



## wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 12:55 pm BST

PDB ID : 9SRA / pdb\_00009sra  
EMDB ID : EMD-55135  
Title : Cryo-EM structure of P. abyssi HibA:ribosome with an SD:antiSD duplex  
Authors : Madru, C.M.; Bourgeois, G.B.; Mechulam, Y.M.; Schmitt, E.S.  
Deposited on : 2025-09-24  
Resolution : 2.20 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.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.50

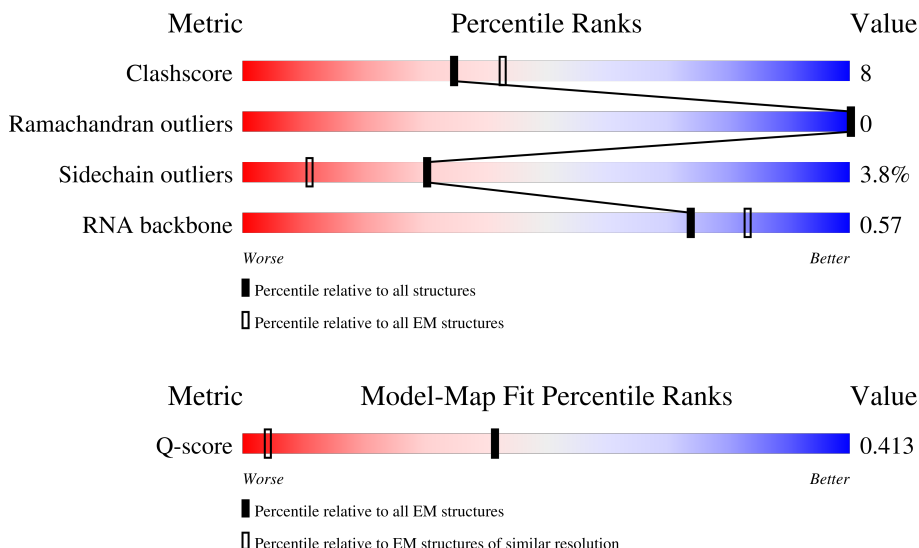
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 3184 ( 1.71 - 2.70 )                                     |

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   | 1     | 3018   |                  |
| 2   | 2     | 1512   |                  |
| 3   | 3     | 128    |                  |

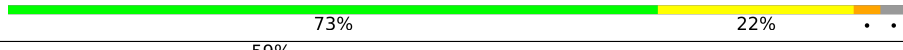
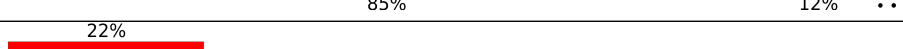
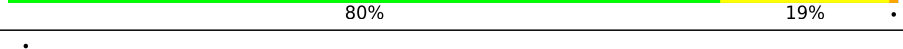
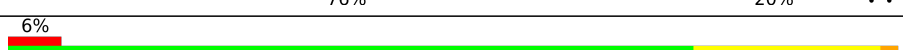
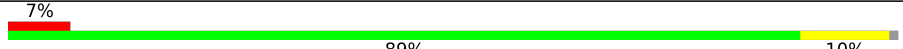
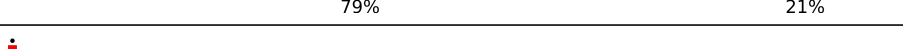
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| Mol | Chain | Length | Quality of chain     |
|-----|-------|--------|----------------------|
| 4   | H     | 392    | <br>66% 76% 20% . .  |
| 5   | AA    | 199    | <br>70% 23% . 6%     |
| 6   | AB    | 202    | <br>83% 14% .        |
| 7   | AC    | 63     | <br>71% 19% 10%      |
| 8   | AD    | 180    | <br>85% 11% .        |
| 9   | AE    | 243    | <br>79% 20%          |
| 10  | AF    | 236    | <br>83% 14% .        |
| 11  | AG    | 125    | <br>72% 26% ..       |
| 12  | AH    | 215    | <br>76% 20% .        |
| 13  | AI    | 130    | <br>85% 14% ..       |
| 14  | AJ    | 127    | <br>87% 9% . .       |
| 15  | AK    | 135    | <br>84% 16%          |
| 16  | AL    | 102    | <br>74% 22% . .      |
| 17  | AM    | 137    | <br>82% 10% . 7%     |
| 18  | AN    | 147    | <br>84% 15% .        |
| 19  | AP    | 56     | <br>62% 34% . .      |
| 20  | AQ    | 158    | <br>85% 13% ..       |
| 21  | AR    | 113    | <br>78% 16% . 5%     |
| 22  | AS    | 67     | <br>70% 25% .        |
| 23  | AU    | 150    | <br>81% 17% ..       |
| 24  | AV    | 99     | <br>85% 12% .        |
| 24  | B6    | 99     | <br>61% 64% 28% . 5% |
| 25  | AW    | 65     | <br>82% 12% 6%       |
| 26  | AX    | 71     | <br>75% 11% 6% 8%    |
| 27  | AY    | 51     | <br>63% 61% 35% .    |

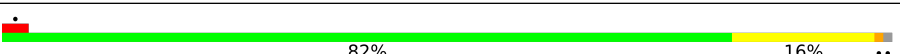
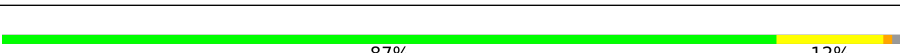
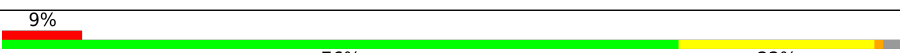
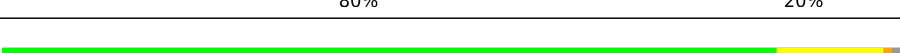
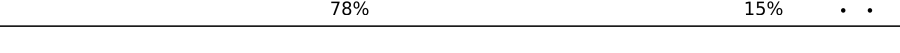
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28  | AZ    | 210    |    |
| 29  | A0    | 37     |    |
| 30  | A3    | 123    |    |
| 30  | B4    | 123    |    |
| 30  | BG    | 123    |    |
| 31  | AT    | 132    |    |
| 32  | AO    | 148    |    |
| 33  | BB    | 239    |    |
| 34  | BY    | 155    |    |
| 35  | BO    | 203    |   |
| 36  | BC    | 361    |  |
| 37  | B5    | 82     |  |
| 37  | BK    | 82     |  |
| 38  | BL    | 147    |  |
| 39  | Bf    | 51     |  |
| 40  | BU    | 121    |  |
| 41  | Bb    | 130    |  |
| 42  | Be    | 62     |  |
| 43  | BE    | 188    |  |
| 44  | Ba    | 94     |  |
| 45  | BT    | 86     |  |
| 46  | BW    | 68     |  |
| 47  | Bi    | 83     |  |
| 48  | BI    | 142    |  |
| 49  | BR    | 97     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 50  | BQ    | 151    |    |
| 51  | BV    | 67     |    |
| 52  | Bj    | 94     |    |
| 53  | BD    | 255    |    |
| 54  | BF    | 184    |    |
| 55  | BZ    | 99     |    |
| 56  | BP    | 120    |    |
| 57  | BM    | 194    |    |
| 58  | BS    | 155    |    |
| 59  | Bd    | 91     |    |
| 60  | BN    | 181    |    |
| 61  | Bg    | 51     |    |
| 62  | Bc    | 87     |  |
| 63  | BJ    | 141    |  |
| 64  | Bl    | 77     |  |
| 65  | Bk    | 65     |  |
| 66  | sd    | 9      |  |

## 2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 170684 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 rRNA 23S.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 1   | 1     | 3018     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 65181 | 29055 | 12094 | 21014 | 3018 |         |       |

- Molecule 2 is a RNA chain called rRNA 16S.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 2   | 2     | 1497     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32311 | 14417 | 5959 | 10438 | 1497 |         |       |

- Molecule 3 is a RNA chain called rRNA 5S.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 3   | 3     | 126      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2703  | 1203 | 498 | 876 | 126 |         |       |

- Molecule 4 is a protein called Dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | H     | 386      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3074  | 1962 | 535 | 567 | 10 |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S3Ae.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | AA    | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1531  | 993 | 268 | 266 | 4 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | AB    | 196      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1571  | 1017 | 269 | 281 | 4 |         |       |

- Molecule 7 is a protein called Zn-ribbon RNA-binding protein involved in translation.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | AC    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 449   | 285 | 80 | 76 | 8 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | AD    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1452  | 913 | 280 | 255 | 4 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S4e.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | AE    | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1983  | 1281 | 358 | 339 | 5 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | AF    | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1808  | 1147 | 334 | 320 | 7 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S6e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | AG    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 977   | 621 | 178 | 176 | 2 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | AH    | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1725  | 1095 | 323 | 300 | 7 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | AI    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 668 | 184 | 180 | 2 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S8e.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14  | AJ    | 125      | Total | C   | N   | O   |         |       |
|     |       |          | 986   | 612 | 205 | 169 | 0       | 0     |

- Molecule 15 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 15  | AK    | 135      | Total | C   | N   | O   | S       |       |
|     |       |          | 1073  | 673 | 207 | 189 | 4       | 0     |

- Molecule 16 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 16  | AL    | 100      | Total | C   | N   | O   | S       |       |
|     |       |          | 809   | 502 | 157 | 147 | 3       | 0     |

- Molecule 17 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17  | AM    | 127      | Total | C   | N   | O   | S       |       |
|     |       |          | 955   | 591 | 190 | 172 | 2       | 0     |

- Molecule 18 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 18  | AN    | 146      | Total | C   | N   | O   | S       |       |
|     |       |          | 1148  | 727 | 224 | 194 | 3       | 0     |

- Molecule 19 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 19  | AP    | 55       | Total | C   | N  | O  | S       |       |
|     |       |          | 455   | 288 | 95 | 67 | 5       | 0     |

- Molecule 20 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 20  | AQ    | 157      | Total | C   | N   | O   | S       |       |
|     |       |          | 1305  | 833 | 249 | 219 | 4       | 0     |

- Molecule 21 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | AR    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 884   | 562 | 172 | 147 | 3 |         |       |

- Molecule 22 is a protein called 30S ribosomal protein S17e.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 22  | AS    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 541   | 343 | 104 | 93 | 1 |         |       |

- Molecule 23 is a protein called 30S ribosomal protein S19e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | AU    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1223  | 790 | 221 | 212 |   |         |       |

- Molecule 24 is a protein called 30S ribosomal protein S24e.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | AV    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 528 | 129 | 148 | 3 |         |       |
| 24  | B6    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 516 | 125 | 146 | 3 |         |       |

- Molecule 25 is a protein called 30S ribosomal protein S27e.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 25  | AW    | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 470   | 294 | 91 | 80 | 5 |         |       |

- Molecule 26 is a protein called 30S ribosomal protein S28e.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 26  | AX    | 65       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 516   | 316 | 103 | 97 |   |         |       |

- Molecule 27 is a protein called 30S ribosomal protein S27ae.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 27  | AY    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 400   | 257 | 76 | 62 | 5 |         |       |

- Molecule 28 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | AZ    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1541  | 983 | 284 | 270 | 4 |         |       |

- Molecule 29 is a protein called eS32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29  | A0    | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 343   | 218 | 84 | 39 | 2 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L7Ae.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | A3    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 594 | 156 | 180 | 3 |         |       |
| 30  | BG    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 932   | 594 | 156 | 179 | 3 |         |       |
| 30  | B4    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 594 | 156 | 180 | 3 |         |       |

- Molecule 31 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | AT    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1057  | 675 | 201 | 174 | 7 |         |       |

- Molecule 32 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | AO    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1116  | 700 | 221 | 190 | 5 |         |       |

- Molecule 33 is a protein called Large ribosomal subunit protein uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 33  | BB    | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1838  | 1163 | 354 | 317 | 4 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein uL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | BY    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1235  | 783 | 234 | 212 | 6 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | BO    | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1607  | 1024 | 302 | 279 | 2 |         |       |

- Molecule 36 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | BC    | 360      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2870  | 1843 | 522 | 494 | 11 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein eL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | B5    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 614   | 388 | 116 | 108 | 2 |         |       |
| 37  | BK    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 607   | 383 | 115 | 107 | 2 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | BL    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1149  | 720 | 224 | 202 | 3 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | Bf    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 435   | 275 | 99 | 60 | 1 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | BU    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 638 | 198 | 170 | 5 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein eL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | Bb    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1095  | 702 | 221 | 171 | 1 |         |       |

- Molecule 42 is a protein called Large ribosomal subunit protein eL37.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | Be    | 61       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 503   | 312 | 112 | 75 | 4 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | BE    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1485  | 934 | 277 | 265 | 9 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein eL31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Ba    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 778   | 503 | 147 | 127 | 1 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | BT    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 696   | 451 | 118 | 126 | 1 |         |       |

- Molecule 46 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 46  | BW    | 68       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 565   | 349 | 111 | 99 | 6 |         |       |

- Molecule 47 is a protein called Large ribosomal subunit protein eL43.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 47  | Bi    | 82       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 620   | 389 | 129 | 97 | 5 |         |       |

- Molecule 48 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | BI    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1148  | 734 | 217 | 194 | 3 |         |       |

- Molecule 49 is a protein called Large ribosomal subunit protein eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | BR    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 797   | 507 | 164 | 125 | 1 |         |       |

- Molecule 50 is a protein called Large ribosomal subunit protein eL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | BQ    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1265  | 795 | 261 | 203 | 6 |         |       |

- Molecule 51 is a protein called Large ribosomal subunit protein eL24.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51  | BV    | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 532   | 339 | 103 | 84 | 6 |         |       |

- Molecule 52 is a protein called Large ribosomal subunit protein eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Bj    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 502 | 163 | 119 | 5 |         |       |

- Molecule 53 is a protein called Large ribosomal subunit protein uL4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | BD    | 255      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2026  | 1290 | 388 | 343 | 5 |         |       |

- Molecule 54 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | BF    | 183      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1456  | 943 | 251 | 261 | 1 |         |       |

- Molecule 55 is a protein called Large ribosomal subunit protein eL30.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 55  | BZ    | 98       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 749   | 486 | 122 | 141 |  |         |       |

- Molecule 56 is a protein called Large ribosomal subunit protein eL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | BP    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 971   | 610 | 188 | 170 | 3 |         |       |

- Molecule 57 is a protein called Large ribosomal subunit protein eL15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | BM    | 193      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1588  | 1014 | 318 | 251 | 5 |         |       |

- Molecule 58 is a protein called Large ribosomal subunit protein uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | BS    | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 786 | 246 | 211 | 4 |         |       |

- Molecule 59 is a protein called Large ribosomal subunit protein eL34.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 59  | Bd    | 91       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 759   | 477 | 163 | 109 | 10 |         |       |

- Molecule 60 is a protein called Large ribosomal subunit protein uL16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | BN    | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1452  | 920 | 281 | 246 | 5 |         |       |

- Molecule 61 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 61  | Bg    | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 387   | 243 | 80 | 60 | 4 |         |       |

- Molecule 62 is a protein called Large ribosomal subunit protein eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | Bc    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 435 | 132 | 115 | 2 |         |       |

- Molecule 63 is a protein called Large ribosomal subunit protein uL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | BJ    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1066  | 664 | 214 | 185 | 3 |         |       |

- Molecule 64 is a protein called Large ribosomal subunit protein eL20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | Bl    | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 659   | 425 | 120 | 113 | 1 |         |       |

- Molecule 65 is a protein called C2H2-type domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 65  | Bk    | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 528   | 339 | 108 | 78 | 3 |         |       |

- Molecule 66 is a RNA chain called antiSD-RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 66  | sd    | 9        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 199   | 88 | 39 | 63 | 9 |         |       |

- Molecule 67 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 67  | 1     | 166      | Total | Mg  | 0       |
|     |       |          | 166   | 166 |         |
| 67  | 2     | 69       | Total | Mg  | 0       |
|     |       |          | 69    | 69  |         |
| 67  | 3     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 67  | AK    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 67  | AN    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 67  | BB    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 67  | Bb    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 67  | BD    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 67  | BM    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 67  | BS    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

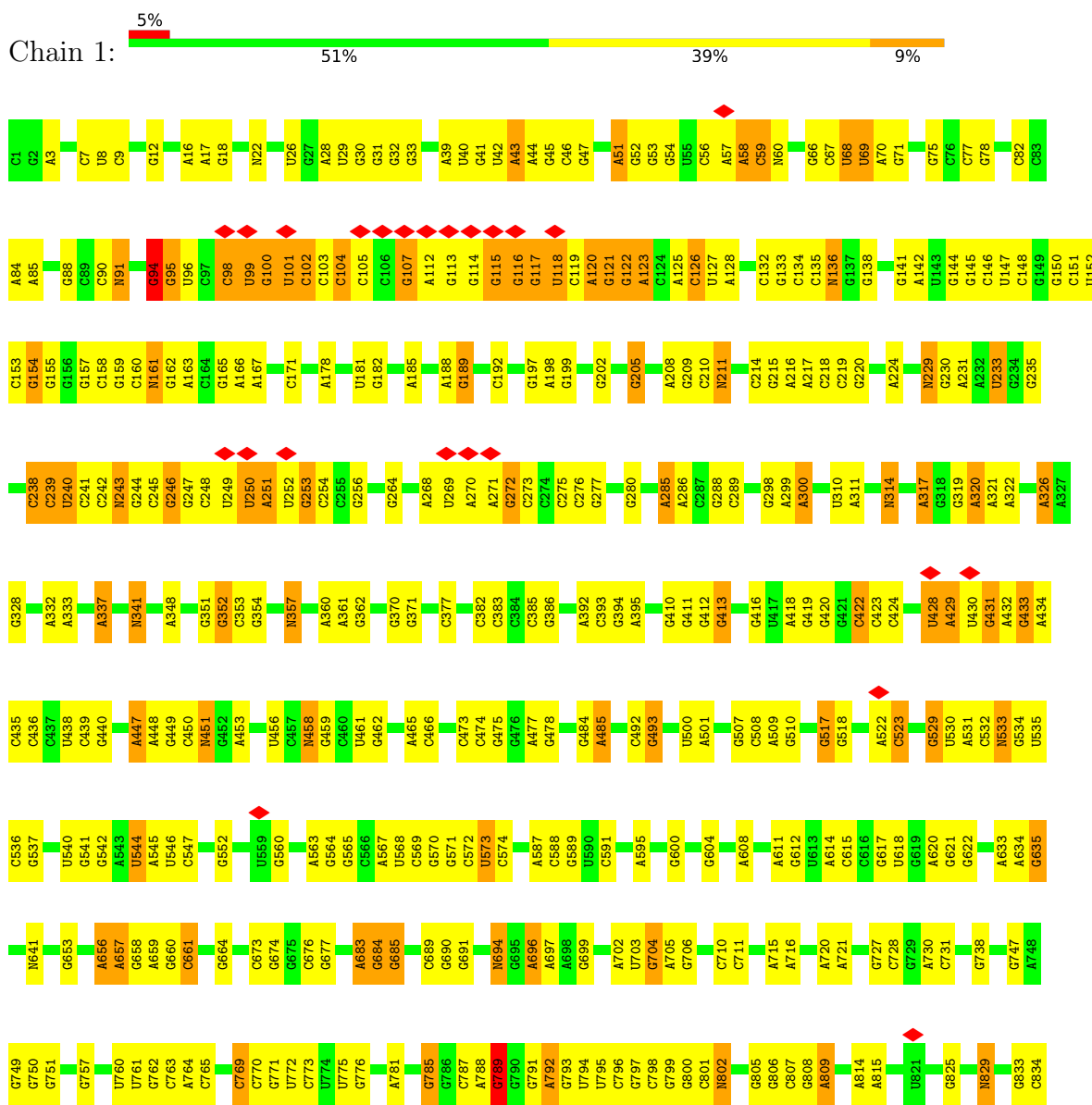
- Molecule 68 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 68  | AC    | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 68  | AF    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | AP    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | AR    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | AW    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Be    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Bi    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | BV    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Bj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Bd    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Bg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 68  | Bk    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

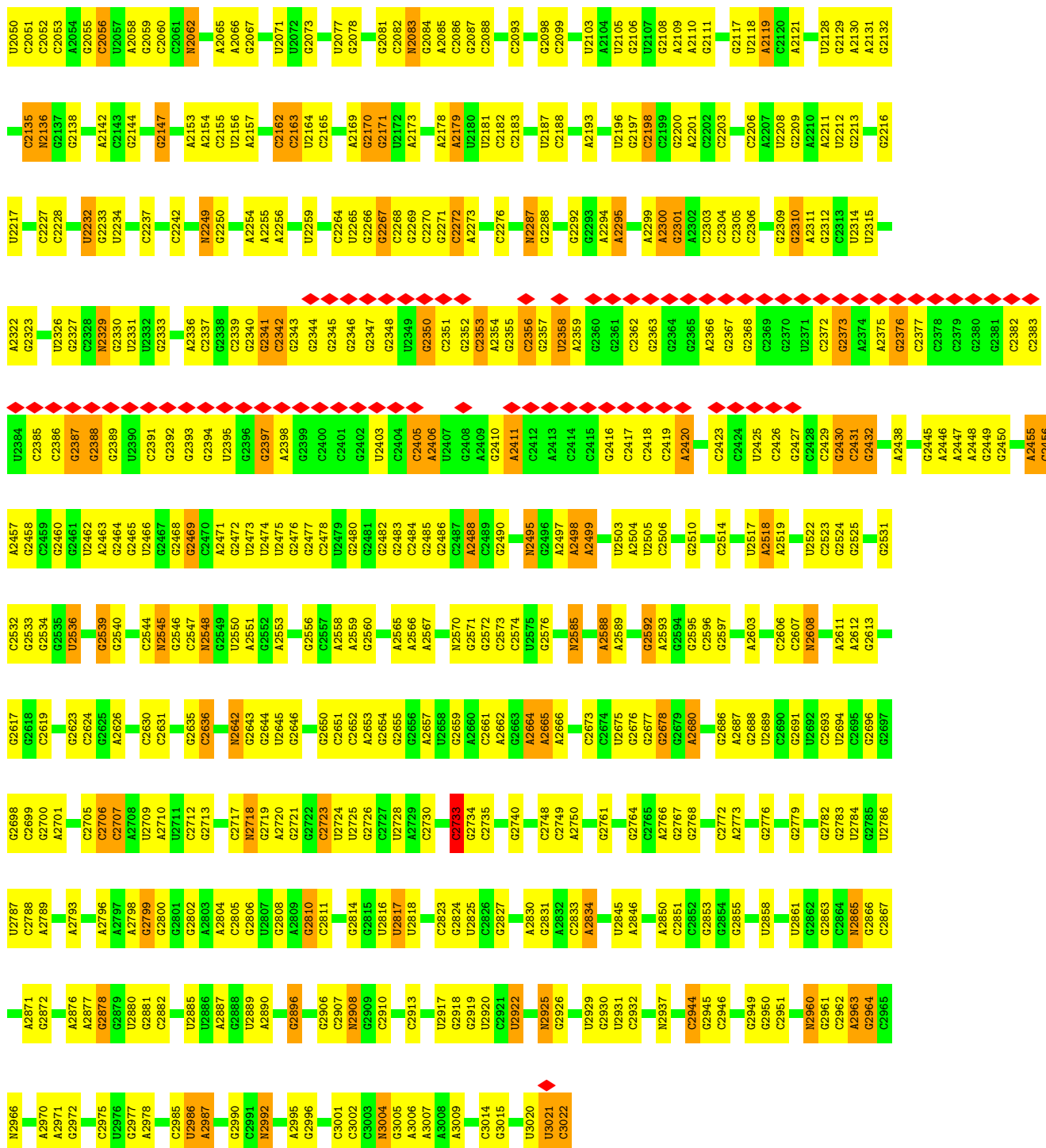
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: rRNA 23S

