | 611 (13%)         | 68 (1%)         |

5 of 611 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 2   | C    |
| 1   | 2     | 8   | A    |
| 1   | 2     | 28  | G    |
| 1   | 2     | 48  | A    |
| 1   | 2     | 54  | G    |

5 of 68 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | 4     | 1162 | A    |
| 3   | 4     | 1178 | A    |
| 3   | 4     | 1444 | G    |
| 2   | 1     | 2420 | G    |
| 2   | 1     | 2361 | G    |

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

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

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMU  | 4     | 15   | 3    | 19,22,23     | 1.33 | 4 (21%)  | 25,31,34    | 1.82 | 4 (16%)  |
| 3   | OMC  | 4     | 1045 | 3    | 19,22,23     | 0.76 | 0        | 25,31,34    | 0.80 | 0        |
| 2   | PSU  | 1     | 1911 | 2    | 18,21,22     | 0.93 | 1 (5%)   | 21,30,33    | 0.78 | 0        |
| 3   | MA6  | 4     | 1478 | 3    | 23,26,27     | 0.34 | 0        | 33,38,41    | 0.78 | 1 (3%)   |
| 2   | OMG  | 1     | 2066 | 2    | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 1.99 | 6 (18%)  |
| 3   | OMG  | 4     | 1202 | 3,70 | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 2.03 | 6 (18%)  |
| 2   | OMC  | 1     | 1976 | 2    | 19,22,23     | 0.83 | 0        | 25,31,34    | 0.91 | 1 (4%)   |
| 2   | OMC  | 1     | 872  | 2    | 19,22,23     | 0.78 | 0        | 25,31,34    | 0.83 | 1 (4%)   |
| 2   | OMC  | 1     | 2555 | 2    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.86 | 1 (4%)   |
| 2   | OMG  | 1     | 2388 | 2    | 23,26,27     | 1.21 | 4 (17%)  | 32,38,41    | 2.05 | 7 (21%)  |
| 2   | OMG  | 1     | 1971 | 2    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.99 | 6 (18%)  |
| 2   | OMC  | 1     | 2115 | 2    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.80 | 0        |
| 2   | OMG  | 1     | 2601 | 2,70 | 23,26,27     | 1.21 | 4 (17%)  | 32,38,41    | 1.99 | 5 (15%)  |
| 2   | G7M  | 1     | 3023 | 2    | 23,26,27     | 1.83 | 2 (8%)   | 34,39,42    | 1.11 | 1 (2%)   |
| 2   | OMC  | 1     | 2538 | 2    | 19,22,23     | 0.78 | 0        | 25,31,34    | 0.79 | 0        |
| 2   | UR3  | 1     | 2698 | 2    | 19,22,23     | 0.93 | 0        | 26,32,35    | 1.72 | 2 (7%)   |
| 3   | OMG  | 4     | 1289 | 3,70 | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.00 | 6 (18%)  |
| 3   | OMG  | 4     | 1211 | 3    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.01 | 6 (18%)  |
| 2   | OMC  | 1     | 2884 | 2    | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.81 | 0        |
| 2   | PSU  | 1     | 2571 | 2    | 18,21,22     | 0.94 | 1 (5%)   | 21,30,33    | 0.73 | 0        |
| 2   | A2M  | 1     | 2011 | 2    | 22,25,26     | 0.20 | 0        | 30,36,39    | 0.38 | 0        |
| 2   | PSU  | 1     | 2044 | 2    | 18,21,22     | 0.90 | 1 (5%)   | 21,30,33    | 0.67 | 0        |
| 3   | MA6  | 4     | 1477 | 3    | 23,26,27     | 0.32 | 0        | 33,38,41    | 0.77 | 1 (3%)   |
| 2   | 5MC  | 1     | 2056 | 2,70 | 19,22,23     | 1.52 | 3 (15%)  | 26,32,35    | 1.16 | 3 (11%)  |
| 2   | OMU  | 1     | 2408 | 2    | 19,22,23     | 1.33 | 4 (21%)  | 25,31,34    | 1.92 | 4 (16%)  |
| 3   | OMC  | 4     | 1184 | 3    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.85 | 1 (4%)   |
| 3   | OMG  | 4     | 1212 | 3    | 23,26,27     | 1.21 | 4 (17%)  | 32,38,41    | 1.99 | 5 (15%)  |
| 2   | OMU  | 1     | 2851 | 2    | 19,22,23     | 1.28 | 4 (21%)  | 25,31,34    | 1.84 | 4 (16%)  |
| 2   | PSU  | 1     | 2610 | 2    | 18,21,22     | 0.90 | 1 (5%)   | 21,30,33    | 0.79 | 0        |
| 2   | OMC  | 1     | 492  | 2    | 19,22,23     | 0.77 | 0        | 25,31,34    | 0.82 | 0        |
| 2   | OMC  | 1     | 2704 | 2    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.88 | 0        |
| 3   | A2M  | 4     | 1060 | 3    | 22,25,26     | 0.20 | 0        | 30,36,39    | 0.47 | 0        |
| 3   | OMG  | 4     | 7    | 3    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.10 | 7 (21%)  |
| 2   | OMC  | 1     | 2885 | 2    | 19,22,23     | 0.81 | 0        | 25,31,34    | 0.78 | 0        |
| 2   | OMG  | 1     | 2608 | 2    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.02 | 5 (15%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMG  | 4     | 467  | 3    | 23,26,27     | 1.19 | 3 (13%)  | 32,38,41    | 1.94 | 6 (18%)  |
| 2   | OMU  | 1     | 2088 | 2    | 19,22,23     | 1.28 | 3 (15%)  | 25,31,34    | 1.80 | 4 (16%)  |
| 2   | OMG  | 1     | 2103 | 2    | 23,26,27     | 1.24 | 3 (13%)  | 32,38,41    | 2.00 | 5 (15%)  |
| 2   | 5MC  | 1     | 38   | 2    | 19,22,23     | 1.46 | 3 (15%)  | 26,32,35    | 1.21 | 3 (11%)  |
| 2   | OMU  | 1     | 2155 | 2    | 19,22,23     | 1.26 | 3 (15%)  | 25,31,34    | 1.86 | 5 (20%)  |
| 3   | 4AC  | 4     | 1318 | 3    | 21,24,25     | 0.39 | 0        | 28,34,37    | 0.70 | 0        |
| 2   | PSU  | 1     | 2607 | 2    | 18,21,22     | 0.96 | 1 (5%)   | 21,30,33    | 0.81 | 0        |
| 2   | OMC  | 1     | 673  | 2    | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.83 | 0        |
| 3   | 4AC  | 4     | 5    | 3    | 21,24,25     | 0.43 | 0        | 28,34,37    | 0.66 | 0        |
| 3   | A2M  | 4     | 880  | 3    | 22,25,26     | 0.20 | 0        | 30,36,39    | 0.51 | 0        |
| 3   | OMG  | 4     | 465  | 3    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.99 | 5 (15%)  |
| 2   | OMG  | 1     | 2667 | 2    | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 1.97 | 6 (18%)  |
| 2   | OMU  | 1     | 2077 | 2    | 19,22,23     | 1.32 | 3 (15%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 2   | OMC  | 1     | 2720 | 2    | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.93 | 1 (4%)   |
| 3   | PSU  | 4     | 263  | 3    | 18,21,22     | 0.93 | 1 (5%)   | 21,30,33    | 0.63 | 0        |
| 2   | PSU  | 1     | 1987 | 2    | 18,21,22     | 0.91 | 1 (5%)   | 21,30,33    | 0.68 | 0        |
| 3   | OMG  | 4     | 511  | 3    | 23,26,27     | 1.20 | 3 (13%)  | 32,38,41    | 1.97 | 6 (18%)  |
| 3   | OMC  | 4     | 1368 | 3    | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.79 | 0        |
| 2   | OMC  | 1     | 2018 | 2    | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.75 | 0        |
| 3   | M7A  | 4     | 508  | 3    | 19,25,26     | 0.29 | 0        | 25,37,40    | 0.57 | 0        |
| 3   | OMG  | 4     | 1163 | 3    | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 2.13 | 6 (18%)  |
| 2   | OMG  | 1     | 2071 | 2    | 23,26,27     | 1.20 | 4 (17%)  | 32,38,41    | 1.94 | 6 (18%)  |
| 2   | OMG  | 1     | 2362 | 2    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.99 | 6 (18%)  |
| 2   | OMU  | 1     | 2707 | 2    | 19,22,23     | 1.28 | 4 (21%)  | 25,31,34    | 1.88 | 5 (20%)  |
| 2   | OMU  | 1     | 2623 | 2    | 19,22,23     | 1.26 | 3 (15%)  | 25,31,34    | 1.85 | 5 (20%)  |
| 2   | OMU  | 1     | 2574 | 2    | 19,22,23     | 1.25 | 3 (15%)  | 25,31,34    | 1.76 | 4 (16%)  |
| 2   | OMG  | 1     | 1949 | 2    | 23,26,27     | 1.20 | 3 (13%)  | 32,38,41    | 1.94 | 6 (18%)  |
| 3   | OMG  | 4     | 19   | 3    | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 2.01 | 7 (21%)  |
| 2   | A2M  | 1     | 2059 | 2,70 | 22,25,26     | 0.27 | 0        | 30,36,39    | 0.59 | 0        |
| 3   | OMC  | 4     | 514  | 3    | 19,22,23     | 0.82 | 0        | 25,31,34    | 0.91 | 1 (4%)   |
| 3   | OMG  | 4     | 908  | 3    | 23,26,27     | 1.19 | 3 (13%)  | 32,38,41    | 1.99 | 6 (18%)  |
| 3   | B8T  | 4     | 1469 | 3    | 19,22,23     | 0.43 | 0        | 25,31,34    | 0.42 | 0        |
| 2   | OMC  | 1     | 1816 | 2    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.71 | 0        |
| 3   | OMU  | 4     | 877  | 3    | 19,22,23     | 1.26 | 3 (15%)  | 25,31,34    | 1.84 | 5 (20%)  |
| 2   | OMU  | 1     | 875  | 2    | 19,22,23     | 1.27 | 3 (15%)  | 25,31,34    | 1.87 | 5 (20%)  |
| 3   | B8T  | 4     | 1035 | 3    | 19,22,23     | 0.41 | 0        | 25,31,34    | 0.56 | 0        |
| 2   | OMG  | 1     | 1957 | 2    | 23,26,27     | 1.22 | 4 (17%)  | 32,38,41    | 2.00 | 6 (18%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | A2M  | 4     | 879  | 3    | 22,25,26     | 0.22 | 0        | 30,36,39    | 0.38 | 0        |
| 2   | B8T  | 1     | 2937 | 2    | 19,22,23     | 0.41 | 0        | 25,31,34    | 0.32 | 0        |
| 2   | OMG  | 1     | 1947 | 2    | 23,26,27     | 1.20 | 4 (17%)  | 32,38,41    | 2.06 | 7 (21%)  |
| 2   | OMU  | 1     | 2666 | 2    | 19,22,23     | 1.26 | 3 (15%)  | 25,31,34    | 1.85 | 5 (20%)  |
| 2   | OMG  | 1     | 2176 | 2,70 | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.97 | 6 (18%)  |
| 3   | OMG  | 4     | 1210 | 3    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.95 | 5 (15%)  |
| 2   | A2M  | 1     | 2691 | 2,70 | 22,25,26     | 0.21 | 0        | 30,36,39    | 0.38 | 0        |
| 2   | OMG  | 1     | 902  | 2,70 | 23,26,27     | 1.20 | 4 (17%)  | 32,38,41    | 2.03 | 7 (21%)  |
| 2   | OMC  | 1     | 2624 | 2    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.85 | 1 (4%)   |
| 2   | OMC  | 1     | 2116 | 2    | 19,22,23     | 0.81 | 0        | 25,31,34    | 0.72 | 0        |
| 2   | OMG  | 1     | 2104 | 2    | 23,26,27     | 1.21 | 4 (17%)  | 32,38,41    | 2.02 | 7 (21%)  |
| 2   | 4AC  | 1     | 2016 | 2    | 21,24,25     | 0.39 | 0        | 28,34,37    | 0.60 | 0        |
| 2   | OMU  | 1     | 2628 | 2    | 19,22,23     | 1.27 | 3 (15%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 3   | A2M  | 4     | 569  | 3,70 | 22,25,26     | 0.19 | 0        | 30,36,39    | 0.42 | 0        |
| 2   | OMG  | 1     | 2366 | 2    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 2.01 | 6 (18%)  |
