



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 09:17 PM UTC

PDB ID : 8APN / pdb\_00008apn  
EMDB ID : EMD-15576  
Title : Structure of the mitochondrial ribosome from *Polytomella magna* with tRNA bound to the P site  
Authors : Tobiasson, V.; Berzina, I.; Amunts, A.  
Deposited on : 2022-08-10  
Resolution : 3.10 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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

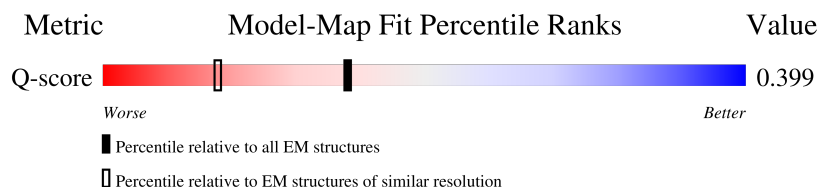
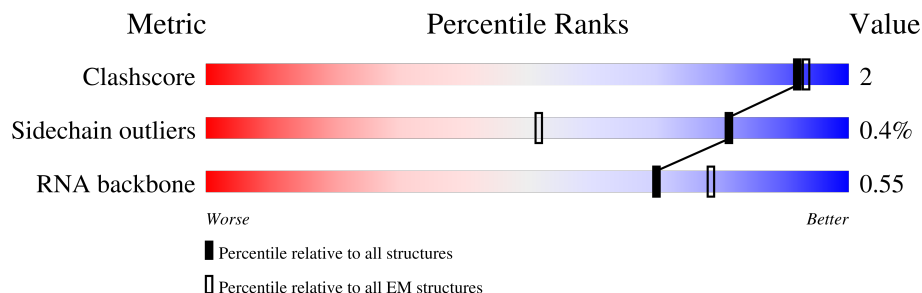
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.



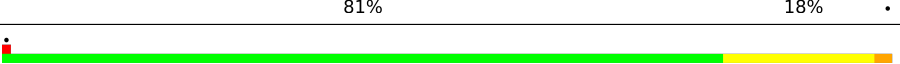
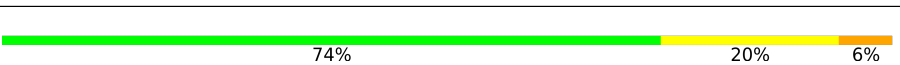
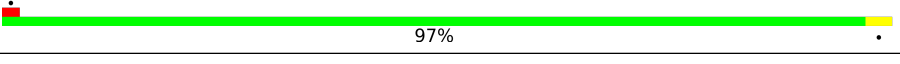
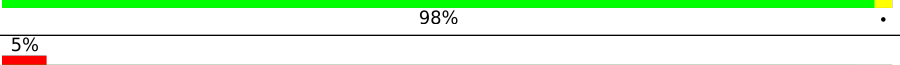
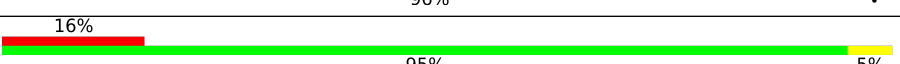
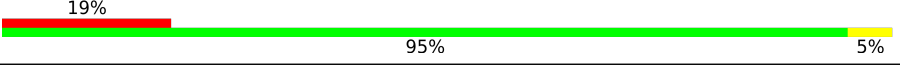
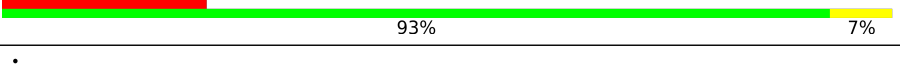
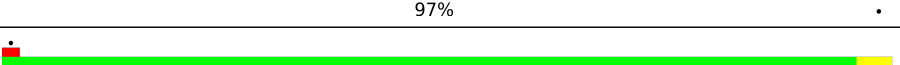
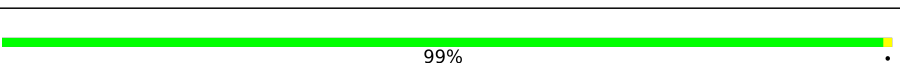
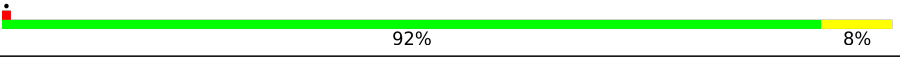
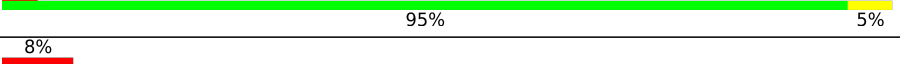
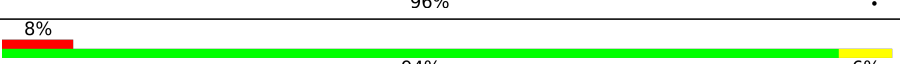
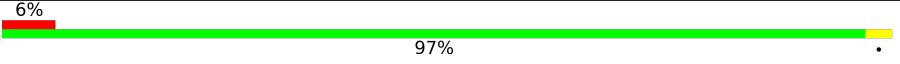
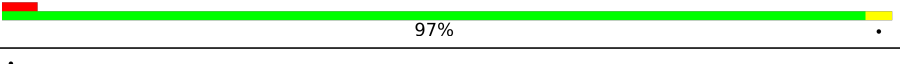
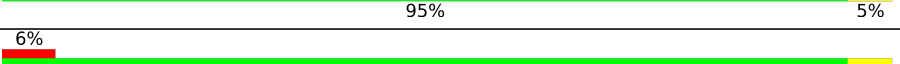
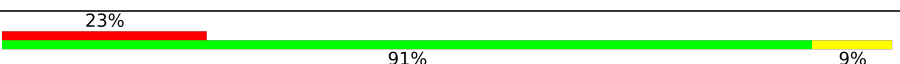
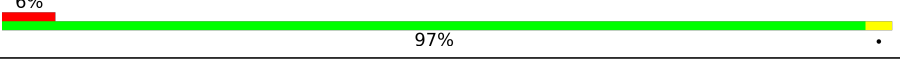
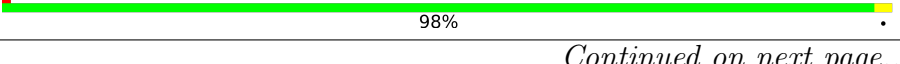
| Metric             | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore         | 229148                      | 23984                       | -                                                        |
| Sidechain outliers | 223484                      | 23102                       | -                                                        |
| RNA backbone       | 8273                        | 3508                        | -                                                        |
| Q-score            | -                           | 25397                       | 14724 ( 2.60 - 3.60 )                                    |

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   | A1    | 109    | <br>5% 75% 22%   |
| 2   | A2    | 81     | <br>5% 75% 22%   |
| 3   | A3    | 207    | <br>84% 15%      |
| 4   | A4    | 73     | <br>79% 21%      |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | A5    | 136    |    |
| 6   | A6    | 109    |    |
| 7   | A7    | 534    |    |
| 8   | A8    | 350    |    |
| 9   | A9    | 69     |    |
| 10  | Aa    | 306    |    |
| 11  | Ab    | 306    |    |
| 12  | Ac    | 303    |    |
| 13  | Ad    | 193    |    |
| 14  | Ae    | 242    |   |
| 15  | Af    | 56     |  |
| 16  | Ah    | 186    |  |
| 17  | Ai    | 121    |  |
| 18  | Aj    | 206    |  |
| 19  | Ak    | 166    |  |
| 20  | Al    | 173    |  |
| 21  | Am    | 114    |  |
| 22  | An    | 170    |  |
| 23  | Ao    | 117    |  |
| 24  | Ap    | 200    |  |
| 25  | Aq    | 188    |  |
| 26  | Ar    | 155    |  |
| 27  | As    | 115    |  |
| 28  | At    | 253    |  |
| 29  | Au    | 142    |  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 30  | Av    | 129    |                  |
| 31  | Aw    | 123    |                  |
| 32  | Ax    | 176    |                  |
| 33  | Ay    | 72     |                  |
| 34  | Az    | 59     |                  |
| 35  | AA    | 50     |                  |
| 36  | AB    | 50     |                  |
| 37  | AC    | 139    |                  |
| 38  | AD    | 47     |                  |
| 39  | AE    | 92     |                  |
| 40  | AF    | 93     |                  |
| 41  | AG    | 121    |                  |
| 42  | AH    | 176    |                  |
| 43  | AI    | 64     |                  |
| 44  | AJ    | 122    |                  |
| 45  | AK    | 139    |                  |
| 46  | AL    | 394    |                  |
| 47  | AM    | 419    |                  |
| 48  | AN    | 420    |                  |
| 49  | AO    | 377    |                  |
| 50  | Xa    | 199    |                  |
| 51  | Xb    | 244    |                  |
| 52  | Xc    | 57     |                  |
| 53  | Xd    | 413    |                  |
| 54  | Xe    | 483    |                  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 55  | Xf    | 201    |                  |
| 56  | Xg    | 410    |                  |
| 57  | Xh    | 143    |                  |
| 58  | Xi    | 24     |                  |
| 59  | Xj    | 71     |                  |
| 60  | B1    | 102    |                  |
| 61  | B2    | 210    |                  |
| 62  | B3    | 379    |                  |
| 63  | B4    | 337    |                  |
| 64  | Ba    | 242    |                  |
| 65  | Bb    | 236    |                  |
| 66  | Bc    | 289    |                  |
| 67  | Bd    | 221    |                  |
| 68  | Be    | 228    |                  |
| 69  | Bf    | 119    |                  |
| 70  | Bg    | 112    |                  |
| 71  | Bh    | 374    |                  |
| 72  | Bi    | 282    |                  |
| 73  | Bj    | 401    |                  |
| 74  | Bk    | 116    |                  |
| 75  | Bl    | 123    |                  |
| 76  | Bm    | 113    |                  |
| 77  | Bn    | 118    |                  |
| 78  | Bo    | 167    |                  |
| 79  | Bp    | 123    |                  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 80  | Bq    | 130    |                  |
| 81  | Br    | 90     |                  |
| 82  | Bs    | 92     |                  |
| 83  | Bt    | 75     |                  |
| 84  | Bu    | 167    |                  |
| 85  | Bv    | 164    |                  |
| 86  | Bw    | 349    |                  |
| 87  | Bx    | 621    |                  |
| 88  | By    | 80     |                  |
| 89  | Bz    | 119    |                  |
| 90  | BA    | 176    |                  |
| 91  | BB    | 84     |                  |
| 92  | BC    | 270    |                  |
| 93  | BD    | 31     |                  |
| 94  | BE    | 171    |                  |
| 95  | BF    | 370    |                  |
| 96  | Ya    | 180    |                  |
| 97  | Yb    | 50     |                  |
| 98  | Yc    | 159    |                  |
| 99  | Yd    | 95     |                  |
| 100 | Ye    | 106    |                  |
| 101 | Yf    | 150    |                  |
| 102 | Yg    | 67     |                  |
| 103 | Yh    | 65     |                  |
| 104 | Yi    | 132    |                  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 105 | Yj    | 386    | 92%<br>          |
| 106 | Yk    | 92     | 98%<br>          |
| 107 | Yl    | 84     | 95%<br>          |
| 108 | C1    | 73     | 59%<br>          |
| 109 | C3    | 4      | 50%<br>          |
| 110 | Ub    | 130    | 88%<br>          |
| 111 | Ua    | 32     | 91%<br>          |
| 112 | Ud    | 43     | 86%<br>          |
| 113 | Ue    | 47     | 100%<br>         |
| 114 | Uf    | 73     | 95%<br>          |
| 115 | Ug    | 63     | 95%<br>          |
| 116 | Uh    | 48     | 100%<br>         |
| 117 | Ui    | 26     | 100%<br>         |
| 118 | Uj    | 9      | 89%<br>          |
| 119 | Uk    | 23     | 87%<br>          |
| 120 | Ul    | 16     | 100%<br>         |
| 121 | Um    | 11     | 55%<br>          |

## 2 Entry composition

There are 126 unique types of molecules in this entry. The entry contains 198407 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 mtLSU-1.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 1   | A1    | 109      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2344  | 1052 | 444 | 739 | 109 |         |       |

- Molecule 2 is a RNA chain called mtLSU-2.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | A2    | 81       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1729  | 777 | 318 | 553 | 81 |         |       |

- Molecule 3 is a RNA chain called mtLSU-3.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | A3    | 207      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 4413  | 1980 | 795 | 1431 | 207 |         |       |

- Molecule 4 is a RNA chain called mtLSU-4.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | A4    | 73       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1572  | 704 | 302 | 493 | 73 |         |       |

- Molecule 5 is a RNA chain called mtLSU-5.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | A5    | 136      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2897  | 1298 | 522 | 941 | 136 |         |       |

- Molecule 6 is a RNA chain called mtLSU-6.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 6   | A6    | 109      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2337  | 1048 | 433 | 747 | 109 |         |       |

- Molecule 7 is a RNA chain called mtLSU-7.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 7   | A7    | 534      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 11387 | 5106 | 2066 | 3681 | 534 |         |       |

- Molecule 8 is a RNA chain called mtLSU-8.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 8   | A8    | 350      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 7452  | 3335 | 1322 | 2445 | 350 |         |       |

- Molecule 9 is a RNA chain called mt-5S.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | A9    | 69       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1466  | 656 | 256 | 485 | 69 |         |       |

- Molecule 10 is a protein called uL2m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | Aa    | 306      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2386  | 1501 | 470 | 410 | 5 |         |       |

- Molecule 11 is a protein called uL3m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | Ab    | 306      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2414  | 1560 | 411 | 432 | 11 |         |       |

- Molecule 12 is a protein called uL4m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | Ac    | 303      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2377  | 1499 | 438 | 435 | 5 |         |       |

- Molecule 13 is a protein called uL5m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | Ad    | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1537  | 991 | 256 | 281 | 9 |         |       |

- Molecule 14 is a protein called uL6m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | Ae    | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1934  | 1260 | 326 | 341 | 7 |         |       |

- Molecule 15 is a protein called uL9m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | Af    | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 432   | 274 | 74 | 83 | 1 |         |       |

- Molecule 16 is a protein called uL13m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Ah    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1517  | 975 | 274 | 260 | 8 |         |       |

- Molecule 17 is a protein called Hypothetical protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Ai    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 952   | 621 | 170 | 158 | 3 |         |       |

- Molecule 18 is a protein called uL15m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | Aj    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1607  | 1027 | 290 | 284 | 6 |         |       |

- Molecule 19 is a protein called uL16m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | Ak    | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1356  | 870 | 261 | 216 | 9 |         |       |

- Molecule 20 is a protein called bL17m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | Al    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1412  | 898 | 272 | 240 | 2 |         |       |

- Molecule 21 is a protein called uL18m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | Am    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 911   | 587 | 166 | 156 | 2 |         |       |

- Molecule 22 is a protein called bL19m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | An    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1392  | 891 | 238 | 255 | 8 |         |       |

- Molecule 23 is a protein called bL20m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Ao    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 964   | 607 | 186 | 168 | 3 |         |       |

- Molecule 24 is a protein called bL21m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | Ap    | 200      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 1003 | 278 | 279 | 6 |         |       |

- Molecule 25 is a protein called uL22m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Aq    | 188      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1533  | 971 | 285 | 273 | 4 |         |       |

- Molecule 26 is a protein called uL23m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Ar    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1283  | 824 | 223 | 232 | 4 |         |       |

- Molecule 27 is a protein called bL24m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | As    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 920   | 590 | 157 | 169 | 4 |         |       |

- Molecule 28 is a protein called bL25m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | At    | 253      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2003  | 1268 | 364 | 361 | 10 |         |       |

- Molecule 29 is a protein called bL27m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | Au    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1149  | 734 | 212 | 200 | 3 |         |       |

- Molecule 30 is a protein called bL28m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Av    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1058  | 670 | 187 | 198 | 3 |         |       |

- Molecule 31 is a protein called uL29m.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 31  | Aw    | 123      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1024  | 646 | 189 | 189 |  |         |       |

- Molecule 32 is a protein called uL30m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Ax    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1472  | 942 | 277 | 250 | 3 |         |       |

- Molecule 33 is a protein called bL31m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Ay    | 72       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 592   | 387 | 103 | 100 | 2 |         |       |

- Molecule 34 is a protein called bL32m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | Az    | 59       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 469   | 306 | 87 | 72 | 4 |         |       |

- Molecule 35 is a protein called bL33m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | AA    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 416   | 276 | 72 | 66 | 2 |         |       |

- Molecule 36 is a protein called bL34m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36  | AB    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 264 | 91 | 68 | 4 |         |       |

- Molecule 37 is a protein called bL35m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | AC    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1180  | 756 | 238 | 184 | 2 |         |       |

- Molecule 38 is a protein called bL36m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | AD    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 375   | 236 | 78 | 57 | 4 |         |       |

- Molecule 39 is a protein called mL40.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39  | AE    | 92       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 771   | 493 | 139 | 139 |         |       |

- Molecule 40 is a protein called mL41.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 40  | AF    | 93       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 765   | 495 | 140 | 130 |         |       |

- Molecule 41 is a protein called mL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | AG    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 994   | 625 | 189 | 173 | 7 |         |       |

- Molecule 42 is a protein called mL46.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | AH    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1412  | 910 | 233 | 262 | 7 |         |       |

- Molecule 43 is a protein called mL63.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | AI    | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 505   | 325 | 92 | 87 | 1 |         |       |

- Molecule 44 is a protein called mL64.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | AJ    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1003  | 646 | 182 | 173 | 2 |         |       |

- Molecule 45 is a protein called mL87.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | AK    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1164  | 751 | 215 | 195 | 3 |         |       |

- Molecule 46 is a protein called mL116.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | AL    | 394      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3093  | 1970 | 548 | 568 | 7 |         |       |

- Molecule 47 is a protein called mL116.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | AM    | 419      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3282  | 2087 | 584 | 604 | 7 |         |       |

- Molecule 48 is a protein called mL116.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | AN    | 420      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3286  | 2089 | 585 | 605 | 7 |         |       |

- Molecule 49 is a protein called mL118.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | AO    | 377      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2881  | 1832 | 516 | 527 | 6 |         |       |

- Molecule 50 is a protein called mL120.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | Xa    | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1568  | 1000 | 268 | 296 | 4 |         |       |

- Molecule 51 is a protein called mL121.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | Xb    | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1956  | 1257 | 320 | 370 | 9 |         |       |

- Molecule 52 is a protein called mL122.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 52  | Xc    | 57       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 496   | 318 | 90 | 88 |         |       |

- Molecule 53 is a protein called mL123.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | Xd    | 413      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3236  | 2064 | 568 | 592 | 12 |         |       |

- Molecule 54 is a protein called mL124.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 54  | Xe    | 483      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3675  | 2334 | 666 | 665 | 10 |         |       |

- Molecule 55 is a protein called mL125.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | Xf    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1615  | 1034 | 289 | 290 | 2 |         |       |

- Molecule 56 is a protein called mL126.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | Xg    | 410      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3081  | 1978 | 538 | 558 | 7 |         |       |

- Molecule 57 is a protein called mL127.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | Xh    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1147  | 736 | 208 | 200 | 3 |         |       |

- Molecule 58 is a protein called mL128.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 58  | Xi    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 206   | 131 | 40 | 34 | 1 |         |       |

- Molecule 59 is a protein called mL129.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | Xj    | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 582   | 362 | 104 | 115 | 1 |         |       |

- Molecule 60 is a RNA chain called mtSSU-1.

| Mol | Chain | Residues | Atoms |     |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| 60  | B1    | 102      | Total | C   | N   | O   | P   | 0       | 0     |
|     |       |          | 2165  | 969 | 376 | 718 | 102 |         |       |

- Molecule 61 is a RNA chain called mtSSU-2.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 61  | B2    | 210      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 4484  | 2008 | 815 | 1451 | 210 |         |       |

- Molecule 62 is a RNA chain called mtSSU-3.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 62  | B3    | 379      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 8096  | 3627 | 1480 | 2610 | 379 |         |       |

- Molecule 63 is a RNA chain called mtSSU-4.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 63  | B4    | 337      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 7186  | 3222 | 1300 | 2327 | 337 |         |       |

- Molecule 64 is a protein called bS1m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 64  | Ba    | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1936  | 1222 | 344 | 361 | 9 |         |       |

- Molecule 65 is a protein called uS2m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | Bb    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1878  | 1215 | 315 | 344 | 4 |         |       |

- Molecule 66 is a protein called uS3m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 66  | Bc    | 289      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2282  | 1451 | 408 | 416 | 7 |         |       |

- Molecule 67 is a protein called uS4m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 67  | Bd    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1793  | 1132 | 338 | 315 | 8 |         |       |

- Molecule 68 is a protein called uS5m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 68  | Be    | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1826  | 1153 | 336 | 330 | 7 |         |       |

- Molecule 69 is a protein called uS6m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | Bf    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 624 | 170 | 171 | 4 |         |       |

- Molecule 70 is a protein called uS7m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | Bg    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 887   | 555 | 168 | 157 | 7 |         |       |

- Molecule 71 is a protein called uS8m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 71  | Bh    | 374      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3037  | 1949 | 549 | 533 | 6 |         |       |

- Molecule 72 is a protein called uS9m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 72  | Bi    | 282      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2271  | 1441 | 406 | 415 | 9 |         |       |

- Molecule 73 is a protein called uS10m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 73  | Bj    | 401      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3174  | 2020 | 543 | 597 | 14 |         |       |

- Molecule 74 is a protein called uS11m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | Bk    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 871   | 550 | 158 | 160 | 3 |         |       |