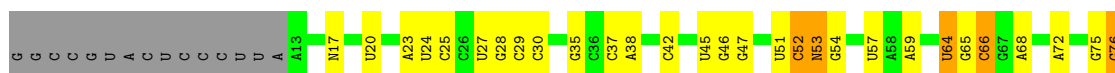


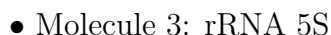
|       |       |       |       |       |       |       |       |       |       |       |       |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|
| G1943 | A1854 | G1759 | N1667 | A1582 | U1482 | G1392 | G1323 | A1251 | C1153 | G1078 | U993  | A919 | N835 |
| G1950 | A1855 | G1668 | C1669 | U1583 | A1484 | G1393 | A1324 | G1252 | C1154 | G1079 |       | C920 | G841 |
| C1951 | U1856 | G1761 | C1669 | C1587 | A1485 | C1394 | A1325 | G1253 | C1155 | A1081 | U998  | N922 | A842 |
| A1952 | C1858 | U1762 | A1676 | C1588 | C1489 | C1395 | G1326 | C1254 | U1159 | A1084 | G1006 | G923 | A843 |
| A1954 | C1859 | G1677 | G1678 | U1589 | G1490 | A1396 | C1327 | C1255 | U1161 | U1085 | C1007 | A924 | A844 |
|       | U1862 | N1765 | G1678 | C1590 | C1498 | A1397 | A1328 | C1256 | A1162 | G1086 | C1011 | A925 | C845 |
| N1962 |       |       |       | A1591 | G1499 | C1401 | G1329 | A1259 | A1163 | G1087 | G1012 | A926 | C846 |
| G1972 | A1769 | U1770 | C1687 | N1593 | C1499 | G1402 | C1330 | U1260 | G1168 |       | U1013 | G929 | A848 |
| A1976 | N1779 |       |       | N1594 | G1508 | G1406 | C1331 | G1261 | C1164 | C1093 | G1014 | G930 | C849 |
| G1979 | N1780 |       |       | G1598 | C1509 | C1407 | C1332 | U1262 | G1169 | C1094 | A1015 | U931 | A850 |
| G1980 | U1875 |       |       | C1599 | C1514 | G1411 | U1333 | G1263 | A1170 | G1095 | C1019 | A854 | U851 |
| G1987 | G1781 |       |       | U1600 | C1515 | C1415 | C1334 | C1265 | C1171 | A1101 | G1020 | U935 | C855 |
| G1989 | G1782 |       |       | U1601 | G1516 |       | G1335 | G1266 | C1172 | G1102 | G1026 | G936 | G856 |
|       | G1783 |       |       | G1606 | G1517 | G1420 | U1337 | U1269 | A1174 | G1103 | G1027 | U937 | A858 |
| G1983 | U1784 |       |       |       |       | G1421 | U1338 | G1272 |       | C1104 |       | G939 |      |
|       | A1787 |       |       | A1612 | G1520 | A1422 | A1339 | G1278 | C1179 | G1105 | G1031 | C940 | G864 |
| U1982 | A1788 |       |       | A1613 | G1524 | A1423 | A1340 | U1279 | G1180 | G1106 | A1032 | C941 | C865 |
| U1986 | G1789 |       |       | C1614 | U1525 | G1424 | A1341 | C1280 | G1186 | U1107 | A1033 | G946 | C866 |
| C1988 | C1790 |       |       | C1615 | A1526 | G1425 | A1342 | C1281 | U1187 | G1108 | A1034 | G947 | U867 |
| U1992 | G1791 |       |       | G1616 | U1533 | A1426 | G1343 | A1282 | U1188 | G1109 | G1035 | C947 | C868 |
| G1993 | G1792 |       |       | U1617 |       |       | A1344 | A1283 | U1207 | G1110 | G1036 | A948 | G869 |
| C1994 | C1707 |       |       | G1618 |       |       |       | A1284 | G1208 | G1111 | C1037 | G949 | A870 |
| A1889 | A1795 |       |       | C1619 | G1540 | U1431 | G1344 | A1285 | A1198 |       | C1038 | G950 | G871 |
| C1890 | U1709 |       |       | G1620 | U1541 | G1432 | U1345 | G1285 | G1199 | A1115 | A1039 | G951 | C872 |
| G1995 | G1796 |       |       | N1621 | U1545 | G1433 | G1346 | U1288 | G1200 | G1116 | A1040 | U952 | G877 |
| U1996 | C1710 |       |       | A1625 | A1546 | U1434 | C1347 | G1289 | G1201 | C1117 | U1041 | G953 | U878 |
| A1997 | G1711 |       |       | C1626 | U1547 | G1435 | U1348 | U1290 | U1202 | C1118 | G1042 | A954 | A879 |
| A1998 | G1712 |       |       | G1630 | U1548 | G1436 | U1349 | G1291 | G1203 | C1119 | G1043 | A955 | G880 |
| C1898 | C1805 |       |       | G1631 | C1549 | G1437 | A1350 | N1293 | C1205 | U1120 | G1046 | U956 |      |
| C1899 | U1807 |       |       | C1632 | N1550 | G1438 | A1351 | G1294 | G1206 | A1121 | C1047 | U957 | G887 |
| U1900 | U1808 |       |       | G1633 | G1551 | G1439 | C1352 | G1295 | G1207 | U1123 | N1048 | C959 | G888 |
| G1901 | A1716 |       |       | C1633 | C1552 |       | A1353 | U1299 | U1208 | U1124 | A1053 | C960 | U889 |
| G1905 | G1726 |       |       |       | C1553 | G1443 | G1354 | U1300 | G1209 | G1125 | A1054 | U961 | G890 |
|       | C1727 |       |       | A1639 | N1554 | G1444 | C1355 | A1301 | U1210 |       | U1054 | C962 | C891 |
| A1908 | U1816 |       |       | A1640 | C1555 | G1445 | U1356 | G1302 | A1211 | G1129 | A1055 | C963 | G892 |
| A1909 | C1822 |       |       | A1641 | C1556 |       | U1357 | A1303 | A1212 | G1130 | G1056 | A964 | A893 |
| G1910 | G1731 |       |       |       | N1557 | G1449 | C1357 | C1304 | G1216 | G1131 | C1057 | C965 | A894 |
| A1914 | A1824 |       |       | A1645 | G1558 | G1450 | A1358 | C1305 |       | C1132 | U1058 | A966 | A895 |
| U1920 | U1825 |       |       | A1646 | C1559 | G1451 | U1359 | A1305 | G1221 | A1133 | G1059 | G896 | G896 |
| C1826 | C1826 |       |       | A1647 | A1560 | G1452 | C1359 | G1306 | G1222 | G1134 | G1060 | U973 | C897 |
| G1735 | G1735 |       |       | C1648 | U1560 |       | C1360 | C1307 | N1222 | G1135 | C1063 | G974 | G898 |
| C1828 | C1736 |       |       | G1649 | G1561 | U1457 | G1361 | G1308 | G1223 | G1136 | C1064 | A976 |      |
| U1830 |       |       |       | G1650 |       | G1458 | C1362 | G1309 | A1224 | G1137 | N1065 | G977 | G903 |
| G1929 | G1739 |       |       |       | A1567 | U1459 | U1362 | G1310 | G1225 | C1138 | G1066 | G978 | U806 |
| C1831 |       |       |       | U1653 | G1568 | C1459 | U1363 | G1311 | A1231 | G1140 | C1067 | C979 | A906 |
| U1929 | A1742 |       |       | A1654 | G1569 | N1460 | C1364 | U1314 | A1234 | A1141 | U1068 | C980 | A908 |
| A1840 | A1743 |       |       | A1655 | G1570 | G1461 | G1365 | U1315 | A1234 | A1142 | A1071 | N981 | C909 |
| A1931 | A1841 |       |       | U1656 | C1574 | G1462 | U1366 | G1316 |       | A1143 | U1072 | G982 | G910 |
| C1932 | A1748 |       |       | A1657 | C1575 |       | G1367 | A1316 | G1240 | G1144 | A1073 | C983 |      |
| A1933 | U1749 |       |       |       | C1576 | A1469 | G1370 | G1317 | A1241 | C1145 | U1074 | U984 | C913 |
| N1934 | A1750 |       |       | C1661 | U1577 | G1470 | C1371 | G1318 | G1242 | A1241 | A1074 |      | G914 |
| C2044 | A1751 |       |       | N1662 | G1578 | G1478 | G1372 | C1319 | C1242 | C1146 | U1075 | U990 | A917 |
| A2045 | G1752 |       |       | G1663 | U1579 | C1479 | G1373 | U1320 | N1243 | C1147 | C1076 | G991 | C918 |
| C2046 | U1755 |       |       | U1664 | C1580 | G1481 | G1374 | U1321 | A1250 | C1148 | C1077 | C992 |      |
| A1940 | G1756 |       |       |       | A1581 |       | G1380 | A1322 |       |       |       |      |      |
|       |       |       |       |       |       |       | G1386 |       |       |       |       |      |      |
|       |       |       |       |       |       |       | G1387 |       |       |       |       |      |      |
|       |       |       |       |       |       |       | A1388 |       |       |       |       |      |      |
|       |       |       |       |       |       |       | C1389 |       |       |       |       |      |      |
|       |       |       |       |       |       |       | G1390 |       |       |       |       |      |      |
|       |       |       |       |       |       |       | G1391 |       |       |       |       |      |      |



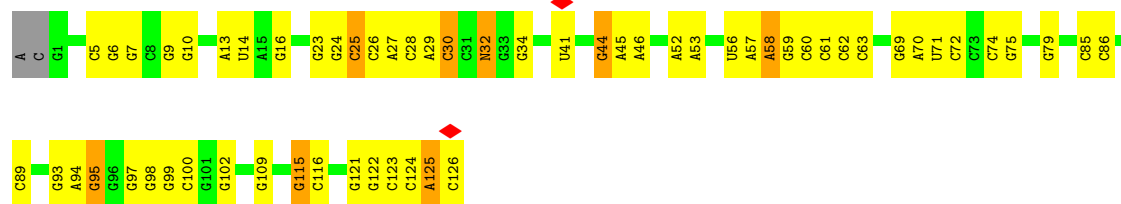
• Molecule 2: rRNA 16S

Chain 2: 58% 34% 7%



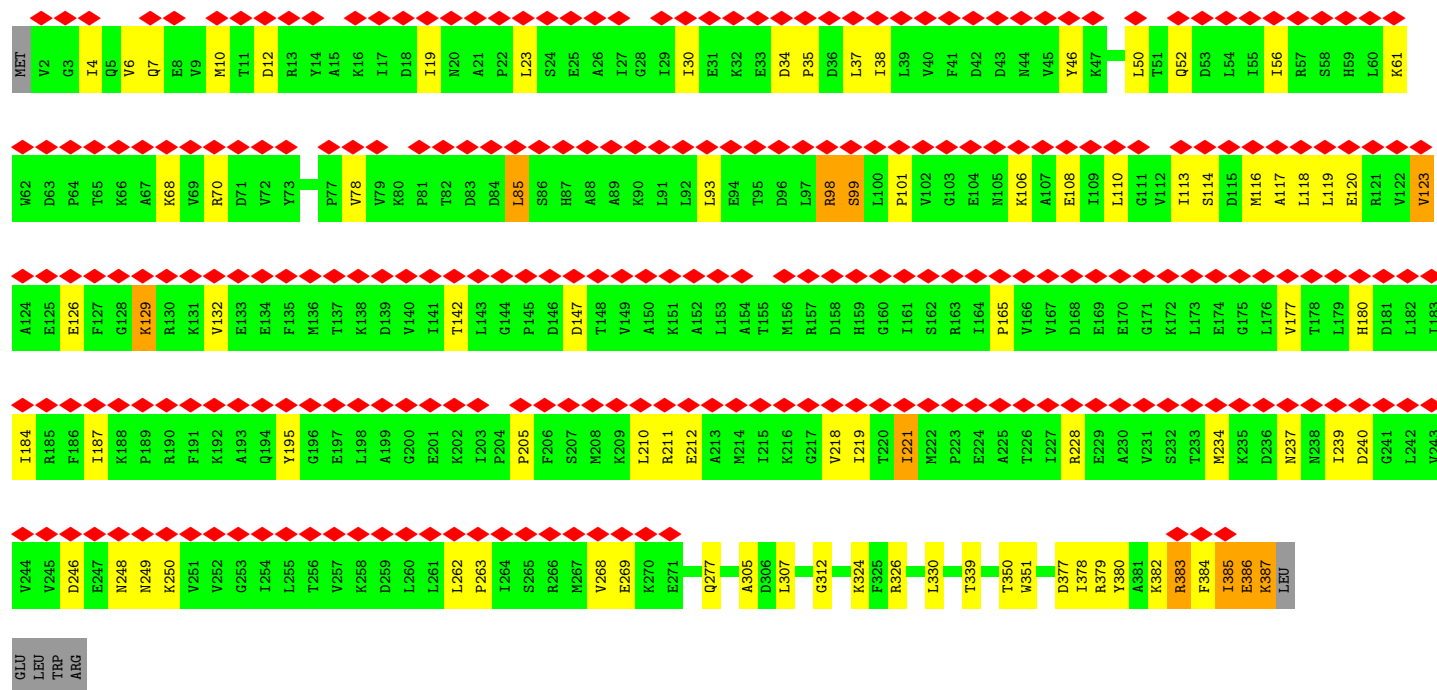


Chain 3: 



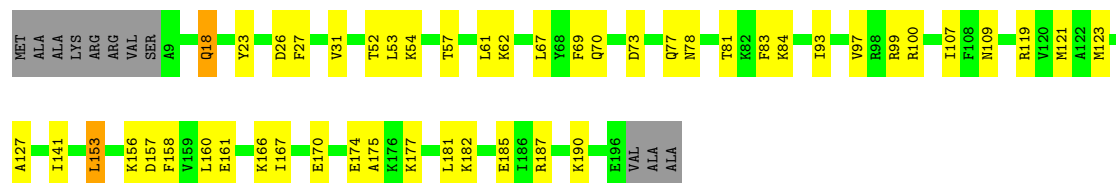
• Molecule 4: Dehydrogenase

Chain H: 



• Molecule 5: 30S ribosomal protein S3Ae

Chain AA: 

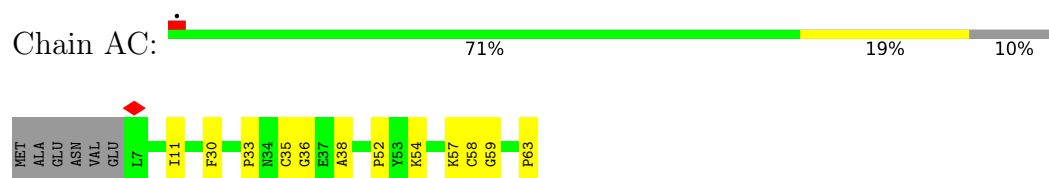


• Molecule 6: 30S ribosomal protein S2

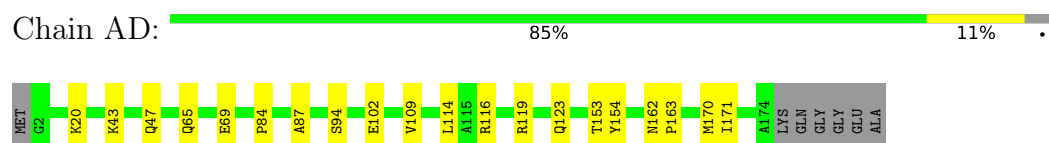
Chain AB: 



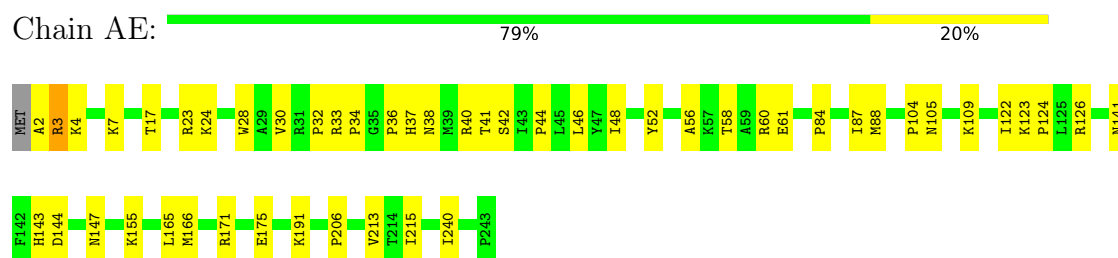
- Molecule 7: Zn-ribbon RNA-binding protein involved in translation



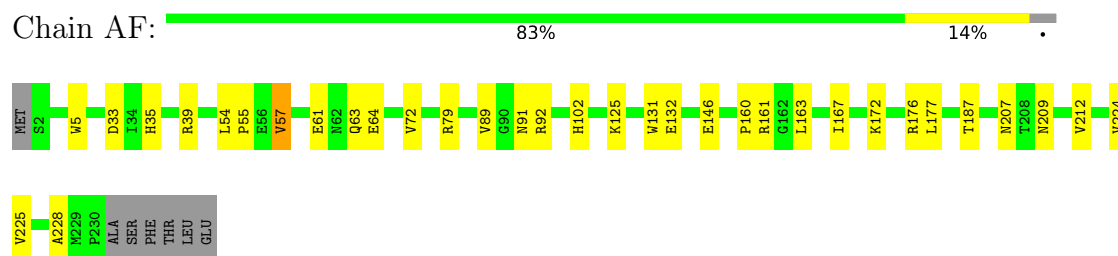
- Molecule 8: 30S ribosomal protein S4



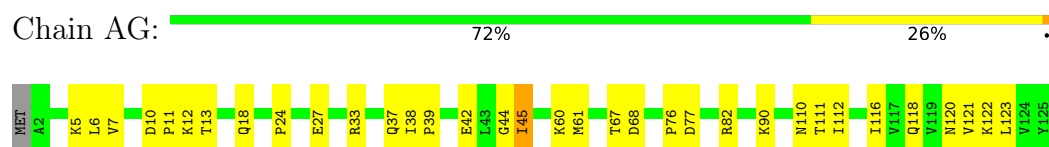
- Molecule 9: 30S ribosomal protein S4e



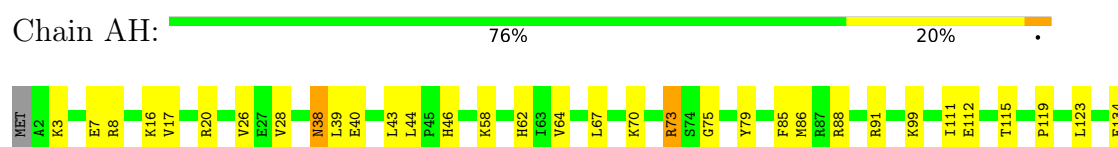
- Molecule 10: 30S ribosomal protein S5



- Molecule 11: 30S ribosomal protein S6e



- Molecule 12: 30S ribosomal protein S7





- Molecule 13: 30S ribosomal protein S8

Chain AI: 85% 14% ..



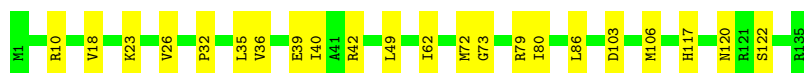
- Molecule 14: 30S ribosomal protein S8e

Chain AJ: 87% 9% ..



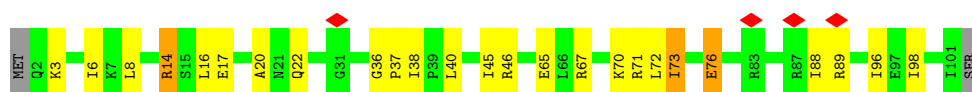
- Molecule 15: 30S ribosomal protein S9

Chain AK: 84% 16%



- Molecule 16: 30S ribosomal protein S10

Chain AL: 74% 22% ..



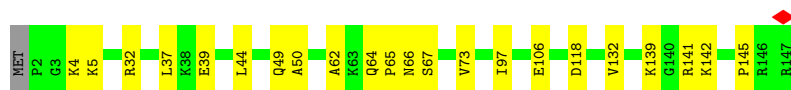
- Molecule 17: 30S ribosomal protein S11

Chain AM: 82% 10% 7%



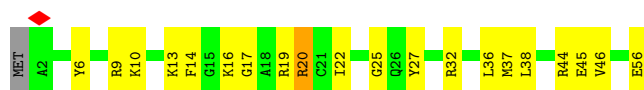
- Molecule 18: 30S ribosomal protein S12

Chain AN: 84% 15%



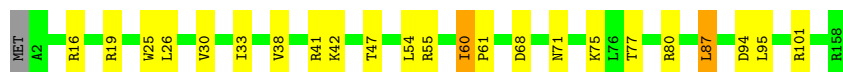
- Molecule 19: 30S ribosomal protein S14 type Z

Chain AP: 62% 34%



- Molecule 20: 30S ribosomal protein S15

Chain AQ: 85% 13% ..