| 2   | OMG  | 1     | 2017 | 2    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.98 | 6 (18%)  |
| 3   | OMC  | 4     | 572  | 3    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.79 | 0        |
| 2   | OMU  | 1     | 908  | 2,70 | 19,22,23     | 1.32 | 4 (21%)  | 25,31,34    | 1.96 | 7 (28%)  |
| 3   | A2M  | 4     | 40   | 3    | 22,25,26     | 0.20 | 0        | 30,36,39    | 0.38 | 0        |
| 3   | OMG  | 4     | 475  | 3    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.97 | 5 (15%)  |
| 3   | 6MZ  | 4     | 1459 | 3,70 | 22,25,26     | 1.44 | 5 (22%)  | 29,36,39    | 2.09 | 7 (24%)  |
| 2   | A2M  | 1     | 1990 | 2    | 22,25,26     | 0.21 | 0        | 30,36,39    | 0.59 | 0        |
| 2   | OMC  | 1     | 493  | 2    | 19,22,23     | 0.79 | 0        | 25,31,34    | 0.81 | 0        |
| 3   | OMG  | 4     | 462  | 3    | 23,26,27     | 1.20 | 3 (13%)  | 32,38,41    | 2.00 | 6 (18%)  |
| 2   | OMC  | 1     | 2143 | 2    | 19,22,23     | 0.27 | 0        | 25,31,34    | 0.30 | 0        |
| 3   | OMG  | 4     | 906  | 3    | 23,26,27     | 1.20 | 3 (13%)  | 32,38,41    | 2.01 | 6 (18%)  |
| 3   | OMC  | 4     | 489  | 3    | 19,22,23     | 0.81 | 0        | 25,31,34    | 0.88 | 0        |
| 2   | B8T  | 1     | 79   | 2    | 19,22,23     | 0.41 | 0        | 25,31,34    | 0.37 | 0        |
| 3   | A2M  | 4     | 496  | 3    | 22,25,26     | 0.21 | 0        | 30,36,39    | 0.46 | 0        |
| 3   | OMC  | 4     | 1034 | 3    | 19,22,23     | 0.80 | 0        | 25,31,34    | 0.81 | 0        |
| 2   | OMG  | 1     | 2537 | 2    | 23,26,27     | 1.22 | 3 (13%)  | 32,38,41    | 1.98 | 6 (18%)  |
| 3   | OMG  | 4     | 674  | 3    | 23,26,27     | 1.21 | 3 (13%)  | 32,38,41    | 1.99 | 6 (18%)  |
| 2   | PSU  | 1     | 2625 | 2    | 18,21,22     | 0.92 | 1 (5%)   | 21,30,33    | 0.71 | 0        |
| 52  | IAS  | BM    | 128  | 52   | 6,7,8        | 1.32 | 1 (16%)  | 3,8,10      | 1.47 | 1 (33%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | OMU  | 4     | 15   | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMC  | 4     | 1045 | 3    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | PSU  | 1     | 1911 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | MA6  | 4     | 1478 | 3    | -       | 2/11/29/30 | 0/3/3/3 |
| 2   | OMG  | 1     | 2066 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 1202 | 3,70 | -       | 3/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 1     | 1976 | 2    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 872  | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 2555 | 2    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2388 | 2    | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 1971 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 1     | 2115 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2601 | 2,70 | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | G7M  | 1     | 3023 | 2    | -       | 1/7/25/26  | 0/3/3/3 |
| 2   | OMC  | 1     | 2538 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | UR3  | 1     | 2698 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 4     | 1289 | 3,70 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 1211 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 1     | 2884 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | PSU  | 1     | 2571 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | A2M  | 1     | 2011 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | 1     | 2044 | 2    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | MA6  | 4     | 1477 | 3    | -       | 0/11/29/30 | 0/3/3/3 |
| 2   | 5MC  | 1     | 2056 | 2,70 | -       | 1/7/25/26  | 0/2/2/2 |
| 2   | OMU  | 1     | 2408 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMC  | 4     | 1184 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | OMG  | 4     | 1212 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMU  | 1     | 2851 | 2    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | PSU  | 1     | 2610 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMC  | 1     | 492  | 2    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 2704 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | 4     | 1060 | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 7    | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 1     | 2885 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2608 | 2    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 467  | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMU  | 1     | 2088 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2103 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 5MC  | 1     | 38   | 2    | -       | 1/7/25/26  | 0/2/2/2 |
| 2   | OMU  | 1     | 2155 | 2    | -       | 2/9/27/28  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | 4AC  | 4     | 1318 | 3    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | PSU  | 1     | 2607 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMC  | 1     | 673  | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | 4AC  | 4     | 5    | 3    | -       | 2/11/29/30 | 0/2/2/2 |
| 3   | A2M  | 4     | 880  | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 465  | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 2667 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMU  | 1     | 2077 | 2    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 2720 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | 4     | 263  | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | PSU  | 1     | 1987 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | 4     | 511  | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | OMC  | 4     | 1368 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 2018 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | M7A  | 4     | 508  | 3    | -       | 3/7/37/38  | 0/3/3/3 |
| 3   | OMG  | 4     | 1163 | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 2071 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 2362 | 2    | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | OMU  | 1     | 2707 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMU  | 1     | 2623 | 2    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | OMU  | 1     | 2574 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 1949 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 19   | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | A2M  | 1     | 2059 | 2,70 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMC  | 4     | 514  | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | OMG  | 4     | 908  | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 3   | B8T  | 4     | 1469 | 3    | -       | 0/7/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 1816 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMU  | 4     | 877  | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMU  | 1     | 875  | 2    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | B8T  | 4     | 1035 | 3    | -       | 0/7/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 1957 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | 4     | 879  | 3    | -       | 4/9/27/28  | 0/3/3/3 |
| 2   | B8T  | 1     | 2937 | 2    | -       | 1/7/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 1947 | 2    | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | OMU  | 1     | 2666 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2176 | 2,70 | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 1210 | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | A2M  | 1     | 2691 | 2,70 | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 902  | 2,70 | -       | 0/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | OMC  | 1     | 2624 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMC  | 1     | 2116 | 2    | -       | 2/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2104 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 4AC  | 1     | 2016 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 1     | 2628 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | 4     | 569  | 3,70 | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 2366 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMG  | 1     | 2017 | 2    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMC  | 4     | 572  | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | OMU  | 1     | 908  | 2,70 | -       | 4/9/27/28  | 0/2/2/2 |
| 3   | A2M  | 4     | 40   | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 475  | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | 6MZ  | 4     | 1459 | 3,70 | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | A2M  | 1     | 1990 | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 1     | 493  | 2    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | OMG  | 4     | 462  | 3    | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 1     | 2143 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | OMG  | 4     | 906  | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMC  | 4     | 489  | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | B8T  | 1     | 79   | 2    | -       | 0/7/27/28  | 0/2/2/2 |
| 3   | A2M  | 4     | 496  | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | OMC  | 4     | 1034 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 1     | 2537 | 2    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMG  | 4     | 674  | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | 1     | 2625 | 2    | -       | 2/7/25/26  | 0/2/2/2 |
| 52  | IAS  | BM    | 128  | 52   | -       | 1/7/7/8    | -       |