- Molecule 75 is a protein called uS12m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | Bl    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 962   | 604 | 190 | 164 | 4 |         |       |

- Molecule 76 is a protein called uS13m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | Bm    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 897   | 560 | 176 | 157 | 4 |         |       |

- Molecule 77 is a protein called uS14m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | Bn    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 978   | 613 | 194 | 167 | 4 |         |       |

- Molecule 78 is a protein called uS15m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | Bo    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1212  | 759 | 234 | 213 | 6 |         |       |

- Molecule 79 is a protein called bS16m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | Bp    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1013  | 655 | 184 | 172 | 2 |         |       |

- Molecule 80 is a protein called uS17m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | Bq    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 662 | 200 | 187 | 4 |         |       |

- Molecule 81 is a protein called bS18m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | Br    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 743   | 465 | 148 | 127 | 3 |         |       |

- Molecule 82 is a protein called bS19m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | Bs    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 734   | 472 | 132 | 128 | 2 |         |       |

- Molecule 83 is a protein called bS21m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | Bt    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 621   | 396 | 117 | 107 | 1 |         |       |

- Molecule 84 is a protein called mS23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | Bu    | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1366  | 874 | 240 | 248 | 4 |         |       |

- Molecule 85 is a protein called mS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 85  | Bv    | 164      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1355  | 846 | 249 | 256 | 4 |         |       |

- Molecule 86 is a protein called mS29.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 86  | Bw    | 349      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2749  | 1748 | 477 | 511 | 13 |         |       |

- Molecule 87 is a protein called mS31.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 87  | Bx    | 621      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4714  | 2990 | 819 | 894 | 11 |         |       |

- Molecule 88 is a protein called mS33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 88  | By    | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 409 | 111 | 114 | 2 |         |       |

- Molecule 89 is a protein called mS34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 89  | Bz    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 648 | 172 | 176 | 1 |         |       |

- Molecule 90 is a protein called mS35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 90  | BA    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1377  | 854 | 253 | 265 | 5 |         |       |

- Molecule 91 is a protein called mS37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 91  | BB    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 663   | 411 | 129 | 118 | 5 |         |       |

- Molecule 92 is a protein called mS45.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 92  | BC    | 270      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2163  | 1364 | 383 | 406 | 10 |         |       |

- Molecule 93 is a protein called mS38.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 93  | BD    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 278   | 176 | 65 | 35 | 2 |         |       |

- Molecule 94 is a protein called mS106.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 94  | BE    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1304  | 824 | 223 | 253 | 4 |         |       |

- Molecule 95 is a protein called mS107.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 95  | BF    | 370      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2980  | 1897 | 541 | 533 | 9 |         |       |

- Molecule 96 is a protein called uS4m-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 96  | Ya    | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1434  | 904 | 252 | 272 | 6 |         |       |

- Molecule 97 is a protein called mS108.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 97  | Yb    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 412   | 260 | 77 | 74 | 1 |         |       |

- Molecule 98 is a protein called mS109.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 98  | Yc    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1297  | 826 | 231 | 237 | 3 |         |       |

- Molecule 99 is a protein called mS110.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 99  | Yd    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 785   | 495 | 147 | 141 | 2 |         |       |

- Molecule 100 is a protein called uS3m-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 100 | Ye    | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 864   | 559 | 156 | 147 | 2 |         |       |

- Molecule 101 is a protein called mS111.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 101 | Yf    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1236  | 792 | 218 | 221 | 5 |         |       |

- Molecule 102 is a protein called mS112.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 102 | Yg    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 553   | 344 | 108 | 97 | 4 |         |       |

- Molecule 103 is a protein called mS113.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 103 | Yh    | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 530   | 339 | 99 | 91 | 1 |         |       |

- Molecule 104 is a protein called mS114.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 104 | Yi    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 692 | 197 | 184 | 2 |         |       |

- Molecule 105 is a protein called mS115.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 105 | Yj    | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2859  | 1796 | 497 | 559 | 7 |         |       |

- Molecule 106 is a protein called mS116.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 106 | Yk    | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 460 | 113 | 133 | 1 |         |       |

- Molecule 107 is a protein called uS7m-2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 107 | Yl    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 673   | 428 | 115 | 127 | 3 |         |       |

- Molecule 108 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 108 | C1    | 73       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1542  | 693 | 268 | 509 | 72 |         |       |

- Molecule 109 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 109 | C3    | 4        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 87    | 39 | 17 | 27 | 4 |         |       |

- Molecule 110 is a protein called mL105.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 110 | Ub    | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 688 | 189 | 207 | 6 |         |       |

- Molecule 111 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 111 | Ua    | 32       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 166   | 99 | 35 | 32 |         |       |

- Molecule 112 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 112 | Ud    | 43       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 215   | 129 | 43 | 43 |         |       |

- Molecule 113 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 113 | Ue    | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 235   | 141 | 47 | 47 |         |       |

- Molecule 114 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 114 | Uf    | 73       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 365   | 219 | 73 | 73 |         |       |

- Molecule 115 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 115 | Ug    | 63       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 315   | 189 | 63 | 63 |         |       |

- Molecule 116 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 116 | Uh    | 48       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 240   | 144 | 48 | 48 |         |       |

- Molecule 117 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 117 | Ui    | 26       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 130   | 78 | 26 | 26 |         |       |

- Molecule 118 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |    |   |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 118 | Uj    | 9        | Total | C  | N | O | 0       | 0     |
|     |       |          | 45    | 27 | 9 | 9 |         |       |

- Molecule 119 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 119 | Uk    | 23       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 115   | 69 | 23 | 23 |         |       |

- Molecule 120 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 120 | U1    | 16       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 80    | 48 | 16 | 16 |         |       |

- Molecule 121 is a protein called Unknown.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 121 | Um    | 11       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 55    | 33 | 11 | 11 |         |       |

- Molecule 122 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 122 | A1    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 122 | A2    | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 122 | A3    | 7        | Total | Mg | 0       |
|     |       |          | 7     | 7  |         |
| 122 | A4    | 10       | Total | Mg | 0       |
|     |       |          | 10    | 10 |         |
| 122 | A5    | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 122 | A6    | 7        | Total | Mg | 0       |
|     |       |          | 7     | 7  |         |
| 122 | A7    | 25       | Total | Mg | 0       |
|     |       |          | 25    | 25 |         |
| 122 | A8    | 14       | Total | Mg | 0       |
|     |       |          | 14    | 14 |         |
| 122 | Ab    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 122 | B1    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 122 | B2    | 8        | Total | Mg | 0       |
|     |       |          | 8     | 8  |         |
| 122 | B3    | 13       | Total | Mg | 0       |
|     |       |          | 13    | 13 |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |          | AltConf |
|-----|-------|----------|-------------|----------|---------|
| 122 | B4    | 15       | Total<br>15 | Mg<br>15 | 0       |
| 122 | Bm    | 1        | Total<br>1  | Mg<br>1  | 0       |
| 122 | Bw    | 1        | Total<br>1  | Mg<br>1  | 0       |

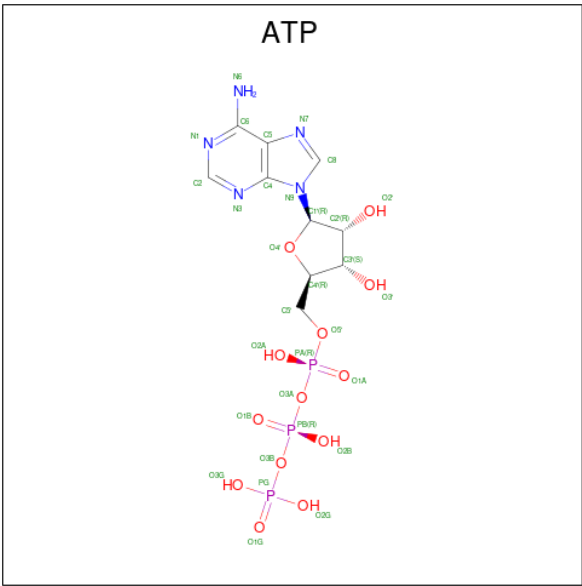
- Molecule 123 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 123 | A1    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | A3    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | A4    | 2        | Total<br>2 | K<br>2 | 0       |
| 123 | A7    | 4        | Total<br>4 | K<br>4 | 0       |
| 123 | A8    | 5        | Total<br>5 | K<br>5 | 0       |
| 123 | Aa    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | Ab    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | Ah    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | AC    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | B1    | 2        | Total<br>2 | K<br>2 | 0       |
| 123 | B2    | 1        | Total<br>1 | K<br>1 | 0       |
| 123 | B3    | 8        | Total<br>8 | K<br>8 | 0       |
| 123 | B4    | 3        | Total<br>3 | K<br>3 | 0       |

- Molecule 124 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 124 | AD    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 125 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



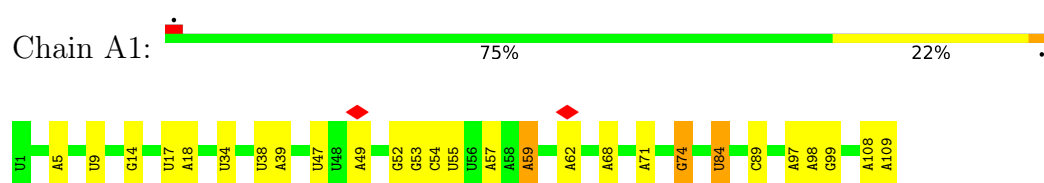
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 126 | Ac    | 1        | Total<br>1  | O<br>1  | 0       |
| 126 | Aj    | 4        | Total<br>4  | O<br>4  | 0       |
| 126 | AA    | 1        | Total<br>1  | O<br>1  | 0       |
| 126 | AC    | 1        | Total<br>1  | O<br>1  | 0       |
| 126 | AI    | 4        | Total<br>4  | O<br>4  | 0       |
| 126 | AK    | 2        | Total<br>2  | O<br>2  | 0       |
| 126 | Xg    | 1        | Total<br>1  | O<br>1  | 0       |
| 126 | B1    | 12       | Total<br>12 | O<br>12 | 0       |
| 126 | B2    | 39       | Total<br>39 | O<br>39 | 0       |
| 126 | B3    | 57       | Total<br>57 | O<br>57 | 0       |
| 126 | B4    | 69       | Total<br>69 | O<br>69 | 0       |
| 126 | Be    | 3        | Total<br>3  | O<br>3  | 0       |
| 126 | Bi    | 2        | Total<br>2  | O<br>2  | 0       |
| 126 | Bl    | 2        | Total<br>2  | O<br>2  | 0       |
| 126 | Bm    | 1        | Total<br>1  | O<br>1  | 0       |
| 126 | Bp    | 1        | Total<br>1  | O<br>1  | 0       |

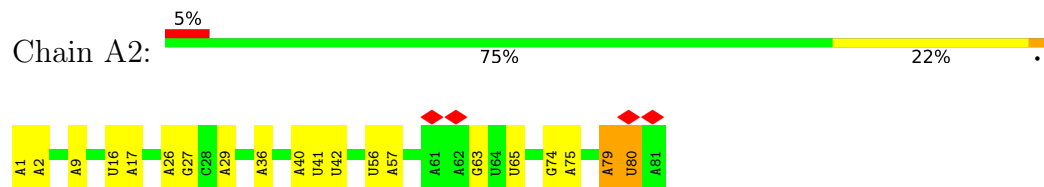
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

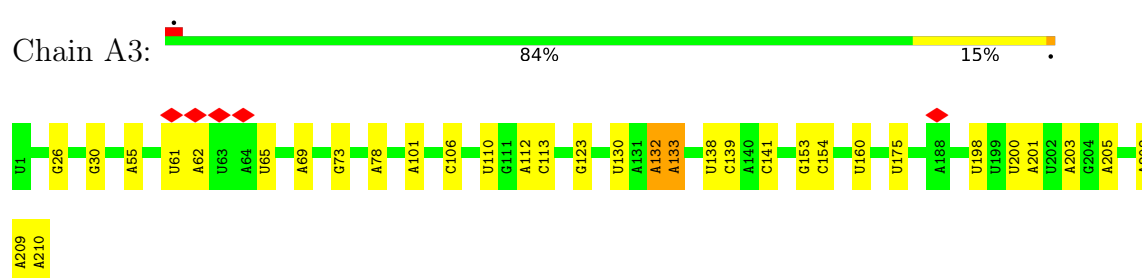
#### • Molecule 1: mtLSU-1



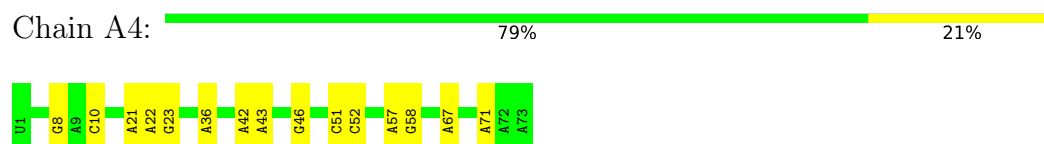
#### • Molecule 2: mtLSU-2



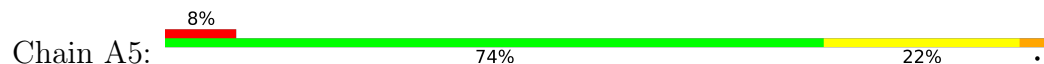
#### • Molecule 3: mtLSU-3



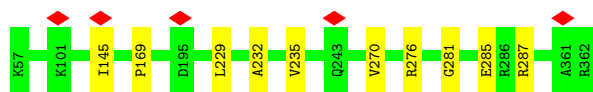
#### • Molecule 4: mtLSU-4



#### • Molecule 5: mtLSU-5



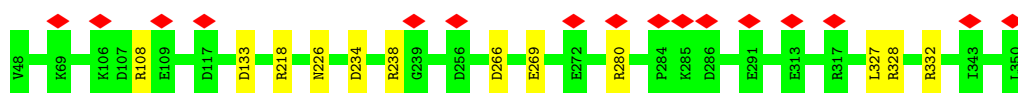




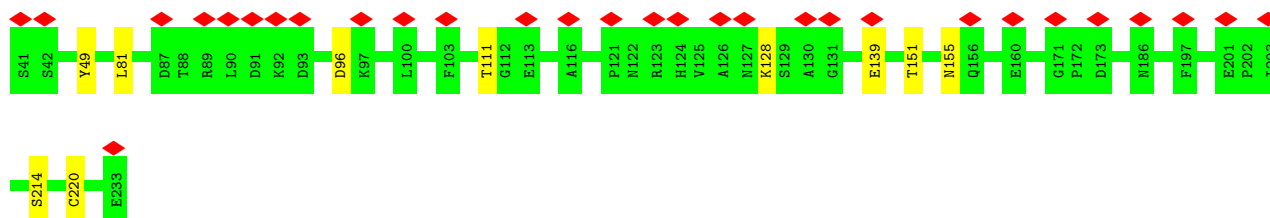
- Molecule 11: uL3m



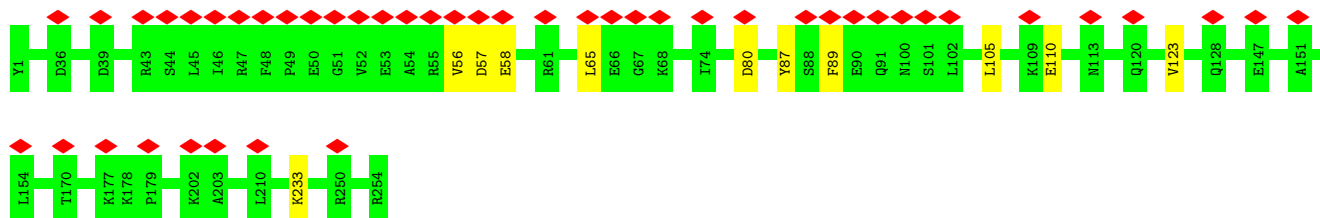
- Molecule 12: uL4m



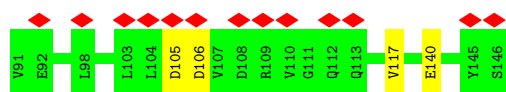
- Molecule 13: uL5m



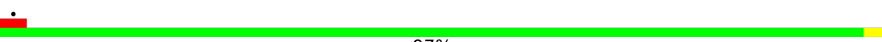
- Molecule 14: uL6m

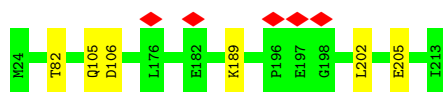


- Molecule 15: uL9m

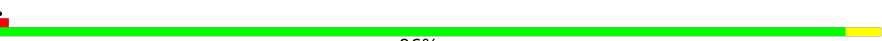


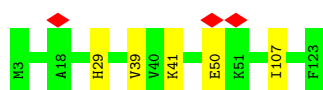
- Molecule 16: uL13m

Chain Ah:  97%

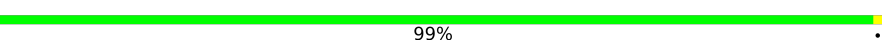


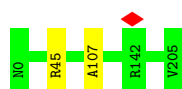
- Molecule 17: Hypothetical protein

Chain Ai:  96%



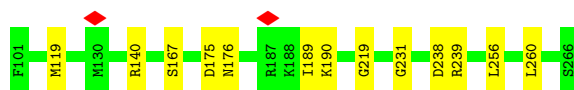
- Molecule 18: uL15m

Chain Aj:  99%

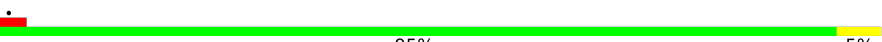


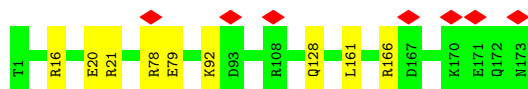
- Molecule 19: uL16m

Chain Ak:  92% 8%

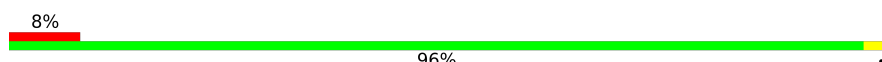


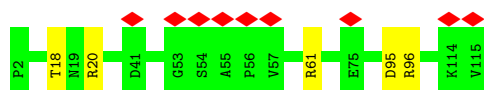
- Molecule 20: bL17m

Chain Al:  95% 5%

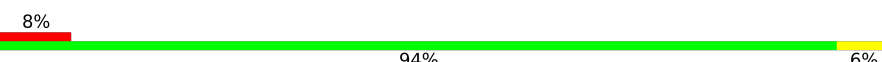


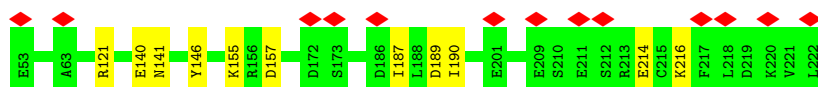
- Molecule 21: uL18m

Chain Am:  96% 8%



- Molecule 22: bL19m

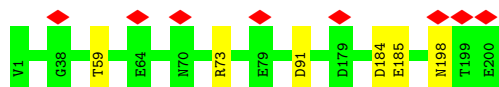
Chain An:  94% 8% 6%



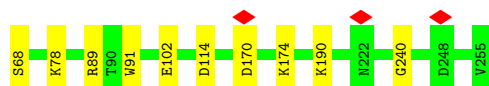
## • Molecule 23: bL20m



## • Molecule 24: bL21m



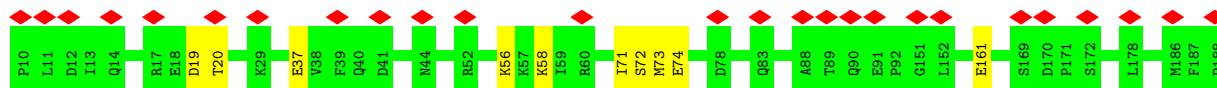
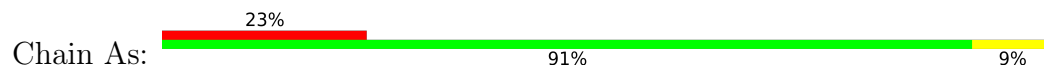
## • Molecule 25: uL22m



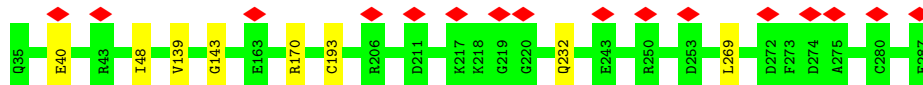
## • Molecule 26: uL23m



## • Molecule 27: bL24m

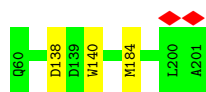


## • Molecule 28: bL25m



## • Molecule 29: bL27m

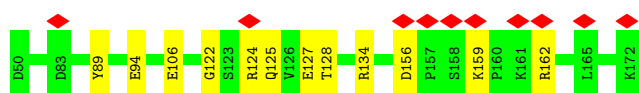
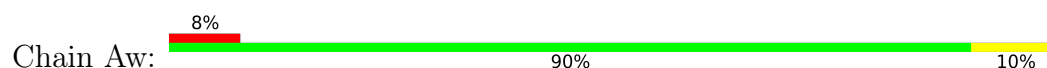




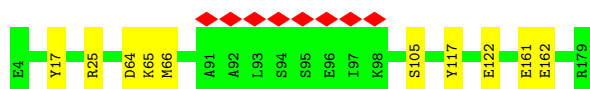
- Molecule 30: bL28m



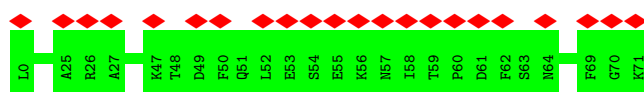
- Molecule 31: uL29m



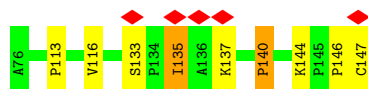
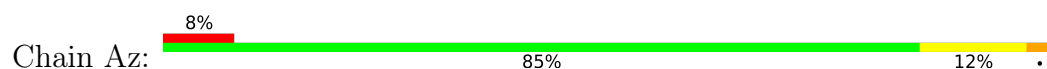
- Molecule 32: uL30m



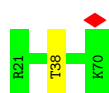
- Molecule 33: bL31m



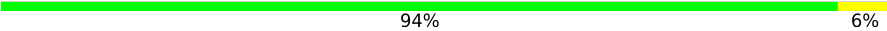
- Molecule 34: bL32m



- Molecule 35: bL33m

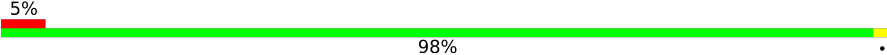


- Molecule 36: bL34m

Chain AB:  94% 6%

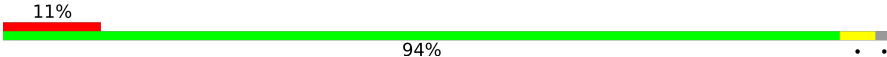


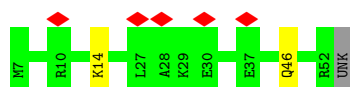
- Molecule 37: bL35m

Chain AC:  5% 98% .