- Molecule 21: 30S ribosomal protein S17

Chain AR: 78% 16% • 5%



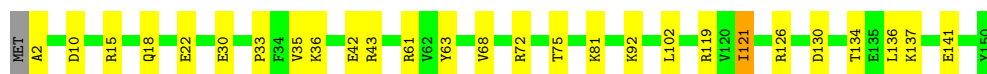
- Molecule 22: 30S ribosomal protein S17e

Chain AS: 70% 25% •



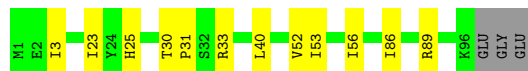
- Molecule 23: 30S ribosomal protein S19e

Chain AU: 81% 17% ..



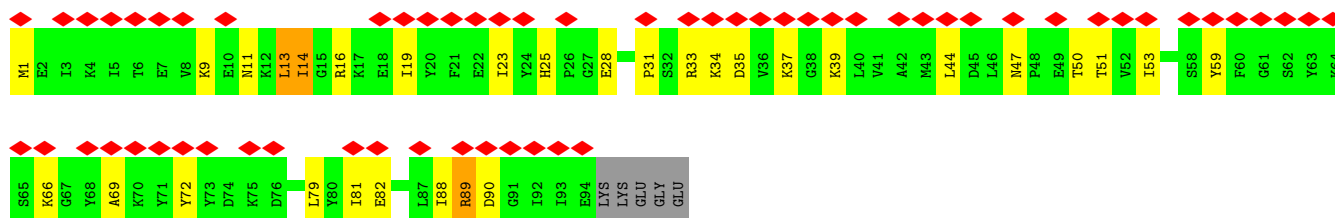
- Molecule 24: 30S ribosomal protein S24e

Chain AV: 85% 12% •



- Molecule 24: 30S ribosomal protein S24e

Chain B6: 61% 64% 28% • 5%



- Molecule 25: 30S ribosomal protein S27e

Chain AW: 



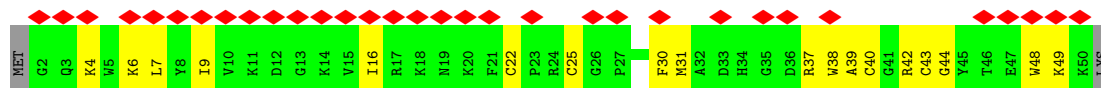
- Molecule 26: 30S ribosomal protein S28e

Chain AX: 



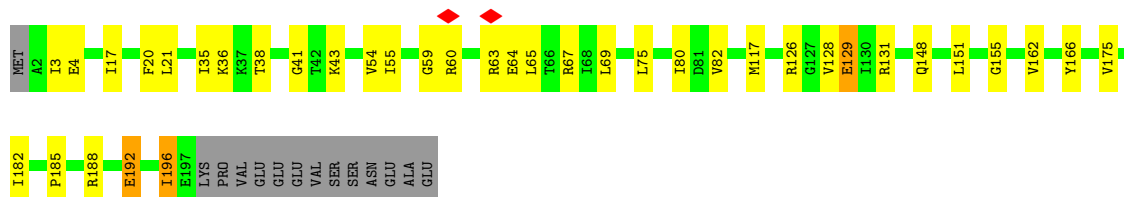
- Molecule 27: 30S ribosomal protein S27ae

Chain AY: 



- Molecule 28: 30S ribosomal protein S3

Chain AZ: 



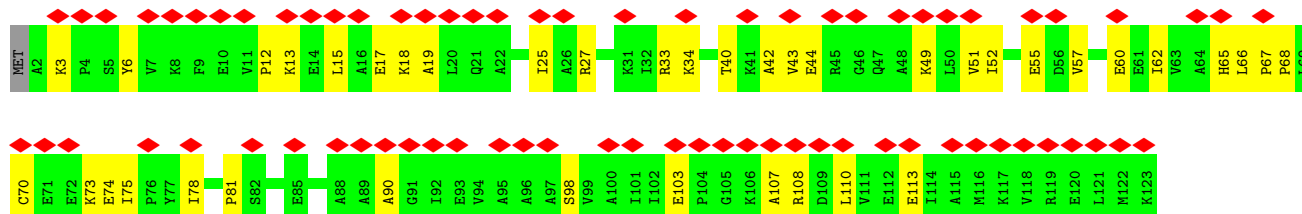
- Molecule 29: eS32

Chain A0: 

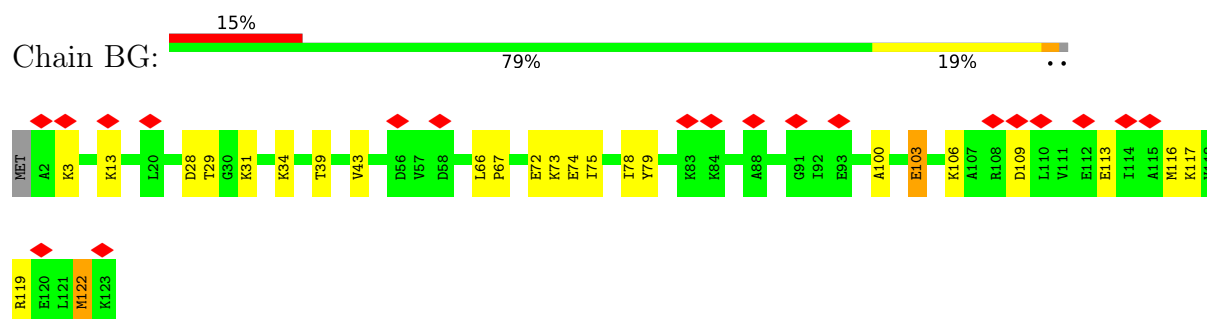


- Molecule 30: 50S ribosomal protein L7Ae

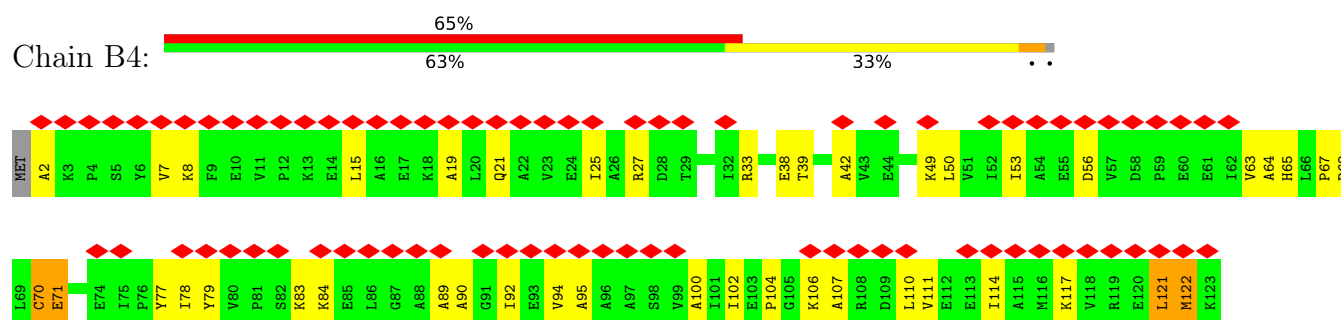
Chain A3: 



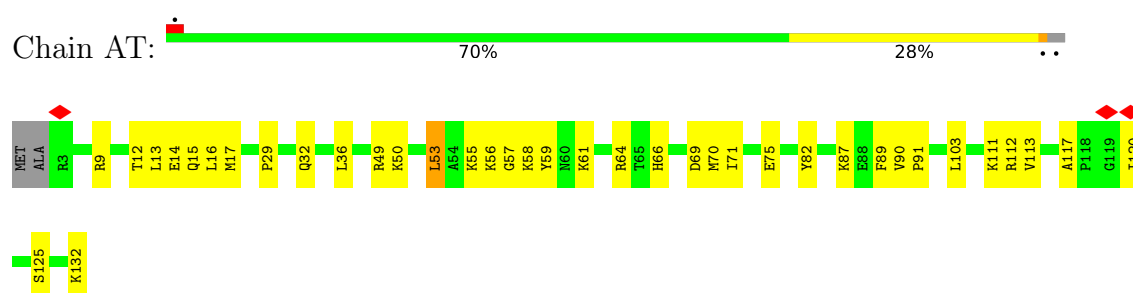
- Molecule 30: 50S ribosomal protein L7Ae



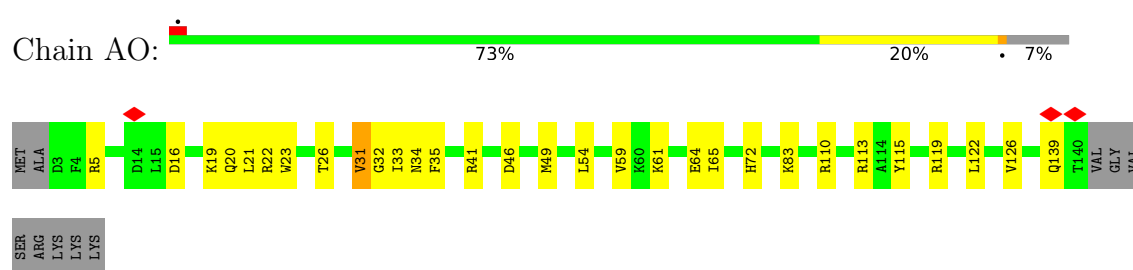
- Molecule 30: 50S ribosomal protein L7Ae



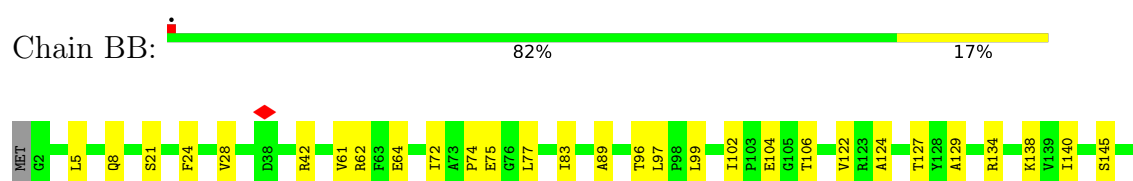
- Molecule 31: 30S ribosomal protein S19



- Molecule 32: 30S ribosomal protein S13

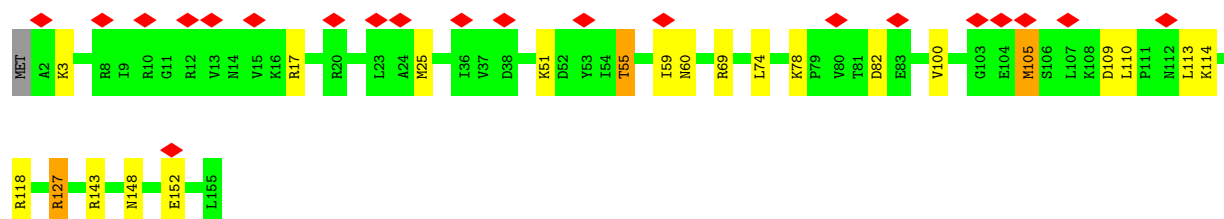
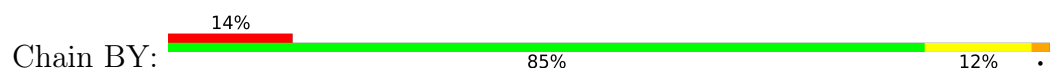


- Molecule 33: Large ribosomal subunit protein uL2

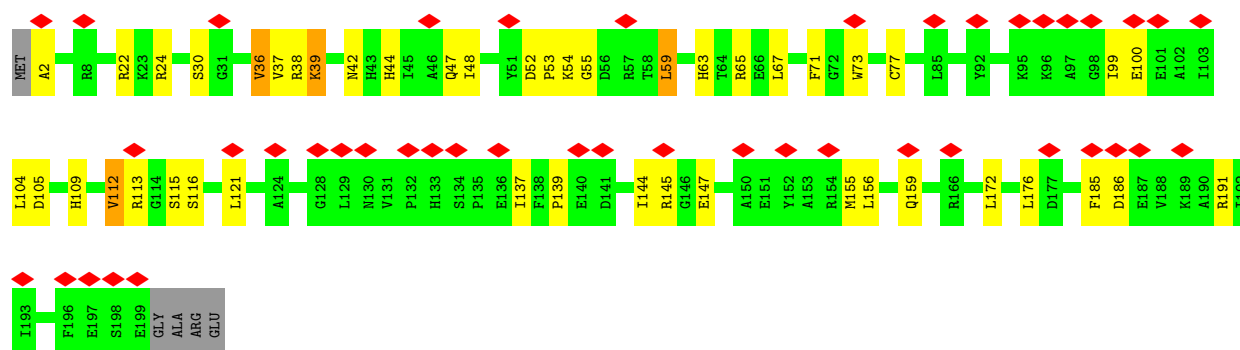
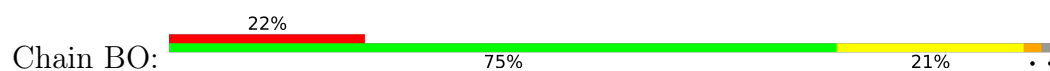




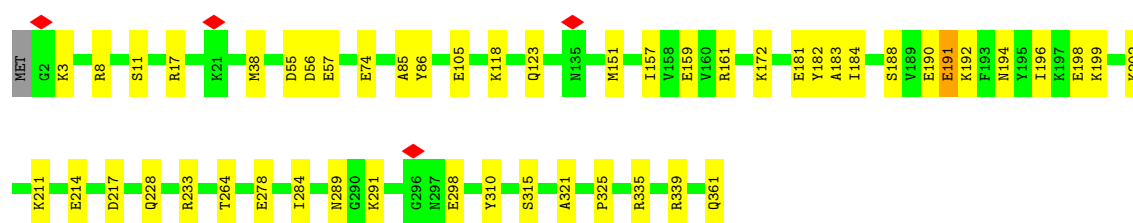
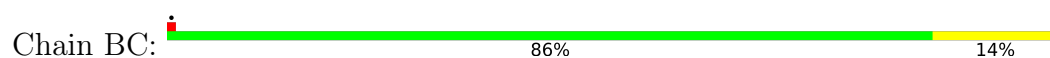
- Molecule 34: Large ribosomal subunit protein uL30



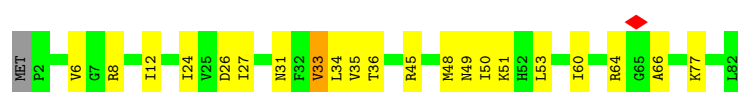
- Molecule 35: Large ribosomal subunit protein uL18



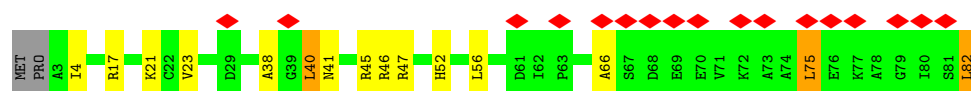
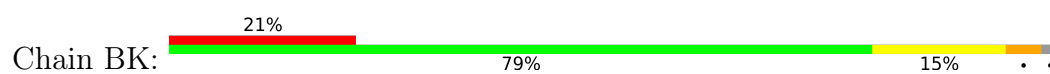
- Molecule 36: Large ribosomal subunit protein uL3



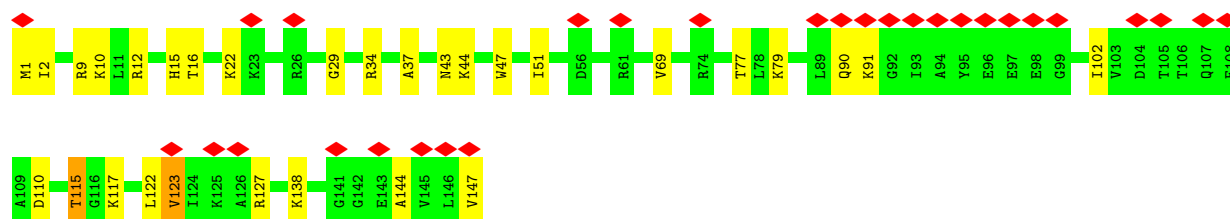
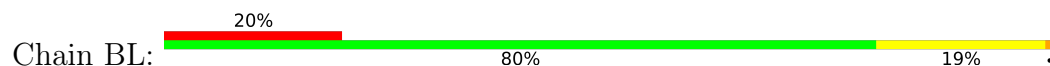
- Molecule 37: Large ribosomal subunit protein eL14



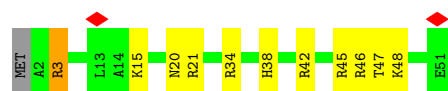
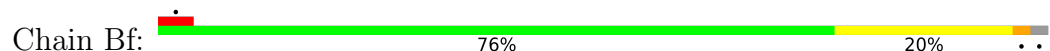
- Molecule 37: Large ribosomal subunit protein eL14



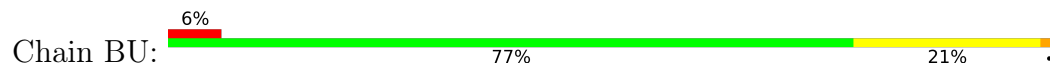
- Molecule 38: Large ribosomal subunit protein uL15



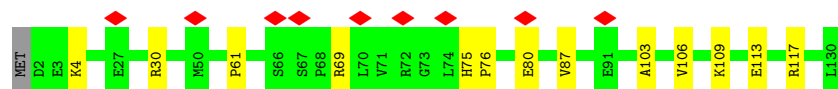
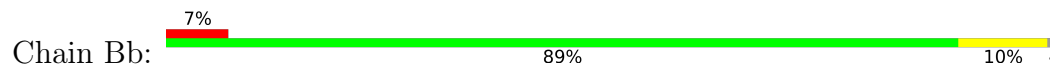
- Molecule 39: Large ribosomal subunit protein eL39



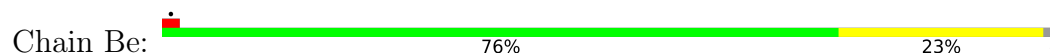
- Molecule 40: Large ribosomal subunit protein uL24



- Molecule 41: Large ribosomal subunit protein eL32

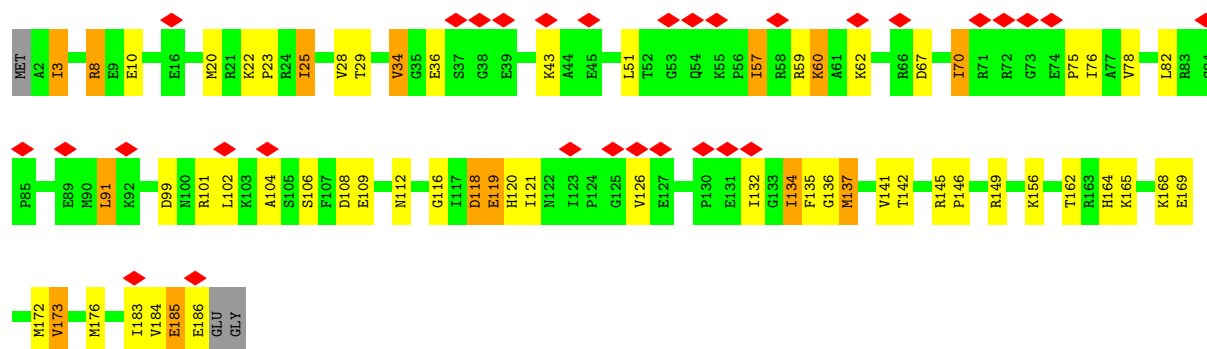


- Molecule 42: Large ribosomal subunit protein eL37

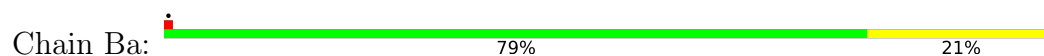


- Molecule 43: Large ribosomal subunit protein uL5

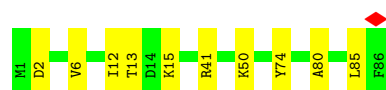




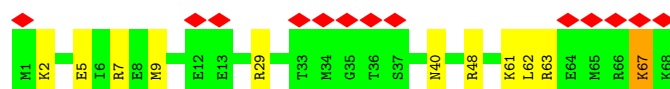
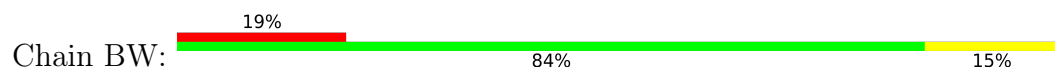
- Molecule 44: Large ribosomal subunit protein eL31



- Molecule 45: Large ribosomal subunit protein uL23



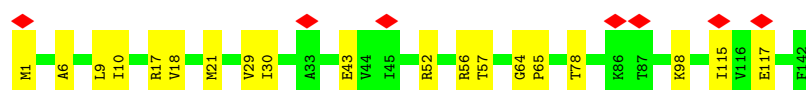
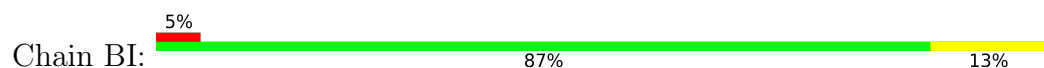
- Molecule 46: Large ribosomal subunit protein uL29



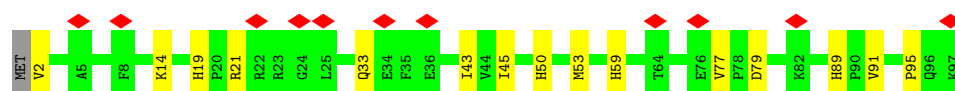
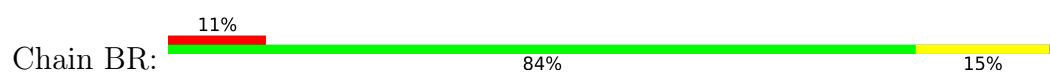
- Molecule 47: Large ribosomal subunit protein eL43



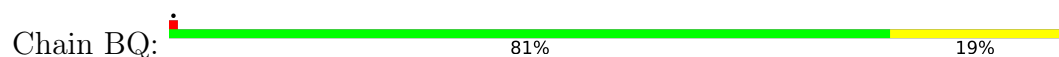
- Molecule 48: Large ribosomal subunit protein uL13



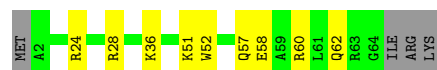
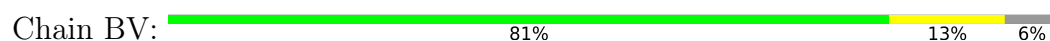
- Molecule 49: Large ribosomal subunit protein eL21