The worst 5 of 179 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | 1     | 3023 | G7M  | C8-N7 | 7.23 | 1.45        | 1.33     |
| 2   | 1     | 2056 | 5MC  | C5-C4 | 5.34 | 1.48        | 1.44     |
| 2   | 1     | 38   | 5MC  | C5-C4 | 5.00 | 1.47        | 1.44     |
| 3   | 4     | 1459 | 6MZ  | C5-C4 | 4.29 | 1.46        | 1.39     |
| 2   | 1     | 3023 | G7M  | C8-N9 | 3.95 | 1.46        | 1.35     |

The worst 5 of 296 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | 1     | 2698 | UR3  | C4-N3-C2 | -6.86 | 119.06      | 124.58   |
| 3   | 4     | 1163 | OMG  | C5-C4-N3 | -6.84 | 117.51      | 128.39   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | 4     | 1202 | OMG  | C5-C4-N3 | -6.41 | 118.19      | 128.39   |
| 3   | 4     | 1289 | OMG  | C5-C4-N3 | -6.37 | 118.25      | 128.39   |
| 2   | 1     | 2667 | OMG  | C5-C4-N3 | -6.35 | 118.29      | 128.39   |

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | 4     | 40   | A2M  | C1'-C2'-O2'-CM' |
| 3   | 4     | 496  | A2M  | C1'-C2'-O2'-CM' |
| 3   | 4     | 879  | A2M  | C3'-C4'-C5'-O5' |
| 3   | 4     | 879  | A2M  | C1'-C2'-O2'-CM' |
| 3   | 4     | 1045 | OMC  | O4'-C4'-C5'-O5' |

There are no ring outliers.