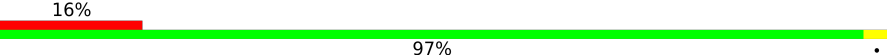


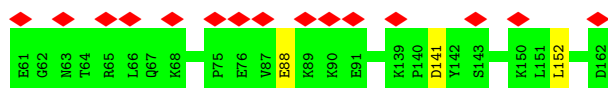
- Molecule 38: bL36m

Chain AD:  11% 94% . .

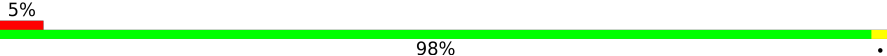


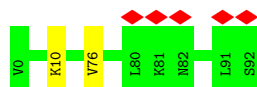
- Molecule 39: mL40

Chain AE:  16% 97% .

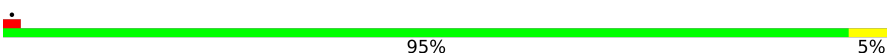


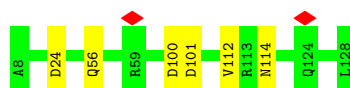
- Molecule 40: mL41

Chain AF:  5% 98% .



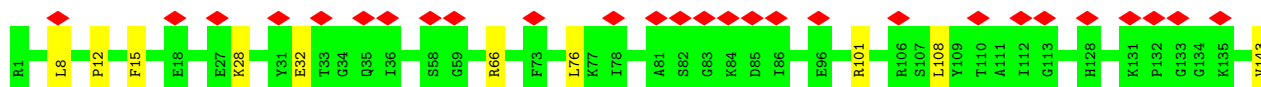
- Molecule 41: mL43

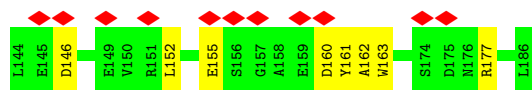
Chain AG:  95% 5%



- Molecule 42: mL46

Chain AH:  22% 90% 10%

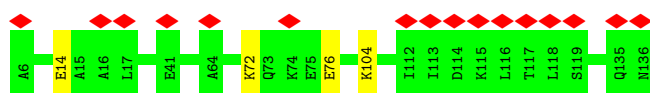




• Molecule 43: mL63



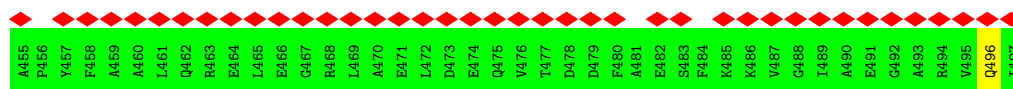
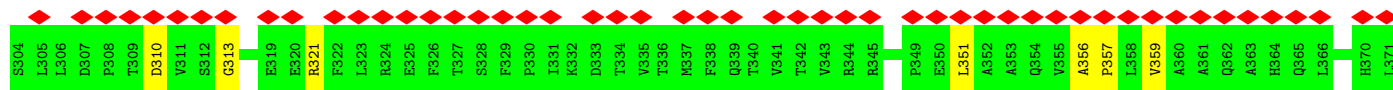
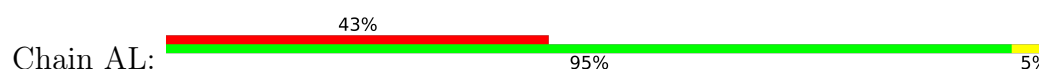
• Molecule 44: mL64