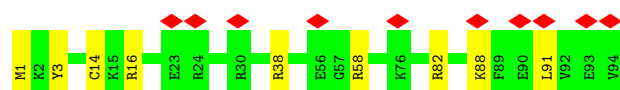
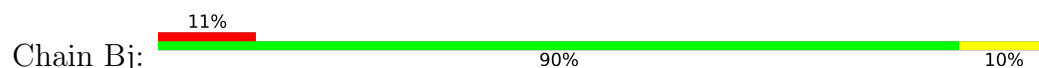
- Molecule 50: Large ribosomal subunit protein eL19



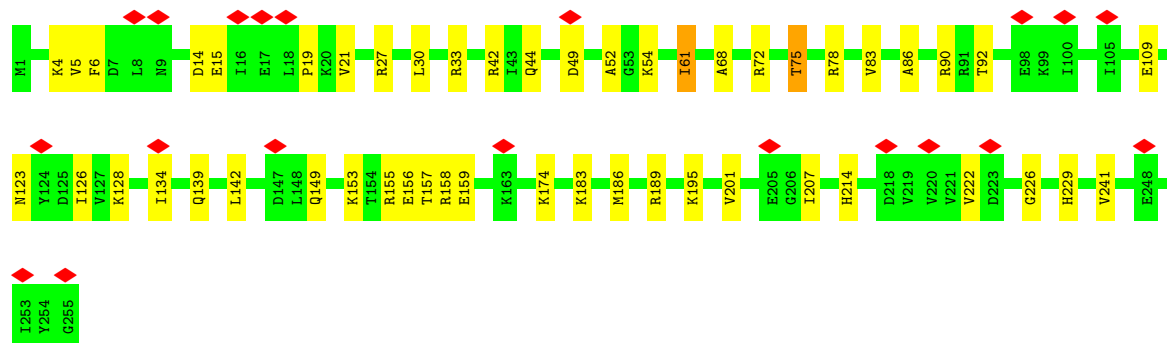
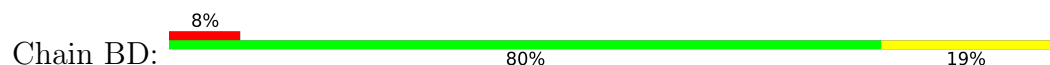
- Molecule 51: Large ribosomal subunit protein eL24



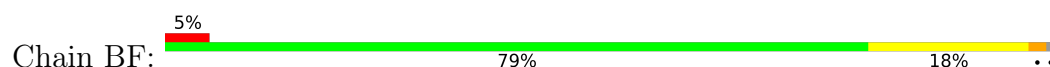
- Molecule 52: Large ribosomal subunit protein eL42



- Molecule 53: Large ribosomal subunit protein uL4

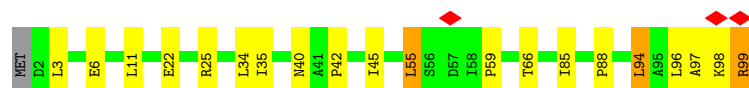
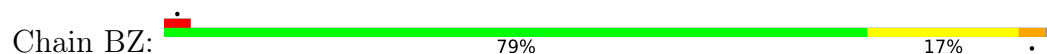


- Molecule 54: Large ribosomal subunit protein uL6

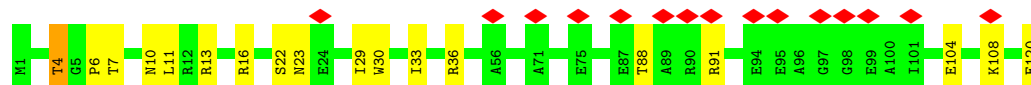
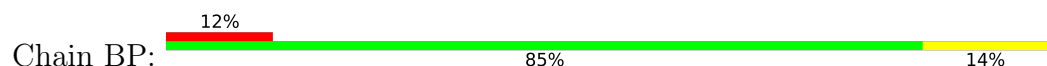




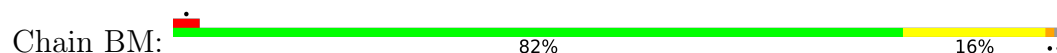
- Molecule 55: Large ribosomal subunit protein eL30



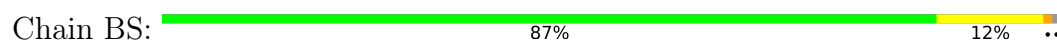
- Molecule 56: Large ribosomal subunit protein eL18



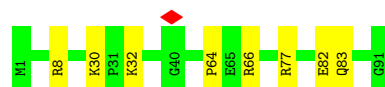
- Molecule 57: Large ribosomal subunit protein eL15



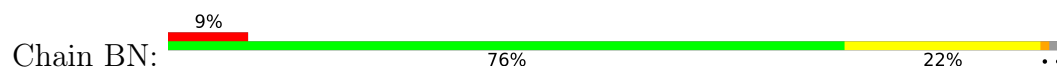
- Molecule 58: Large ribosomal subunit protein uL22

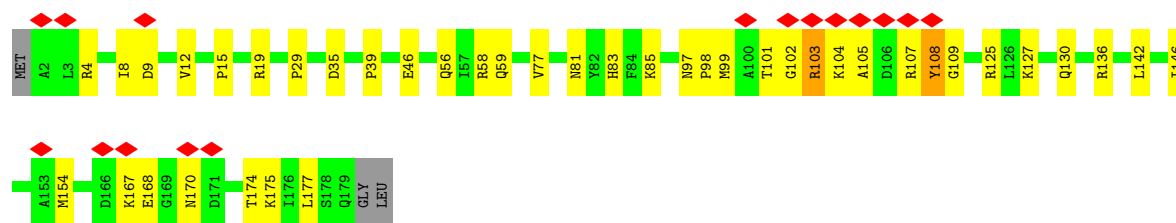


- Molecule 59: Large ribosomal subunit protein eL34

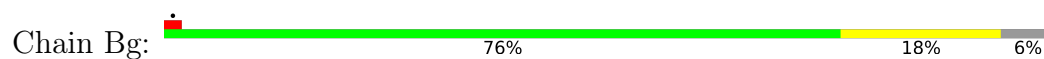


- Molecule 60: Large ribosomal subunit protein uL16

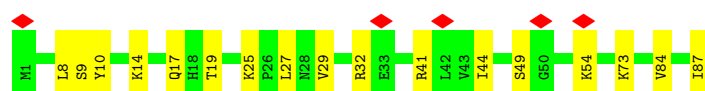
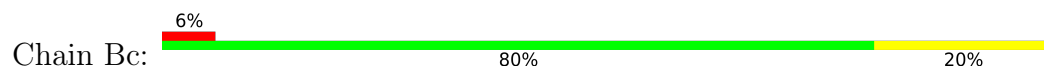




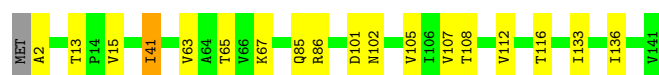
- Molecule 61: Large ribosomal subunit protein eL40



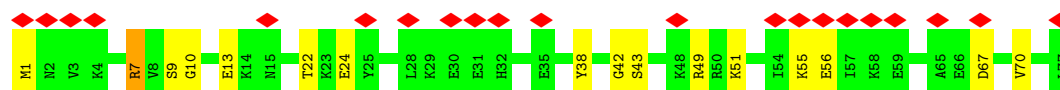
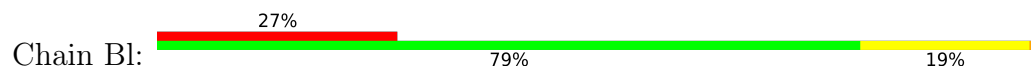
- Molecule 62: Large ribosomal subunit protein eL33



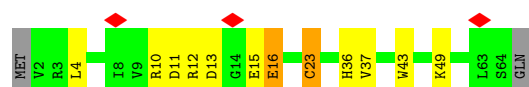
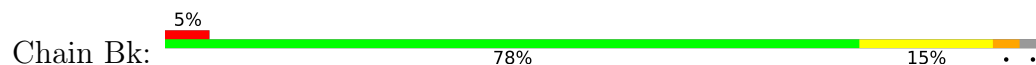
- Molecule 63: Large ribosomal subunit protein uL14



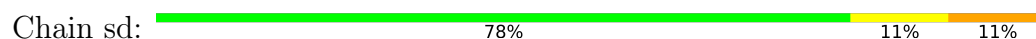
- Molecule 64: Large ribosomal subunit protein eL20



- Molecule 65: C2H2-type domain-containing protein



- Molecule 66: antiSD-RNA





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 182000                                  | 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)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.891                                   | Depositor |
| Minimum map value                    | -0.355                                  | Depositor |
| Average map value                    | 0.007                                   | Depositor |
| Map value standard deviation         | 0.050                                   | Depositor |
| Recommended contour level            | 0.07                                    | Depositor |
| Map size (Å)                         | 302.04, 302.04, 302.04                  | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.83900005, 0.83900005, 0.83900005      | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, A2M, UR3, OMG, ZN, OMU, 4AC, MG, 6MZ, OMC, LHH, MA6, B8H

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   | 1     | 0.14         | 3/70601 (0.0%) | 0.32        | 0/110066       |
| 2   | 2     | 0.18         | 0/34457        | 0.30        | 2/53715 (0.0%) |
| 3   | 3     | 0.16         | 0/2995         | 0.34        | 0/4669         |
| 4   | H     | 0.31         | 1/3120 (0.0%)  | 0.49        | 3/4209 (0.1%)  |
| 5   | AA    | 0.13         | 0/1557         | 0.28        | 0/2087         |
| 6   | AB    | 0.12         | 0/1602         | 0.26        | 0/2165         |
| 7   | AC    | 0.11         | 0/463          | 0.27        | 0/628          |
| 8   | AD    | 0.12         | 0/1476         | 0.23        | 0/1980         |
| 9   | AE    | 0.13         | 0/2032         | 0.29        | 0/2742         |
| 10  | AF    | 0.12         | 0/1838         | 0.25        | 0/2478         |
| 11  | AG    | 0.12         | 0/993          | 0.29        | 0/1329         |
| 12  | AH    | 0.21         | 0/1762         | 0.37        | 0/2366         |
| 13  | AI    | 0.13         | 0/1055         | 0.25        | 0/1415         |
| 14  | AJ    | 0.13         | 0/995          | 0.24        | 0/1327         |
| 15  | AK    | 0.12         | 0/1089         | 0.26        | 0/1459         |
| 16  | AL    | 0.11         | 0/817          | 0.28        | 0/1097         |
| 17  | AM    | 0.14         | 0/973          | 0.28        | 0/1311         |
| 18  | AN    | 0.12         | 0/1165         | 0.27        | 0/1547         |
| 19  | AP    | 0.13         | 0/465          | 0.32        | 0/613          |
| 20  | AQ    | 0.13         | 0/1333         | 0.26        | 0/1791         |
| 21  | AR    | 0.13         | 0/907          | 0.27        | 0/1225         |
| 22  | AS    | 0.12         | 0/548          | 0.28        | 0/725          |
| 23  | AU    | 0.11         | 0/1253         | 0.26        | 0/1689         |
| 24  | AV    | 0.11         | 0/826          | 0.24        | 0/1108         |
| 24  | B6    | 0.15         | 0/808          | 0.35        | 0/1086         |
| 25  | AW    | 0.12         | 0/476          | 0.27        | 0/641          |
| 26  | AX    | 0.10         | 0/518          | 0.23        | 0/694          |
| 27  | AY    | 0.09         | 0/412          | 0.25        | 0/549          |
| 28  | AZ    | 0.10         | 0/1563         | 0.24        | 0/2099         |
| 29  | A0    | 0.15         | 0/349          | 0.37        | 0/451          |
| 30  | A3    | 0.11         | 0/945          | 0.31        | 0/1274         |
| 30  | B4    | 0.17         | 0/945          | 0.36        | 0/1274         |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 30  | BG    | 0.18         | 0/944           | 0.33        | 0/1274          |
| 31  | AT    | 0.14         | 0/1077          | 0.29        | 0/1439          |
| 32  | AO    | 0.10         | 0/1135          | 0.28        | 0/1526          |
| 33  | BB    | 0.12         | 0/1882          | 0.31        | 0/2538          |
| 34  | BY    | 0.10         | 0/1254          | 0.26        | 0/1677          |
| 35  | BO    | 0.17         | 0/1645          | 0.33        | 0/2209          |
| 36  | BC    | 0.11         | 0/2933          | 0.30        | 0/3943          |
| 37  | B5    | 0.14         | 0/619           | 0.30        | 0/830           |
| 37  | BK    | 0.11         | 0/611           | 0.32        | 0/819           |
| 38  | BL    | 0.13         | 0/1167          | 0.32        | 0/1552          |
| 39  | Bf    | 0.11         | 0/443           | 0.26        | 0/589           |
| 40  | BU    | 0.31         | 0/1027          | 0.45        | 1/1368 (0.1%)   |
| 41  | Bb    | 0.10         | 0/1120          | 0.27        | 0/1494          |
| 42  | Be    | 0.09         | 0/514           | 0.29        | 0/676           |
| 43  | BE    | 0.21         | 0/1509          | 0.40        | 0/2022          |
| 44  | Ba    | 0.10         | 0/793           | 0.28        | 0/1064          |
| 45  | BT    | 0.11         | 0/705           | 0.28        | 0/945           |
| 46  | BW    | 0.13         | 0/566           | 0.28        | 0/747           |
| 47  | Bi    | 0.11         | 0/630           | 0.32        | 0/839           |
| 48  | BI    | 0.08         | 0/1166          | 0.25        | 0/1559          |
| 49  | BR    | 0.10         | 0/819           | 0.27        | 0/1098          |
| 50  | BQ    | 0.09         | 0/1281          | 0.25        | 0/1689          |
| 51  | BV    | 0.09         | 0/547           | 0.34        | 0/729           |
| 52  | Bj    | 0.11         | 0/807           | 0.26        | 0/1070          |
| 53  | BD    | 0.13         | 0/2069          | 0.31        | 0/2787          |
| 54  | BF    | 0.15         | 0/1485          | 0.30        | 0/2003          |
| 55  | BZ    | 0.14         | 0/759           | 0.32        | 0/1023          |
| 56  | BP    | 0.09         | 0/984           | 0.25        | 0/1314          |
| 57  | BM    | 0.11         | 0/1627          | 0.26        | 0/2170          |
| 58  | BS    | 0.13         | 0/1275          | 0.32        | 0/1715          |
| 59  | Bd    | 0.10         | 0/778           | 0.27        | 0/1036          |
| 60  | BN    | 0.12         | 0/1483          | 0.30        | 0/1992          |
| 61  | Bg    | 0.11         | 0/396           | 0.25        | 0/526           |
| 62  | Bc    | 0.11         | 0/693           | 0.30        | 0/926           |
| 63  | BJ    | 0.12         | 0/1080          | 0.30        | 0/1456          |
| 64  | Bl    | 0.14         | 0/669           | 0.29        | 0/886           |
| 65  | Bk    | 0.14         | 0/538           | 0.28        | 0/709           |
| 66  | sd    | 0.24         | 0/223           | 0.49        | 0/347           |
| All | All   | 0.15         | 4/179591 (0.0%) | 0.31        | 6/264395 (0.0%) |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 4   | H     | 377  | ASP  | C-N    | 14.46  | 1.54        | 1.33     |
| 1   | 1     | 94   | G    | O3'-P  | -10.51 | 1.45        | 1.61     |
| 1   | 1     | 96   | U    | C1'-N1 | 5.73   | 1.57        | 1.48     |
| 1   | 1     | 2173 | A2M  | O3'-P  | 5.03   | 1.61        | 1.56     |

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

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 4   | H     | 377  | ASP  | CA-C-N      | -15.23 | 101.77      | 123.10   |
| 4   | H     | 377  | ASP  | C-N-CA      | -15.23 | 101.77      | 123.10   |
| 4   | H     | 383  | ARG  | N-CA-C      | 6.30   | 120.58      | 113.01   |
| 40  | BU    | 115  | ILE  | CB-CA-C     | -5.83  | 104.27      | 112.14   |
| 2   | 2     | 1499 | G    | C2'-C3'-O3' | -5.44  | 105.54      | 113.70   |

There are no chirality outliers.

There are no planarity outliers.

## 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   | 1     | 65181 | 0        | 32950    | 1072    | 0            |
| 2   | 2     | 32311 | 0        | 16352    | 422     | 0            |
| 3   | 3     | 2703  | 0        | 1375     | 44      | 0            |
| 4   | H     | 3074  | 0        | 3190     | 85      | 0            |
| 5   | AA    | 1531  | 0        | 1623     | 28      | 0            |
| 6   | AB    | 1571  | 0        | 1630     | 19      | 0            |
| 7   | AC    | 449   | 0        | 435      | 8       | 0            |
| 8   | AD    | 1452  | 0        | 1521     | 10      | 0            |
| 9   | AE    | 1983  | 0        | 2060     | 28      | 0            |
| 10  | AF    | 1808  | 0        | 1879     | 27      | 0            |
| 11  | AG    | 977   | 0        | 1037     | 21      | 0            |
| 12  | AH    | 1725  | 0        | 1780     | 35      | 0            |
| 13  | AI    | 1034  | 0        | 1069     | 15      | 0            |
| 14  | AJ    | 986   | 0        | 1070     | 9       | 0            |
| 15  | AK    | 1073  | 0        | 1133     | 15      | 0            |
| 16  | AL    | 809   | 0        | 859      | 17      | 0            |
| 17  | AM    | 955   | 0        | 981      | 26      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | AN    | 1148  | 0        | 1248     | 14      | 0            |
| 19  | AP    | 455   | 0        | 475      | 18      | 0            |
| 20  | AQ    | 1305  | 0        | 1388     | 18      | 0            |
| 21  | AR    | 884   | 0        | 906      | 11      | 0            |
| 22  | AS    | 541   | 0        | 573      | 10      | 0            |
| 23  | AU    | 1223  | 0        | 1263     | 18      | 0            |
| 24  | AV    | 808   | 0        | 832      | 9       | 0            |
| 24  | B6    | 790   | 0        | 806      | 16      | 0            |
| 25  | AW    | 470   | 0        | 495      | 7       | 0            |
| 26  | AX    | 516   | 0        | 544      | 9       | 0            |
| 27  | AY    | 400   | 0        | 401      | 8       | 0            |
| 28  | AZ    | 1541  | 0        | 1624     | 20      | 0            |
| 29  | A0    | 343   | 0        | 407      | 7       | 0            |
| 30  | A3    | 933   | 0        | 982      | 25      | 0            |
| 30  | B4    | 933   | 0        | 982      | 30      | 0            |
| 30  | BG    | 932   | 0        | 982      | 9       | 0            |
| 31  | AT    | 1057  | 0        | 1131     | 26      | 0            |
| 32  | AO    | 1116  | 0        | 1152     | 20      | 0            |
| 33  | BB    | 1838  | 0        | 1903     | 30      | 0            |
| 34  | BY    | 1235  | 0        | 1314     | 15      | 0            |
| 35  | BO    | 1607  | 0        | 1638     | 30      | 0            |
| 36  | BC    | 2870  | 0        | 3020     | 30      | 0            |
| 37  | B5    | 614   | 0        | 671      | 13      | 0            |
| 37  | BK    | 607   | 0        | 663      | 10      | 0            |
| 38  | BL    | 1149  | 0        | 1218     | 23      | 0            |
| 39  | Bf    | 435   | 0        | 494      | 9       | 0            |
| 40  | BU    | 1011  | 0        | 1078     | 26      | 0            |
| 41  | Bb    | 1095  | 0        | 1190     | 8       | 0            |
| 42  | Be    | 503   | 0        | 533      | 12      | 0            |
| 43  | BE    | 1485  | 0        | 1539     | 41      | 0            |
| 44  | Ba    | 778   | 0        | 851      | 14      | 0            |
| 45  | BT    | 696   | 0        | 758      | 7       | 0            |
| 46  | BW    | 565   | 0        | 628      | 6       | 0            |
| 47  | Bi    | 620   | 0        | 668      | 3       | 0            |
| 48  | BI    | 1148  | 0        | 1237     | 15      | 0            |
| 49  | BR    | 797   | 0        | 835      | 12      | 0            |
| 50  | BQ    | 1265  | 0        | 1392     | 26      | 0            |
| 51  | BV    | 532   | 0        | 523      | 6       | 0            |
| 52  | Bj    | 789   | 0        | 842      | 7       | 0            |
| 53  | BD    | 2026  | 0        | 2131     | 34      | 0            |
| 54  | BF    | 1456  | 0        | 1514     | 20      | 0            |
| 55  | BZ    | 749   | 0        | 796      | 14      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56  | BP    | 971    | 0        | 1039     | 10      | 0            |
| 57  | BM    | 1588   | 0        | 1683     | 20      | 0            |
| 58  | BS    | 1247   | 0        | 1280     | 10      | 0            |
| 59  | Bd    | 759    | 0        | 825      | 6       | 0            |
| 60  | BN    | 1452   | 0        | 1491     | 29      | 0            |
| 61  | Bg    | 387    | 0        | 397      | 6       | 0            |
| 62  | Bc    | 684    | 0        | 748      | 10      | 0            |
| 63  | BJ    | 1066   | 0        | 1133     | 11      | 0            |
| 64  | Bl    | 659    | 0        | 702      | 12      | 0            |
| 65  | Bk    | 528    | 0        | 575      | 9       | 0            |
| 66  | sd    | 199    | 0        | 98       | 7       | 0            |
| 67  | 1     | 166    | 0        | 0        | 0       | 0            |
| 67  | 2     | 69     | 0        | 0        | 0       | 0            |
| 67  | 3     | 1      | 0        | 0        | 0       | 0            |
| 67  | AK    | 1      | 0        | 0        | 0       | 0            |
| 67  | AN    | 1      | 0        | 0        | 0       | 0            |
| 67  | BB    | 2      | 0        | 0        | 0       | 0            |
| 67  | BD    | 1      | 0        | 0        | 0       | 0            |
| 67  | BM    | 1      | 0        | 0        | 0       | 0            |
| 67  | BS    | 1      | 0        | 0        | 0       | 0            |
| 67  | Bb    | 1      | 0        | 0        | 0       | 0            |
| 68  | AC    | 2      | 0        | 0        | 0       | 0            |
| 68  | AF    | 1      | 0        | 0        | 0       | 0            |
| 68  | AP    | 1      | 0        | 0        | 0       | 0            |
| 68  | AR    | 1      | 0        | 0        | 0       | 0            |
| 68  | AW    | 1      | 0        | 0        | 0       | 0            |
| 68  | BV    | 1      | 0        | 0        | 0       | 0            |
| 68  | Bd    | 1      | 0        | 0        | 0       | 0            |
| 68  | Be    | 1      | 0        | 0        | 0       | 0            |
| 68  | Bg    | 1      | 0        | 0        | 0       | 0            |
| 68  | Bi    | 1      | 0        | 0        | 0       | 0            |
| 68  | Bj    | 1      | 0        | 0        | 0       | 0            |
| 68  | Bk    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 170684 | 0        | 124542   | 2351    | 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 8.