77 monomers are involved in 118 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | 4     | 1045 | OMC  | 1       | 0            |
| 3   | 4     | 1478 | MA6  | 2       | 0            |
| 3   | 4     | 1202 | OMG  | 3       | 0            |
| 2   | 1     | 1976 | OMC  | 1       | 0            |
| 2   | 1     | 872  | OMC  | 1       | 0            |
| 2   | 1     | 2555 | OMC  | 1       | 0            |
| 2   | 1     | 3023 | G7M  | 2       | 0            |
| 2   | 1     | 2538 | OMC  | 1       | 0            |
| 2   | 1     | 2698 | UR3  | 1       | 0            |
| 3   | 4     | 1289 | OMG  | 2       | 0            |
| 3   | 4     | 1211 | OMG  | 3       | 0            |
| 2   | 1     | 2884 | OMC  | 1       | 0            |
| 2   | 1     | 2011 | A2M  | 1       | 0            |
| 2   | 1     | 2044 | PSU  | 3       | 0            |
| 3   | 4     | 1477 | MA6  | 2       | 0            |
| 2   | 1     | 2056 | 5MC  | 2       | 0            |
| 3   | 4     | 1184 | OMC  | 2       | 0            |
| 3   | 4     | 1212 | OMG  | 2       | 0            |
| 2   | 1     | 2851 | OMU  | 1       | 0            |
| 2   | 1     | 2610 | PSU  | 2       | 0            |
| 2   | 1     | 492  | OMC  | 2       | 0            |
| 2   | 1     | 2704 | OMC  | 3       | 0            |
| 3   | 4     | 1060 | A2M  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | 4     | 7    | OMG  | 3       | 0            |
| 2   | 1     | 2885 | OMC  | 1       | 0            |
| 2   | 1     | 2608 | OMG  | 1       | 0            |
| 3   | 4     | 467  | OMG  | 2       | 0            |
| 2   | 1     | 2088 | OMU  | 1       | 0            |
| 2   | 1     | 2103 | OMG  | 1       | 0            |
| 2   | 1     | 2155 | OMU  | 1       | 0            |
| 3   | 4     | 1318 | 4AC  | 1       | 0            |
| 2   | 1     | 673  | OMC  | 1       | 0            |
| 3   | 4     | 5    | 4AC  | 1       | 0            |
| 3   | 4     | 880  | A2M  | 5       | 0            |
| 3   | 4     | 465  | OMG  | 2       | 0            |
| 2   | 1     | 2667 | OMG  | 2       | 0            |
| 2   | 1     | 2077 | OMU  | 1       | 0            |
| 2   | 1     | 2720 | OMC  | 2       | 0            |
| 3   | 4     | 263  | PSU  | 1       | 0            |
| 2   | 1     | 1987 | PSU  | 1       | 0            |
| 3   | 4     | 511  | OMG  | 2       | 0            |
| 3   | 4     | 1368 | OMC  | 1       | 0            |
| 2   | 1     | 2018 | OMC  | 1       | 0            |
| 3   | 4     | 508  | M7A  | 2       | 0            |
| 3   | 4     | 1163 | OMG  | 2       | 0            |
| 2   | 1     | 2362 | OMG  | 1       | 0            |
| 2   | 1     | 2707 | OMU  | 1       | 0            |
| 2   | 1     | 2623 | OMU  | 4       | 0            |
| 2   | 1     | 1949 | OMG  | 1       | 0            |
| 2   | 1     | 2059 | A2M  | 1       | 0            |
| 3   | 4     | 514  | OMC  | 1       | 0            |
| 3   | 4     | 908  | OMG  | 1       | 0            |
| 3   | 4     | 877  | OMU  | 1       | 0            |
| 2   | 1     | 875  | OMU  | 2       | 0            |
| 3   | 4     | 1035 | B8T  | 1       | 0            |
| 2   | 1     | 1957 | OMG  | 2       | 0            |
| 3   | 4     | 879  | A2M  | 3       | 0            |
| 2   | 1     | 1947 | OMG  | 3       | 0            |
| 2   | 1     | 2176 | OMG  | 1       | 0            |
| 3   | 4     | 1210 | OMG  | 2       | 0            |
| 2   | 1     | 2691 | A2M  | 1       | 0            |
| 2   | 1     | 2624 | OMC  | 3       | 0            |
| 2   | 1     | 2116 | OMC  | 1       | 0            |
| 2   | 1     | 2104 | OMG  | 3       | 0            |
| 2   | 1     | 2016 | 4AC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | 1     | 2628 | OMU  | 2       | 0            |
| 2   | 1     | 2366 | OMG  | 3       | 0            |
| 3   | 4     | 572  | OMC  | 1       | 0            |
| 3   | 4     | 40   | A2M  | 1       | 0            |
| 3   | 4     | 475  | OMG  | 2       | 0            |
| 2   | 1     | 493  | OMC  | 1       | 0            |
| 3   | 4     | 462  | OMG  | 4       | 0            |
| 3   | 4     | 906  | OMG  | 1       | 0            |
| 3   | 4     | 489  | OMC  | 1       | 0            |
| 2   | 1     | 2537 | OMG  | 1       | 0            |
| 3   | 4     | 674  | OMG  | 1       | 0            |
| 52  | BM    | 128  | IAS  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 327 ligands modelled in this entry, 263 are monoatomic - leaving 64 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 69  | SPM  | 1     | 3111 | -    | 13,13,13     | 0.15 | 0           | 12,12,12    | 0.25 | 0           |
| 69  | SPM  | 1     | 3102 | -    | 13,13,13     | 0.16 | 0           | 12,12,12    | 0.43 | 0           |
| 69  | SPM  | 1     | 3142 | -    | 13,13,13     | 0.18 | 0           | 12,12,12    | 0.34 | 0           |
| 69  | SPM  | 4     | 3016 | -    | 13,13,13     | 0.16 | 0           | 12,12,12    | 0.22 | 0           |
| 69  | SPM  | 1     | 3105 | -    | 13,13,13     | 0.15 | 0           | 12,12,12    | 0.16 | 0           |
| 69  | SPM  | 1     | 3101 | -    | 13,13,13     | 0.18 | 0           | 12,12,12    | 0.66 | 0           |
| 69  | SPM  | 1     | 3106 | -    | 13,13,13     | 0.17 | 0           | 12,12,12    | 0.19 | 0           |
| 69  | SPM  | 1     | 3107 | -    | 13,13,13     | 0.18 | 0           | 12,12,12    | 0.19 | 0           |
| 69  | SPM  | 1     | 3143 | -    | 13,13,13     | 0.21 | 0           | 12,12,12    | 0.46 | 0           |
| 69  | SPM  | 4     | 3013 | -    | 13,13,13     | 0.16 | 0           | 12,12,12    | 0.28 | 0           |
| 69  | SPM  | 1     | 3112 | -    | 13,13,13     | 0.17 | 0           | 12,12,12    | 0.32 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 69  | SPM  | 4     | 3002 | -    | 13,13,13     | 0.21 | 0        | 12,12,12    | 0.47 | 0        |
| 69  | SPM  | 1     | 3136 | -    | 13,13,13     | 0.14 | 0        | 12,12,12    | 0.29 | 0        |
| 69  | SPM  | 1     | 3144 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.40 | 0        |
| 69  | SPM  | 1     | 3134 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.43 | 0        |
| 69  | SPM  | 1     | 3124 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.23 | 0        |
| 69  | SPM  | 4     | 3011 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.43 | 0        |
| 69  | SPM  | 4     | 3017 | -    | 13,13,13     | 0.21 | 0        | 12,12,12    | 1.70 | 1 (8%)   |
| 69  | SPM  | AL    | 201  | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.40 | 0        |
| 69  | SPM  | 4     | 3018 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.32 | 0        |
| 69  | SPM  | 4     | 3008 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.27 | 0        |
| 69  | SPM  | 1     | 3130 | -    | 13,13,13     | 0.14 | 0        | 12,12,12    | 0.18 | 0        |
| 69  | SPM  | 4     | 3012 | -    | 13,13,13     | 0.19 | 0        | 12,12,12    | 0.20 | 0        |
| 69  | SPM  | 1     | 3121 | -    | 13,13,13     | 0.24 | 0        | 12,12,12    | 0.30 | 0        |
| 69  | SPM  | 4     | 3001 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.33 | 0        |
| 69  | SPM  | 1     | 3114 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.19 | 0        |
| 69  | SPM  | 1     | 3116 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.26 | 0        |
| 69  | SPM  | 1     | 3109 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.36 | 0        |
| 69  | SPM  | 1     | 3141 | -    | 13,13,13     | 0.20 | 0        | 12,12,12    | 0.62 | 0        |
| 69  | SPM  | 1     | 3113 | -    | 13,13,13     | 0.18 | 0        | 12,12,12    | 0.19 | 0        |
| 69  | SPM  | 1     | 3138 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.82 | 0        |
| 69  | SPM  | 1     | 3117 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.36 | 0        |
| 69  | SPM  | 4     | 3005 | -    | 13,13,13     | 0.14 | 0        | 12,12,12    | 0.16 | 0        |
| 69  | SPM  | 1     | 3133 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.37 | 0        |
| 69  | SPM  | 1     | 3115 | -    | 13,13,13     | 0.18 | 0        | 12,12,12    | 0.45 | 0        |
| 69  | SPM  | 1     | 3131 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.34 | 0        |
| 69  | SPM  | 1     | 3120 | -    | 13,13,13     | 0.18 | 0        | 12,12,12    | 0.22 | 0        |
| 69  | SPM  | 1     | 3137 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.43 | 0        |
| 69  | SPM  | 1     | 3110 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.29 | 0        |
| 69  | SPM  | 4     | 3007 | -    | 13,13,13     | 0.24 | 0        | 12,12,12    | 0.53 | 0        |
| 69  | SPM  | 1     | 3108 | -    | 13,13,13     | 0.19 | 0        | 12,12,12    | 0.66 | 0        |
| 69  | SPM  | 1     | 3119 | -    | 13,13,13     | 0.21 | 0        | 12,12,12    | 0.26 | 0        |
| 69  | SPM  | 1     | 3126 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.59 | 0        |
| 69  | SPM  | 1     | 3128 | -    | 13,13,13     | 0.18 | 0        | 12,12,12    | 0.21 | 0        |
| 69  | SPM  | 4     | 3006 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.24 | 0        |
| 69  | SPM  | 1     | 3123 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.36 | 0        |
| 69  | SPM  | 1     | 3118 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.17 | 0        |
| 69  | SPM  | 1     | 3125 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.29 | 0        |
| 69  | SPM  | 4     | 3004 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.26 | 0        |
| 69  | SPM  | 1     | 3129 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.37 | 0        |
| 69  | SPM  | 4     | 3010 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.69 | 0        |
| 69  | SPM  | 1     | 3104 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.31 | 0        |
| 69  | SPM  | 4     | 3009 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.35 | 0        |
| 69  | SPM  | 4     | 3003 | -    | 13,13,13     | 0.18 | 0        | 12,12,12    | 0.38 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 69  | SPM  | 1     | 3139 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.25 | 0        |
| 69  | SPM  | Ah    | 101  | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.19 | 0        |
| 69  | SPM  | 4     | 3014 | -    | 13,13,13     | 0.19 | 0        | 12,12,12    | 0.57 | 0        |
| 69  | SPM  | 1     | 3103 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.44 | 0        |
| 69  | SPM  | 1     | 3127 | -    | 13,13,13     | 0.17 | 0        | 12,12,12    | 0.30 | 0        |
| 69  | SPM  | 1     | 3132 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.40 | 0        |
| 69  | SPM  | 1     | 3135 | -    | 13,13,13     | 0.16 | 0        | 12,12,12    | 0.64 | 0        |
| 69  | SPM  | 4     | 3015 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.35 | 0        |
| 69  | SPM  | 1     | 3140 | -    | 13,13,13     | 0.15 | 0        | 12,12,12    | 0.39 | 0        |
| 69  | SPM  | 1     | 3122 | -    | 13,13,13     | 0.18 | 0        | 12,12,12    | 0.25 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 69  | SPM  | 1     | 3111 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3102 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3142 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 4     | 3016 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3105 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3101 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3106 | -    | -       | 5/11/11/11 | -     |
| 69  | SPM  | 1     | 3107 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3143 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 4     | 3013 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3112 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 4     | 3002 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3136 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3144 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 1     | 3134 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 1     | 3124 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 4     | 3011 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3017 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | AL    | 201  | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 4     | 3018 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 4     | 3008 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3130 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 4     | 3012 | -    | -       | 4/11/11/11 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 69  | SPM  | 1     | 3121 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 4     | 3001 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3114 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3116 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3109 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3141 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3113 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3138 | -    | -       | 6/11/11/11 | -     |
| 69  | SPM  | 1     | 3117 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3005 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3133 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 1     | 3115 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3131 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3120 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3137 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3110 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 4     | 3007 | -    | -       | 5/11/11/11 | -     |
| 69  | SPM  | 1     | 3108 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 1     | 3119 | -    | -       | 4/11/11/11 | -     |
| 69  | SPM  | 1     | 3126 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 1     | 3128 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3006 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3123 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3118 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3125 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 4     | 3004 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 1     | 3129 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3010 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3104 | -    | -       | 3/11/11/11 | -     |
| 69  | SPM  | 4     | 3009 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3003 | -    | -       | 5/11/11/11 | -     |
| 69  | SPM  | 1     | 3139 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | Ah    | 101  | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3014 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3103 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3127 | -    | -       | 0/11/11/11 | -     |
| 69  | SPM  | 1     | 3132 | -    | -       | 3/11/11/11 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 69  | SPM  | 1     | 3135 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 4     | 3015 | -    | -       | 2/11/11/11 | -     |
| 69  | SPM  | 1     | 3140 | -    | -       | 1/11/11/11 | -     |
| 69  | SPM  | 1     | 3122 | -    | -       | 1/11/11/11 | -     |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 69  | 4     | 3017 | SPM  | C7-C8-C9 | 5.69 | 139.82      | 113.56   |

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 69  | 1     | 3106 | SPM  | C12-C11-N10-C9 |
| 69  | 4     | 3017 | SPM  | C6-C7-C8-C9    |
| 69  | 1     | 3101 | SPM  | C7-C8-C9-N10   |
| 69  | 4     | 3007 | SPM  | C7-C8-C9-N10   |
| 69  | 1     | 3134 | SPM  | N5-C6-C7-C8    |

There are no ring outliers.