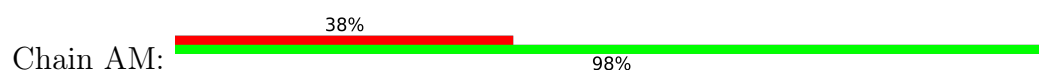
• Molecule 45: mL87

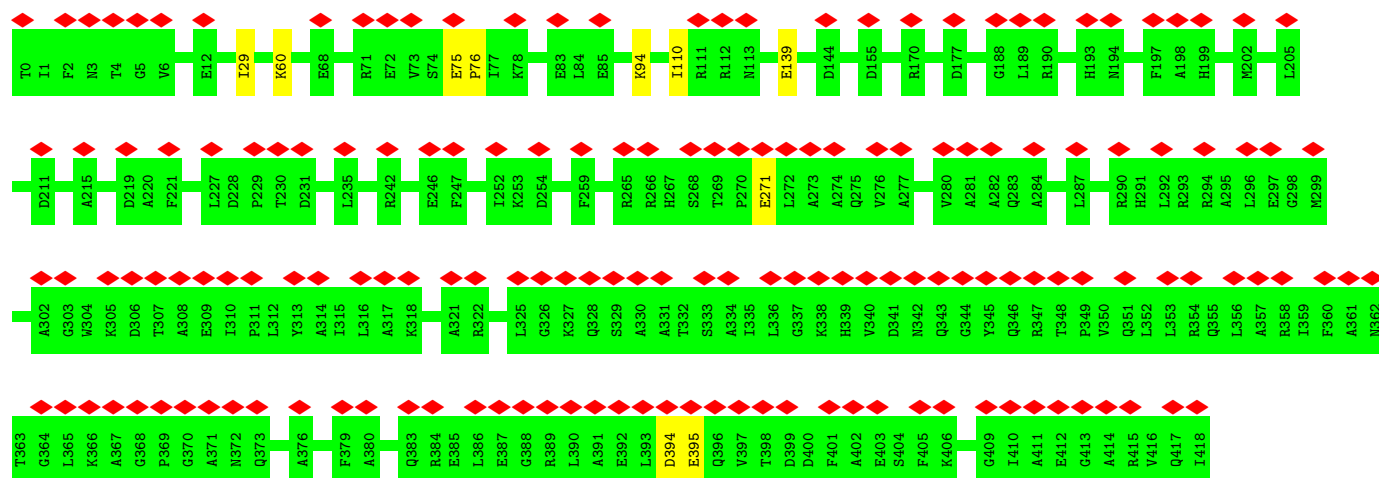


• Molecule 46: mL116

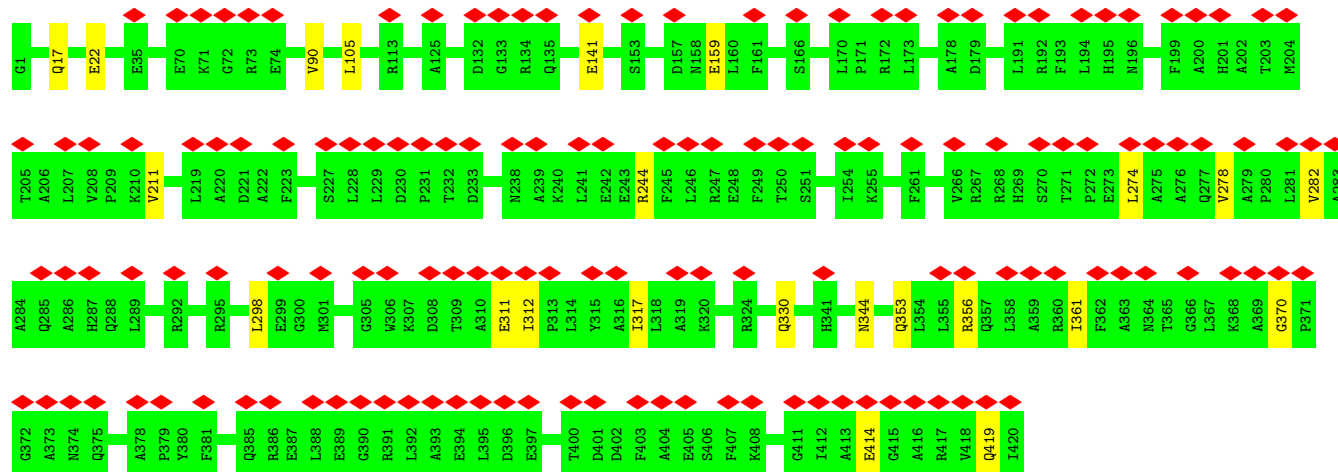


• Molecule 47: mL116

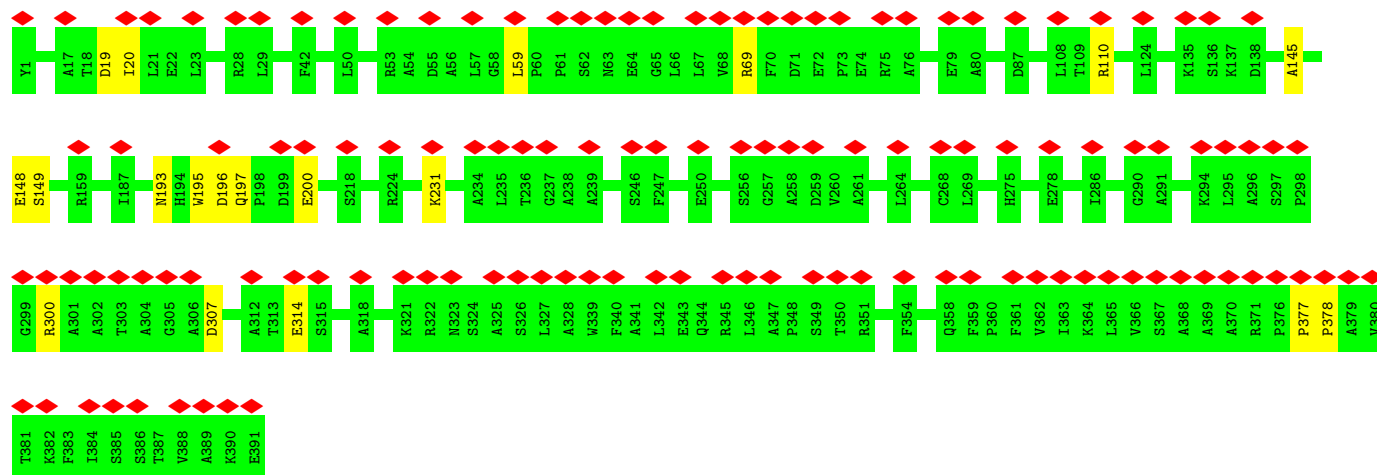




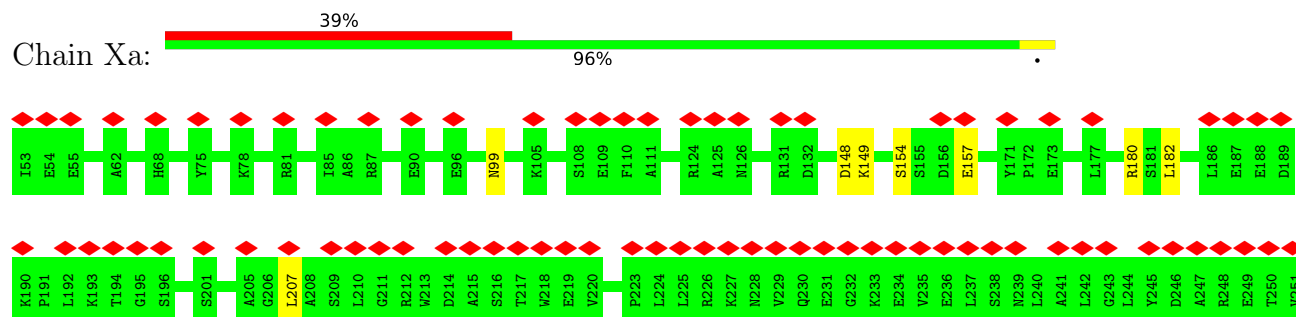
• Molecule 48: mL116



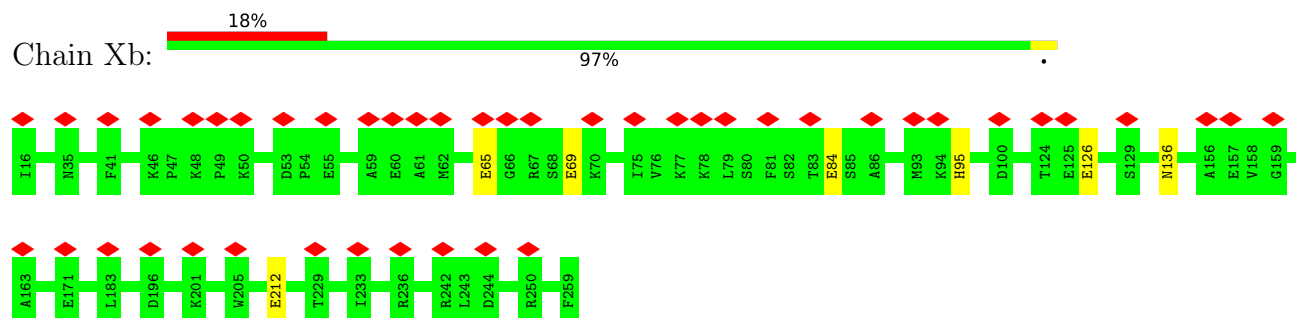
• Molecule 49: mL118



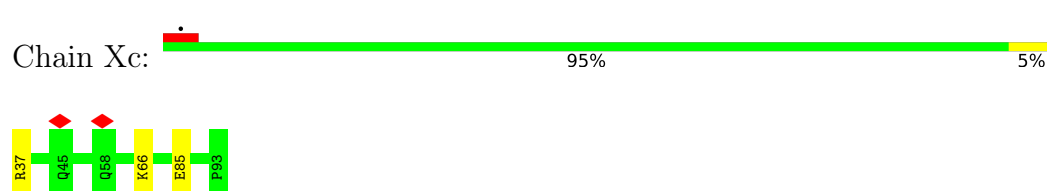
- Molecule 50: mL120



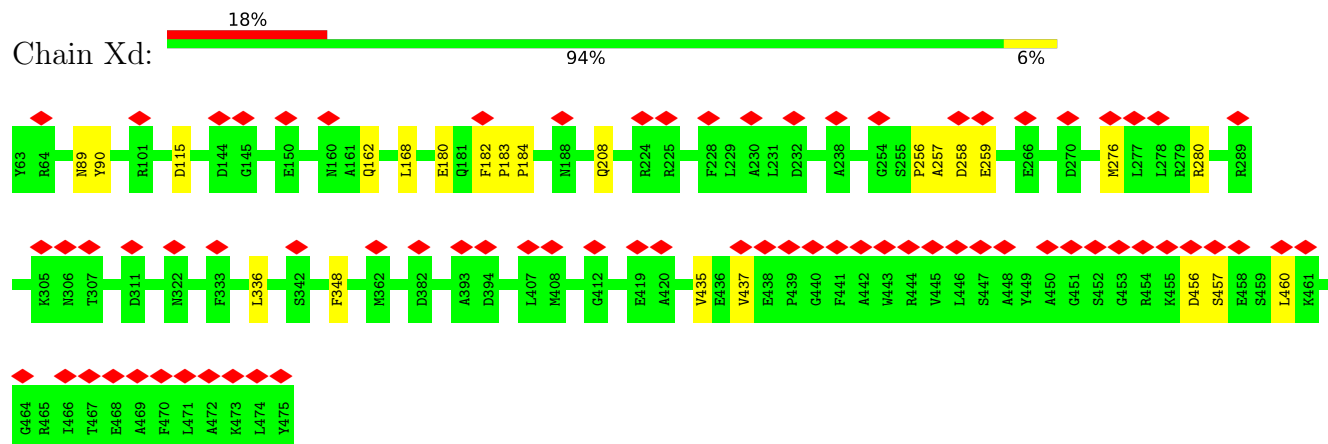
- Molecule 51: mL121



- Molecule 52: mL122

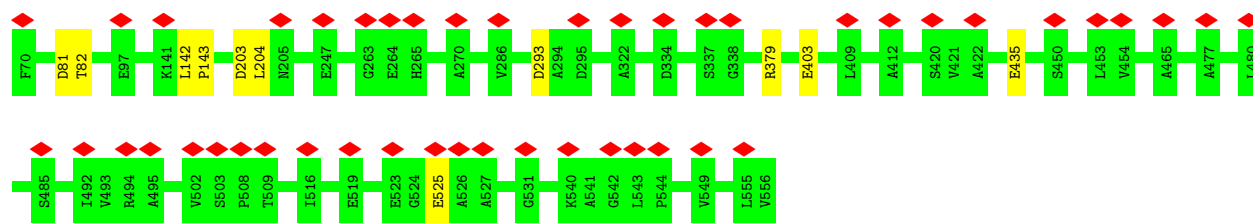


- Molecule 53: mL123

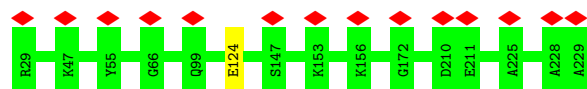


- Molecule 54: mL124

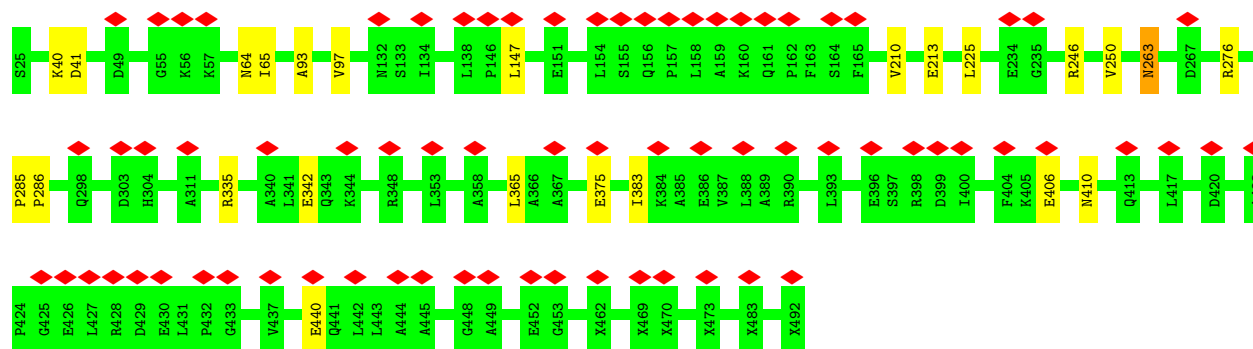




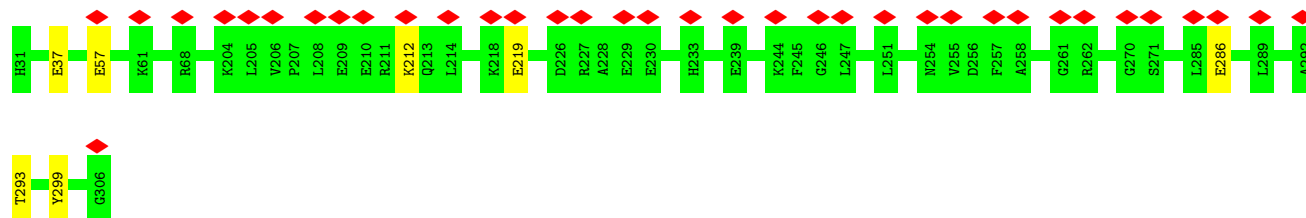
• Molecule 55: mL125



• Molecule 56: mL126



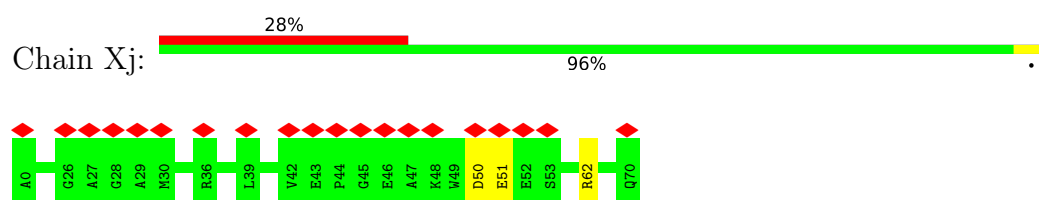
• Molecule 57: mL127



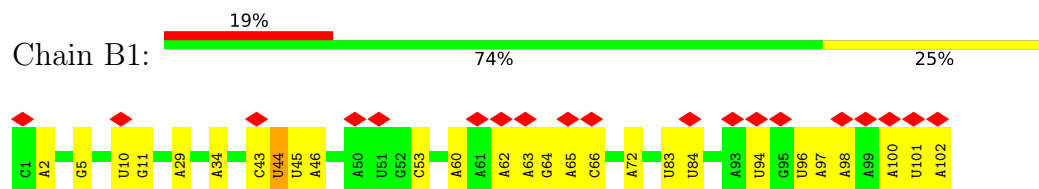
• Molecule 58: mL128



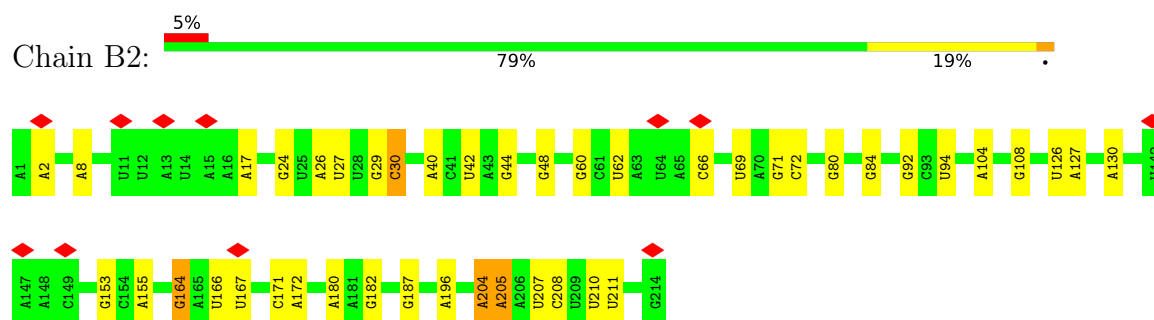
• Molecule 59: mL129



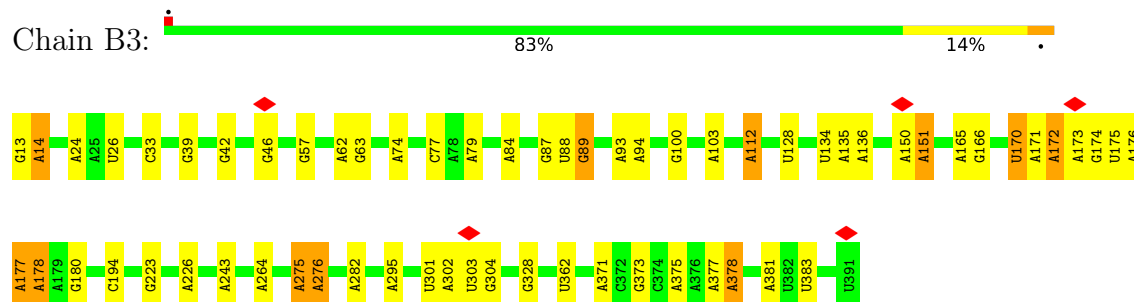
• Molecule 60: mtSSU-1



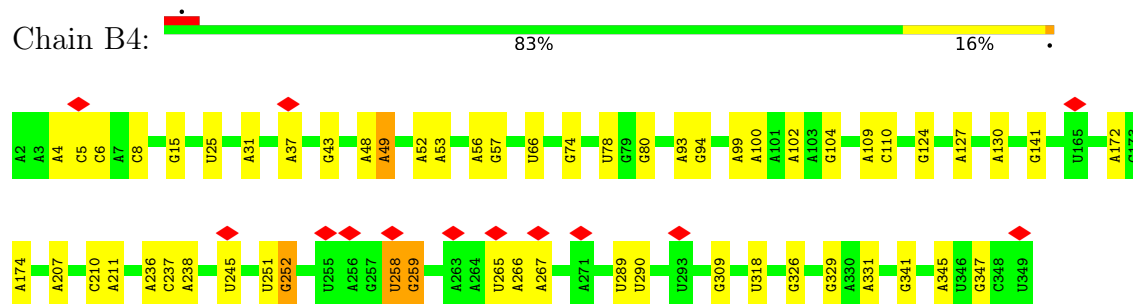
• Molecule 61: mtSSU-2



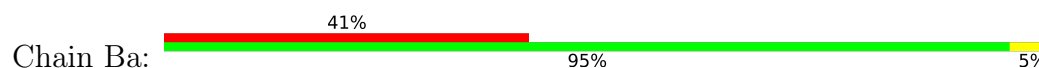
• Molecule 62: mtSSU-3

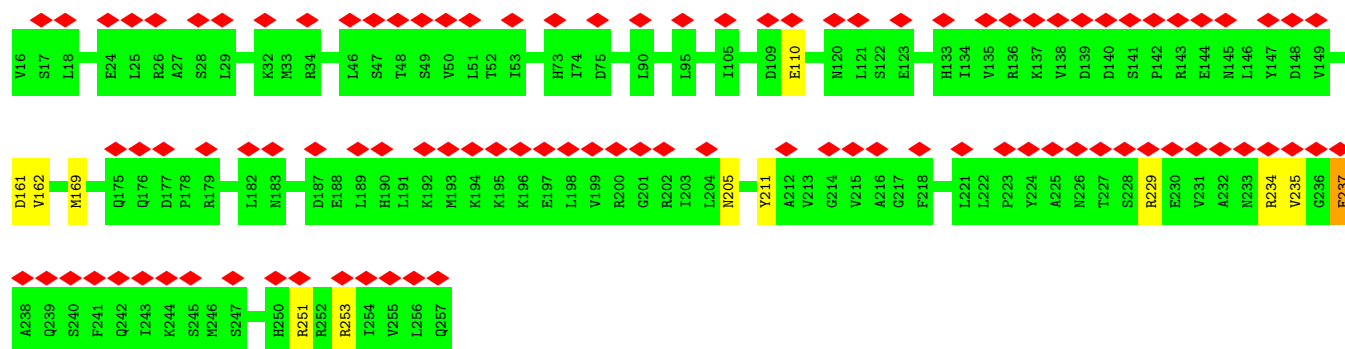


• Molecule 63: mtSSU-4

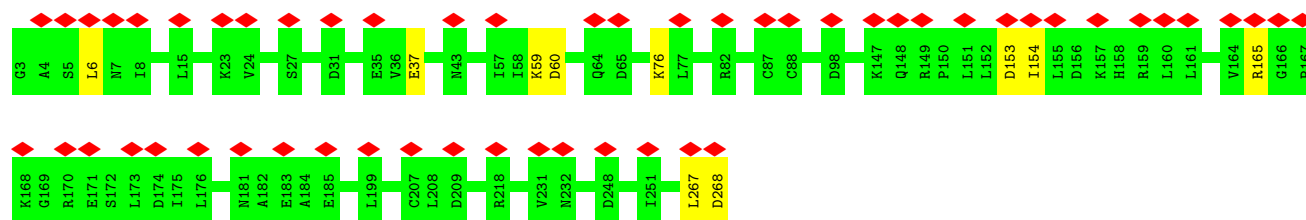


• Molecule 64: bS1m

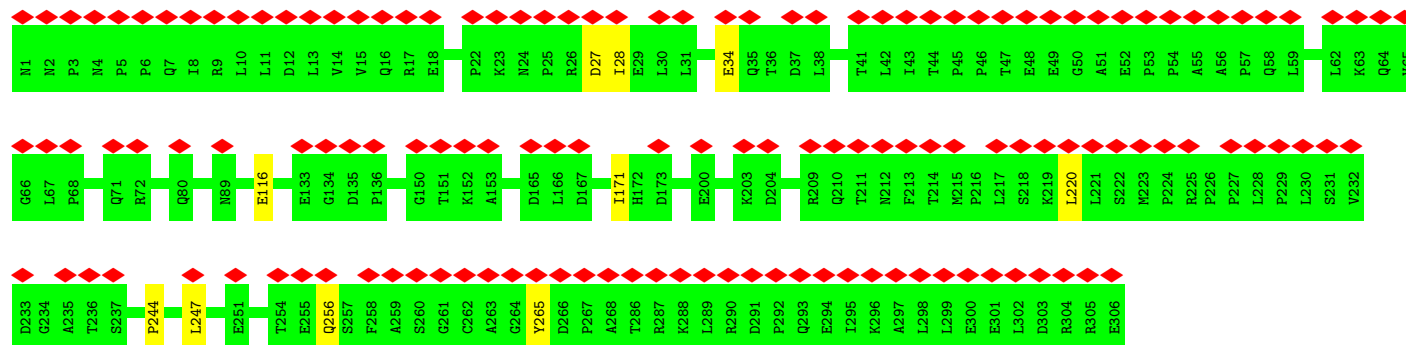




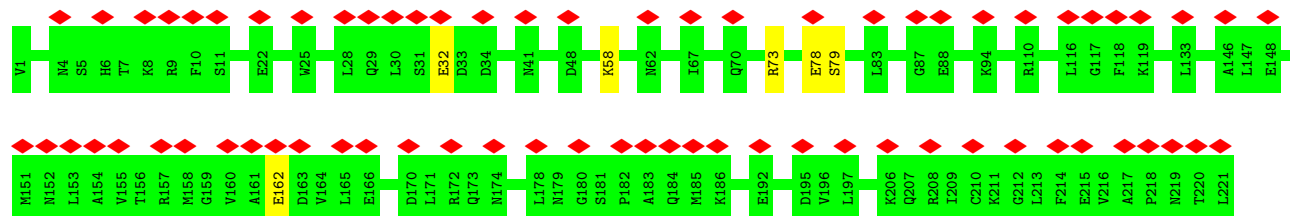
• Molecule 65: uS2m



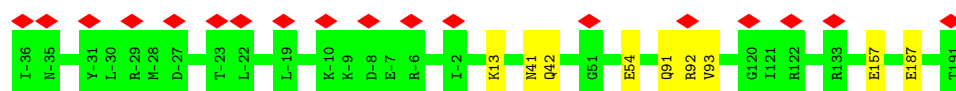
• Molecule 66: uS3m



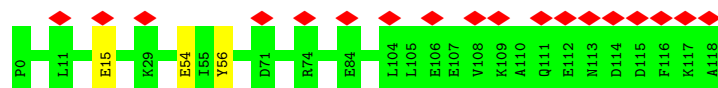
• Molecule 67: uS4m



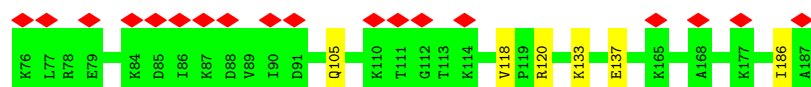
• Molecule 68: uS5m



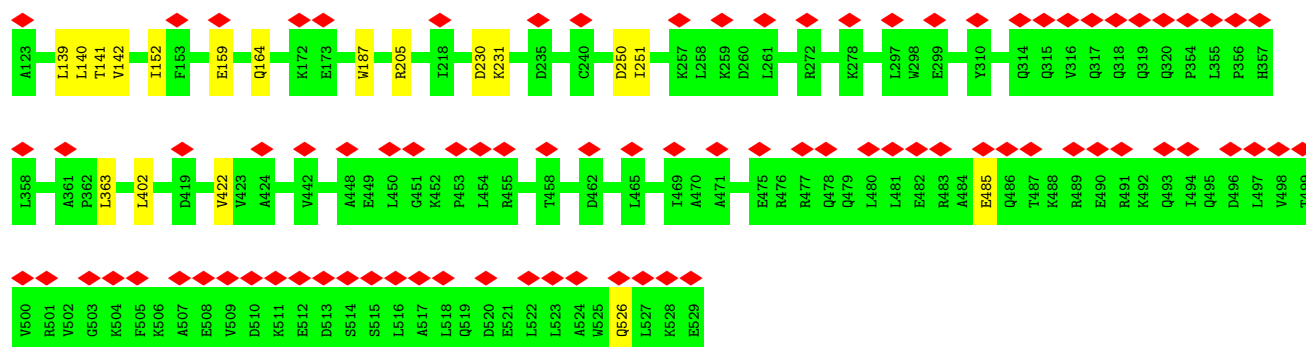
• Molecule 69: uS6m



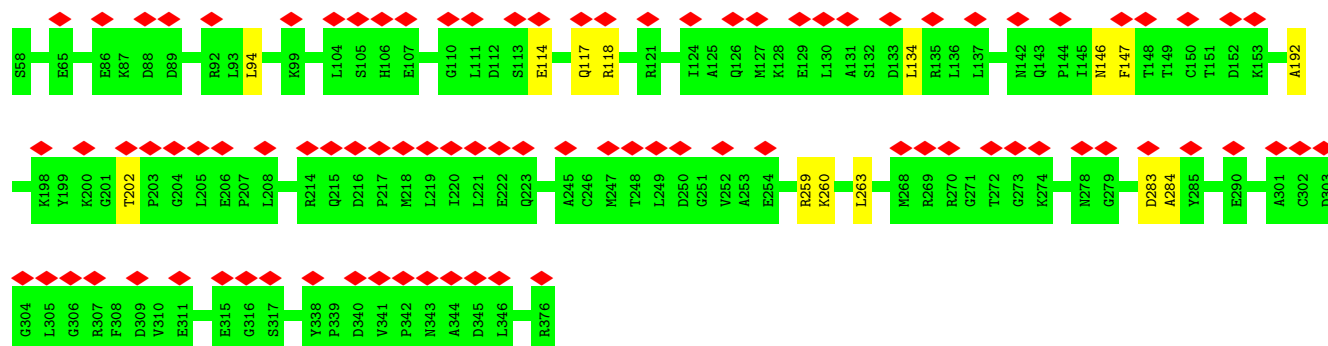
• Molecule 70: uS7m



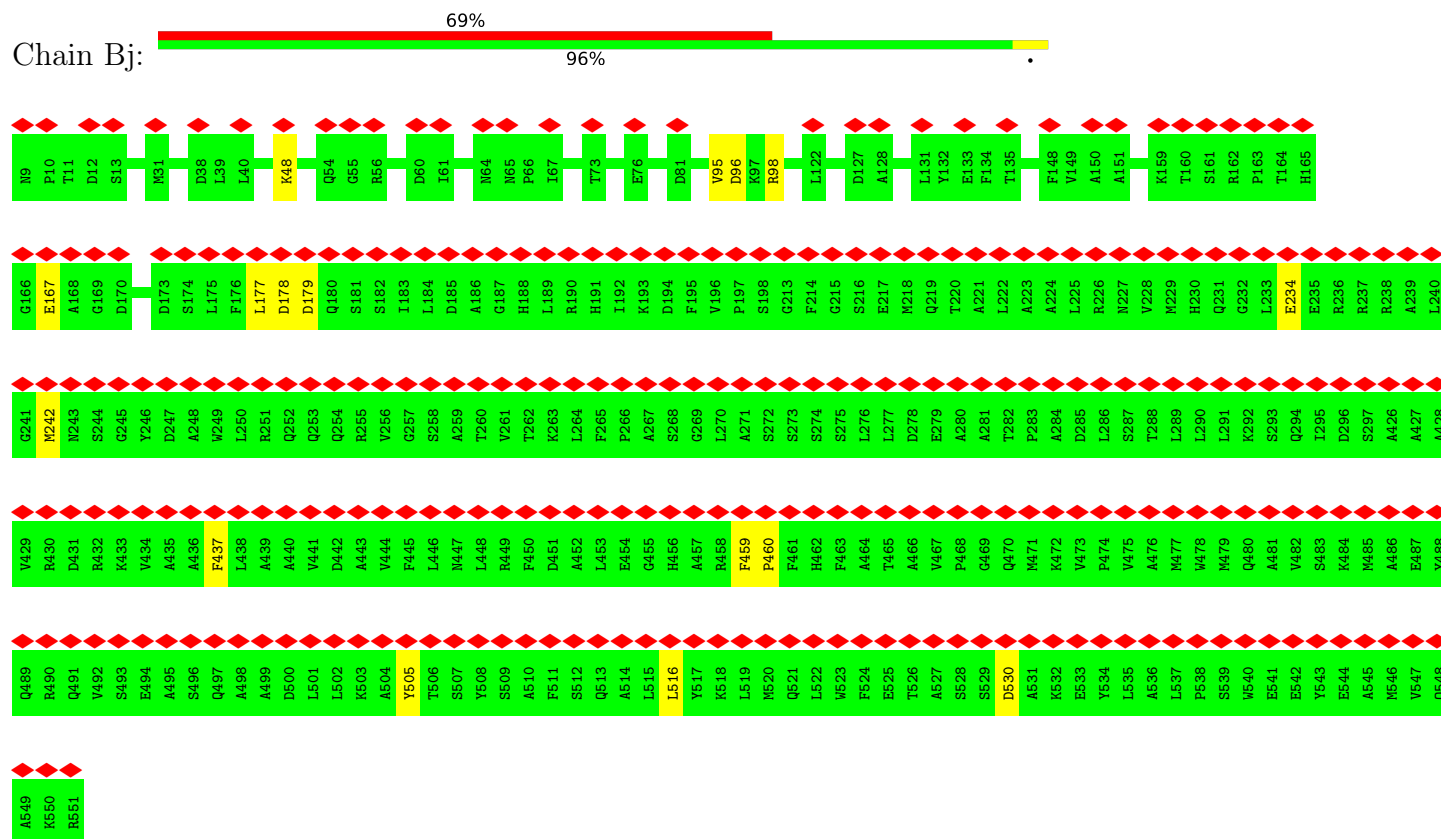
• Molecule 71: uS8m



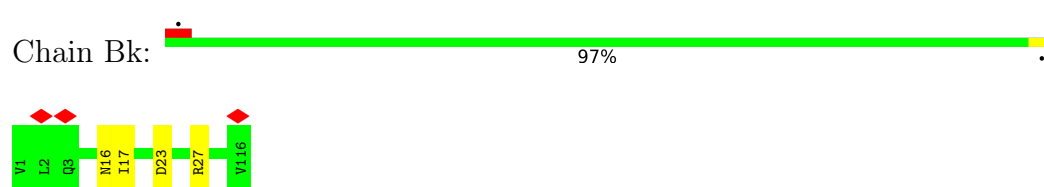
• Molecule 72: uS9m



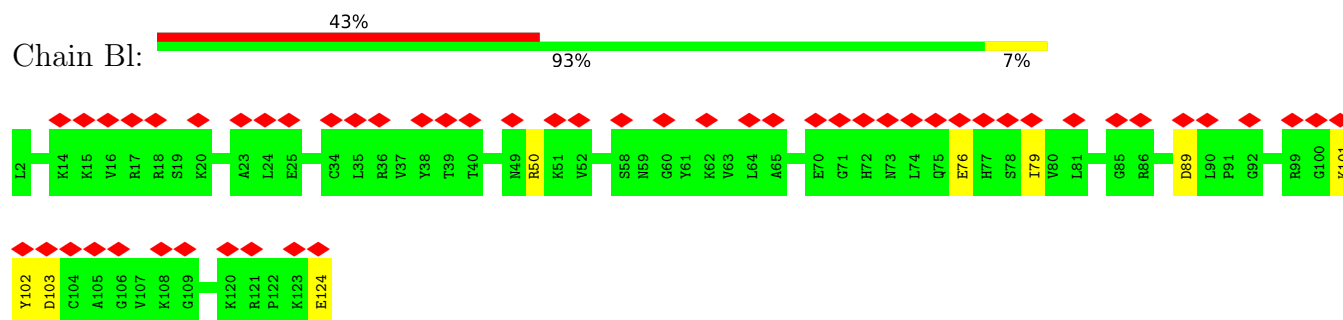
## ● Molecule 73: uS10m



## ● Molecule 74: uS11m

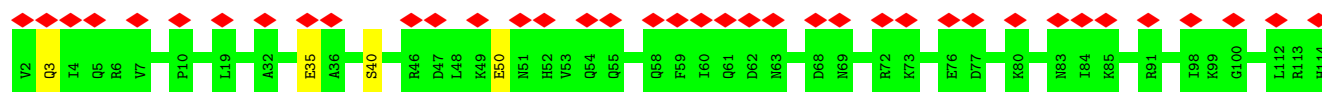


## ● Molecule 75: uS12m

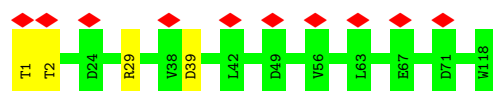