The worst 5 of 2351 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) |
|-----------------|---------------|--------------------------|-------------------|
| 1:1:107:G:N2    | 1:1:112:A:N7  | 1.85                     | 1.20              |
| 1:1:107:G:N2    | 1:1:112:A:C8  | 2.14                     | 1.15              |
| 1:1:117:G:O2'   | 1:1:118:U:OP1 | 1.67                     | 1.12              |
| 1:1:100:G:N2    | 1:1:119:C:O2  | 1.82                     | 1.12              |
| 1:1:2887:A:HO2' | 63:BJ:2:ALA:N | 1.50                     | 1.07              |

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   | H     | 384/392 (98%) | 382 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 5   | AA    | 186/199 (94%) | 181 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 6   | AB    | 194/202 (96%) | 193 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 7   | AC    | 55/63 (87%)   | 53 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 8   | AD    | 171/180 (95%) | 169 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 9   | AE    | 240/243 (99%) | 236 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 10  | AF    | 227/236 (96%) | 222 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 11  | AG    | 122/125 (98%) | 117 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 12  | AH    | 212/215 (99%) | 210 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 13  | AI    | 127/130 (98%) | 125 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 14  | AJ    | 123/127 (97%) | 122 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 15  | AK    | 133/135 (98%) | 129 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 16  | AL    | 98/102 (96%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 17  | AM    | 125/137 (91%) | 122 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 18  | AN    | 144/147 (98%) | 143 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 19  | AP    | 53/56 (95%)   | 53 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 20  | AQ    | 155/158 (98%) | 152 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 21  | AR    | 105/113 (93%) | 101 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 22  | AS    | 62/67 (92%)   | 58 (94%)   | 4 (6%)  | 0        | 100         | 100 |
| 23  | AU    | 147/150 (98%) | 147 (100%) | 0       | 0        | 100         | 100 |
| 24  | AV    | 94/99 (95%)   | 92 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 24  | B6    | 92/99 (93%)   | 91 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 25  | AW    | 59/65 (91%)   | 58 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 26  | AX    | 63/71 (89%)   | 63 (100%)  | 0       | 0        | 100         | 100 |
| 27  | AY    | 47/51 (92%)   | 41 (87%)   | 6 (13%) | 0        | 100         | 100 |
| 28  | AZ    | 194/210 (92%) | 182 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 29  | A0    | 34/37 (92%)   | 33 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 30  | A3    | 120/123 (98%) | 113 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 30  | B4    | 120/123 (98%) | 116 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 30  | BG    | 120/123 (98%) | 120 (100%) | 0       | 0        | 100         | 100 |
| 31  | AT    | 128/132 (97%) | 127 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 32  | AO    | 136/148 (92%) | 128 (94%)  | 8 (6%)  | 0        | 100         | 100 |
| 33  | BB    | 236/239 (99%) | 230 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 34  | BY    | 152/155 (98%) | 152 (100%) | 0       | 0        | 100         | 100 |
| 35  | BO    | 196/203 (97%) | 195 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 36  | BC    | 358/361 (99%) | 349 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 37  | B5    | 79/82 (96%)   | 79 (100%)  | 0       | 0        | 100         | 100 |
| 37  | BK    | 78/82 (95%)   | 75 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 38  | BL    | 145/147 (99%) | 139 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 39  | Bf    | 48/51 (94%)   | 46 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 40  | BU    | 119/121 (98%) | 118 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 41  | Bb    | 127/130 (98%) | 127 (100%) | 0       | 0        | 100         | 100 |
| 42  | Be    | 59/62 (95%)   | 58 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 43  | BE    | 183/188 (97%) | 183 (100%) | 0       | 0        | 100         | 100 |
| 44  | Ba    | 92/94 (98%)   | 92 (100%)  | 0       | 0        | 100         | 100 |
| 45  | BT    | 84/86 (98%)   | 83 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 46  | BW    | 66/68 (97%)   | 66 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 47  | Bi    | 80/83 (96%)     | 77 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 48  | BI    | 140/142 (99%)   | 137 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 49  | BR    | 94/97 (97%)     | 94 (100%)  | 0        | 0        | 100         | 100 |
| 50  | BQ    | 148/151 (98%)   | 148 (100%) | 0        | 0        | 100         | 100 |
| 51  | BV    | 61/67 (91%)     | 60 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 52  | Bj    | 92/94 (98%)     | 91 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 53  | BD    | 253/255 (99%)   | 248 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 54  | BF    | 181/184 (98%)   | 180 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 55  | BZ    | 96/99 (97%)     | 95 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 56  | BP    | 118/120 (98%)   | 118 (100%) | 0        | 0        | 100         | 100 |
| 57  | BM    | 191/194 (98%)   | 188 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 58  | BS    | 152/155 (98%)   | 151 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 59  | Bd    | 89/91 (98%)     | 89 (100%)  | 0        | 0        | 100         | 100 |
| 60  | BN    | 176/181 (97%)   | 169 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 61  | Bg    | 46/51 (90%)     | 46 (100%)  | 0        | 0        | 100         | 100 |
| 62  | Bc    | 85/87 (98%)     | 84 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 63  | BJ    | 138/141 (98%)   | 138 (100%) | 0        | 0        | 100         | 100 |
| 64  | Bl    | 75/77 (97%)     | 75 (100%)  | 0        | 0        | 100         | 100 |
| 65  | Bk    | 61/65 (94%)     | 60 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| All | All   | 8568/8861 (97%) | 8416 (98%) | 152 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | H     | 332/338 (98%) | 306 (92%) | 26 (8%)  | 11          | 13 |
| 5   | AA    | 160/167 (96%) | 151 (94%) | 9 (6%)   | 19          | 24 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 6   | AB    | 168/173 (97%)  | 163 (97%) | 5 (3%)   | 36          | 49  |
| 7   | AC    | 50/55 (91%)    | 50 (100%) | 0        | 100         | 100 |
| 8   | AD    | 156/160 (98%)  | 153 (98%) | 3 (2%)   | 50          | 66  |
| 9   | AE    | 213/214 (100%) | 210 (99%) | 3 (1%)   | 59          | 75  |
| 10  | AF    | 192/198 (97%)  | 190 (99%) | 2 (1%)   | 68          | 81  |
| 11  | AG    | 107/108 (99%)  | 102 (95%) | 5 (5%)   | 23          | 31  |
| 12  | AH    | 183/184 (100%) | 166 (91%) | 17 (9%)  | 8           | 9   |
| 13  | AI    | 106/107 (99%)  | 105 (99%) | 1 (1%)   | 70          | 84  |
| 14  | AJ    | 101/103 (98%)  | 97 (96%)  | 4 (4%)   | 28          | 38  |
| 15  | AK    | 111/111 (100%) | 109 (98%) | 2 (2%)   | 51          | 68  |
| 16  | AL    | 89/91 (98%)    | 84 (94%)  | 5 (6%)   | 19          | 24  |
| 17  | AM    | 94/104 (90%)   | 91 (97%)  | 3 (3%)   | 34          | 47  |
| 18  | AN    | 120/121 (99%)  | 119 (99%) | 1 (1%)   | 73          | 85  |
| 19  | AP    | 45/46 (98%)    | 41 (91%)  | 4 (9%)   | 9           | 10  |
| 20  | AQ    | 142/143 (99%)  | 139 (98%) | 3 (2%)   | 47          | 63  |
| 21  | AR    | 96/102 (94%)   | 94 (98%)  | 2 (2%)   | 47          | 63  |
| 22  | AS    | 58/61 (95%)    | 54 (93%)  | 4 (7%)   | 14          | 16  |
| 23  | AU    | 126/127 (99%)  | 122 (97%) | 4 (3%)   | 34          | 47  |
| 24  | AV    | 88/90 (98%)    | 87 (99%)  | 1 (1%)   | 65          | 79  |
| 24  | B6    | 86/90 (96%)    | 78 (91%)  | 8 (9%)   | 8           | 9   |
| 25  | AW    | 53/56 (95%)    | 53 (100%) | 0        | 100         | 100 |
| 26  | AX    | 55/60 (92%)    | 49 (89%)  | 6 (11%)  | 6           | 6   |
| 27  | AY    | 40/42 (95%)    | 38 (95%)  | 2 (5%)   | 22          | 28  |
| 28  | AZ    | 155/168 (92%)  | 147 (95%) | 8 (5%)   | 21          | 26  |
| 29  | A0    | 34/35 (97%)    | 33 (97%)  | 1 (3%)   | 37          | 51  |
| 30  | A3    | 98/99 (99%)    | 97 (99%)  | 1 (1%)   | 68          | 81  |
| 30  | B4    | 98/99 (99%)    | 93 (95%)  | 5 (5%)   | 21          | 27  |
| 30  | BG    | 98/99 (99%)    | 88 (90%)  | 10 (10%) | 7           | 7   |
| 31  | AT    | 113/114 (99%)  | 108 (96%) | 5 (4%)   | 25          | 34  |
| 32  | AO    | 115/123 (94%)  | 111 (96%) | 4 (4%)   | 32          | 43  |
| 33  | BB    | 188/189 (100%) | 185 (98%) | 3 (2%)   | 55          | 71  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 34  | BY    | 132/133 (99%)  | 128 (97%)  | 4 (3%)   | 36          | 49  |
| 35  | BO    | 167/170 (98%)  | 156 (93%)  | 11 (7%)  | 15          | 18  |
| 36  | BC    | 306/307 (100%) | 302 (99%)  | 4 (1%)   | 61          | 76  |
| 37  | B5    | 65/66 (98%)    | 62 (95%)   | 3 (5%)   | 24          | 32  |
| 37  | BK    | 64/66 (97%)    | 59 (92%)   | 5 (8%)   | 11          | 13  |
| 38  | BL    | 118/118 (100%) | 110 (93%)  | 8 (7%)   | 14          | 17  |
| 39  | Bf    | 46/47 (98%)    | 44 (96%)   | 2 (4%)   | 26          | 35  |
| 40  | BU    | 109/109 (100%) | 105 (96%)  | 4 (4%)   | 30          | 41  |
| 41  | Bb    | 117/118 (99%)  | 115 (98%)  | 2 (2%)   | 53          | 69  |
| 42  | Be    | 52/53 (98%)    | 52 (100%)  | 0        | 100         | 100 |
| 43  | BE    | 158/160 (99%)  | 134 (85%)  | 24 (15%) | 3           | 2   |
| 44  | Ba    | 84/84 (100%)   | 82 (98%)   | 2 (2%)   | 43          | 58  |
| 45  | BT    | 77/77 (100%)   | 76 (99%)   | 1 (1%)   | 61          | 76  |
| 46  | BW    | 63/63 (100%)   | 60 (95%)   | 3 (5%)   | 23          | 30  |
| 47  | Bi    | 61/62 (98%)    | 59 (97%)   | 2 (3%)   | 33          | 45  |
| 48  | BI    | 122/122 (100%) | 122 (100%) | 0        | 100         | 100 |
| 49  | BR    | 86/87 (99%)    | 86 (100%)  | 0        | 100         | 100 |
| 50  | BQ    | 132/133 (99%)  | 132 (100%) | 0        | 100         | 100 |
| 51  | BV    | 54/58 (93%)    | 53 (98%)   | 1 (2%)   | 50          | 66  |
| 52  | Bj    | 83/84 (99%)    | 83 (100%)  | 0        | 100         | 100 |
| 53  | BD    | 212/212 (100%) | 208 (98%)  | 4 (2%)   | 50          | 66  |
| 54  | BF    | 156/157 (99%)  | 145 (93%)  | 11 (7%)  | 13          | 16  |
| 55  | BZ    | 79/80 (99%)    | 72 (91%)   | 7 (9%)   | 9           | 10  |
| 56  | BP    | 102/102 (100%) | 99 (97%)   | 3 (3%)   | 37          | 51  |
| 57  | BM    | 160/161 (99%)  | 157 (98%)  | 3 (2%)   | 50          | 66  |
| 58  | BS    | 130/131 (99%)  | 128 (98%)  | 2 (2%)   | 57          | 73  |
| 59  | Bd    | 82/82 (100%)   | 80 (98%)   | 2 (2%)   | 43          | 58  |
| 60  | BN    | 149/151 (99%)  | 145 (97%)  | 4 (3%)   | 39          | 53  |
| 61  | Bg    | 37/39 (95%)    | 37 (100%)  | 0        | 100         | 100 |
| 62  | Bc    | 74/74 (100%)   | 71 (96%)   | 3 (4%)   | 27          | 37  |
| 63  | BJ    | 108/109 (99%)  | 105 (97%)  | 3 (3%)   | 38          | 52  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 64  | Bl    | 72/72 (100%)    | 70 (97%)   | 2 (3%)   | 38 52       |
| 65  | Bk    | 55/57 (96%)     | 52 (94%)   | 3 (6%)   | 19 24       |
| All | All   | 7382/7521 (98%) | 7102 (96%) | 280 (4%) | 30 40       |

5 of 280 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | BF    | 136 | GLU  |
| 55  | BZ    | 55  | LEU  |
| 60  | BN    | 103 | ARG  |
| 22  | AS    | 61  | LYS  |
| 21  | AR    | 48  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 166 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | BR    | 89  | HIS  |
| 57  | BM    | 174 | ASN  |
| 50  | BQ    | 75  | HIS  |
| 54  | BF    | 74  | HIS  |
| 60  | BN    | 59  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1     | 3016/3018 (99%) | 472 (15%)         | 25 (0%)         |
| 2   | 2     | 1496/1512 (98%) | 165 (11%)         | 3 (0%)          |
| 3   | 3     | 125/128 (97%)   | 16 (12%)          | 0               |
| 66  | sd    | 8/9 (88%)       | 1 (12%)           | 0               |
| All | All   | 4645/4667 (99%) | 654 (14%)         | 28 (0%)         |

5 of 654 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 12  | G    |
| 1   | 1     | 28  | A    |
| 1   | 1     | 39  | A    |
| 1   | 1     | 43  | A    |
| 1   | 1     | 51  | A    |

5 of 28 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1     | 1288 | U    |
| 2   | 2     | 1106 | C    |
| 1   | 1     | 1364 | C    |
| 1   | 1     | 3021 | U    |
| 1   | 1     | 1363 | U    |