25 monomers are involved in 36 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 69  | 1     | 3102 | SPM  | 1       | 0            |
| 69  | 1     | 3105 | SPM  | 1       | 0            |
| 69  | 1     | 3106 | SPM  | 2       | 0            |
| 69  | 1     | 3112 | SPM  | 1       | 0            |
| 69  | 4     | 3002 | SPM  | 2       | 0            |
| 69  | 1     | 3136 | SPM  | 1       | 0            |
| 69  | 1     | 3134 | SPM  | 1       | 0            |
| 69  | 1     | 3124 | SPM  | 2       | 0            |
| 69  | 4     | 3017 | SPM  | 2       | 0            |
| 69  | 4     | 3008 | SPM  | 1       | 0            |
| 69  | 1     | 3130 | SPM  | 1       | 0            |
| 69  | 4     | 3012 | SPM  | 4       | 0            |
| 69  | 1     | 3116 | SPM  | 2       | 0            |
| 69  | 1     | 3113 | SPM  | 2       | 0            |
| 69  | 1     | 3115 | SPM  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 69  | 4     | 3007 | SPM  | 1       | 0            |
| 69  | 1     | 3108 | SPM  | 2       | 0            |
| 69  | 1     | 3128 | SPM  | 1       | 0            |
| 69  | 1     | 3123 | SPM  | 1       | 0            |
| 69  | 1     | 3125 | SPM  | 1       | 0            |
| 69  | 1     | 3129 | SPM  | 1       | 0            |
| 69  | 4     | 3014 | SPM  | 1       | 0            |
| 69  | 1     | 3132 | SPM  | 1       | 0            |
| 69  | 4     | 3015 | SPM  | 2       | 0            |
| 69  | 1     | 3140 | SPM  | 1       | 0            |

## 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.

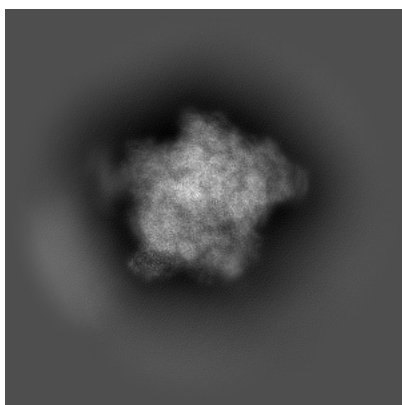
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47628. These allow visual inspection of the internal detail of the map and identification of artifacts.

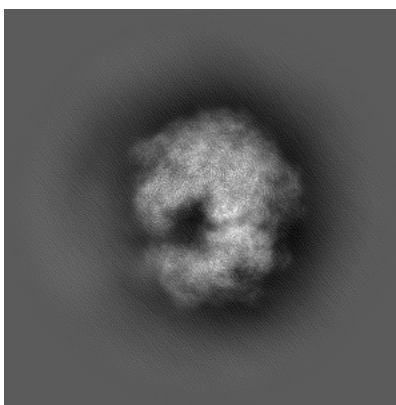
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

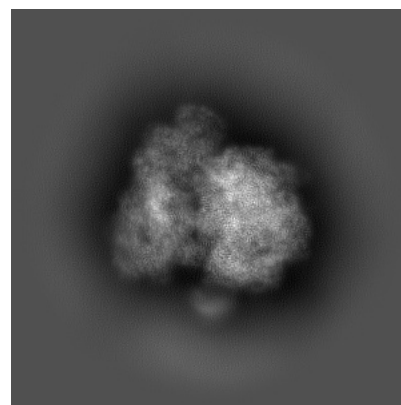
#### 6.1.1 Primary map



X



Y

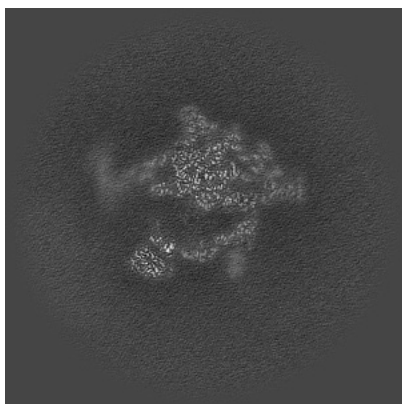


Z

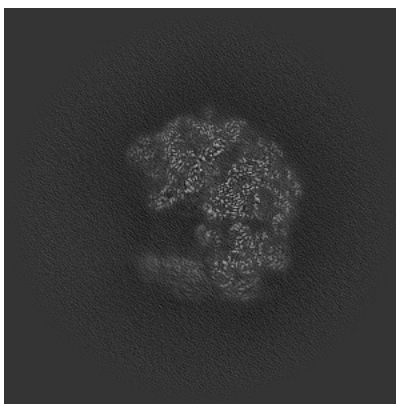
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

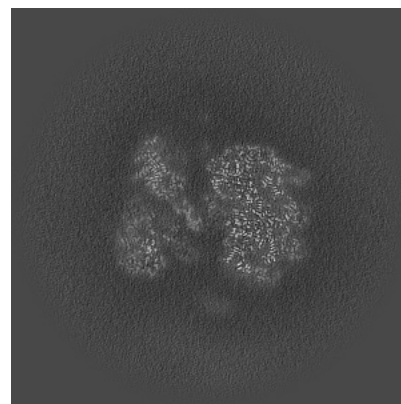
#### 6.2.1 Primary map



X Index: 304



Y Index: 304

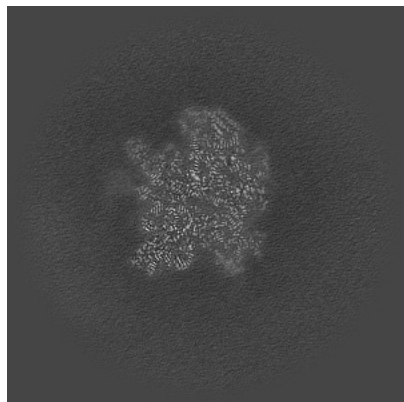


Z Index: 304

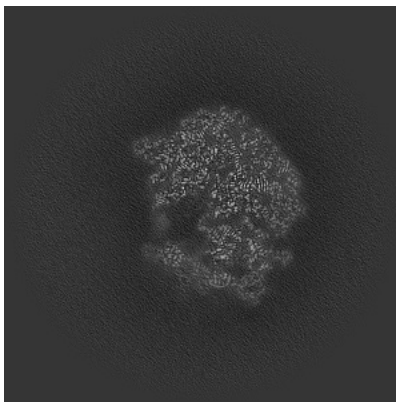
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

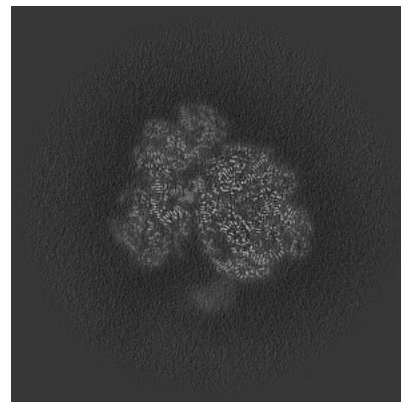
### 6.3.1 Primary map



X Index: 334



Y Index: 288

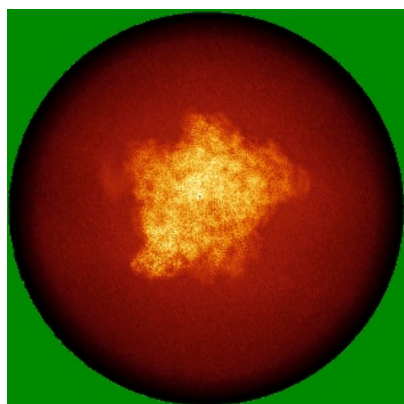


Z Index: 326

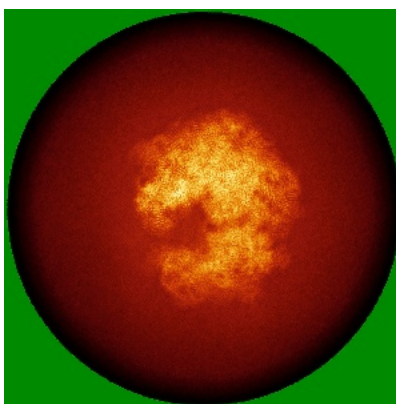
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