## ● Molecule 76: uS13m

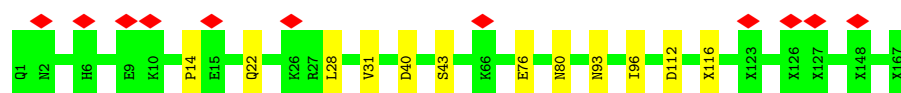




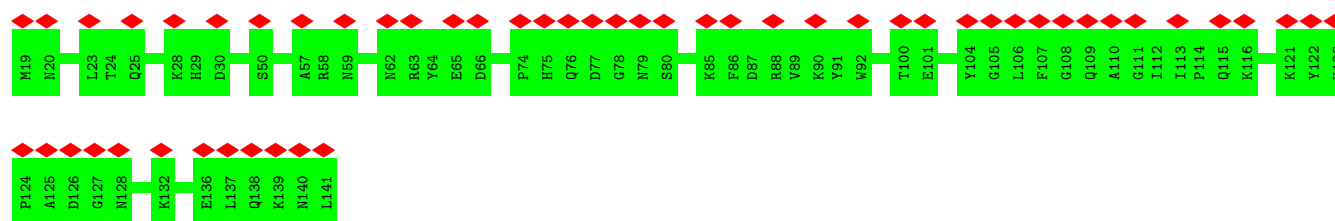
• Molecule 77: uS14m



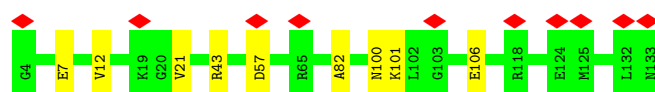
• Molecule 78: uS15m



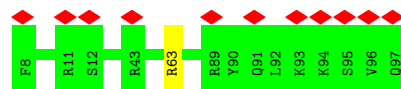
• Molecule 79: bS16m



• Molecule 80: uS17m

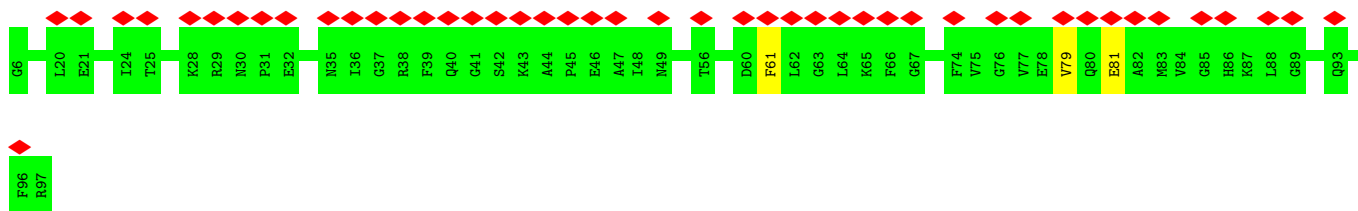


• Molecule 81: bS18m

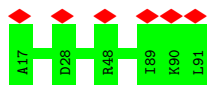


• Molecule 82: bS19m

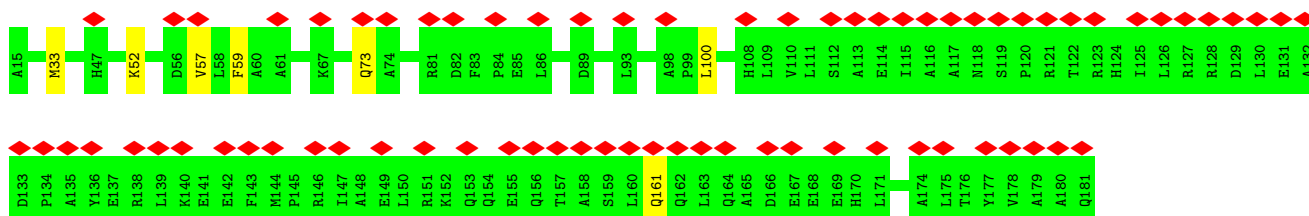




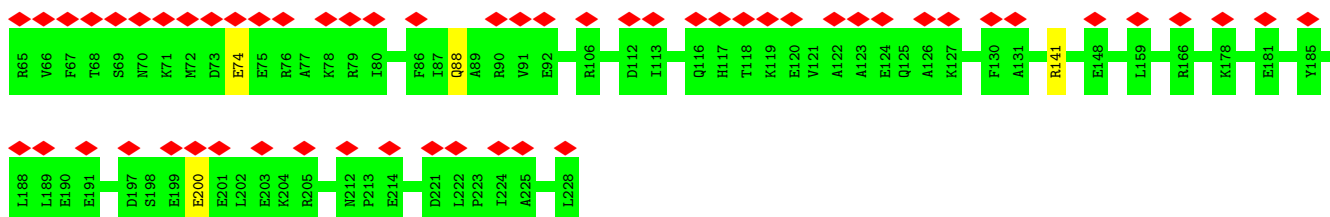
• Molecule 83: bS21m



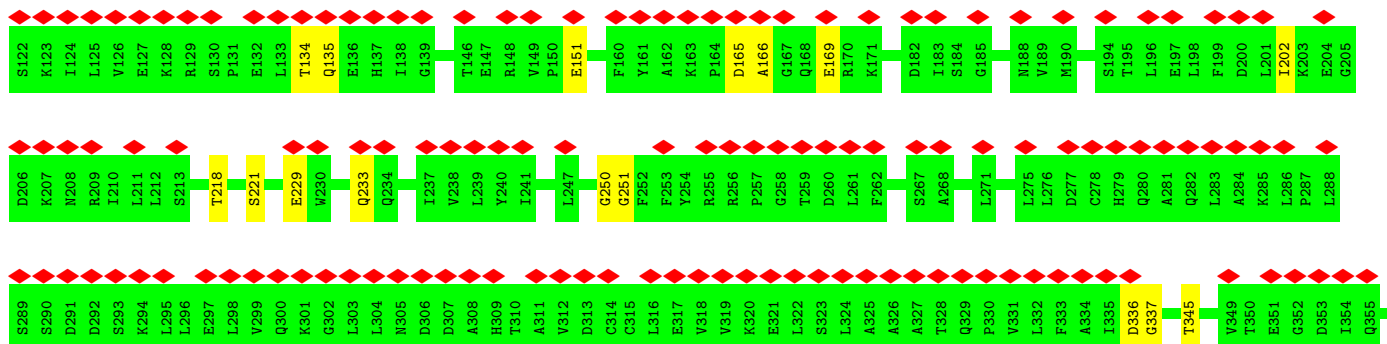
• Molecule 84: mS23

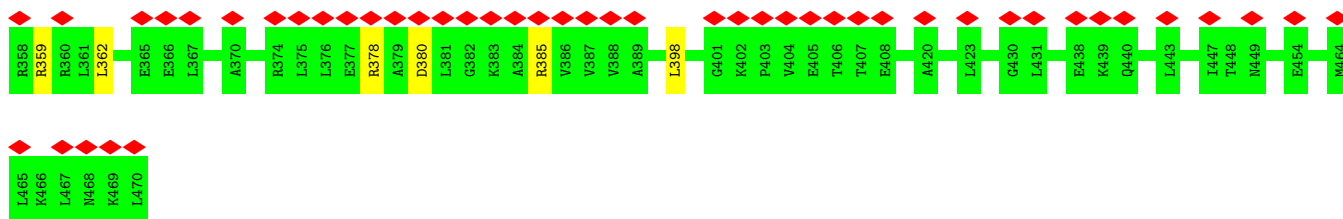


• Molecule 85: mS26

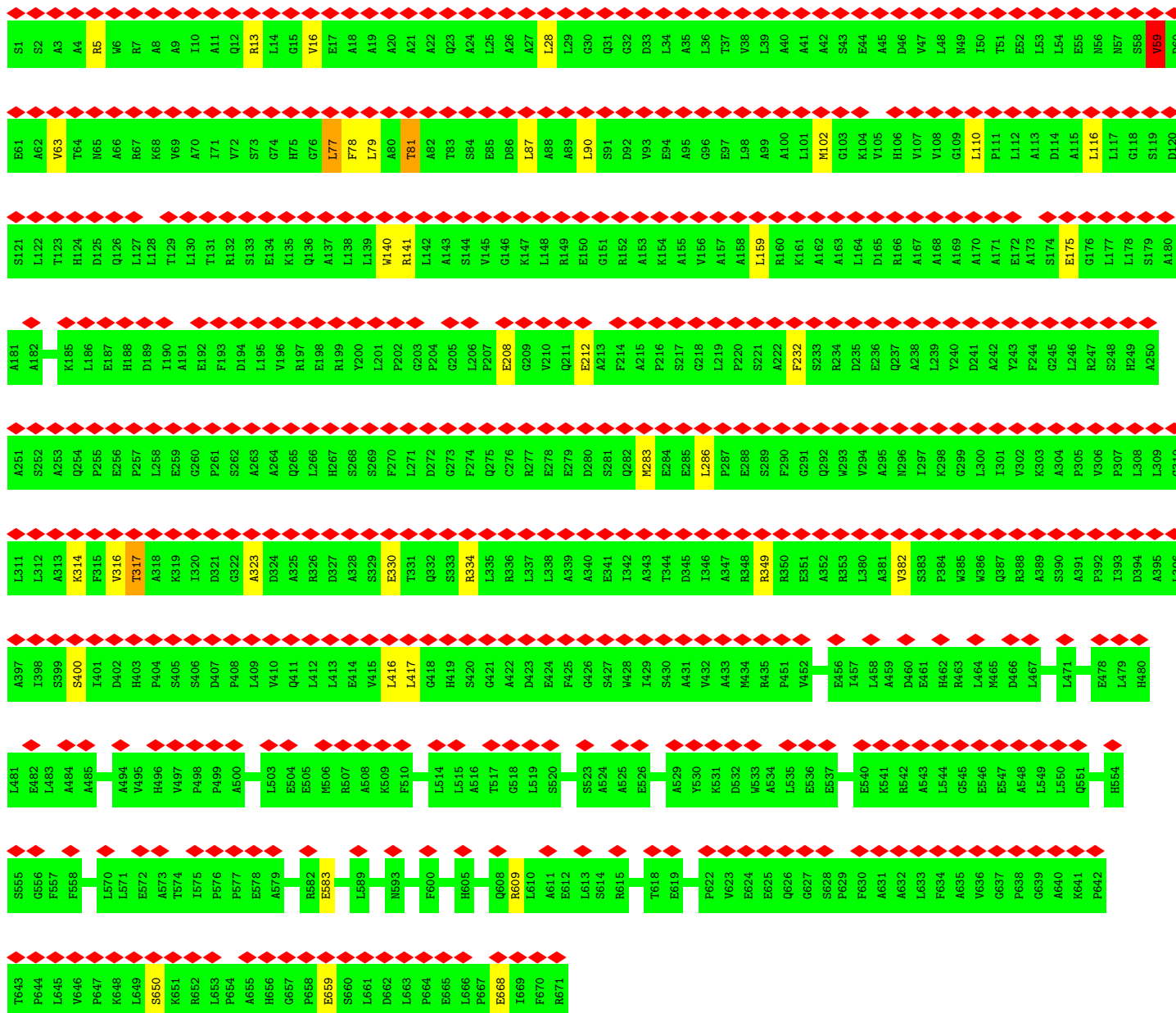
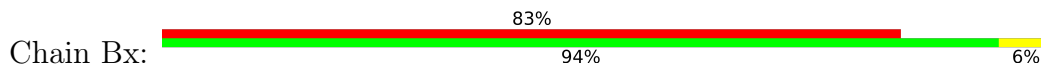


• Molecule 86: mS29

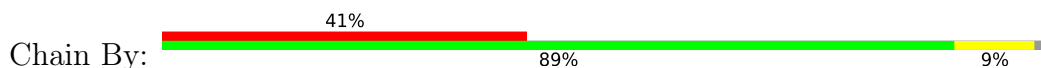


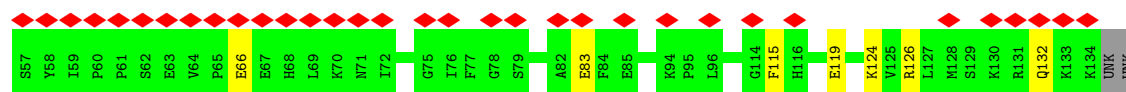


• Molecule 87: mS31

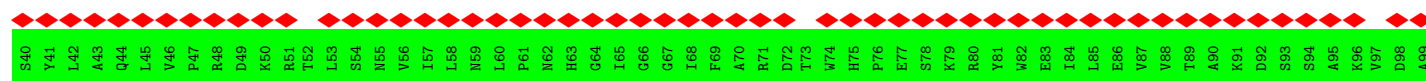
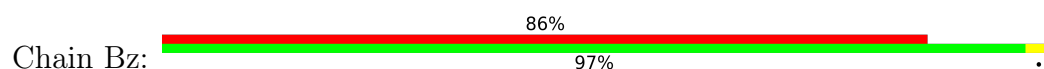


• Molecule 88: mS33

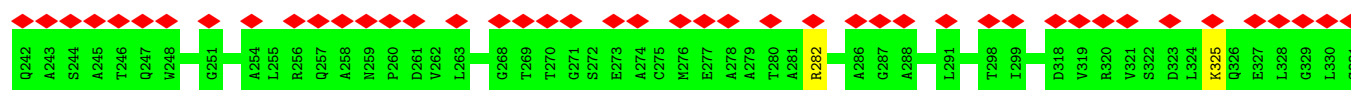




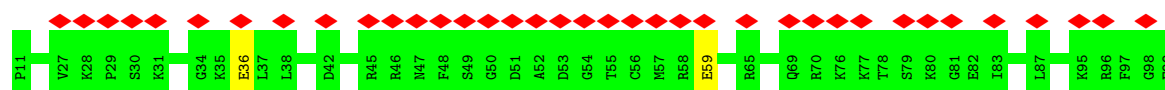
• Molecule 89: mS34



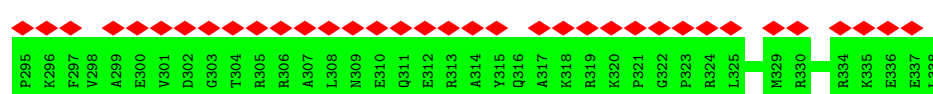
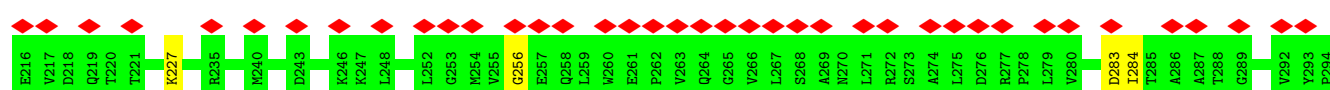
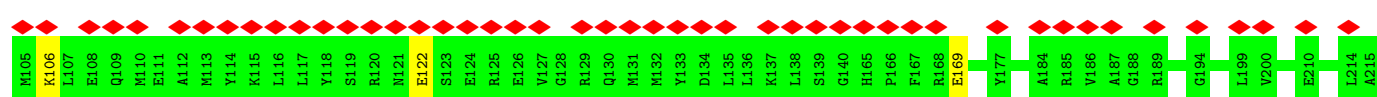
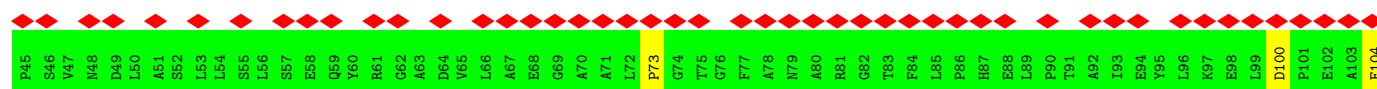
• Molecule 90: mS35



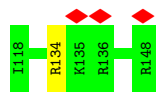
• Molecule 91: mS37



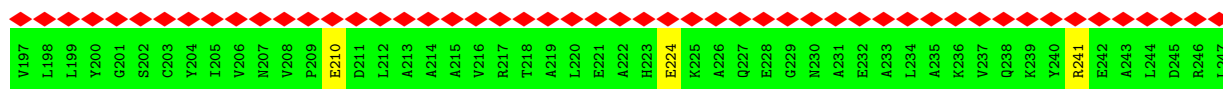
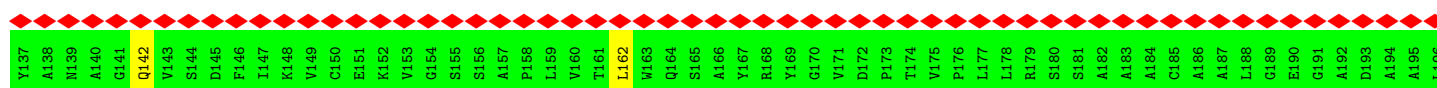
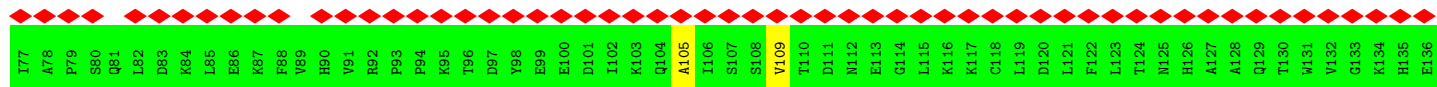
• Molecule 92: mS45



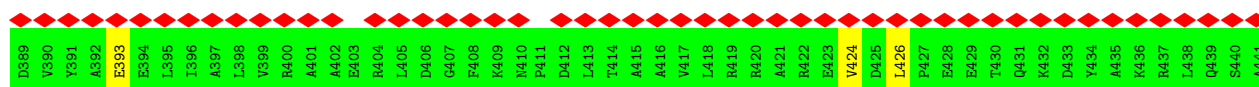
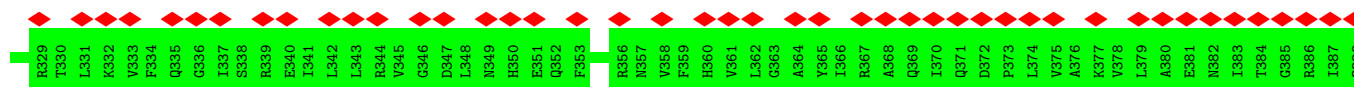
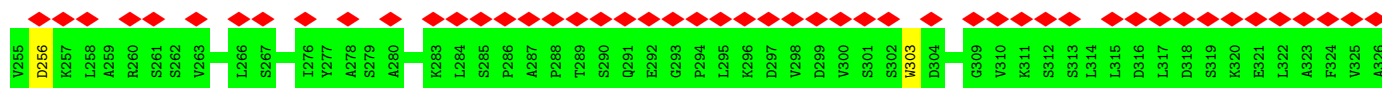
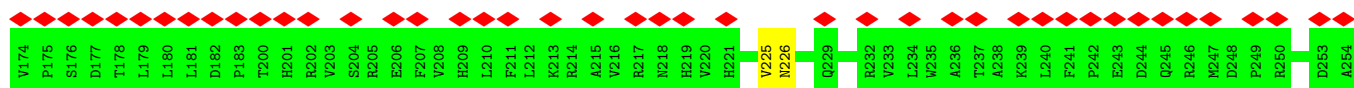
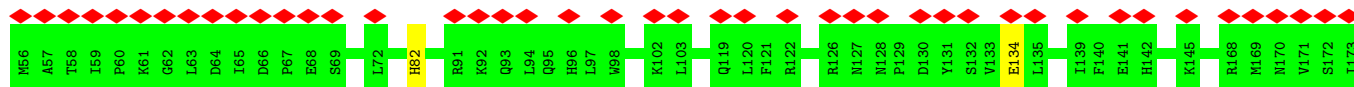
- Molecule 93: mS38



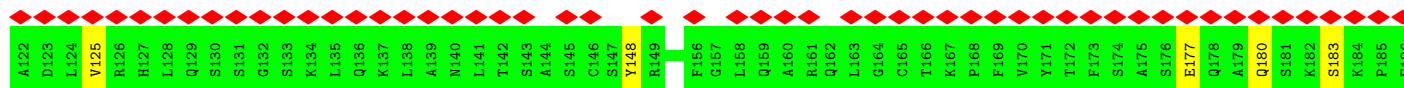
- Molecule 94: mS106

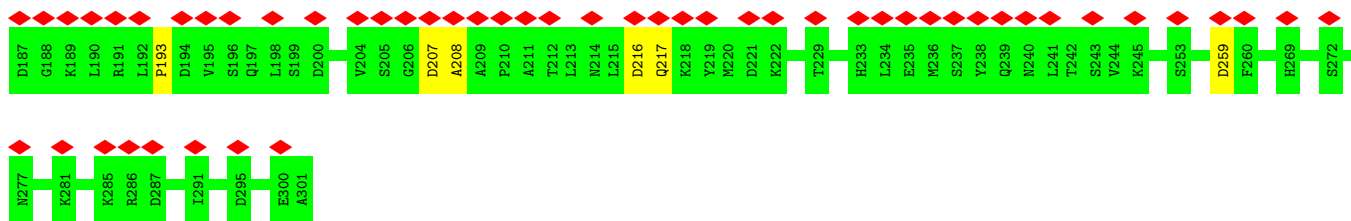


- Molecule 95: mS107

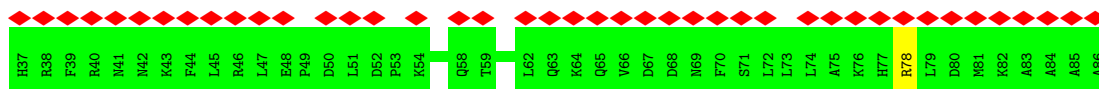
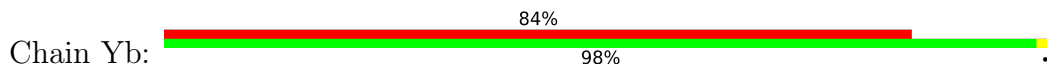


- Molecule 96: uS4m-2

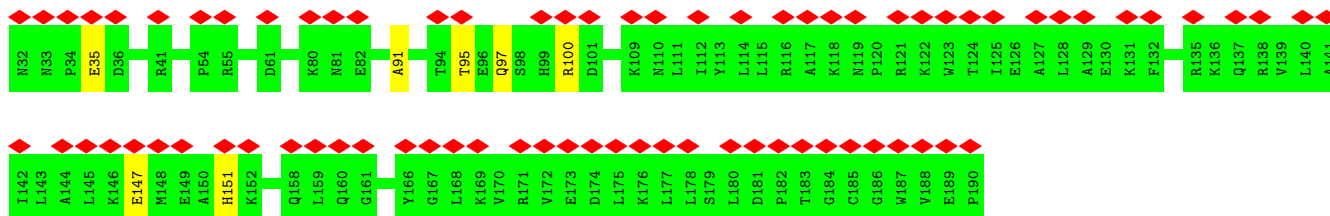




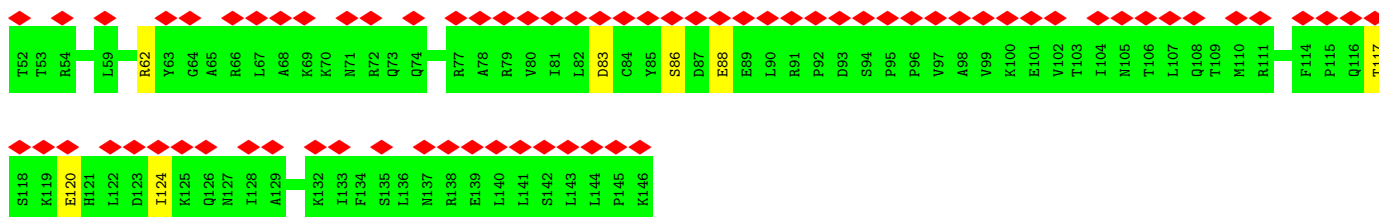
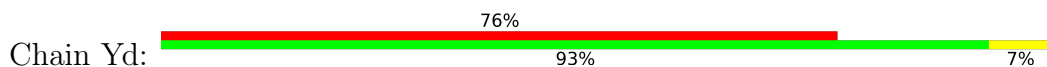
• Molecule 97: mS108