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

159 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 |
| 2   | 6MZ  | 2     | 1469 | 67,2 | 22,25,26     | 1.48 | 4 (18%)  | 30,36,39    | 2.22 | 10 (33%) |
| 1   | 4AC  | 1     | 1557 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.34 | 4 (13%)  |
| 2   | 4AC  | 2     | 379  | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 1   | 4AC  | 1     | 2027 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 2   | OMG  | 2     | 657  | 2    | 23,26,27     | 1.23 | 3 (13%)  | 33,38,41    | 1.97 | 6 (18%)  |
| 1   | 4AC  | 1     | 229  | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 2   | 4AC  | 2     | 751  | 2    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.34 | 4 (13%)  |
| 1   | 4AC  | 1     | 694  | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 4AC  | 1     | 357  | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | 4AC  | 2     | 731  | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 2   | UR3  | 2     | 1467 | 2    | 19,22,23     | 0.97 | 0        | 26,32,35    | 1.47 | 2 (7%)   |
| 1   | 4AC  | 1     | 2585 | 1    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.79 | 6 (20%)  |
| 2   | OMG  | 2     | 680  | 2    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.96 | 6 (18%)  |
| 2   | 4AC  | 2     | 1479 | 2    | 21,24,25     | 1.00 | 2 (9%)   | 29,34,37    | 1.43 | 4 (13%)  |
| 1   | 4AC  | 1     | 981  | 1    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.41 | 4 (13%)  |
| 1   | 4AC  | 1     | 1765 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 2   | 4AC  | 2     | 839  | 2    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.53 | 5 (17%)  |
| 2   | OMG  | 2     | 519  | 2    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.96 | 6 (18%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | 5MC  | 2     | 1202 | 2    | 18,22,23     | 0.98 | 2 (11%)  | 26,32,35    | 1.25 | 3 (11%)  |
| 2   | 4AC  | 2     | 848  | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 4AC  | 1     | 922  | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.49 | 4 (13%)  |
| 1   | 4AC  | 1     | 2495 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | OMU  | 1     | 2784 | 1    | 19,22,23     | 1.18 | 2 (10%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 1   | 4AC  | 1     | 1755 | 1    | 21,24,25     | 1.01 | 1 (4%)   | 29,34,37    | 1.67 | 4 (13%)  |
| 2   | OMG  | 2     | 471  | 2    | 23,26,27     | 1.22 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 2   | 5MC  | 2     | 1505 | 66,2 | 18,22,23     | 0.98 | 2 (11%)  | 26,32,35    | 1.17 | 3 (11%)  |
| 2   | 5MC  | 2     | 535  | 2    | 18,22,23     | 0.93 | 2 (11%)  | 26,32,35    | 1.15 | 2 (7%)   |
| 1   | 4AC  | 1     | 1621 | 1    | 21,24,25     | 1.03 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 1293 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.35 | 4 (13%)  |
| 2   | 5MC  | 2     | 1025 | 2    | 18,22,23     | 0.95 | 2 (11%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 2   | 4AC  | 2     | 718  | 2    | 21,24,25     | 1.00 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 1   | 5MC  | 1     | 2733 | 1    | 18,22,23     | 0.98 | 1 (5%)   | 26,32,35    | 1.34 | 4 (15%)  |
| 1   | 4AC  | 1     | 136  | 1    | 21,24,25     | 1.03 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 1048 | 1    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.44 | 4 (13%)  |
| 2   | 5MC  | 2     | 875  | 2    | 18,22,23     | 0.94 | 2 (11%)  | 26,32,35    | 1.17 | 3 (11%)  |
| 1   | 4AC  | 1     | 22   | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 1460 | 1    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | OMG  | 1     | 789  | 1    | 23,26,27     | 1.25 | 3 (13%)  | 33,38,41    | 2.00 | 7 (21%)  |
| 2   | 4AC  | 2     | 319  | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 1   | 4AC  | 1     | 829  | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | OMC  | 1     | 615  | 1    | 19,22,23     | 0.80 | 0        | 26,31,34    | 0.80 | 0        |
| 1   | 4AC  | 1     | 2570 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 4AC  | 1     | 1243 | 1    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.44 | 4 (13%)  |
| 2   | 4AC  | 2     | 286  | 2    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.34 | 4 (13%)  |
| 2   | 5MC  | 2     | 1374 | 2    | 18,22,23     | 0.93 | 2 (11%)  | 26,32,35    | 1.10 | 2 (7%)   |
| 1   | 4AC  | 1     | 533  | 1    | 21,24,25     | 1.03 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 2   | 5MC  | 2     | 1498 | 2    | 18,22,23     | 0.94 | 2 (11%)  | 26,32,35    | 1.25 | 4 (15%)  |
| 2   | 4AC  | 2     | 626  | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 2925 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.42 | 4 (13%)  |
| 1   | 4AC  | 1     | 1662 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 1885 | 1    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 1   | 4AC  | 1     | 1934 | 1    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | 4AC  | 2     | 1147 | 2    | 21,24,25     | 1.04 | 1 (4%)   | 29,34,37    | 1.54 | 5 (17%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | 4AC  | 1     | 835  | 1    | 21,24,25     | 1.03 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 2   | OMG  | 2     | 934  | 2    | 23,26,27     | 1.22 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | 5MC  | 1     | 2163 | 1    | 18,22,23     | 0.94 | 2 (11%)  | 26,32,35    | 1.26 | 2 (7%)   |
| 2   | 5MC  | 2     | 1496 | 2    | 18,22,23     | 0.94 | 2 (11%)  | 26,32,35    | 1.18 | 2 (7%)   |
| 1   | 4AC  | 1     | 161  | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 2   | OMU  | 2     | 830  | 2    | 19,22,23     | 1.27 | 4 (21%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 2   | 4AC  | 2     | 590  | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 1   | 4AC  | 1     | 2908 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 4AC  | 1     | 2287 | 1    | 21,24,25     | 1.01 | 1 (4%)   | 29,34,37    | 1.43 | 4 (13%)  |
| 1   | 5MC  | 1     | 2183 | 1    | 18,22,23     | 0.93 | 2 (11%)  | 26,32,35    | 1.17 | 2 (7%)   |
| 2   | OMG  | 2     | 873  | 2    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.96 | 6 (18%)  |
| 2   | 4AC  | 2     | 1028 | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.34 | 4 (13%)  |
| 2   | MA6  | 2     | 1488 | 2    | 23,26,27     | 1.45 | 4 (17%)  | 34,38,41    | 2.11 | 10 (29%) |
| 1   | OMG  | 1     | 2138 | 1    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.91 | 6 (18%)  |
| 2   | OMU  | 2     | 20   | 2    | 19,22,23     | 1.23 | 2 (10%)  | 26,31,34    | 1.81 | 5 (19%)  |
| 1   | OMG  | 1     | 2678 | 1    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.92 | 6 (18%)  |
| 1   | 4AC  | 1     | 1222 | 67,1 | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.44 | 4 (13%)  |
| 2   | OMU  | 2     | 774  | 2    | 19,22,23     | 1.22 | 3 (15%)  | 26,31,34    | 1.73 | 4 (15%)  |
| 1   | LHH  | 1     | 616  | 1    | 22,25,26     | 0.30 | 0        | 29,35,38    | 0.46 | 0        |
| 1   | 4AC  | 1     | 1617 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 211  | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.41 | 4 (13%)  |
| 2   | LHH  | 2     | 250  | 2    | 22,25,26     | 0.30 | 0        | 29,35,38    | 0.49 | 0        |
| 2   | OMG  | 2     | 1069 | 2    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 1   | OMG  | 1     | 328  | 1    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.91 | 6 (18%)  |
| 2   | OMC  | 2     | 773  | 2    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.83 | 0        |
| 1   | 4AC  | 1     | 1594 | 67,1 | 21,24,25     | 1.01 | 1 (4%)   | 29,34,37    | 1.43 | 4 (13%)  |
| 1   | 5MC  | 1     | 2203 | 1    | 18,22,23     | 0.95 | 2 (11%)  | 26,32,35    | 1.20 | 2 (7%)   |
| 2   | 4AC  | 2     | 546  | 2    | 21,24,25     | 0.99 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 1   | 4AC  | 1     | 243  | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | LHH  | 2     | 1041 | 2    | 22,25,26     | 0.31 | 0        | 29,35,38    | 0.49 | 0        |
| 3   | 4AC  | 3     | 32   | 3    | 21,24,25     | 1.04 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 2   | 4AC  | 2     | 868  | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.36 | 4 (13%)  |
| 2   | OMU  | 2     | 1380 | 2    | 19,22,23     | 1.28 | 4 (21%)  | 26,31,34    | 1.71 | 4 (15%)  |
| 1   | OMC  | 1     | 1948 | 1    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.74 | 0        |
| 1   | 4AC  | 1     | 2865 | 1    | 21,24,25     | 1.03 | 1 (4%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | 4AC  | 2     | 851  | 2    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.36 | 4 (13%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | 1     | 2144 | 1    | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.95 | 6 (18%)  |
| 2   | OMC  | 2     | 1376 | 2    | 19,22,23     | 0.81 | 0        | 26,31,34    | 0.76 | 0        |
| 2   | OMG  | 2     | 913  | 2    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.92 | 6 (18%)  |
| 1   | 4AC  | 1     | 1873 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | 4AC  | 2     | 1184 | 2    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.56 | 4 (13%)  |
| 1   | OMG  | 1     | 2147 | 1    | 23,26,27     | 1.20 | 3 (13%)  | 33,38,41    | 1.93 | 6 (18%)  |
| 1   | 4AC  | 1     | 2992 | 1    | 21,24,25     | 1.06 | 1 (4%)   | 29,34,37    | 0.86 | 2 (6%)   |
| 1   | A2M  | 1     | 2173 | 1    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.02 | 8 (25%)  |
| 1   | 4AC  | 1     | 91   | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.58 | 4 (13%)  |
| 1   | 4AC  | 1     | 2001 | 1    | 21,24,25     | 1.07 | 2 (9%)   | 29,34,37    | 1.50 | 4 (13%)  |
| 2   | OMU  | 2     | 787  | 2    | 19,22,23     | 1.23 | 2 (10%)  | 26,31,34    | 1.80 | 5 (19%)  |
| 1   | 4AC  | 1     | 1867 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | A2M  | 1     | 1055 | 1    | 22,25,26     | 1.47 | 4 (18%)  | 31,36,39    | 2.11 | 10 (32%) |
| 2   | OMC  | 2     | 846  | 2    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.79 | 0        |
| 1   | 4AC  | 1     | 2642 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.35 | 4 (13%)  |
| 1   | 4AC  | 1     | 2329 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | 4AC  | 2     | 511  | 2    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.34 | 4 (13%)  |
| 2   | 4AC  | 2     | 17   | 2    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.36 | 4 (13%)  |
| 1   | 4AC  | 1     | 2249 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.41 | 4 (13%)  |
| 1   | 4AC  | 1     | 2608 | 1    | 21,24,25     | 1.07 | 2 (9%)   | 29,34,37    | 1.76 | 6 (20%)  |
| 2   | OMC  | 2     | 1040 | 2    | 19,22,23     | 0.84 | 0        | 26,31,34    | 0.96 | 1 (3%)   |
| 1   | 4AC  | 1     | 2083 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.39 | 5 (17%)  |
| 2   | OMU  | 2     | 64   | 2    | 19,22,23     | 1.22 | 3 (15%)  | 26,31,34    | 1.70 | 5 (19%)  |
| 1   | 4AC  | 1     | 2718 | 1    | 21,24,25     | 1.01 | 1 (4%)   | 29,34,37    | 1.43 | 4 (13%)  |
| 1   | 4AC  | 1     | 1962 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.35 | 4 (13%)  |
| 1   | 4AC  | 1     | 641  | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 4AC  | 1     | 1554 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.41 | 4 (13%)  |
| 1   | 4AC  | 1     | 458  | 1    | 21,24,25     | 1.00 | 1 (4%)   | 29,34,37    | 1.40 | 4 (13%)  |
| 1   | 4AC  | 1     | 1938 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 2   | 4AC  | 2     | 394  | 2    | 21,24,25     | 1.00 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 1   | 4AC  | 1     | 1878 | 1    | 21,24,25     | 1.01 | 1 (4%)   | 29,34,37    | 1.53 | 4 (13%)  |
| 2   | 4AC  | 2     | 53   | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 1   | 4AC  | 1     | 1695 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 2   | A2M  | 2     | 373  | 2    | 22,25,26     | 1.46 | 4 (18%)  | 31,36,39    | 2.11 | 9 (29%)  |
| 2   | 4AC  | 2     | 1233 | 2    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.42 | 4 (13%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | 4AC  | 2     | 636  | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.48 | 4 (13%)  |
| 2   | 4AC  | 2     | 828  | 2    | 21,24,25     | 1.00 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 4AC  | 1     | 802  | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.45 | 4 (13%)  |
| 1   | 4AC  | 1     | 2548 | 1    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.50 | 4 (13%)  |
| 1   | 5MC  | 1     | 2198 | 1    | 18,22,23     | 0.95 | 2 (11%)  | 26,32,35    | 1.11 | 2 (7%)   |
| 1   | 4AC  | 1     | 341  | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 2   | 4AC  | 2     | 957  | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.35 | 4 (13%)  |
| 2   | 4AC  | 2     | 303  | 2    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 1   | 5MC  | 1     | 2093 | 1    | 18,22,23     | 0.94 | 2 (11%)  | 26,32,35    | 1.12 | 2 (7%)   |
| 1   | 5MC  | 1     | 2162 | 1    | 18,22,23     | 0.96 | 2 (11%)  | 26,32,35    | 1.23 | 2 (7%)   |
| 1   | 4AC  | 1     | 3004 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.35 | 4 (13%)  |
| 1   | 4AC  | 1     | 1068 | 1    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.54 | 4 (13%)  |
| 1   | 4AC  | 1     | 451  | 1    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.47 | 4 (13%)  |
| 1   | 4AC  | 1     | 1780 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.62 | 4 (13%)  |
| 2   | 4AC  | 2     | 703  | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.43 | 4 (13%)  |
| 1   | 4AC  | 1     | 60   | 1    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.43 | 5 (17%)  |
| 1   | 4AC  | 1     | 1065 | 1    | 21,24,25     | 1.01 | 1 (4%)   | 29,34,37    | 1.41 | 4 (13%)  |
| 1   | 4AC  | 1     | 2960 | 1    | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.36 | 4 (13%)  |
| 1   | 4AC  | 1     | 2937 | 67,1 | 21,24,25     | 1.02 | 2 (9%)   | 29,34,37    | 1.61 | 4 (13%)  |
| 2   | OMU  | 2     | 1177 | 2    | 19,22,23     | 1.22 | 3 (15%)  | 26,31,34    | 1.69 | 5 (19%)  |
| 1   | 4AC  | 1     | 2062 | 1    | 21,24,25     | 1.03 | 2 (9%)   | 29,34,37    | 1.38 | 4 (13%)  |
| 2   | 4AC  | 2     | 1239 | 2    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.35 | 4 (13%)  |
| 1   | OMG  | 1     | 923  | 67,1 | 23,26,27     | 1.21 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | 4AC  | 1     | 1667 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.37 | 4 (13%)  |
| 2   | 4AC  | 2     | 479  | 2    | 21,24,25     | 1.01 | 2 (9%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | B8H  | 2     | 938  | 2    | 19,22,23     | 0.63 | 1 (5%)   | 22,32,35    | 0.71 | 1 (4%)   |
| 1   | 4AC  | 1     | 1550 | 1    | 21,24,25     | 1.02 | 1 (4%)   | 29,34,37    | 1.39 | 4 (13%)  |
| 2   | OMG  | 2     | 467  | 2    | 23,26,27     | 1.19 | 3 (13%)  | 33,38,41    | 1.94 | 6 (18%)  |
| 1   | 4AC  | 1     | 2136 | 1    | 21,24,25     | 1.04 | 1 (4%)   | 29,34,37    | 1.46 | 5 (17%)  |
| 2   | OMC  | 2     | 129  | 2    | 19,22,23     | 0.82 | 0        | 26,31,34    | 0.80 | 0        |
| 1   | 4AC  | 1     | 2545 | 1    | 21,24,25     | 1.05 | 2 (9%)   | 29,34,37    | 1.46 | 4 (13%)  |
| 2   | 5MC  | 2     | 693  | 2    | 18,22,23     | 0.93 | 2 (11%)  | 26,32,35    | 1.10 | 2 (7%)   |
| 2   | MA6  | 2     | 1487 | 2    | 23,26,27     | 1.50 | 4 (17%)  | 34,38,41    | 2.18 | 11 (32%) |
| 1   | 4AC  | 1     | 2966 | 1    | 21,24,25     | 1.04 | 2 (9%)   | 29,34,37    | 1.49 | 4 (13%)  |
| 1   | 4AC  | 1     | 314  | 1    | 21,24,25     | 1.03 | 1 (4%)   | 29,34,37    | 1.39 | 4 (13%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | 6MZ  | 2     | 1469 | 67,2 | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 1557 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 379  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2027 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMG  | 2     | 657  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 229  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 751  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 694  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 357  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 731  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | UR3  | 2     | 1467 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2585 | 1    | -       | 3/11/29/30 | 0/2/2/2 |
| 2   | OMG  | 2     | 680  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 4AC  | 2     | 1479 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 981  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1765 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 839  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMG  | 2     | 519  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 5MC  | 2     | 1202 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 4AC  | 2     | 848  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 922  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2495 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMU  | 1     | 2784 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 1755 | 1    | -       | 1/11/29/30 | 0/2/2/2 |
| 2   | OMG  | 2     | 471  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 5MC  | 2     | 1505 | 66,2 | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | 2     | 535  | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 1621 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1293 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 5MC  | 2     | 1025 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 4AC  | 2     | 718  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 5MC  | 1     | 2733 | 1    | -       | 6/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 136  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1048 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 5MC  | 2     | 875  | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 22   | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1460 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMG  | 1     | 789  | 1    | -       | 2/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | 4AC  | 2     | 319  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 829  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMC  | 1     | 615  | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2570 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1243 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 286  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 5MC  | 2     | 1374 | 2    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 533  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 5MC  | 2     | 1498 | 2    | -       | 3/7/25/26  | 0/2/2/2 |
| 2   | 4AC  | 2     | 626  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2925 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1662 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1885 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1934 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 1147 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 835  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMG  | 2     | 934  | 2    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | 5MC  | 1     | 2163 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 5MC  | 2     | 1496 | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 161  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 2     | 830  | 2    | -       | 1/9/27/28  | 0/2/2/2 |
| 2   | 4AC  | 2     | 590  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2908 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2287 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 5MC  | 1     | 2183 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | OMG  | 2     | 873  | 2    | -       | 1/9/27/28  | 0/3/3/3 |
| 2   | 4AC  | 2     | 1028 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | MA6  | 2     | 1488 | 2    | -       | 2/11/29/30 | 0/3/3/3 |
| 1   | OMG  | 1     | 2138 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMU  | 2     | 20   | 2    | -       | 6/9/27/28  | 0/2/2/2 |
| 1   | OMG  | 1     | 2678 | 1    | -       | 1/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 1222 | 67,1 | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 2     | 774  | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | LHH  | 1     | 616  | 1    | -       | 0/13/31/32 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1617 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 211  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | LHH  | 2     | 250  | 2    | -       | 0/13/31/32 | 0/2/2/2 |
| 2   | OMG  | 2     | 1069 | 2    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | OMG  | 1     | 328  | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 2     | 773  | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 1594 | 67,1 | -       | 0/11/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 1   | 5MC  | 1     | 2203 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | 4AC  | 2     | 546  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 243  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | LHH  | 2     | 1041 | 2    | -       | 0/13/31/32 | 0/2/2/2 |
| 3   | 4AC  | 3     | 32   | 3    | -       | 1/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 868  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 2     | 1380 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMC  | 1     | 1948 | 1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2865 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 851  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMG  | 1     | 2144 | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 2     | 1376 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 2   | OMG  | 2     | 913  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 1873 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 1184 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMG  | 1     | 2147 | 1    | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 2992 | 1    | -       | 2/11/29/30 | 0/2/2/2 |
| 1   | A2M  | 1     | 2173 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 91   | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2001 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 2     | 787  | 2    | -       | 4/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 1867 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | A2M  | 1     | 1055 | 1    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | OMC  | 2     | 846  | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2642 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2329 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 511  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 17   | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2249 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2608 | 1    | -       | 3/11/29/30 | 0/2/2/2 |
| 2   | OMC  | 2     | 1040 | 2    | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2083 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 2     | 64   | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2718 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1962 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 641  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1554 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 458  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1938 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 394  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1878 | 1    | -       | 0/11/29/30 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 2   | 4AC  | 2     | 53   | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1695 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | A2M  | 2     | 373  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 4AC  | 2     | 1233 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 636  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 828  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 802  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2548 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 5MC  | 1     | 2198 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 341  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 957  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 303  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 5MC  | 1     | 2093 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 5MC  | 1     | 2162 | 1    | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 3004 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1068 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 451  | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1780 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 703  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 60   | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 1065 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2960 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 2937 | 67,1 | -       | 1/11/29/30 | 0/2/2/2 |
| 2   | OMU  | 2     | 1177 | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2062 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 1239 | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | OMG  | 1     | 923  | 67,1 | -       | 2/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 1667 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 4AC  | 2     | 479  | 2    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | B8H  | 2     | 938  | 2    | -       | 1/7/25/26  | 0/2/2/2 |
| 1   | 4AC  | 1     | 1550 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMG  | 2     | 467  | 2    | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | 4AC  | 1     | 2136 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | OMC  | 2     | 129  | 2    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | 4AC  | 1     | 2545 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 2   | 5MC  | 2     | 693  | 2    | -       | 0/7/25/26  | 0/2/2/2 |
| 2   | MA6  | 2     | 1487 | 2    | -       | 0/11/29/30 | 0/3/3/3 |
| 1   | 4AC  | 1     | 2966 | 1    | -       | 0/11/29/30 | 0/2/2/2 |
| 1   | 4AC  | 1     | 314  | 1    | -       | 0/11/29/30 | 0/2/2/2 |

The worst 5 of 298 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | 2     | 1469 | 6MZ  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 2   | 2     | 1487 | MA6  | C5-C4 | 4.52 | 1.47        | 1.39     |
| 1   | 1     | 1055 | A2M  | C5-C4 | 4.52 | 1.47        | 1.39     |
| 1   | 1     | 2173 | A2M  | C5-C4 | 4.50 | 1.47        | 1.39     |
| 2   | 2     | 1488 | MA6  | C5-C4 | 4.41 | 1.47        | 1.39     |

The worst 5 of 647 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | 2     | 657  | OMG  | C5-C4-N3 | -6.59 | 117.77      | 128.46   |
| 2   | 2     | 471  | OMG  | C5-C4-N3 | -6.38 | 118.12      | 128.46   |
| 2   | 2     | 680  | OMG  | C5-C4-N3 | -6.37 | 118.13      | 128.46   |
| 1   | 1     | 789  | OMG  | C5-C4-N3 | -6.33 | 118.18      | 128.46   |
| 1   | 1     | 2144 | OMG  | C5-C4-N3 | -6.26 | 118.30      | 128.46   |

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1     | 789  | OMG  | C3'-C4'-C5'-O5' |
| 1   | 1     | 2147 | OMG  | C3'-C4'-C5'-O5' |
| 1   | 1     | 2585 | 4AC  | O4'-C1'-N1-C2   |
| 1   | 1     | 2585 | 4AC  | O4'-C1'-N1-C6   |
| 1   | 1     | 2608 | 4AC  | O4'-C1'-N1-C2   |

There are no ring outliers.

107 monomers are involved in 177 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1     | 1557 | 4AC  | 1       | 0            |
| 2   | 2     | 379  | 4AC  | 1       | 0            |
| 1   | 1     | 2027 | 4AC  | 1       | 0            |
| 1   | 1     | 229  | 4AC  | 2       | 0            |
| 1   | 1     | 694  | 4AC  | 1       | 0            |
| 1   | 1     | 357  | 4AC  | 1       | 0            |
| 2   | 2     | 731  | 4AC  | 2       | 0            |
| 1   | 1     | 2585 | 4AC  | 2       | 0            |
| 2   | 2     | 680  | OMG  | 1       | 0            |
| 2   | 2     | 1479 | 4AC  | 2       | 0            |
| 1   | 1     | 981  | 4AC  | 1       | 0            |
| 1   | 1     | 1765 | 4AC  | 2       | 0            |
| 2   | 2     | 839  | 4AC  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | 2     | 848  | 4AC  | 1       | 0            |
| 1   | 1     | 922  | 4AC  | 2       | 0            |
| 1   | 1     | 2495 | 4AC  | 1       | 0            |
| 1   | 1     | 1755 | 4AC  | 3       | 0            |
| 2   | 2     | 471  | OMG  | 1       | 0            |
| 1   | 1     | 1621 | 4AC  | 1       | 0            |
| 1   | 1     | 1293 | 4AC  | 1       | 0            |
| 2   | 2     | 1025 | 5MC  | 1       | 0            |
| 2   | 2     | 718  | 4AC  | 1       | 0            |
| 1   | 1     | 2733 | 5MC  | 2       | 0            |
| 1   | 1     | 136  | 4AC  | 1       | 0            |
| 1   | 1     | 1048 | 4AC  | 2       | 0            |
| 1   | 1     | 1460 | 4AC  | 3       | 0            |
| 1   | 1     | 789  | OMG  | 2       | 0            |
| 2   | 2     | 319  | 4AC  | 1       | 0            |
| 1   | 1     | 829  | 4AC  | 1       | 0            |
| 1   | 1     | 615  | OMC  | 1       | 0            |
| 1   | 1     | 1243 | 4AC  | 1       | 0            |
| 1   | 1     | 533  | 4AC  | 2       | 0            |
| 2   | 2     | 626  | 4AC  | 2       | 0            |
| 1   | 1     | 2925 | 4AC  | 2       | 0            |
| 1   | 1     | 1662 | 4AC  | 2       | 0            |
| 1   | 1     | 1934 | 4AC  | 2       | 0            |
| 2   | 2     | 1147 | 4AC  | 1       | 0            |
| 1   | 1     | 835  | 4AC  | 2       | 0            |
| 1   | 1     | 2163 | 5MC  | 3       | 0            |
| 2   | 2     | 1496 | 5MC  | 1       | 0            |
| 1   | 1     | 161  | 4AC  | 1       | 0            |
| 2   | 2     | 590  | 4AC  | 1       | 0            |
| 1   | 1     | 2908 | 4AC  | 2       | 0            |
| 1   | 1     | 2287 | 4AC  | 5       | 0            |
| 2   | 2     | 873  | OMG  | 1       | 0            |
| 2   | 2     | 1488 | MA6  | 1       | 0            |
| 1   | 1     | 2678 | OMG  | 2       | 0            |
| 1   | 1     | 1222 | 4AC  | 2       | 0            |
| 1   | 1     | 1617 | 4AC  | 4       | 0            |
| 1   | 1     | 211  | 4AC  | 2       | 0            |
| 2   | 2     | 1069 | OMG  | 1       | 0            |
| 1   | 1     | 1594 | 4AC  | 1       | 0            |
| 2   | 2     | 546  | 4AC  | 1       | 0            |
| 1   | 1     | 243  | 4AC  | 1       | 0            |
| 3   | 3     | 32   | 4AC  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | 2     | 868  | 4AC  | 1       | 0            |
| 2   | 2     | 1380 | OMU  | 2       | 0            |
| 1   | 1     | 2865 | 4AC  | 1       | 0            |
| 2   | 2     | 1376 | OMC  | 2       | 0            |
| 2   | 2     | 913  | OMG  | 1       | 0            |
| 2   | 2     | 1184 | 4AC  | 2       | 0            |
| 1   | 1     | 2992 | 4AC  | 1       | 0            |
| 1   | 1     | 91   | 4AC  | 2       | 0            |
| 1   | 1     | 2001 | 4AC  | 4       | 0            |
| 1   | 1     | 1867 | 4AC  | 1       | 0            |
| 1   | 1     | 1055 | A2M  | 1       | 0            |
| 1   | 1     | 2642 | 4AC  | 1       | 0            |
| 1   | 1     | 2329 | 4AC  | 1       | 0            |
| 2   | 2     | 511  | 4AC  | 1       | 0            |
| 1   | 1     | 2249 | 4AC  | 2       | 0            |
| 1   | 1     | 2608 | 4AC  | 3       | 0            |
| 1   | 1     | 2083 | 4AC  | 2       | 0            |
| 2   | 2     | 64   | OMU  | 1       | 0            |
| 1   | 1     | 2718 | 4AC  | 2       | 0            |
| 1   | 1     | 1554 | 4AC  | 1       | 0            |
| 1   | 1     | 458  | 4AC  | 3       | 0            |
| 1   | 1     | 1938 | 4AC  | 1       | 0            |
| 2   | 2     | 394  | 4AC  | 1       | 0            |
| 1   | 1     | 1878 | 4AC  | 2       | 0            |
| 2   | 2     | 53   | 4AC  | 2       | 0            |
| 1   | 1     | 1695 | 4AC  | 1       | 0            |
| 2   | 2     | 373  | A2M  | 2       | 0            |
| 2   | 2     | 1233 | 4AC  | 1       | 0            |
| 2   | 2     | 636  | 4AC  | 2       | 0            |
| 2   | 2     | 828  | 4AC  | 1       | 0            |
| 1   | 1     | 802  | 4AC  | 2       | 0            |
| 1   | 1     | 2548 | 4AC  | 2       | 0            |
| 1   | 1     | 2198 | 5MC  | 1       | 0            |
| 1   | 1     | 341  | 4AC  | 1       | 0            |
| 2   | 2     | 957  | 4AC  | 1       | 0            |
| 1   | 1     | 2162 | 5MC  | 2       | 0            |
| 1   | 1     | 3004 | 4AC  | 2       | 0            |
| 1   | 1     | 1068 | 4AC  | 2       | 0            |
| 1   | 1     | 451  | 4AC  | 3       | 0            |
| 1   | 1     | 1780 | 4AC  | 3       | 0            |
| 2   | 2     | 703  | 4AC  | 4       | 0            |
| 1   | 1     | 1065 | 4AC  | 3       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1   | 1     | 2960 | 4AC  | 2       | 0            |
| 2   | 2     | 1177 | OMU  | 2       | 0            |
| 1   | 1     | 2062 | 4AC  | 1       | 0            |
| 2   | 2     | 1239 | 4AC  | 1       | 0            |
| 1   | 1     | 1667 | 4AC  | 4       | 0            |
| 2   | 2     | 479  | 4AC  | 2       | 0            |
| 1   | 1     | 1550 | 4AC  | 2       | 0            |
| 1   | 1     | 2136 | 4AC  | 2       | 0            |
| 1   | 1     | 2545 | 4AC  | 3       | 0            |
| 1   | 1     | 314  | 4AC  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 257 ligands modelled in this entry, 257 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 1     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 1     | 107:G     | O3'    | 112:A     | P      | 11.57        |

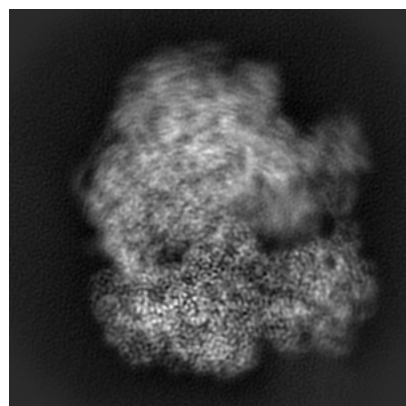
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55135. These allow visual inspection of the internal detail of the map and identification of artifacts.