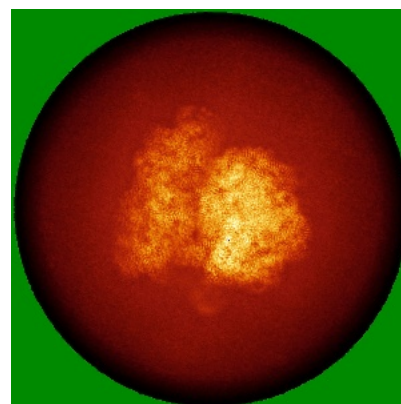
### 6.4.1 Primary map



X



Y

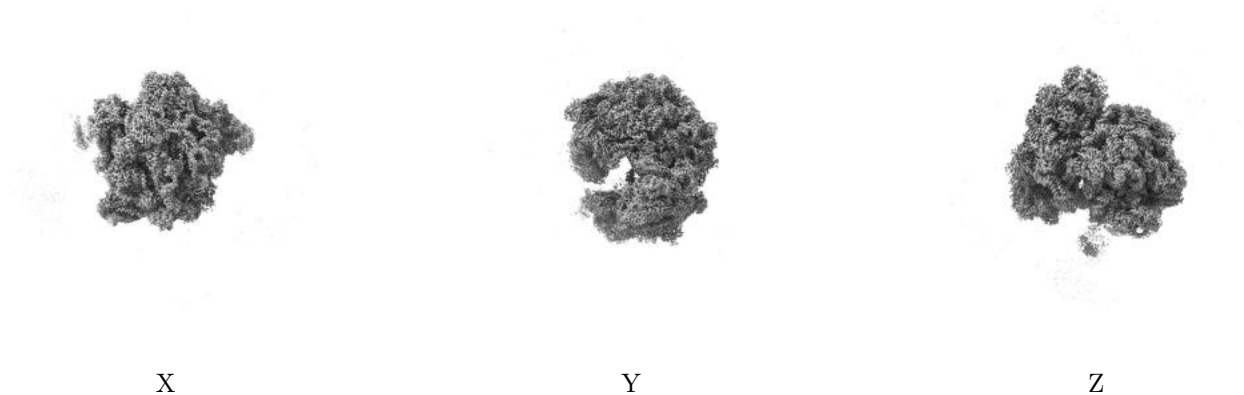


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

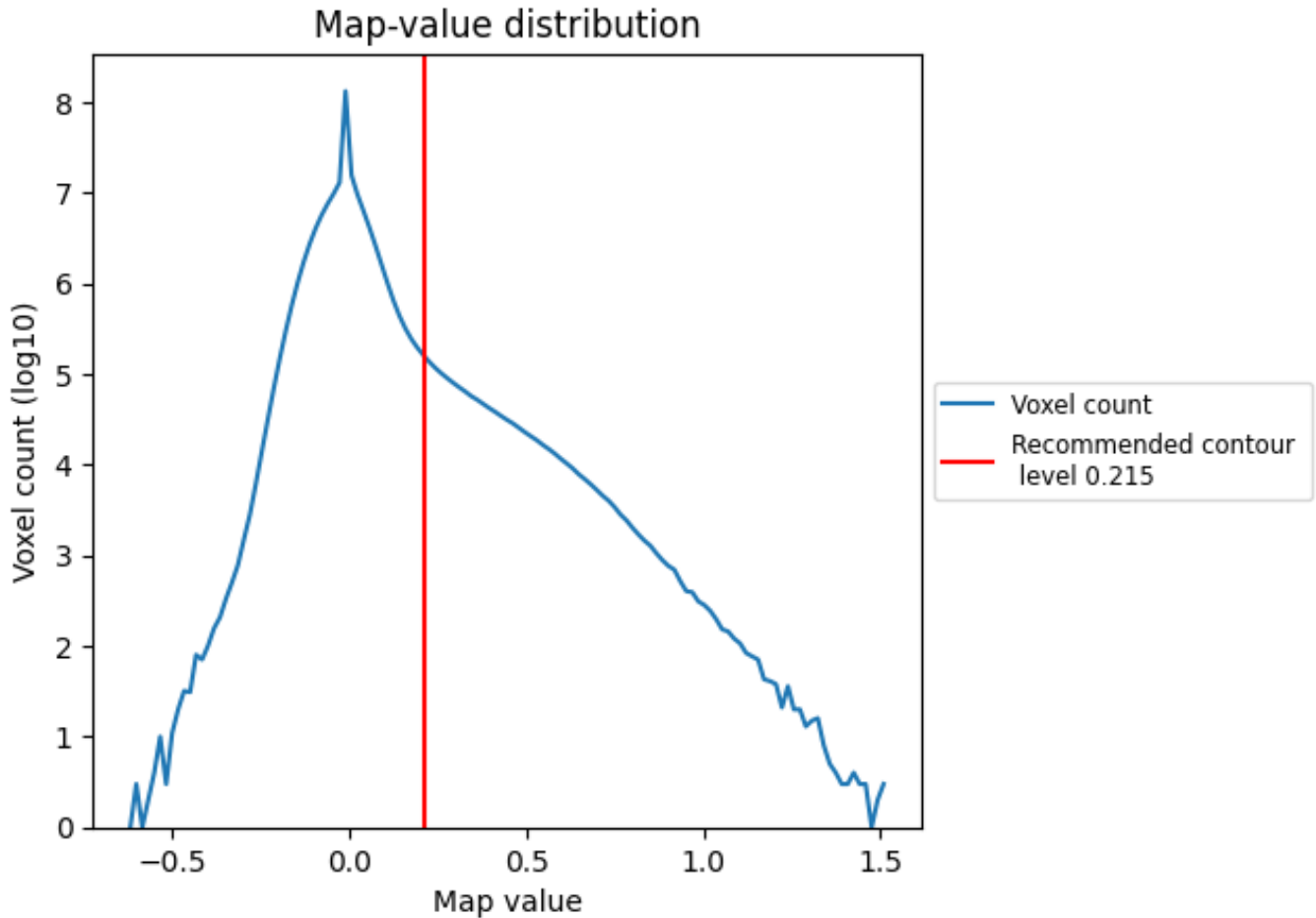
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

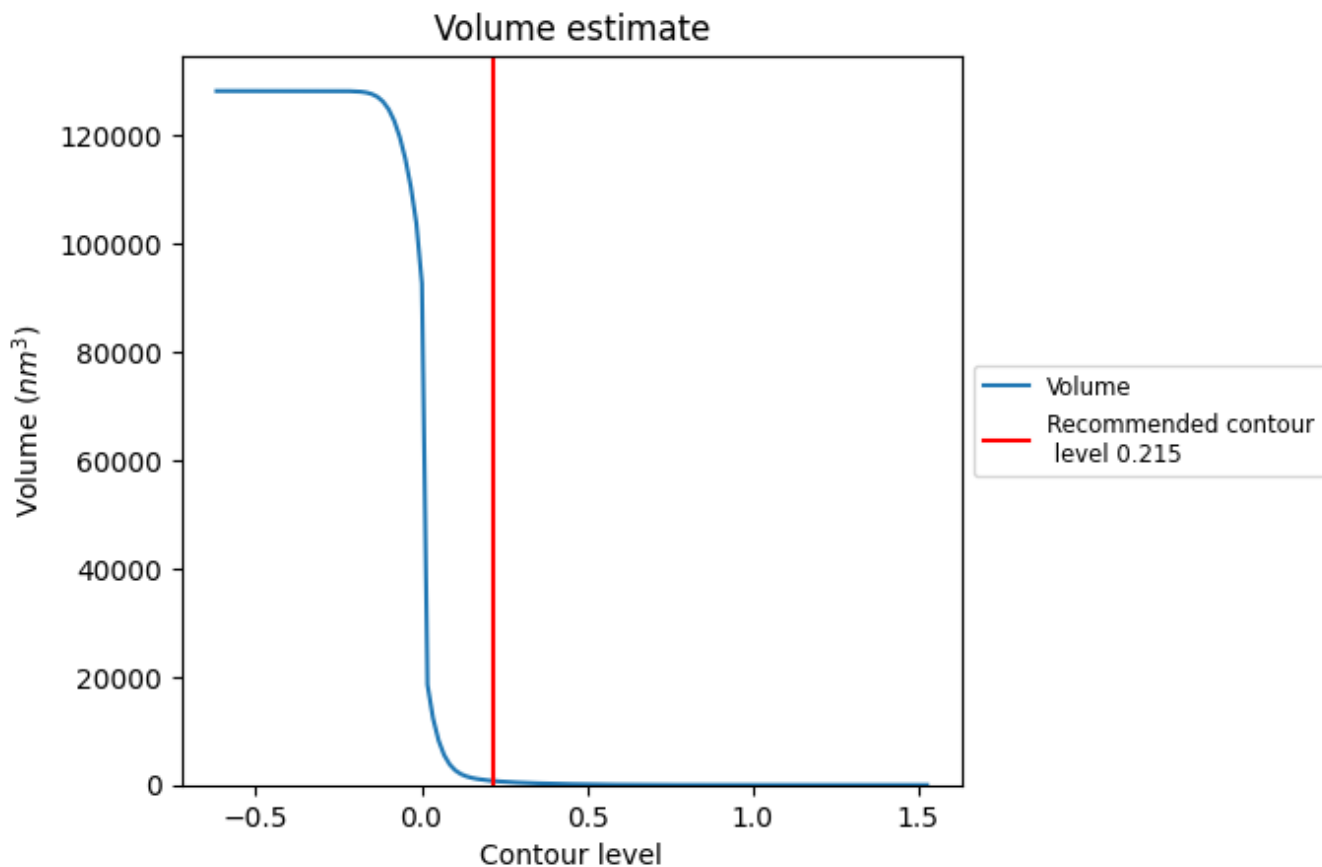
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