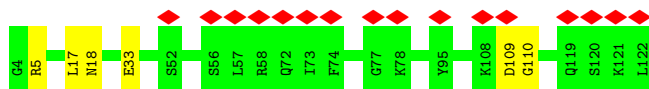
• Molecule 98: mS109



• Molecule 99: mS110

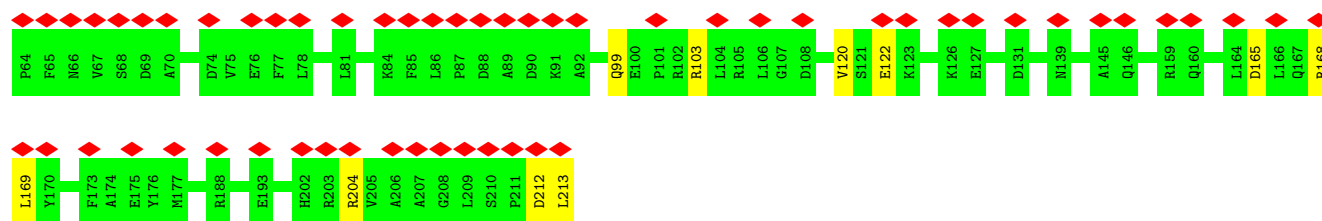


• Molecule 100: uS3m-2

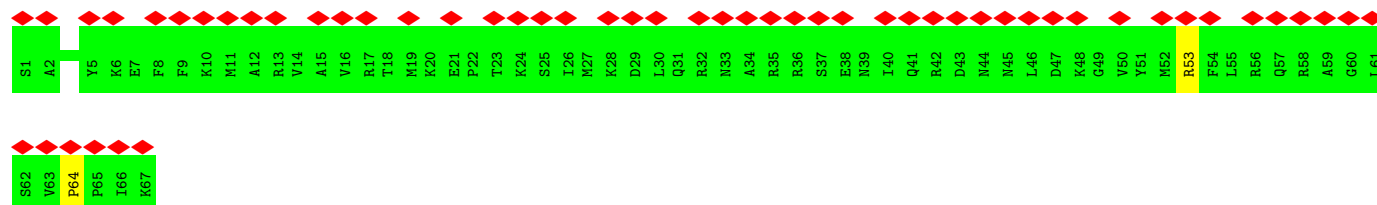
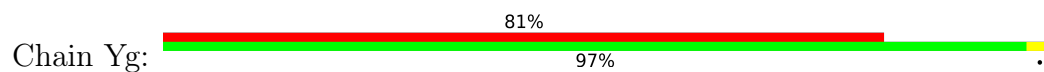


• Molecule 101: mS111

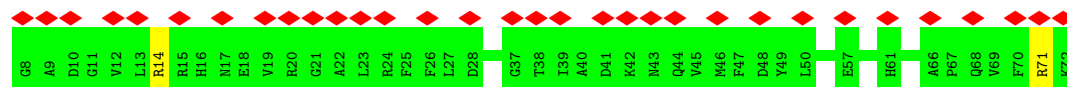




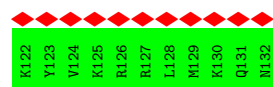
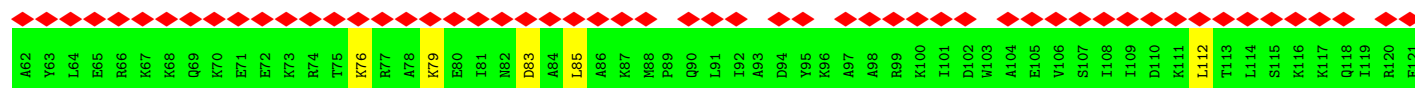
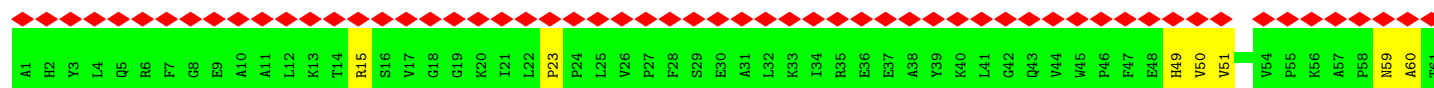
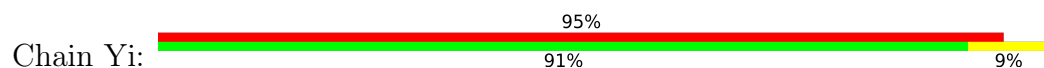
• Molecule 102: mS112



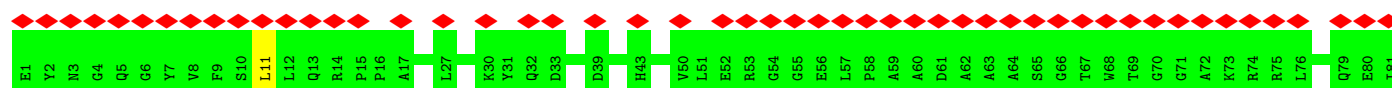
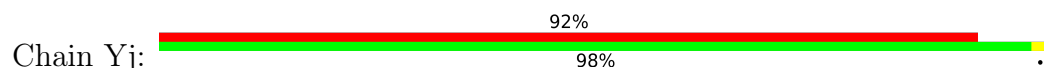
• Molecule 103: mS113

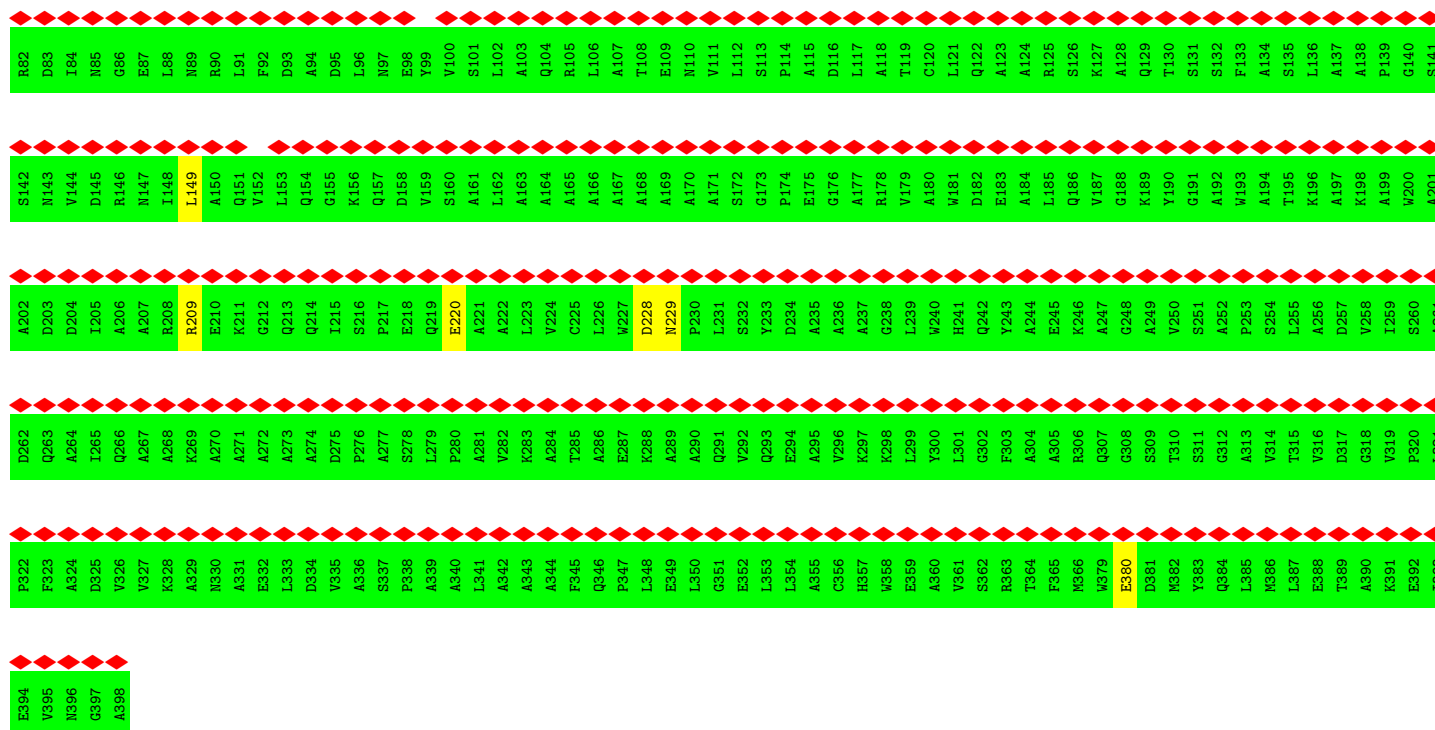


• Molecule 104: mS114

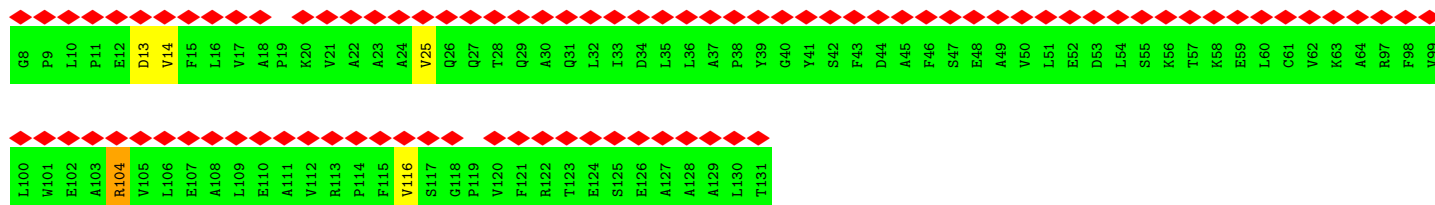


• Molecule 105: mS115

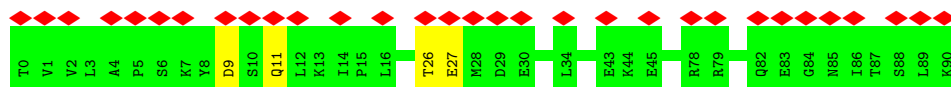




• Molecule 106: mS116



• Molecule 107: uS7m-2



• Molecule 108: P-site tRNA

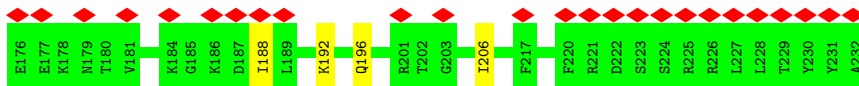
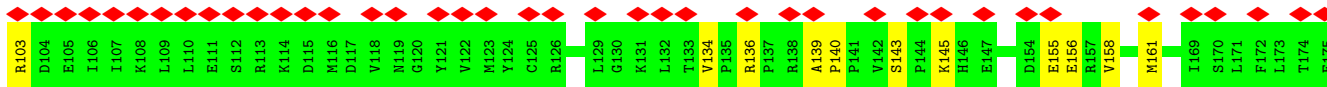
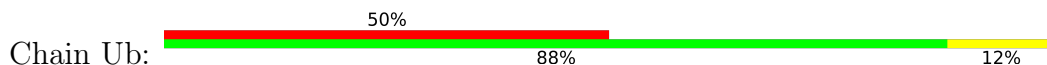


• Molecule 109: mRNA

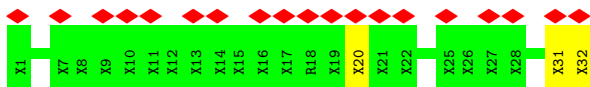




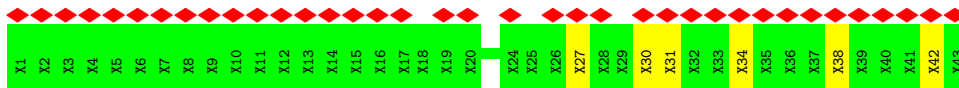
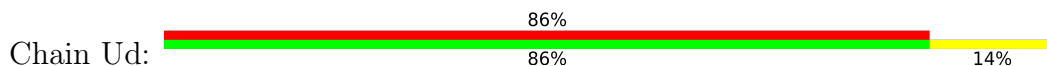
- Molecule 110: mL105



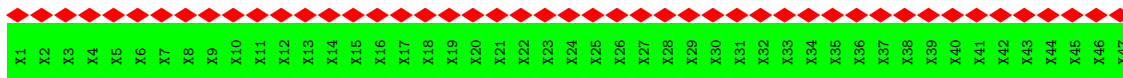
- Molecule 111: Unknown



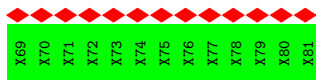
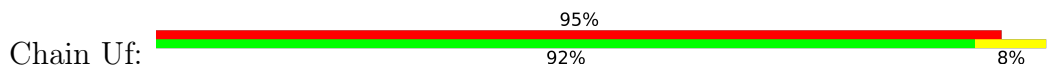
- Molecule 112: Unknown



- Molecule 113: Unknown

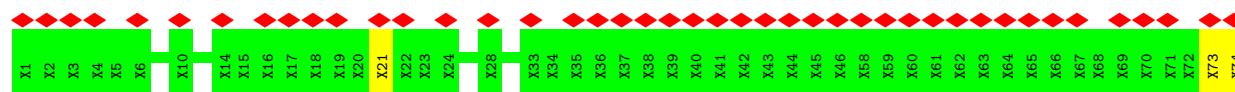


- Molecule 114: Unknown

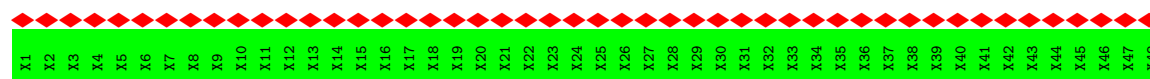


- Molecule 115: Unknown

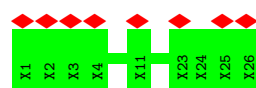




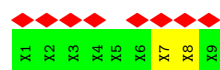
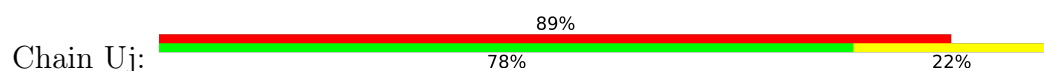
- Molecule 116: Unknown



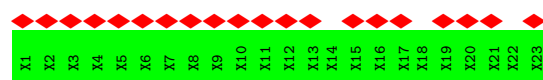
- Molecule 117: Unknown



- Molecule 118: Unknown



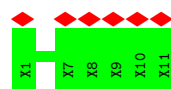
- Molecule 119: Unknown



- Molecule 120: Unknown



- Molecule 121: Unknown



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 59000                                   | Depositor |
| Resolution determination method      | OTHER                                   | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 130000                                  | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.048                                   | Depositor |
| Minimum map value                    | -0.018                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.01                                    | Depositor |
| Map size (Å)                         | 592.2, 592.2, 592.2                     | wwPDB     |
| Map dimensions                       | 700, 700, 700                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.846, 0.846, 0.846                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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   | A1    | 0.09         | 0/2632      | 0.18        | 0/4101      |
| 2   | A2    | 0.11         | 0/1938      | 0.21        | 0/3016      |
| 3   | A3    | 0.11         | 0/4942      | 0.21        | 0/7693      |
| 4   | A4    | 0.12         | 0/1764      | 0.23        | 0/2749      |
| 5   | A5    | 0.07         | 0/3239      | 0.17        | 0/5036      |
| 6   | A6    | 0.10         | 0/2619      | 0.19        | 0/4075      |
| 7   | A7    | 0.10         | 0/12753     | 0.19        | 0/19862     |
| 8   | A8    | 0.10         | 0/8336      | 0.20        | 0/12985     |
| 9   | A9    | 0.08         | 0/1637      | 0.16        | 0/2545      |
| 10  | Aa    | 0.11         | 0/2439      | 0.27        | 0/3287      |
| 11  | Ab    | 0.11         | 0/2483      | 0.26        | 0/3369      |
| 12  | Ac    | 0.11         | 0/2431      | 0.25        | 0/3290      |
| 13  | Ad    | 0.08         | 0/1574      | 0.22        | 0/2136      |
| 14  | Ae    | 0.10         | 0/1982      | 0.22        | 0/2683      |
| 15  | Af    | 0.08         | 0/437       | 0.21        | 0/589       |
| 16  | Ah    | 0.10         | 0/1555      | 0.25        | 0/2098      |
| 17  | Ai    | 0.10         | 0/972       | 0.22        | 0/1303      |
| 18  | Aj    | 0.12         | 0/1643      | 0.25        | 0/2220      |
| 19  | Ak    | 0.12         | 0/1389      | 0.27        | 0/1869      |
| 20  | Al    | 0.12         | 0/1438      | 0.27        | 0/1938      |
| 21  | Am    | 0.09         | 0/931       | 0.22        | 0/1258      |
| 22  | An    | 0.09         | 0/1420      | 0.24        | 0/1914      |
| 23  | Ao    | 0.11         | 0/981       | 0.24        | 0/1314      |
| 24  | Ap    | 0.12         | 0/1600      | 0.27        | 0/2176      |
| 25  | Aq    | 0.11         | 0/1566      | 0.25        | 0/2106      |
| 26  | Ar    | 0.09         | 0/1309      | 0.24        | 0/1759      |
| 27  | As    | 0.08         | 0/938       | 0.21        | 0/1263      |
| 28  | At    | 0.09         | 0/2041      | 0.23        | 0/2755      |
| 29  | Au    | 0.10         | 0/1182      | 0.23        | 0/1596      |
| 30  | Av    | 0.08         | 0/1073      | 0.19        | 0/1443      |
| 31  | Aw    | 0.10         | 0/1043      | 0.22        | 0/1401      |
| 32  | Ax    | 0.11         | 0/1508      | 0.23        | 0/2028      |