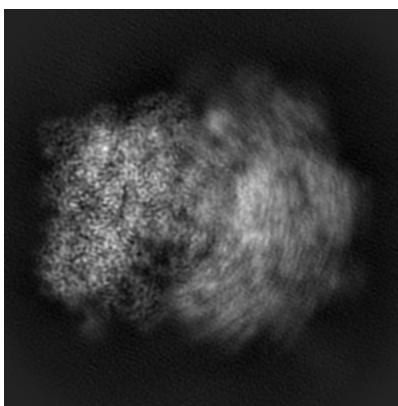
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

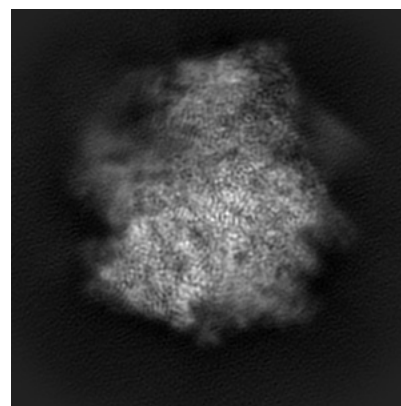
#### 6.1.1 Primary map



X

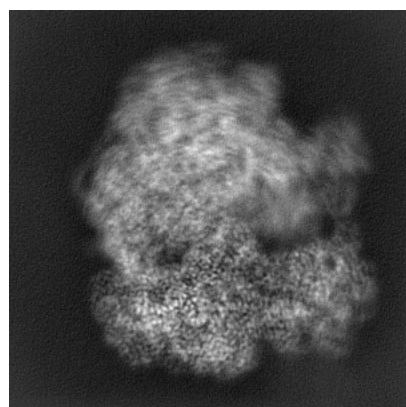


Y

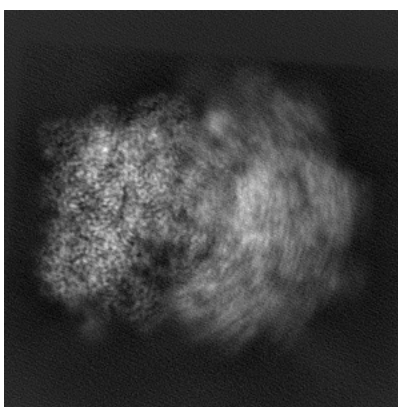


Z

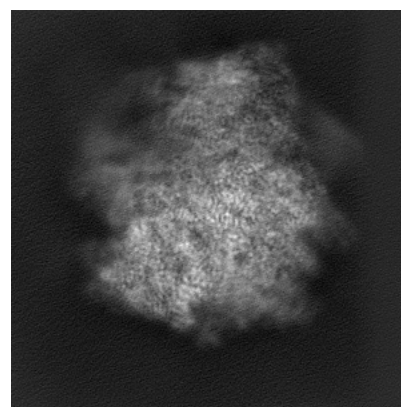
#### 6.1.2 Raw map



X



Y

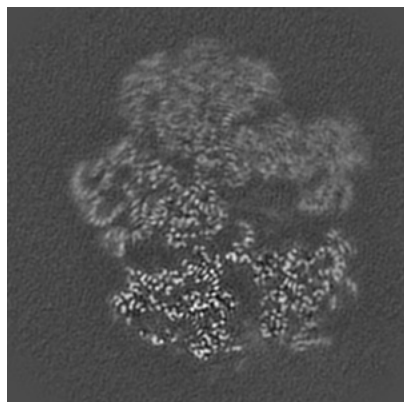


Z

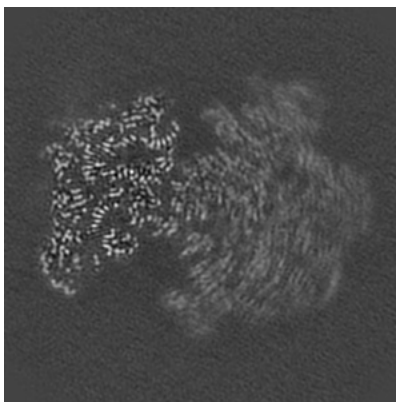
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

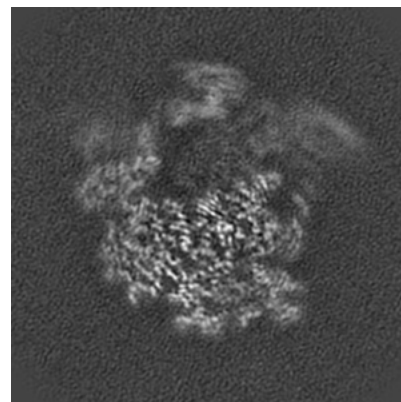
### 6.2.1 Primary map



X Index: 180

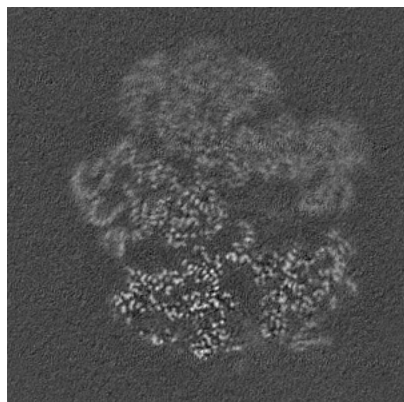


Y Index: 180

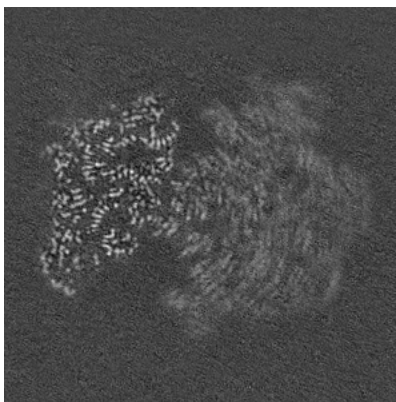


Z Index: 180

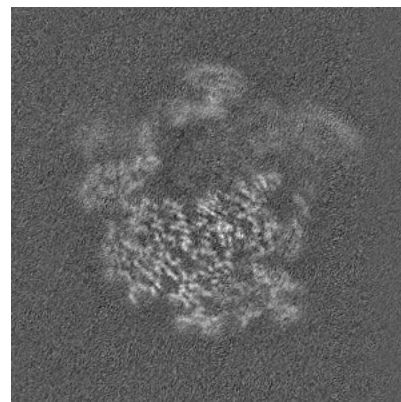
### 6.2.2 Raw map



X Index: 180



Y Index: 180

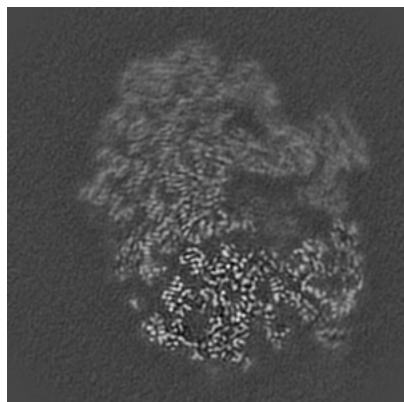


Z Index: 180

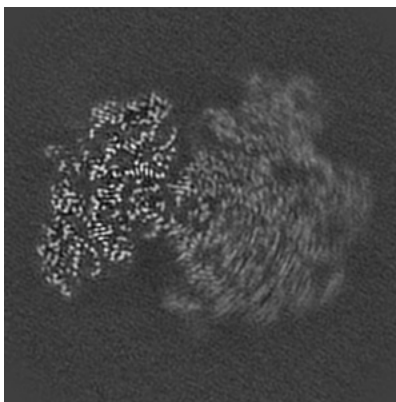
The images above show central slices of the map in three orthogonal directions.

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

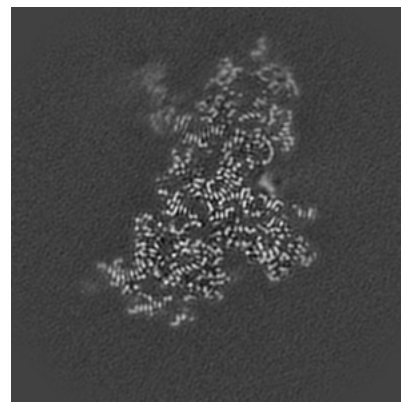
### 6.3.1 Primary map



X Index: 196

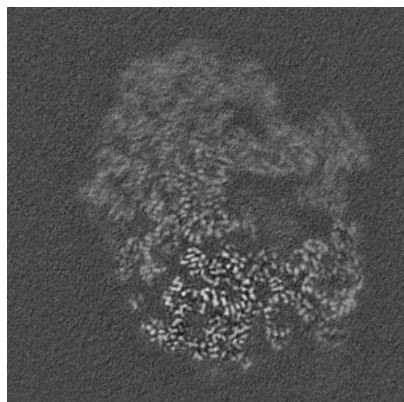


Y Index: 175

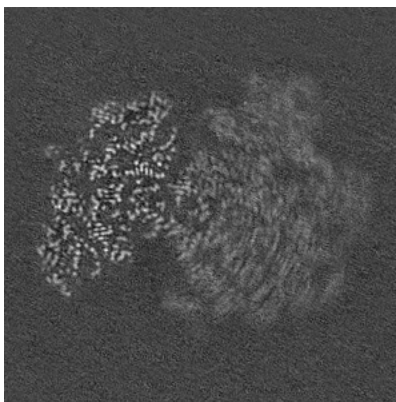


Z Index: 91

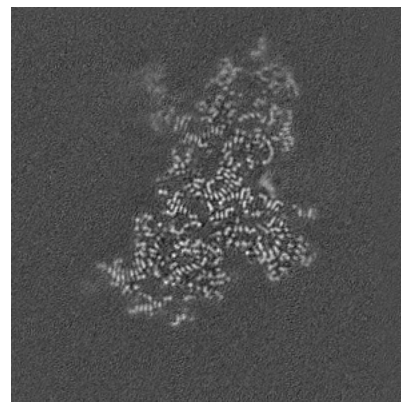
### 6.3.2 Raw map



X Index: 195



Y Index: 175

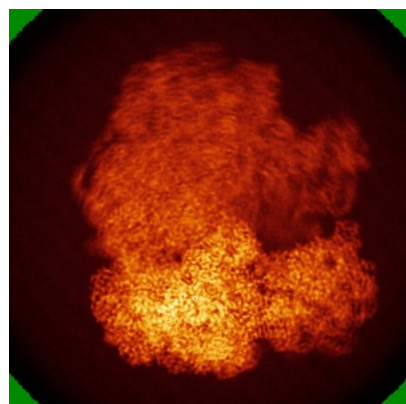


Z Index: 91

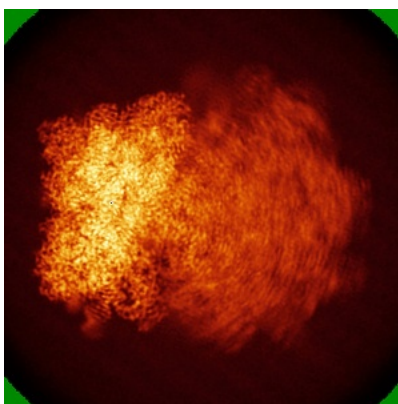
The images above show the largest variance slices of the map in three orthogonal directions.

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

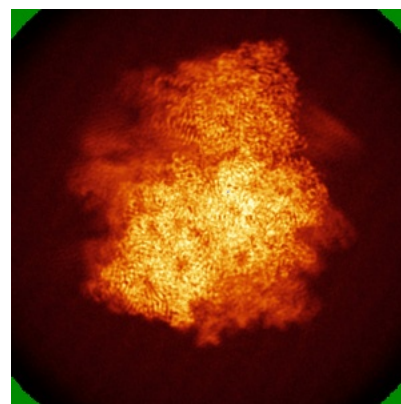
### 6.4.1 Primary map



X

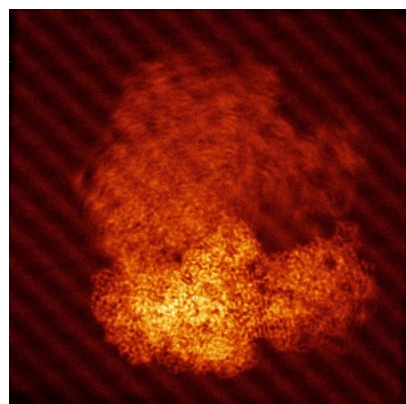


Y

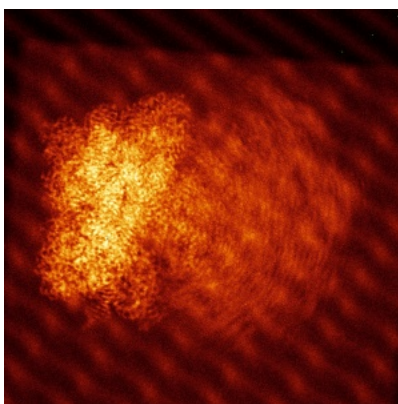


Z

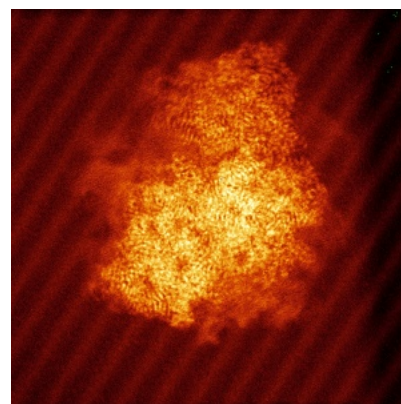
### 6.4.2 Raw map



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



X



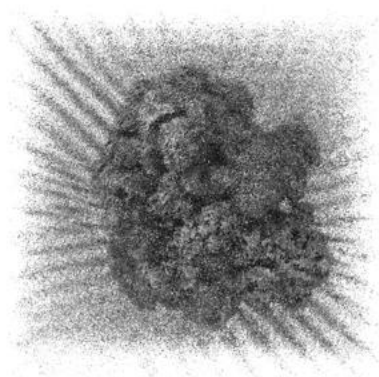
Y



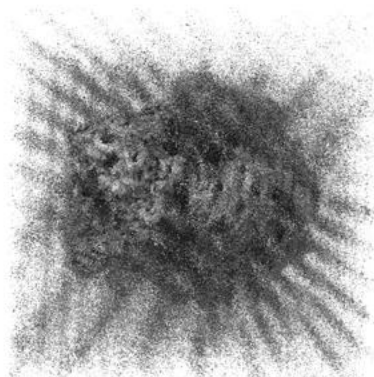
Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

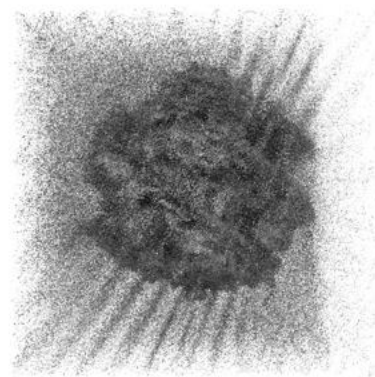
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

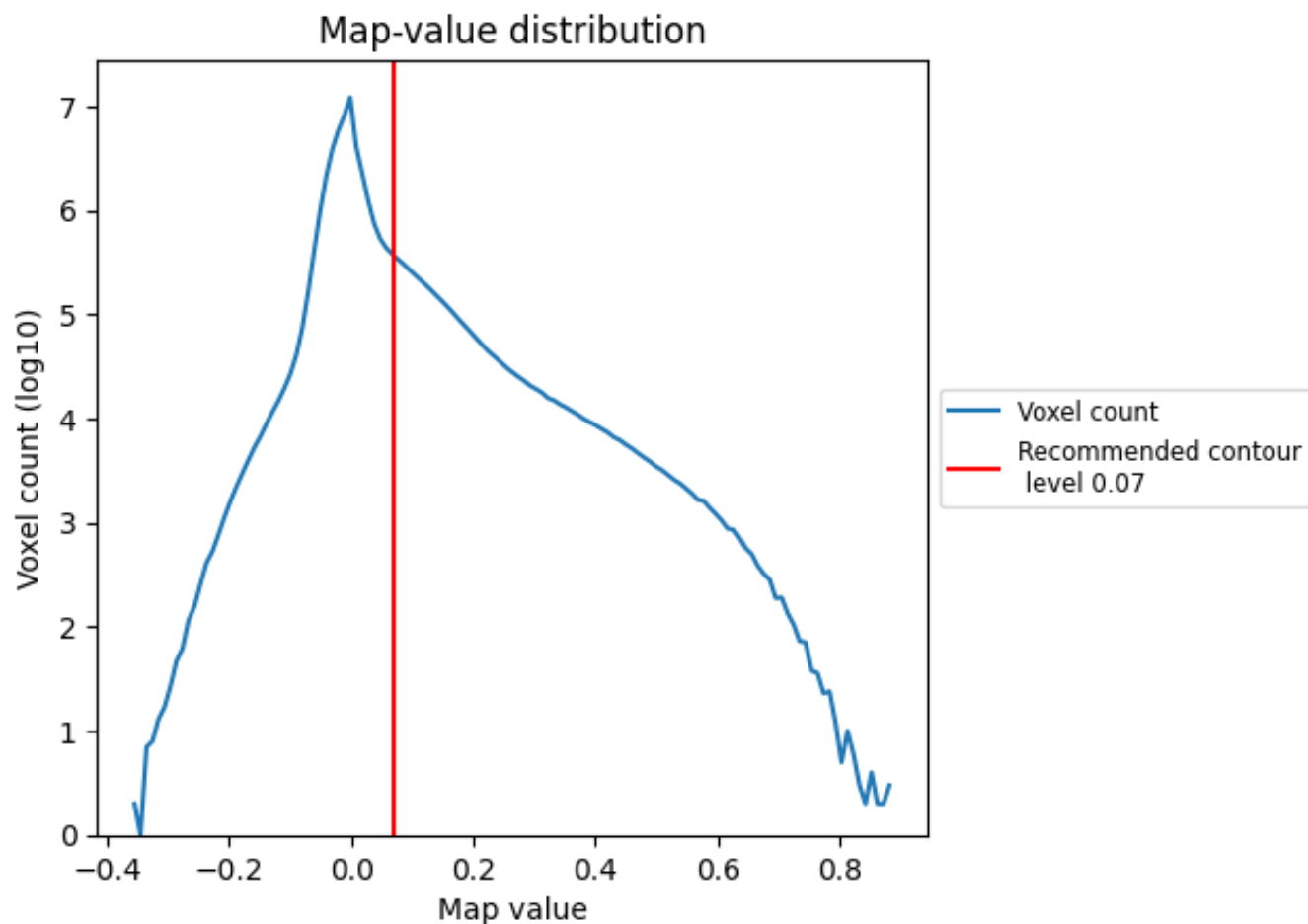
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

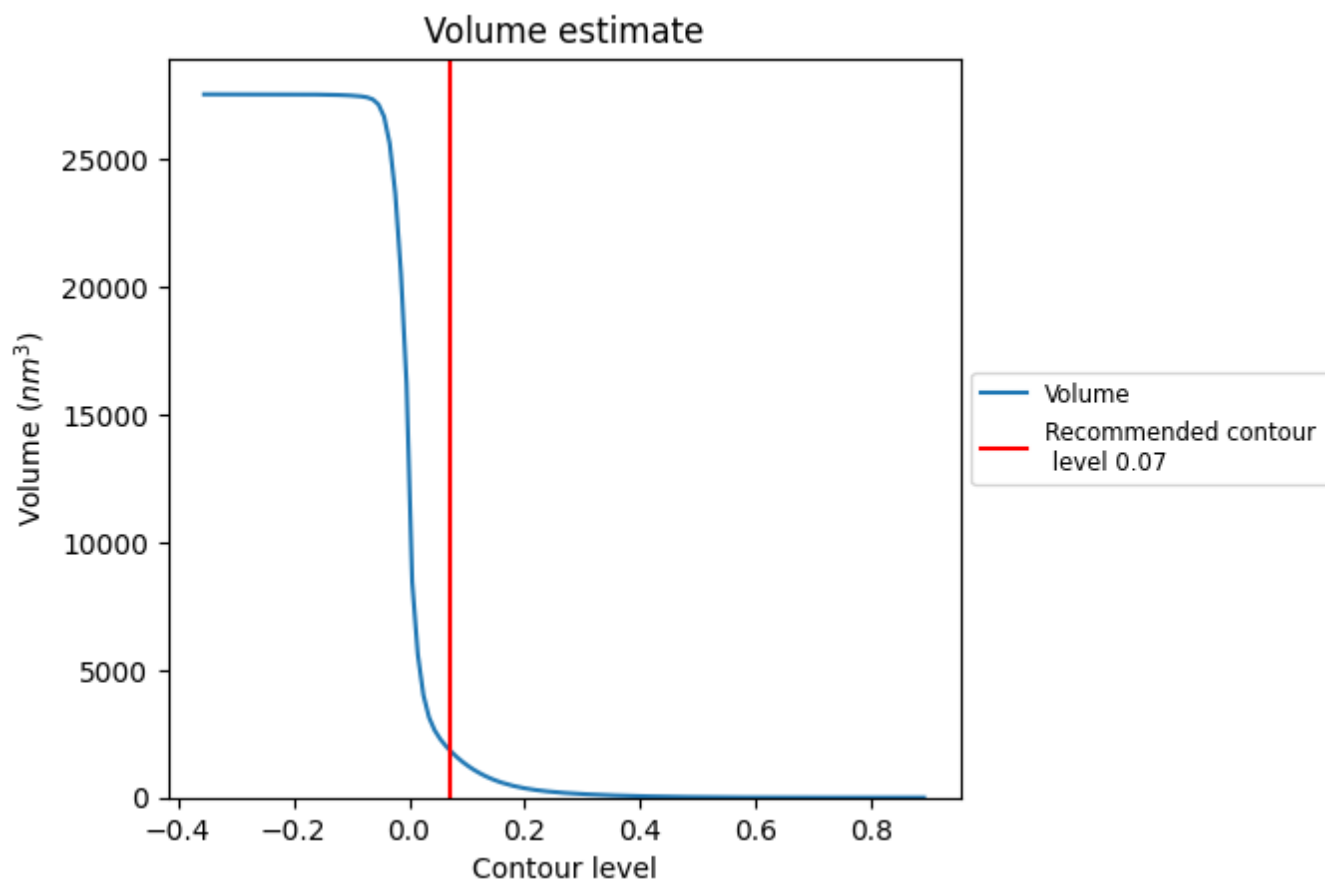
This section contains the results of statistical analysis of the map.