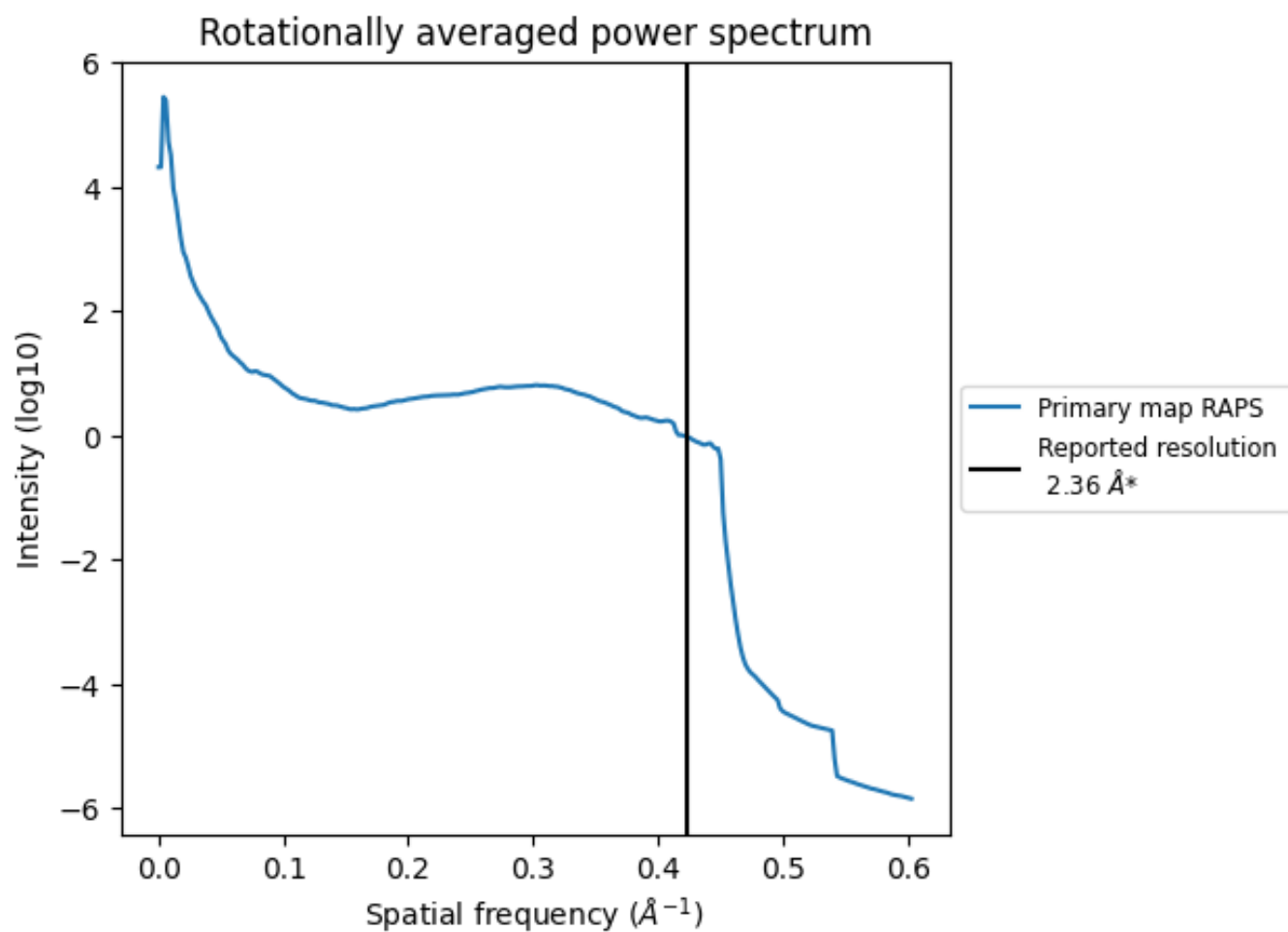
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 756 nm<sup>3</sup>; this corresponds to an approximate mass of 683 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.424 \text{\AA}^{-1}$

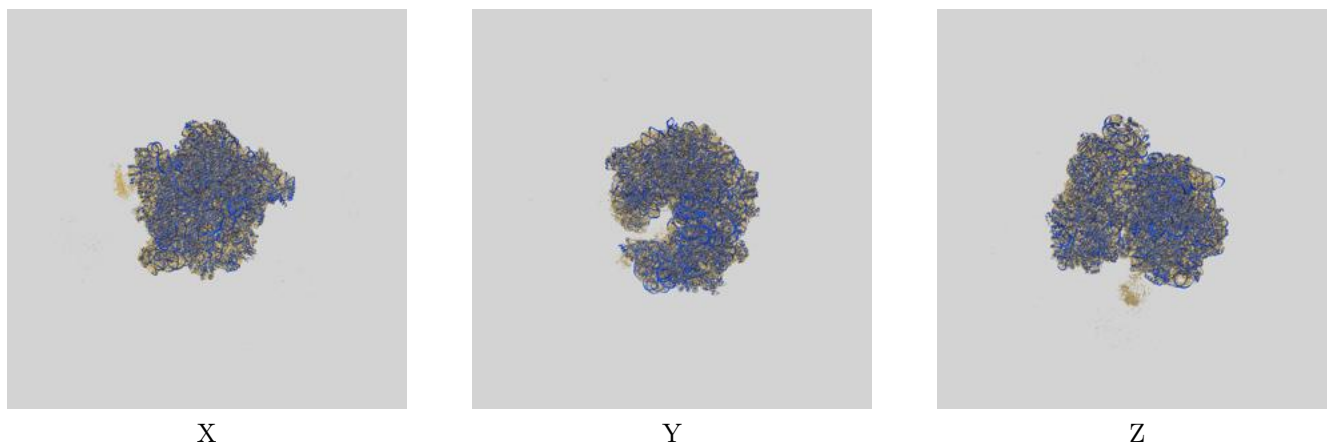
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

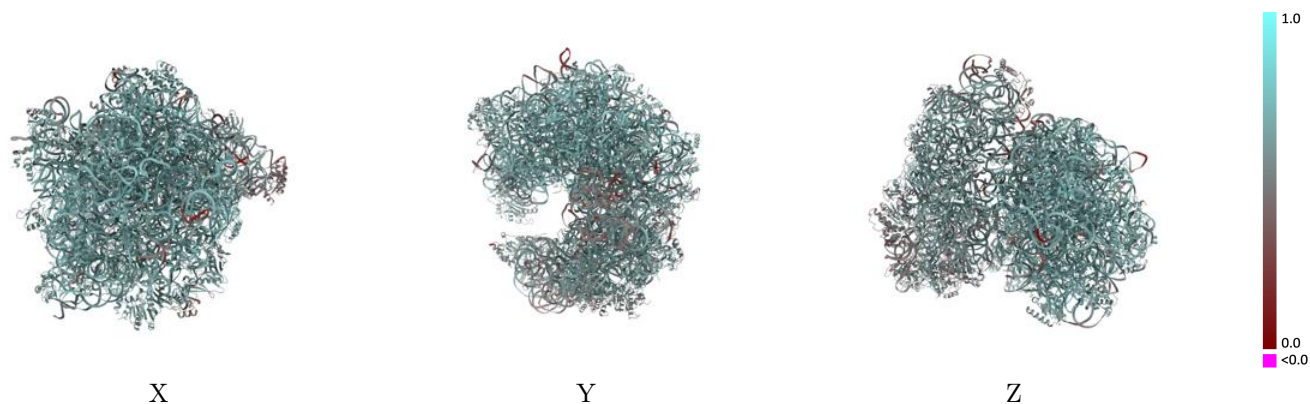
This section contains information regarding the fit between EMDB map EMD-47628 and PDB model 9E71. Per-residue inclusion information can be found in section 3 on page 23.