| Mol | Chain | Bond lengths |         | Bond angles |              |
|-----|-------|--------------|---------|-------------|--------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5      |
| 33  | Ay    | 0.11         | 0/610   | 0.17        | 0/827        |
| 34  | Az    | 0.48         | 0/484   | 0.69        | 1/652 (0.2%) |
| 35  | AA    | 0.08         | 0/426   | 0.21        | 0/572        |
| 36  | AB    | 0.14         | 0/432   | 0.28        | 0/568        |
| 37  | AC    | 0.12         | 0/1217  | 0.27        | 0/1639       |
| 38  | AD    | 0.10         | 0/379   | 0.24        | 0/500        |
| 39  | AE    | 0.09         | 0/790   | 0.20        | 0/1066       |
| 40  | AF    | 0.11         | 0/782   | 0.24        | 0/1053       |
| 41  | AG    | 0.11         | 0/1019  | 0.25        | 0/1373       |
| 42  | AH    | 0.10         | 0/1444  | 0.27        | 0/1945       |
| 43  | AI    | 0.09         | 0/515   | 0.22        | 0/696        |
| 44  | AJ    | 0.09         | 0/1023  | 0.21        | 0/1370       |
| 45  | AK    | 0.11         | 0/1206  | 0.22        | 0/1635       |
| 46  | AL    | 0.08         | 0/3152  | 0.21        | 0/4271       |
| 47  | AM    | 0.09         | 0/3345  | 0.21        | 0/4532       |
| 48  | AN    | 0.10         | 0/3349  | 0.21        | 0/4537       |
| 49  | AO    | 0.09         | 0/2941  | 0.22        | 0/4000       |
| 50  | Xa    | 0.08         | 0/1600  | 0.21        | 0/2178       |
| 51  | Xb    | 0.07         | 0/1999  | 0.18        | 0/2701       |
| 52  | Xc    | 0.09         | 0/509   | 0.23        | 0/684        |
| 53  | Xd    | 0.09         | 0/3305  | 0.22        | 0/4478       |
| 54  | Xe    | 0.08         | 0/3748  | 0.21        | 0/5096       |
| 55  | Xf    | 0.09         | 0/1659  | 0.22        | 0/2253       |
| 56  | Xg    | 0.08         | 0/3018  | 0.21        | 0/4098       |
| 57  | Xh    | 0.10         | 0/1169  | 0.22        | 0/1578       |
| 58  | Xi    | 0.10         | 0/209   | 0.23        | 0/273        |
| 59  | Xj    | 0.12         | 0/596   | 0.22        | 0/802        |
| 60  | B1    | 0.08         | 0/2419  | 0.16        | 0/3765       |
| 61  | B2    | 0.08         | 0/5020  | 0.18        | 0/7818       |
| 62  | B3    | 0.09         | 0/9069  | 0.19        | 0/14130      |
| 63  | B4    | 0.08         | 0/8046  | 0.16        | 0/12527      |
| 64  | Ba    | 0.09         | 0/1967  | 0.23        | 0/2662       |
| 65  | Bb    | 0.08         | 0/1920  | 0.21        | 0/2615       |
| 66  | Bc    | 0.10         | 0/2340  | 0.23        | 0/3182       |
| 67  | Bd    | 0.10         | 0/1825  | 0.24        | 0/2459       |
| 68  | Be    | 0.11         | 0/1863  | 0.22        | 0/2521       |
| 69  | Bf    | 0.09         | 0/989   | 0.21        | 0/1334       |
| 70  | Bg    | 0.08         | 0/898   | 0.20        | 0/1205       |
| 71  | Bh    | 0.10         | 0/3109  | 0.23        | 0/4215       |
| 72  | Bi    | 0.10         | 0/2317  | 0.24        | 0/3119       |
| 73  | Bj    | 0.09         | 0/3243  | 0.22        | 0/4384       |
| 74  | Bk    | 0.11         | 0/882   | 0.26        | 0/1193       |
| 75  | Bl    | 0.10         | 0/977   | 0.26        | 0/1303       |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 76  | Bm    | 0.09         | 0/910           | 0.24        | 0/1223           |
| 77  | Bn    | 0.12         | 0/995           | 0.28        | 0/1336           |
| 78  | Bo    | 0.11         | 0/963           | 0.26        | 0/1284           |
| 79  | Bp    | 0.10         | 0/1046          | 0.26        | 0/1414           |
| 80  | Bq    | 0.09         | 0/1068          | 0.22        | 0/1434           |
| 81  | Br    | 0.10         | 0/754           | 0.23        | 0/1009           |
| 82  | Bs    | 0.09         | 0/754           | 0.24        | 0/1019           |
| 83  | Bt    | 0.09         | 0/630           | 0.20        | 0/840            |
| 84  | Bu    | 0.08         | 0/1395          | 0.20        | 0/1878           |
| 85  | Bv    | 0.09         | 0/1372          | 0.18        | 0/1835           |
| 86  | Bw    | 0.09         | 0/2804          | 0.23        | 0/3791           |
| 87  | Bx    | 0.12         | 0/4813          | 0.29        | 1/6545 (0.0%)    |
| 88  | By    | 0.09         | 0/655           | 0.22        | 0/883            |
| 89  | Bz    | 0.08         | 0/1030          | 0.23        | 0/1400           |
| 90  | BA    | 0.09         | 0/1405          | 0.24        | 0/1907           |
| 91  | BB    | 0.09         | 0/673           | 0.19        | 0/896            |
| 92  | BC    | 0.09         | 0/2207          | 0.22        | 0/2977           |
| 93  | BD    | 0.11         | 0/280           | 0.26        | 0/365            |
| 94  | BE    | 0.06         | 0/1328          | 0.17        | 0/1805           |
| 95  | BF    | 0.08         | 0/3039          | 0.21        | 0/4111           |
| 96  | Ya    | 0.09         | 0/1466          | 0.21        | 0/1979           |
| 97  | Yb    | 0.24         | 0/419           | 0.32        | 0/562            |
| 98  | Yc    | 0.08         | 0/1328          | 0.22        | 0/1799           |
| 99  | Yd    | 0.09         | 0/797           | 0.24        | 0/1069           |
| 100 | Ye    | 0.10         | 0/887           | 0.23        | 0/1191           |
| 101 | Yf    | 0.09         | 0/1276          | 0.21        | 0/1735           |
| 102 | Yg    | 0.12         | 0/560           | 0.21        | 0/744            |
| 103 | Yh    | 0.09         | 0/543           | 0.19        | 0/730            |
| 104 | Yi    | 0.10         | 0/1096          | 0.22        | 0/1470           |
| 105 | Yj    | 0.08         | 0/2911          | 0.18        | 0/3966           |
| 106 | Yk    | 0.13         | 0/721           | 0.21        | 0/982            |
| 107 | Yl    | 0.11         | 0/680           | 0.19        | 0/911            |
| 108 | C1    | 0.11         | 0/1723          | 0.30        | 0/2681           |
| 109 | C3    | 0.08         | 0/97            | 0.20        | 0/149            |
| 110 | Ub    | 0.89         | 2/1110 (0.2%)   | 1.09        | 9/1490 (0.6%)    |
| 111 | Ua    | 0.26         | 0/10            | 0.55        | 0/11             |
| All | All   | 0.12         | 2/205350 (0.0%) | 0.23        | 11/291087 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 110 | Ub    | 103 | ARG  | NE-CZ | 5.25 | 1.38        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 110 | Ub    | 103 | ARG  | CD-NE | 5.10 | 1.53        | 1.46     |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 34  | Az    | 140 | PRO  | CA-N-CD | -9.52 | 98.67       | 112.00   |
| 110 | Ub    | 143 | SER  | CA-C-N  | 7.56  | 127.27      | 119.56   |
| 110 | Ub    | 143 | SER  | C-N-CA  | 7.56  | 127.27      | 119.56   |
| 110 | Ub    | 140 | PRO  | CA-C-N  | 6.96  | 127.11      | 119.87   |
| 110 | Ub    | 140 | PRO  | C-N-CA  | 6.96  | 127.11      | 119.87   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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   | A1    | 2344  | 0        | 1175     | 11      | 0            |
| 2   | A2    | 1729  | 0        | 871      | 5       | 0            |
| 3   | A3    | 4413  | 0        | 2219     | 5       | 0            |
| 4   | A4    | 1572  | 0        | 793      | 4       | 0            |
| 5   | A5    | 2897  | 0        | 1466     | 6       | 0            |
| 6   | A6    | 2337  | 0        | 1174     | 1       | 0            |
| 7   | A7    | 11387 | 0        | 5738     | 18      | 0            |
| 8   | A8    | 7452  | 0        | 3753     | 11      | 0            |
| 9   | A9    | 1466  | 0        | 740      | 6       | 0            |
| 10  | Aa    | 2386  | 0        | 2474     | 7       | 0            |
| 11  | Ab    | 2414  | 0        | 2446     | 5       | 0            |
| 12  | Ac    | 2377  | 0        | 2406     | 7       | 0            |
| 13  | Ad    | 1537  | 0        | 1560     | 5       | 0            |
| 14  | Ae    | 1934  | 0        | 2006     | 11      | 0            |
| 15  | Af    | 432   | 0        | 444      | 2       | 0            |
| 16  | Ah    | 1517  | 0        | 1544     | 7       | 0            |
| 17  | Ai    | 952   | 0        | 1020     | 4       | 0            |
| 18  | Aj    | 1607  | 0        | 1644     | 2       | 0            |
| 19  | Ak    | 1356  | 0        | 1458     | 7       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | Al    | 1412  | 0        | 1501     | 16      | 0            |
| 21  | Am    | 911   | 0        | 952      | 4       | 0            |
| 22  | An    | 1392  | 0        | 1419     | 6       | 0            |
| 23  | Ao    | 964   | 0        | 975      | 4       | 0            |
| 24  | Ap    | 1566  | 0        | 1647     | 4       | 0            |
| 25  | Aq    | 1533  | 0        | 1562     | 10      | 0            |
| 26  | Ar    | 1283  | 0        | 1321     | 5       | 0            |
| 27  | As    | 920   | 0        | 942      | 14      | 0            |
| 28  | At    | 2003  | 0        | 2068     | 5       | 0            |
| 29  | Au    | 1149  | 0        | 1138     | 2       | 0            |
| 30  | Av    | 1058  | 0        | 1098     | 4       | 0            |
| 31  | Aw    | 1024  | 0        | 1044     | 13      | 0            |
| 32  | Ax    | 1472  | 0        | 1513     | 8       | 0            |
| 33  | Ay    | 592   | 0        | 605      | 0       | 0            |
| 34  | Az    | 469   | 0        | 490      | 21      | 0            |
| 35  | AA    | 416   | 0        | 451      | 1       | 0            |
| 36  | AB    | 427   | 0        | 459      | 3       | 0            |
| 37  | AC    | 1180  | 0        | 1225     | 1       | 0            |
| 38  | AD    | 375   | 0        | 413      | 1       | 0            |
| 39  | AE    | 771   | 0        | 776      | 4       | 0            |
| 40  | AF    | 765   | 0        | 798      | 2       | 0            |
| 41  | AG    | 994   | 0        | 990      | 4       | 0            |
| 42  | AH    | 1412  | 0        | 1430     | 15      | 0            |
| 43  | AI    | 505   | 0        | 538      | 1       | 0            |
| 44  | AJ    | 1003  | 0        | 1059     | 3       | 0            |
| 45  | AK    | 1164  | 0        | 1143     | 2       | 0            |
| 46  | AL    | 3093  | 0        | 3152     | 12      | 0            |
| 47  | AM    | 3282  | 0        | 3344     | 7       | 0            |
| 48  | AN    | 3286  | 0        | 3347     | 18      | 0            |
| 49  | AO    | 2881  | 0        | 2923     | 10      | 0            |
| 50  | Xa    | 1568  | 0        | 1596     | 6       | 0            |
| 51  | Xb    | 1956  | 0        | 1944     | 7       | 0            |
| 52  | Xc    | 496   | 0        | 501      | 3       | 0            |
| 53  | Xd    | 3236  | 0        | 3251     | 13      | 0            |
| 54  | Xe    | 3675  | 0        | 3783     | 7       | 0            |
| 55  | Xf    | 1615  | 0        | 1627     | 1       | 0            |
| 56  | Xg    | 3081  | 0        | 3082     | 14      | 0            |
| 57  | Xh    | 1147  | 0        | 1210     | 8       | 0            |
| 58  | Xi    | 206   | 0        | 216      | 0       | 0            |
| 59  | Xj    | 582   | 0        | 563      | 2       | 0            |
| 60  | B1    | 2165  | 0        | 1090     | 4       | 0            |
| 61  | B2    | 4484  | 0        | 2261     | 5       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 62  | B3    | 8096  | 0        | 4079     | 20      | 0            |
| 63  | B4    | 7186  | 0        | 3621     | 10      | 0            |
| 64  | Ba    | 1936  | 0        | 2000     | 5       | 0            |
| 65  | Bb    | 1878  | 0        | 1922     | 7       | 0            |
| 66  | Bc    | 2282  | 0        | 2286     | 7       | 0            |
| 67  | Bd    | 1793  | 0        | 1852     | 5       | 0            |
| 68  | Be    | 1826  | 0        | 1838     | 4       | 0            |
| 69  | Bf    | 969   | 0        | 993      | 2       | 0            |
| 70  | Bg    | 887   | 0        | 942      | 2       | 0            |
| 71  | Bh    | 3037  | 0        | 3099     | 14      | 0            |
| 72  | Bi    | 2271  | 0        | 2284     | 11      | 0            |
| 73  | Bj    | 3174  | 0        | 3135     | 15      | 0            |
| 74  | Bk    | 871   | 0        | 937      | 2       | 0            |
| 75  | Bl    | 962   | 0        | 1042     | 5       | 0            |
| 76  | Bm    | 897   | 0        | 935      | 4       | 0            |
| 77  | Bn    | 978   | 0        | 1018     | 3       | 0            |
| 78  | Bo    | 1212  | 0        | 1057     | 7       | 0            |
| 79  | Bp    | 1013  | 0        | 1014     | 0       | 0            |
| 80  | Bq    | 1053  | 0        | 1086     | 6       | 0            |
| 81  | Br    | 743   | 0        | 784      | 1       | 0            |
| 82  | Bs    | 734   | 0        | 720      | 2       | 0            |
| 83  | Bt    | 621   | 0        | 656      | 0       | 0            |
| 84  | Bu    | 1366  | 0        | 1380     | 6       | 0            |
| 85  | Bv    | 1355  | 0        | 1372     | 3       | 0            |
| 86  | Bw    | 2749  | 0        | 2765     | 14      | 0            |
| 87  | Bx    | 4714  | 0        | 4716     | 26      | 0            |
| 88  | By    | 636   | 0        | 631      | 7       | 0            |
| 89  | Bz    | 997   | 0        | 985      | 2       | 0            |
| 90  | BA    | 1377  | 0        | 1350     | 2       | 0            |
| 91  | BB    | 663   | 0        | 684      | 2       | 0            |
| 92  | BC    | 2163  | 0        | 2135     | 7       | 0            |
| 93  | BD    | 278   | 0        | 333      | 1       | 0            |
| 94  | BE    | 1304  | 0        | 1299     | 5       | 0            |
| 95  | BF    | 2980  | 0        | 3056     | 5       | 0            |
| 96  | Ya    | 1434  | 0        | 1426     | 8       | 0            |
| 97  | Yb    | 412   | 0        | 416      | 0       | 0            |
| 98  | Yc    | 1297  | 0        | 1295     | 4       | 0            |
| 99  | Yd    | 785   | 0        | 823      | 6       | 0            |
| 100 | Ye    | 864   | 0        | 870      | 3       | 0            |
| 101 | Yf    | 1236  | 0        | 1195     | 8       | 0            |
| 102 | Yg    | 553   | 0        | 581      | 1       | 0            |
| 103 | Yh    | 530   | 0        | 527      | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 104 | Yi    | 1075  | 0        | 1150     | 6       | 0            |
| 105 | Yj    | 2859  | 0        | 2822     | 6       | 0            |
| 106 | Yk    | 707   | 0        | 712      | 4       | 0            |
| 107 | Yl    | 673   | 0        | 707      | 2       | 0            |
| 108 | C1    | 1542  | 0        | 779      | 3       | 0            |
| 109 | C3    | 87    | 0        | 44       | 2       | 0            |
| 110 | Ub    | 1090  | 0        | 1086     | 24      | 0            |
| 111 | Ua    | 166   | 0        | 47       | 2       | 0            |
| 112 | Ud    | 215   | 0        | 45       | 4       | 0            |
| 113 | Ue    | 235   | 0        | 49       | 0       | 0            |
| 114 | Uf    | 365   | 0        | 79       | 3       | 0            |
| 115 | Ug    | 315   | 0        | 68       | 4       | 0            |
| 116 | Uh    | 240   | 0        | 51       | 0       | 0            |
| 117 | Ui    | 130   | 0        | 30       | 0       | 0            |
| 118 | Uj    | 45    | 0        | 14       | 1       | 0            |
| 119 | Uk    | 115   | 0        | 25       | 0       | 0            |
| 120 | Ul    | 80    | 0        | 18       | 0       | 0            |
| 121 | Um    | 55    | 0        | 13       | 0       | 0            |
| 122 | A1    | 3     | 0        | 0        | 0       | 0            |
| 122 | A2    | 2     | 0        | 0        | 0       | 0            |
| 122 | A3    | 7     | 0        | 0        | 0       | 0            |
| 122 | A4    | 10    | 0        | 0        | 0       | 0            |
| 122 | A5    | 2     | 0        | 0        | 0       | 0            |
| 122 | A6    | 7     | 0        | 0        | 0       | 0            |
| 122 | A7    | 25    | 0        | 0        | 0       | 0            |
| 122 | A8    | 14    | 0        | 0        | 0       | 0            |
| 122 | Ab    | 1     | 0        | 0        | 0       | 0            |
| 122 | B1    | 3     | 0        | 0        | 0       | 0            |
| 122 | B2    | 8     | 0        | 0        | 0       | 0            |
| 122 | B3    | 13    | 0        | 0        | 0       | 0            |
| 122 | B4    | 15    | 0        | 0        | 0       | 0            |
| 122 | Bm    | 1     | 0        | 0        | 0       | 0            |
| 122 | Bw    | 1     | 0        | 0        | 0       | 0            |
| 123 | A1    | 1     | 0        | 0        | 0       | 0            |
| 123 | A3    | 1     | 0        | 0        | 0       | 0            |
| 123 | A4    | 2     | 0        | 0        | 0       | 0            |
| 123 | A7    | 4     | 0        | 0        | 0       | 0            |
| 123 | A8    | 5     | 0        | 0        | 0       | 0            |
| 123 | AC    | 1     | 0        | 0        | 0       | 0            |
| 123 | Aa    | 1     | 0        | 0        | 0       | 0            |
| 123 | Ab    | 1     | 0        | 0        | 0       | 0            |
| 123 | Ah    | 1     | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 123 | B1    | 2      | 0        | 0        | 0       | 0            |
| 123 | B2    | 1      | 0        | 0        | 0       | 0            |
| 123 | B3    | 8      | 0        | 0        | 0       | 0            |
| 123 | B4    | 3      | 0        | 0        | 0       | 0            |
| 124 | AD    | 1      | 0        | 0        | 0       | 0            |
| 125 | Bw    | 31     | 0        | 12       | 1       | 0            |
| 126 | A1    | 15     | 0        | 0        | 2       | 0            |
| 126 | A2    | 9      | 0        | 0        | 0       | 0            |
| 126 | A3    | 30     | 0        | 0        | 1       | 0            |
| 126 | A4    | 33     | 0        | 0        | 0       | 0            |
| 126 | A5    | 9      | 0        | 0        | 0       | 0            |
| 126 | A6    | 22     | 0        | 0        | 0       | 0            |
| 126 | A7    | 110    | 0        | 0        | 5       | 0            |
| 126 | A8    | 70     | 0        | 0        | 2       | 0            |
| 126 | AA    | 1      | 0        | 0        | 0       | 0            |
| 126 | AC    | 1      | 0        | 0        | 0       | 0            |
| 126 | AI    | 4      | 0        | 0        | 0       | 0            |
| 126 | AK    | 2      | 0        | 0        | 0       | 0            |
| 126 | Aa    | 2      | 0        | 0        | 0       | 0            |
| 126 | Ab    | 4      | 0        | 0        | 0       | 0            |
| 126 | Ac    | 1      | 0        | 0        | 0       | 0            |
| 126 | Aj    | 4      | 0        | 0        | 0       | 0            |
| 126 | B1    | 12     | 0        | 0        | 0       | 0            |
| 126 | B2    | 39     | 0        | 0        | 1       | 0            |
| 126 | B3    | 57     | 0        | 0        | 2       | 0            |
| 126 | B4    | 69     | 0        | 0        | 4       | 0            |
| 126 | Be    | 3      | 0        | 0        | 0       | 0            |
| 126 | Bi    | 2      | 0        | 0        | 0       | 0            |
| 126 | Bl    | 2      | 0        | 0        | 0       | 0            |
| 126 | Bm    | 1      | 0        | 0        | 0       | 0            |
| 126 | Bp    | 1      | 0        | 0        | 0       | 0            |
| 126 | Xg    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 198407 | 0        | 169268   | 555     | 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 2.