### 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.

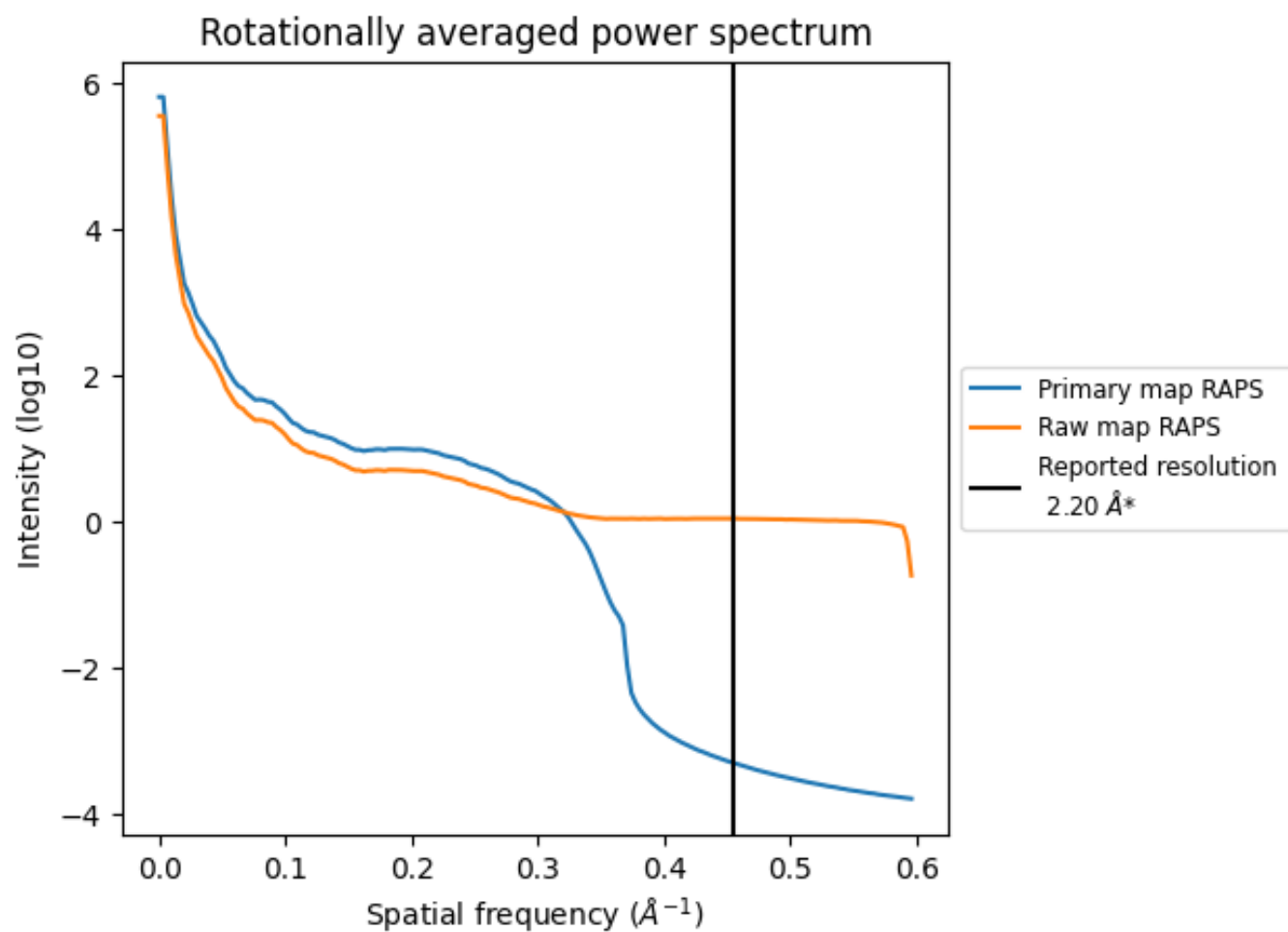
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1867  $\text{nm}^3$ ; this corresponds to an approximate mass of 1686 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 ⓘ

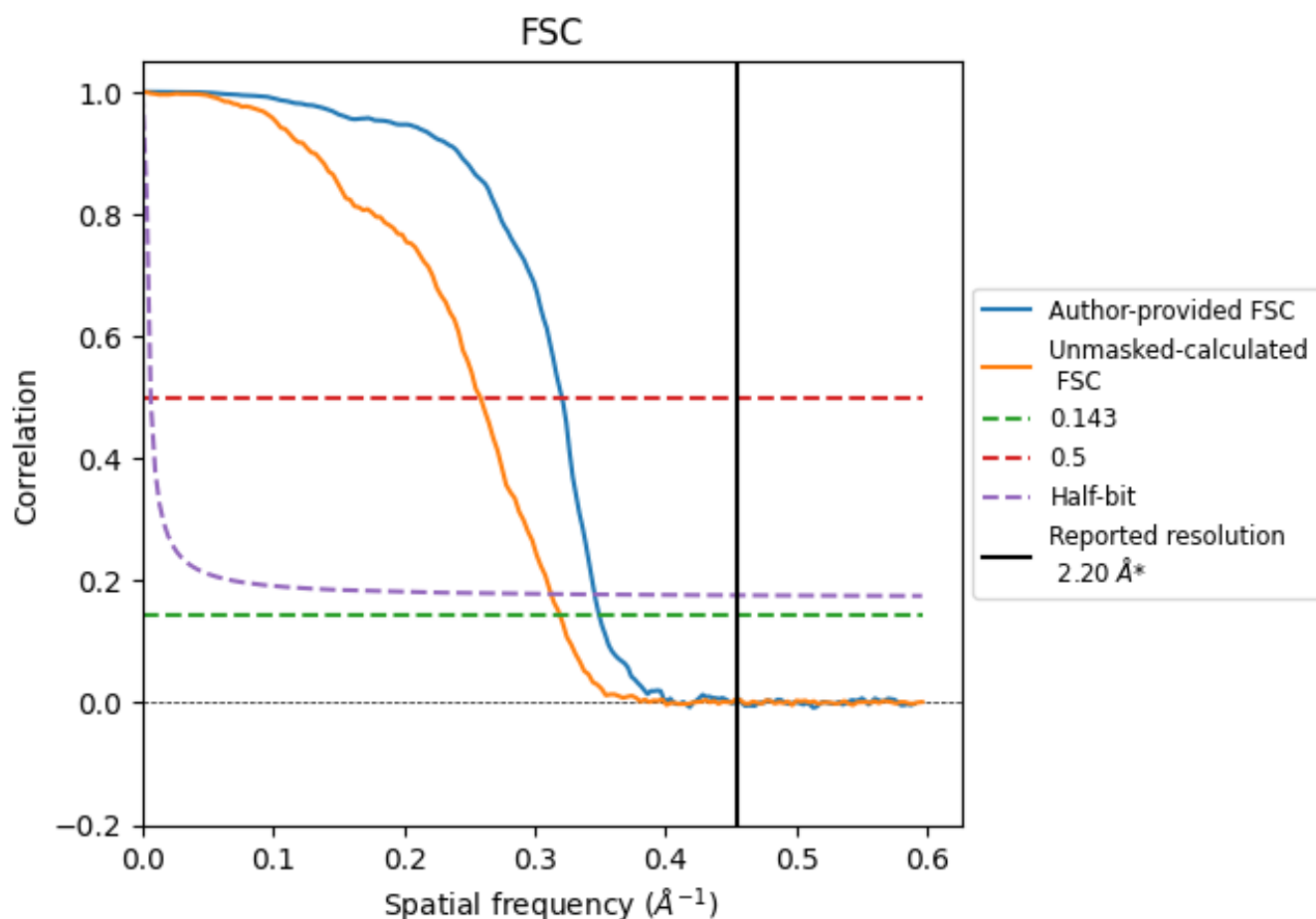


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8.2 Resolution estimates

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.20                               | -    | -        |
| Author-provided FSC curve | 2.86                               | 3.12 | 2.89     |
| Unmasked-calculated*      | 3.13                               | 3.87 | 3.20     |

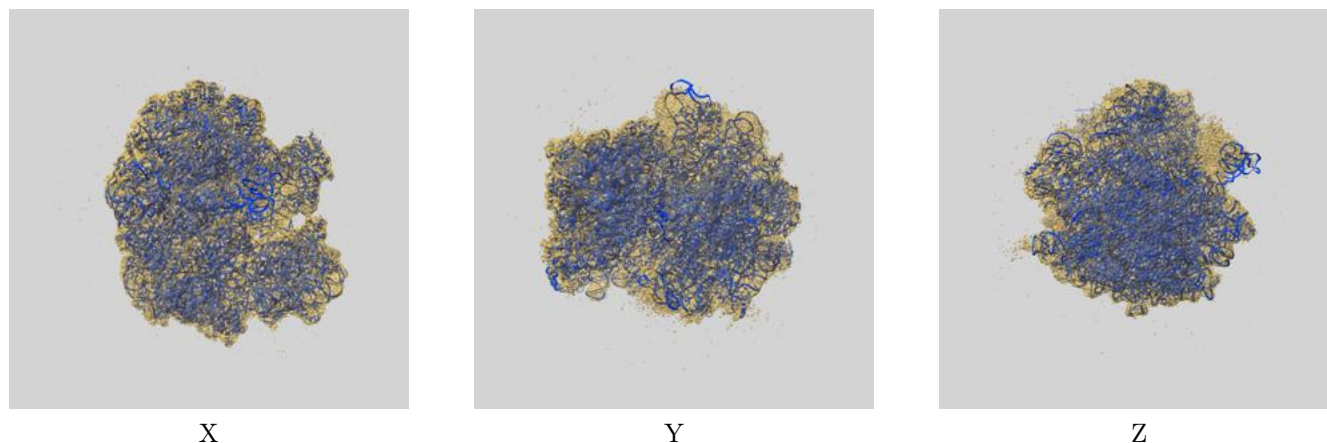
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.86 differs from the reported value 2.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.2 by more than 10 %

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

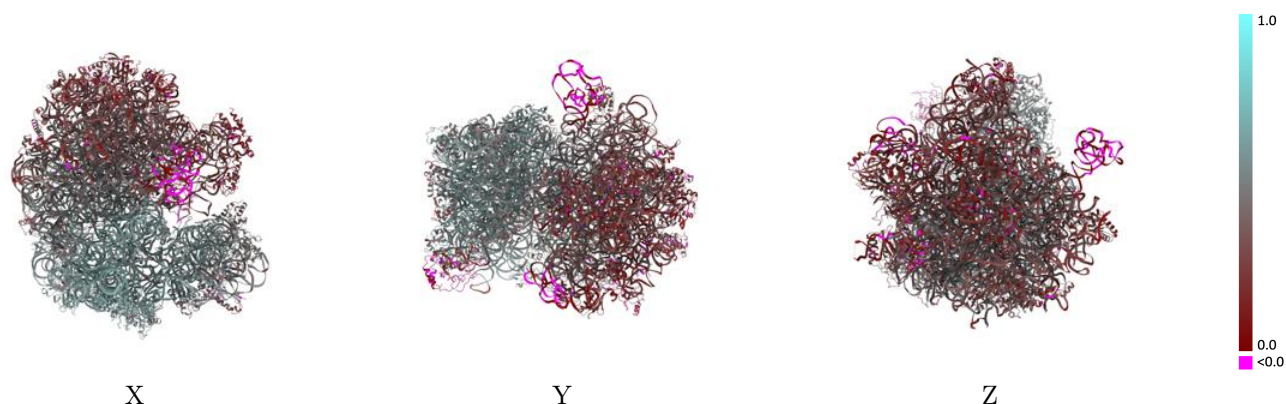
This section contains information regarding the fit between EMDB map EMD-55135 and PDB model 9SRA. Per-residue inclusion information can be found in section 3 on page 17.

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



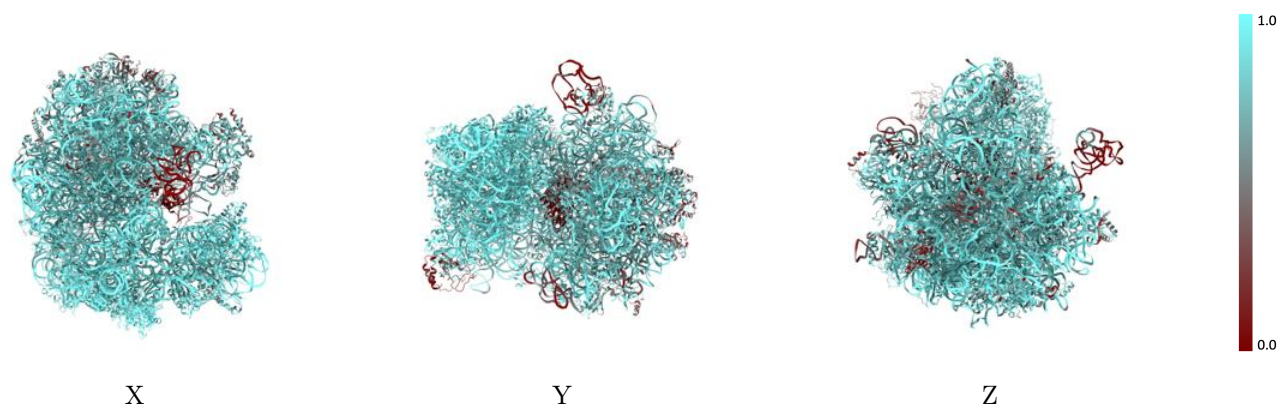
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



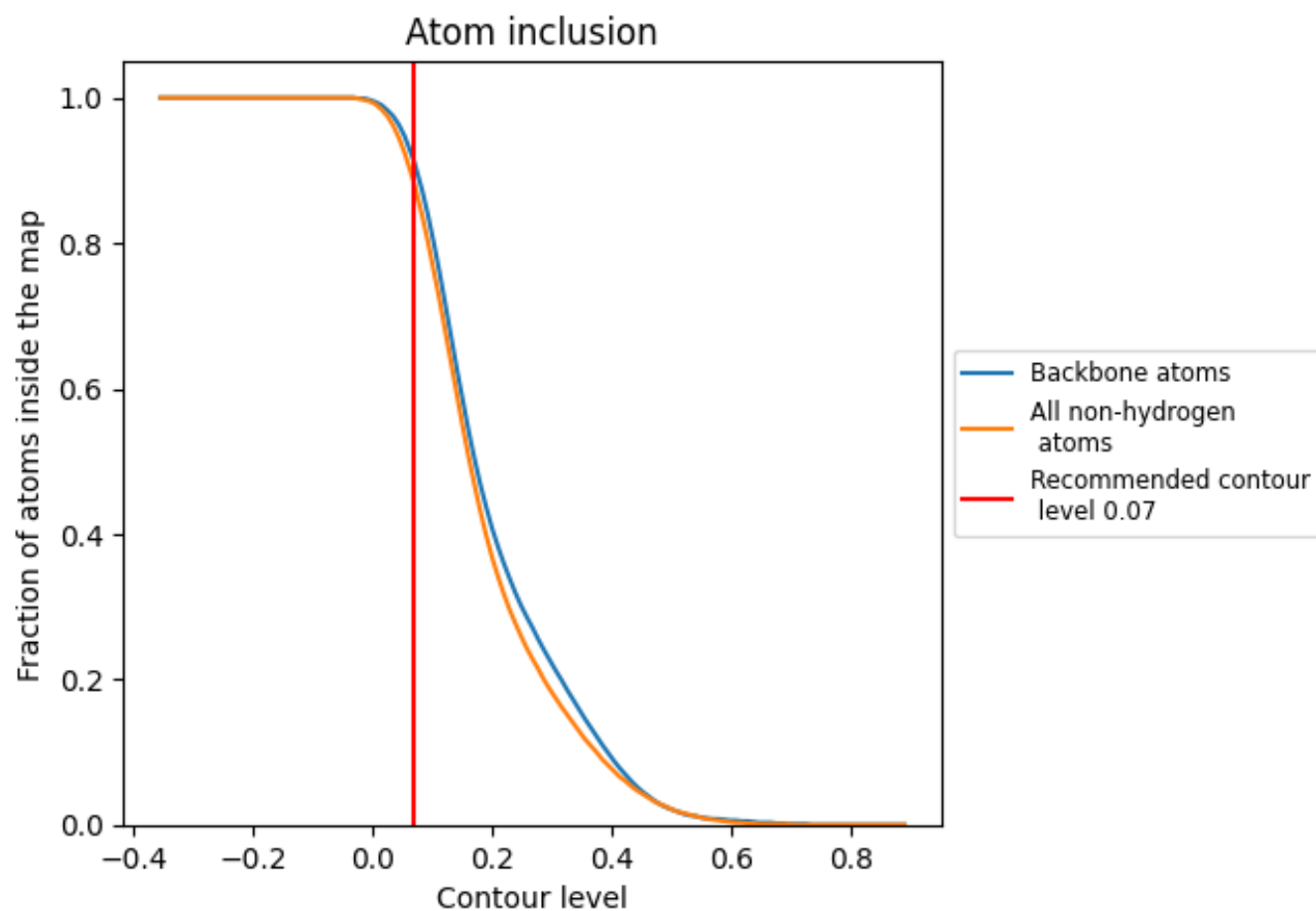
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 88% 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 (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8820   |  0.4130   |
| 1     |  0.9040   |  0.3630   |
| 2     |  0.9930   |  0.5590   |
| 3     |  0.9120   |  0.2480   |
| A0    |  0.9500   |  0.5960   |
| A3    |  0.3670   |  0.0910   |
| AA    |  0.9400   |  0.5430   |
| AB    |  0.9630   |  0.5590   |
| AC    |  0.9660   |  0.5740   |
| AD    |  0.9680   |  0.5590   |
| AE    |  0.9680   |  0.5650   |
| AF    |  0.9620   |  0.5750   |
| AG    |  0.9380   |  0.5040   |
| AH    |  0.9670   |  0.5550   |
| AI    |  0.9790  |  0.5980  |
| AJ    |  0.9540 |  0.5500 |
| AK    |  0.9420 |  0.5120 |
| AL    |  0.8550 |  0.4280 |
| AM    |  0.9440 |  0.5610 |
| AN    |  0.9540 |  0.5760 |
| AO    |  0.9010 |  0.4330 |
| AP    |  0.9290 |  0.5180 |
| AQ    |  0.9590 |  0.5670 |
| AR    |  0.9700 |  0.5860 |
| AS    |  0.9330 |  0.4910 |
| AT    |  0.8780 |  0.4330 |
| AU    |  0.9380 |  0.4730 |
| AV    |  0.9390 |  0.5140 |
| AW    |  0.9740 |  0.5280 |
| AX    |  0.8970 |  0.4850 |
| AY    |  0.2330 |  0.0680 |
| AZ    |  0.8930 |  0.4620 |
| B4    |  0.3280 |  0.1520 |
| B5    |  0.8530 |  0.4050 |
| B6    |  0.3360 |  0.1680 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| BB    |  0.8710   |  0.4790   |
| BC    |  0.8510   |  0.3840   |
| BD    |  0.7510   |  0.2670   |
| BE    |  0.7160   |  0.1880   |
| BF    |  0.8040   |  0.2580   |
| BG    |  0.6820   |  0.2780   |
| BI    |  0.7730   |  0.3000   |
| BJ    |  0.8560   |  0.4420   |
| BK    |  0.7020   |  0.1860   |
| BL    |  0.6410   |  0.2590   |
| BM    |  0.8230   |  0.3600   |
| BN    |  0.7610   |  0.2940   |
| BO    |  0.6370   |  0.2020   |
| BP    |  0.7400   |  0.2220   |
| BQ    |  0.8810   |  0.4570   |
| BR    |  0.7500   |  0.2660   |
| BS    |  0.8760   |  0.4130   |
| BT    |  0.7910   |  0.3520   |
| BU    |  0.7700   |  0.2700   |
| BV    |  0.9100  |  0.4140  |
| BW    |  0.6870 |  0.2640 |
| BY    |  0.7130 |  0.2530 |
| BZ    |  0.8630 |  0.4450 |
| Ba    |  0.8820 |  0.4430 |
| Bb    |  0.7500 |  0.2990 |
| Bc    |  0.7190 |  0.2510 |
| Bd    |  0.9000 |  0.4510 |
| Be    |  0.8310 |  0.4000 |
| Bf    |  0.8380 |  0.3500 |
| Bg    |  0.8730 |  0.2910 |
| Bi    |  0.8790 |  0.5000 |
| Bj    |  0.6700 |  0.3110 |
| Bk    |  0.7950 |  0.2740 |
| Bl    |  0.5770 |  0.1920 |
| H     |  0.3280 |  0.3540 |
| sd    |  0.9400 |  0.4010 |