### 9.1 Map-model overlay [i](#)



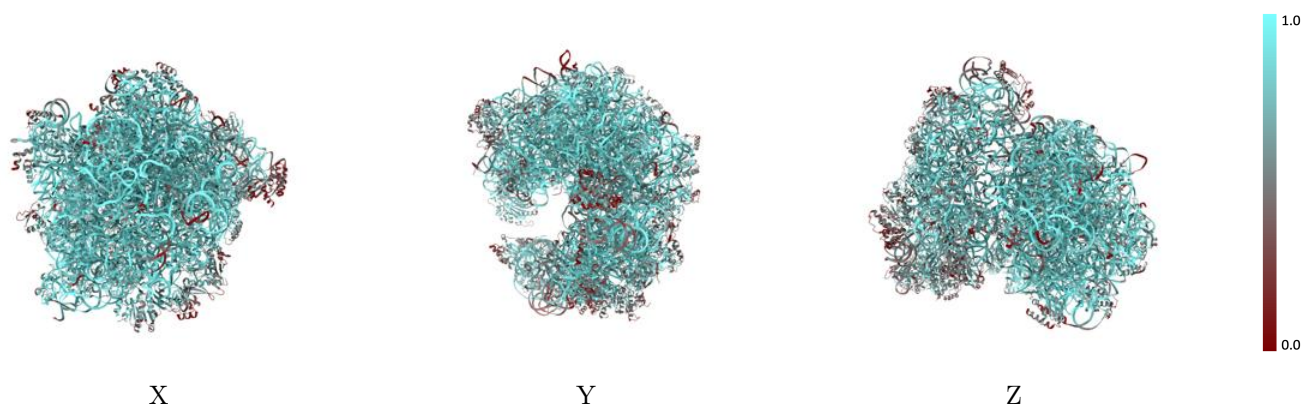
The images above show the 3D surface view of the map at the recommended contour level 0.215 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



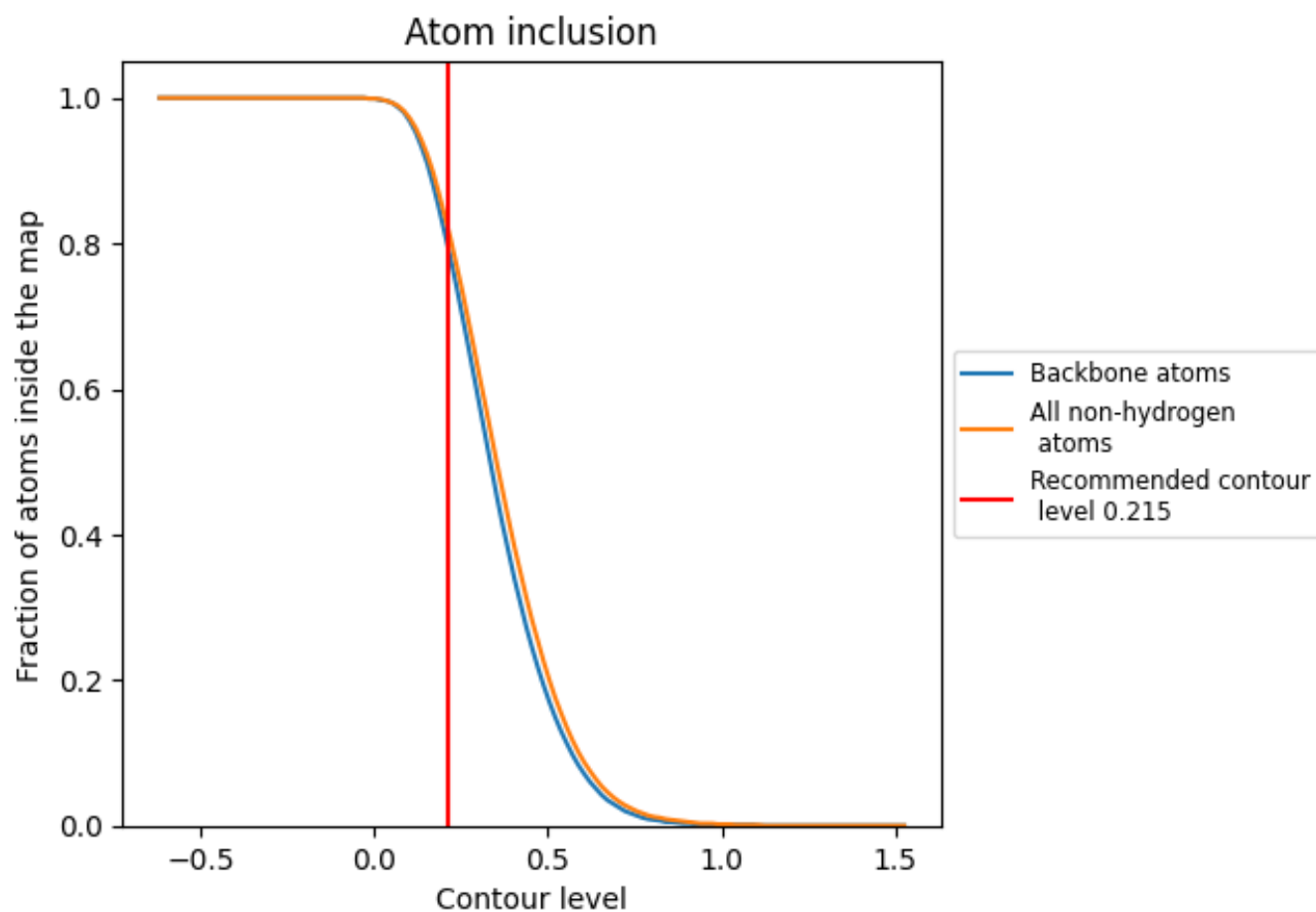
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.215).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary







































































The table lists the average atom inclusion at the recommended contour level (0.215) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8160   |  0.6140   |
| 1     |  0.9300   |  0.6510   |
| 2     |  0.9230   |  0.6430   |
| 4     |  0.8380   |  0.5700   |
| AA    |  0.8830   |  0.6710   |
| AB    |  0.8490   |  0.6750   |
| AC    |  0.8070   |  0.6490   |
| AD    |  0.7750   |  0.6090   |
| AE    |  0.5900   |  0.5970   |
| AF    |  0.5750   |  0.5870   |
| AG    |  0.8080   |  0.6520   |
| AH    |  0.8180   |  0.6540   |
| AI    |  0.8270   |  0.6530   |
| AJ    |  0.5520   |  0.5570   |
| AK    |  0.5190  |  0.5690  |
| AL    |  0.7420 |  0.6260 |
| AM    |  0.8600 |  0.6640 |
| AN    |  0.7920 |  0.6340 |
| AO    |  0.8770 |  0.6530 |
| AP    |  0.8330 |  0.6490 |
| AQ    |  0.8250 |  0.6440 |
| AR    |  0.6960 |  0.6010 |
| AS    |  0.9430 |  0.6800 |
| AT    |  0.8680 |  0.6700 |
| AU    |  0.8050 |  0.6680 |
| AV    |  0.7400 |  0.6280 |
| AW    |  0.8320 |  0.6530 |
| AX    |  0.6420 |  0.6150 |
| AY    |  0.8380 |  0.6470 |
| AZ    |  0.6670 |  0.5790 |
| Aa    |  0.8080 |  0.6560 |
| Ab    |  0.8120 |  0.6530 |
| Ac    |  0.9160 |  0.6590 |
| Ad    |  0.9830 |  0.7140 |
| Ae    |  0.7110 |  0.6450 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Af    |  0.9470   |  0.6810   |
| Ag    |  0.6910   |  0.6150   |
| Ah    |  0.9020   |  0.6710   |
| Ai    |  0.7920   |  0.6270   |
| Aj    |  0.6470   |  0.6020   |
| Ak    |  0.6880   |  0.6160   |
| BA    |  0.5200   |  0.5220   |
| BB    |  0.4950   |  0.5050   |
| BC    |  0.1640   |  0.3990   |
| BD    |  0.7110   |  0.5830   |
| BE    |  0.6780   |  0.5840   |
| BF    |  0.6980   |  0.5740   |
| BG    |  0.3720   |  0.4690   |
| BH    |  0.6510   |  0.5460   |
| BI    |  0.7930   |  0.5960   |
| BJ    |  0.7190   |  0.5880   |
| BK    |  0.6360   |  0.5360   |
| BL    |  0.1690  |  0.4480  |
| BM    |  0.6630 |  0.5330 |
| BN    |  0.7040 |  0.5810 |
| BO    |  0.5280 |  0.5410 |
| BP    |  0.1730 |  0.4250 |
| BQ    |  0.6570 |  0.5710 |
| BR    |  0.6460 |  0.5780 |
| BS    |  0.2220 |  0.4030 |
| BT    |  0.5290 |  0.5350 |
| BU    |  0.6990 |  0.5720 |
| BV    |  0.4610 |  0.5190 |
| BW    |  0.5220 |  0.5330 |
| BX    |  0.2220 |  0.4380 |
| BY    |  0.6210 |  0.5710 |
| BZ    |  0.5230 |  0.5050 |
| Ba    |  0.5900 |  0.5470 |
| Bb    |  0.2760 |  0.4360 |
| Bc    |  0.6180 |  0.5340 |