The worst 5 of 555 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) |
|------------------|------------------|--------------------------|-------------------|
| 20:Al:78:ARG:HG3 | 34:Az:147:CYS:SG | 1.70                     | 1.31              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:Al:78:ARG:CG   | 34:Az:147:CYS:SG   | 2.46                     | 1.03              |
| 20:Al:128:GLN:NE2 | 34:Az:137:LYS:HD2  | 1.74                     | 1.02              |
| 27:As:73:MET:HA   | 110:Ub:161:MET:HE2 | 1.42                     | 1.00              |
| 62:B3:63:G:O6     | 126:B3:501:HOH:O   | 1.84                     | 0.95              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 10  | Aa    | 248/248 (100%) | 248 (100%) | 0        | 100         | 100 |
| 11  | Ab    | 261/261 (100%) | 261 (100%) | 0        | 100         | 100 |
| 12  | Ac    | 259/259 (100%) | 258 (100%) | 1 (0%)   | 84          | 86  |
| 13  | Ad    | 176/176 (100%) | 175 (99%)  | 1 (1%)   | 78          | 83  |
| 14  | Ae    | 211/211 (100%) | 211 (100%) | 0        | 100         | 100 |
| 15  | Af    | 47/47 (100%)   | 46 (98%)   | 1 (2%)   | 47          | 71  |
| 16  | Ah    | 161/161 (100%) | 159 (99%)  | 2 (1%)   | 63          | 78  |
| 17  | Ai    | 103/103 (100%) | 102 (99%)  | 1 (1%)   | 68          | 79  |
| 18  | Aj    | 172/172 (100%) | 172 (100%) | 0        | 100         | 100 |
| 19  | Ak    | 146/146 (100%) | 145 (99%)  | 1 (1%)   | 76          | 82  |
| 20  | Al    | 150/150 (100%) | 149 (99%)  | 1 (1%)   | 76          | 82  |
| 21  | Am    | 102/102 (100%) | 102 (100%) | 0        | 100         | 100 |
| 22  | An    | 157/157 (100%) | 157 (100%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 23  | Ao    | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 24  | Ap    | 177/177 (100%) | 177 (100%) | 0        | 100         | 100 |
| 25  | Aq    | 161/161 (100%) | 161 (100%) | 0        | 100         | 100 |
| 26  | Ar    | 142/142 (100%) | 141 (99%)  | 1 (1%)   | 76          | 82  |
| 27  | As    | 105/105 (100%) | 105 (100%) | 0        | 100         | 100 |
| 28  | At    | 223/223 (100%) | 223 (100%) | 0        | 100         | 100 |
| 29  | Au    | 121/121 (100%) | 121 (100%) | 0        | 100         | 100 |
| 30  | Av    | 120/120 (100%) | 120 (100%) | 0        | 100         | 100 |
| 31  | Aw    | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 32  | Ax    | 161/161 (100%) | 161 (100%) | 0        | 100         | 100 |
| 33  | Ay    | 66/66 (100%)   | 66 (100%)  | 0        | 100         | 100 |
| 34  | Az    | 51/51 (100%)   | 49 (96%)   | 2 (4%)   | 28          | 60  |
| 35  | AA    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 36  | AB    | 45/45 (100%)   | 45 (100%)  | 0        | 100         | 100 |
| 37  | AC    | 125/125 (100%) | 123 (98%)  | 2 (2%)   | 55          | 75  |
| 38  | AD    | 42/42 (100%)   | 42 (100%)  | 0        | 100         | 100 |
| 39  | AE    | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 40  | AF    | 82/82 (100%)   | 82 (100%)  | 0        | 100         | 100 |
| 41  | AG    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 42  | AH    | 155/155 (100%) | 155 (100%) | 0        | 100         | 100 |
| 43  | AI    | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 44  | AJ    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 45  | AK    | 117/117 (100%) | 117 (100%) | 0        | 100         | 100 |
| 46  | AL    | 332/332 (100%) | 331 (100%) | 1 (0%)   | 86          | 87  |
| 47  | AM    | 351/351 (100%) | 351 (100%) | 0        | 100         | 100 |
| 48  | AN    | 351/351 (100%) | 351 (100%) | 0        | 100         | 100 |
| 49  | AO    | 293/293 (100%) | 292 (100%) | 1 (0%)   | 86          | 87  |
| 50  | Xa    | 173/173 (100%) | 173 (100%) | 0        | 100         | 100 |
| 51  | Xb    | 217/217 (100%) | 217 (100%) | 0        | 100         | 100 |
| 52  | Xc    | 54/54 (100%)   | 54 (100%)  | 0        | 100         | 100 |
| 53  | Xd    | 339/339 (100%) | 337 (99%)  | 2 (1%)   | 78          | 83  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 54  | Xe    | 385/385 (100%) | 385 (100%) | 0        | 100         | 100 |
| 55  | Xf    | 172/172 (100%) | 172 (100%) | 0        | 100         | 100 |
| 56  | Xg    | 312/312 (100%) | 308 (99%)  | 4 (1%)   | 61          | 77  |
| 57  | Xh    | 127/127 (100%) | 127 (100%) | 0        | 100         | 100 |
| 58  | Xi    | 21/21 (100%)   | 21 (100%)  | 0        | 100         | 100 |
| 59  | Xj    | 62/62 (100%)   | 62 (100%)  | 0        | 100         | 100 |
| 64  | Ba    | 220/220 (100%) | 216 (98%)  | 4 (2%)   | 51          | 73  |
| 65  | Bb    | 214/214 (100%) | 213 (100%) | 1 (0%)   | 81          | 85  |
| 66  | Bc    | 247/247 (100%) | 246 (100%) | 1 (0%)   | 84          | 86  |
| 67  | Bd    | 196/196 (100%) | 196 (100%) | 0        | 100         | 100 |
| 68  | Be    | 196/196 (100%) | 191 (97%)  | 5 (3%)   | 40          | 68  |
| 69  | Bf    | 103/103 (100%) | 103 (100%) | 0        | 100         | 100 |
| 70  | Bg    | 97/97 (100%)   | 95 (98%)   | 2 (2%)   | 47          | 71  |
| 71  | Bh    | 327/327 (100%) | 327 (100%) | 0        | 100         | 100 |
| 72  | Bi    | 242/242 (100%) | 242 (100%) | 0        | 100         | 100 |
| 73  | Bj    | 334/334 (100%) | 334 (100%) | 0        | 100         | 100 |
| 74  | Bk    | 95/95 (100%)   | 95 (100%)  | 0        | 100         | 100 |
| 75  | Bl    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 76  | Bm    | 100/100 (100%) | 99 (99%)   | 1 (1%)   | 68          | 79  |
| 77  | Bn    | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 78  | Bo    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 79  | Bp    | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 80  | Bq    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 81  | Br    | 81/81 (100%)   | 81 (100%)  | 0        | 100         | 100 |
| 82  | Bs    | 77/77 (100%)   | 77 (100%)  | 0        | 100         | 100 |
| 83  | Bt    | 66/66 (100%)   | 66 (100%)  | 0        | 100         | 100 |
| 84  | Bu    | 142/142 (100%) | 142 (100%) | 0        | 100         | 100 |
| 85  | Bv    | 140/140 (100%) | 139 (99%)  | 1 (1%)   | 76          | 82  |
| 86  | Bw    | 298/298 (100%) | 297 (100%) | 1 (0%)   | 86          | 87  |
| 87  | Bx    | 481/481 (100%) | 467 (97%)  | 14 (3%)  | 37          | 66  |
| 88  | By    | 69/69 (100%)   | 69 (100%)  | 0        | 100         | 100 |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Analysed           | Rotameric    | Outliers | Percentiles |     |
|-----|-------|--------------------|--------------|----------|-------------|-----|
| 89  | Bz    | 107/107 (100%)     | 107 (100%)   | 0        | 100         | 100 |
| 90  | BA    | 143/143 (100%)     | 143 (100%)   | 0        | 100         | 100 |
| 91  | BB    | 72/72 (100%)       | 72 (100%)    | 0        | 100         | 100 |
| 92  | BC    | 225/225 (100%)     | 224 (100%)   | 1 (0%)   | 84          | 86  |
| 93  | BD    | 30/30 (100%)       | 30 (100%)    | 0        | 100         | 100 |
| 94  | BE    | 136/136 (100%)     | 136 (100%)   | 0        | 100         | 100 |
| 95  | BF    | 326/326 (100%)     | 325 (100%)   | 1 (0%)   | 86          | 87  |
| 96  | Ya    | 161/161 (100%)     | 161 (100%)   | 0        | 100         | 100 |
| 97  | Yb    | 44/44 (100%)       | 43 (98%)     | 1 (2%)   | 44          | 70  |
| 98  | Yc    | 140/140 (100%)     | 140 (100%)   | 0        | 100         | 100 |
| 99  | Yd    | 88/88 (100%)       | 88 (100%)    | 0        | 100         | 100 |
| 100 | Ye    | 91/91 (100%)       | 89 (98%)     | 2 (2%)   | 45          | 71  |
| 101 | Yf    | 132/132 (100%)     | 132 (100%)   | 0        | 100         | 100 |
| 102 | Yg    | 60/60 (100%)       | 60 (100%)    | 0        | 100         | 100 |
| 103 | Yh    | 54/54 (100%)       | 54 (100%)    | 0        | 100         | 100 |
| 104 | Yi    | 112/112 (100%)     | 110 (98%)    | 2 (2%)   | 51          | 73  |
| 105 | Yj    | 278/278 (100%)     | 278 (100%)   | 0        | 100         | 100 |
| 106 | Yk    | 74/74 (100%)       | 73 (99%)     | 1 (1%)   | 59          | 76  |
| 107 | Yl    | 76/76 (100%)       | 76 (100%)    | 0        | 100         | 100 |
| 110 | Ub    | 122/122 (100%)     | 122 (100%)   | 0        | 100         | 100 |
| 111 | Ua    | 1/1 (100%)         | 1 (100%)     | 0        | 100         | 100 |
| All | All   | 14618/14618 (100%) | 14559 (100%) | 59 (0%)  | 81          | 86  |

5 of 59 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | Be    | 42  | GLN  |
| 100 | Ye    | 18  | ASN  |
| 85  | Bv    | 88  | GLN  |
| 100 | Ye    | 5   | ARG  |
| 87  | Bx    | 317 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 87  | Bx    | 332 | GLN  |
| 90  | BA    | 247 | GLN  |
| 99  | Yd    | 126 | GLN  |
| 46  | AL    | 365 | GLN  |
| 46  | AL    | 278 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A1    | 108/109 (99%)   | 25 (23%)          | 0               |
| 108 | C1    | 72/73 (98%)     | 29 (40%)          | 2 (2%)          |
| 109 | C3    | 3/4 (75%)       | 1 (33%)           | 0               |
| 2   | A2    | 80/81 (98%)     | 16 (20%)          | 1 (1%)          |
| 3   | A3    | 205/207 (99%)   | 29 (14%)          | 1 (0%)          |
| 4   | A4    | 72/73 (98%)     | 9 (12%)           | 1 (1%)          |
| 5   | A5    | 132/136 (97%)   | 32 (24%)          | 0               |
| 6   | A6    | 106/109 (97%)   | 21 (19%)          | 0               |
| 60  | B1    | 101/102 (99%)   | 22 (21%)          | 0               |
| 61  | B2    | 208/210 (99%)   | 40 (19%)          | 0               |
| 62  | B3    | 378/379 (99%)   | 49 (12%)          | 2 (0%)          |
| 63  | B4    | 334/337 (99%)   | 47 (14%)          | 0               |
| 7   | A7    | 532/534 (99%)   | 80 (15%)          | 1 (0%)          |
| 8   | A8    | 349/350 (99%)   | 58 (16%)          | 0               |
| 9   | A9    | 67/69 (97%)     | 15 (22%)          | 0               |
| All | All   | 2747/2773 (99%) | 473 (17%)         | 8 (0%)          |

5 of 473 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 5   | A    |
| 1   | A1    | 9   | U    |
| 1   | A1    | 17  | U    |
| 1   | A1    | 18  | A    |
| 1   | A1    | 34  | U    |

5 of 8 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 108 | C1    | 20  | U    |
| 108 | C1    | 16  | C    |
| 62  | B3    | 177 | A    |
| 7   | A7    | 192 | A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | B3    | 275 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 145 ligands modelled in this entry, 144 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 125 | ATP  | Bw    | 502 | 122  | 32,33,33     | 1.34 | 5 (15%)     | 48,52,52    | 1.73 | 8 (16%)     |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 125 | ATP  | Bw    | 502 | 122  | -       | 6/22/38/38 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 125 | Bw    | 502 | ATP  | C5-C4 | 4.30  | 1.46        | 1.39     |
| 125 | Bw    | 502 | ATP  | C5-N7 | -2.41 | 1.34        | 1.39     |
| 125 | Bw    | 502 | ATP  | C5-C6 | 2.39  | 1.47        | 1.41     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 125 | Bw    | 502 | ATP  | C8-N7 | 2.19  | 1.35        | 1.31     |
| 125 | Bw    | 502 | ATP  | C4-N9 | -2.10 | 1.33        | 1.37     |

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 125 | Bw    | 502 | ATP  | C5-C4-N3 | -5.44 | 119.22      | 126.72   |
| 125 | Bw    | 502 | ATP  | N3-C4-N9 | 4.57  | 134.94      | 127.17   |
| 125 | Bw    | 502 | ATP  | C2-N3-C4 | 3.73  | 120.94      | 111.83   |
| 125 | Bw    | 502 | ATP  | N3-C2-N1 | -3.66 | 123.04      | 128.58   |
| 125 | Bw    | 502 | ATP  | C4-N9-C8 | 3.07  | 108.97      | 105.74   |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

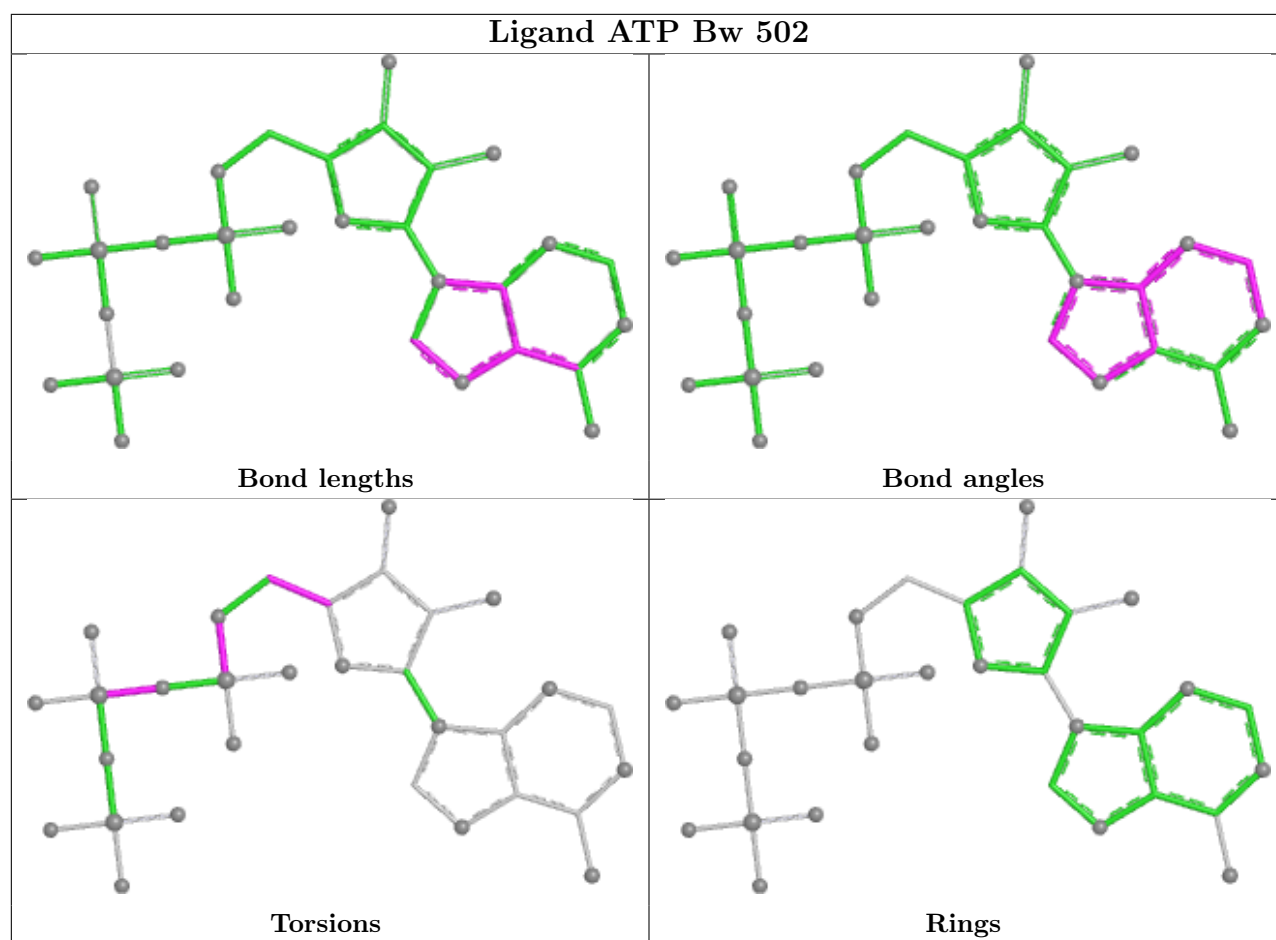
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 125 | Bw    | 502 | ATP  | C5'-O5'-PA-O1A  |
| 125 | Bw    | 502 | ATP  | C5'-O5'-PA-O3A  |
| 125 | Bw    | 502 | ATP  | O4'-C4'-C5'-O5' |
| 125 | Bw    | 502 | ATP  | C3'-C4'-C5'-O5' |
| 125 | Bw    | 502 | ATP  | PA-O3A-PB-O1B   |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 125 | Bw    | 502 | ATP  | 1       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 56  | Xg    | 4                |
| 5   | A5    | 3                |
| 87  | Bx    | 3                |
| 27  | As    | 2                |
| 72  | Bi    | 2                |
| 6   | A6    | 2                |
| 73  | Bj    | 2                |
| 49  | AO    | 2                |
| 63  | B4    | 2                |
| 14  | Ae    | 2                |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 42  | AH    | 1                |
| 66  | Bc    | 1                |
| 57  | Xh    | 1                |
| 71  | Bh    | 1                |
| 65  | Bb    | 1                |
| 92  | BC    | 1                |
| 105 | Yj    | 1                |
| 9   | A9    | 1                |
| 107 | Yl    | 1                |
| 26  | Ar    | 1                |
| 39  | AE    | 1                |
| 91  | BB    | 1                |
| 61  | B2    | 1                |
| 115 | Ug    | 1                |
| 3   | A3    | 1                |
| 114 | Uf    | 1                |
| 34  | Az    | 1                |
| 95  | BF    | 1                |
| 100 | Ye    | 1                |
| 7   | A7    | 1                |
| 16  | Ah    | 1                |
| 106 | Yk    | 1                |
| 46  | AL    | 1                |
| 44  | AJ    | 1                |
| 54  | Xe    | 1                |

The worst 5 of 49 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | Xg    | 165:PHE   | C      | 206:LYS   | N      | 58.01        |
| 1     | As    | 92:PRO    | C      | 151:GLY   | N      | 44.12        |
| 1     | Bi    | 223:GLN   | C      | 243:ALA   | N      | 41.07        |
| 1     | A6    | 114:A     | O3'    | 127:A     | P      | 35.38        |
| 1     | Bj    | 297:SER   | C      | 426:ALA   | N      | 32.85        |

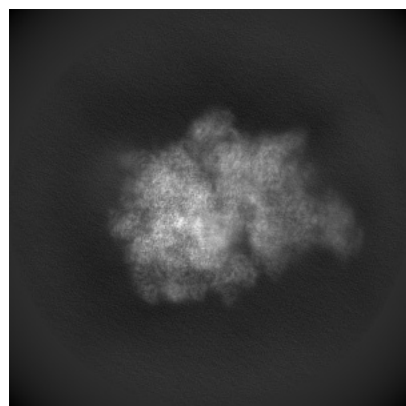
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15576. These allow visual inspection of the internal detail of the map and identification of artifacts.

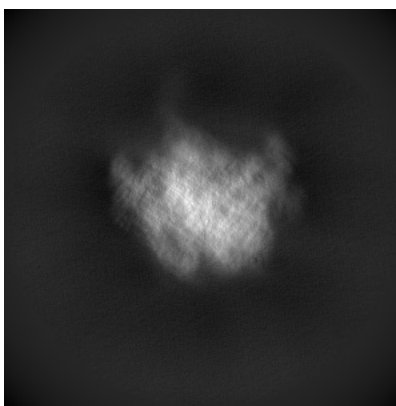
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

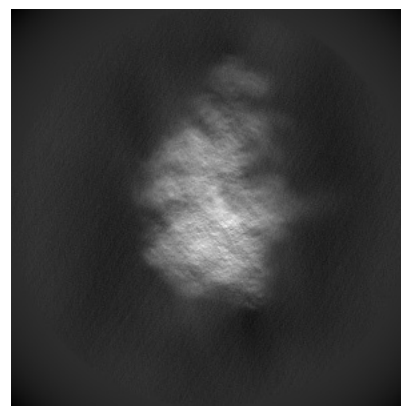
#### 6.1.1 Primary map



X

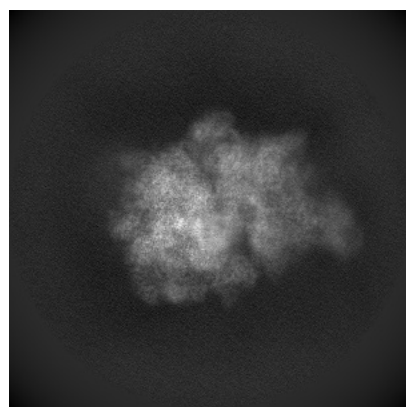


Y

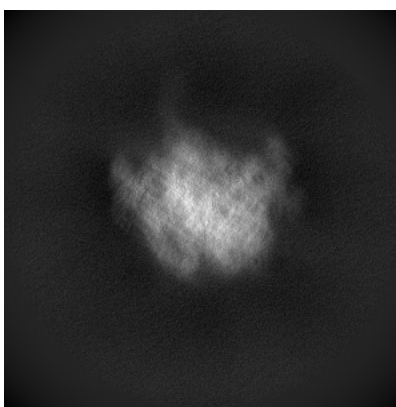


Z

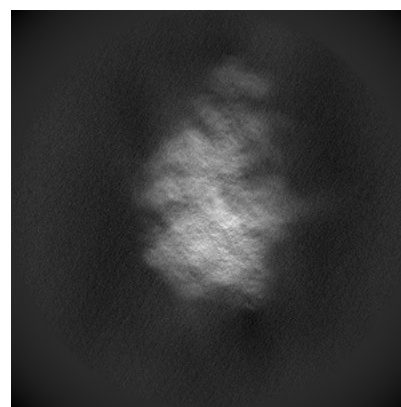
#### 6.1.2 Raw map



X



Y

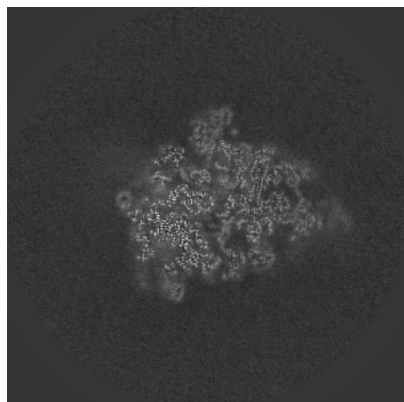


Z

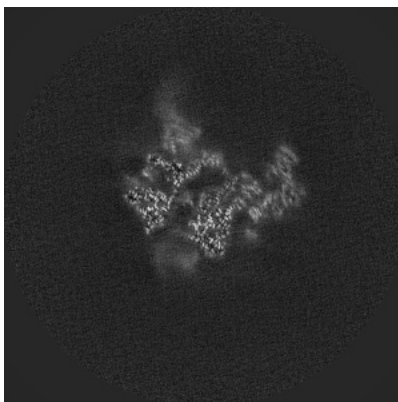
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

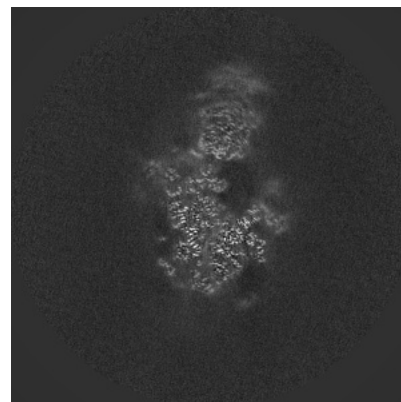
### 6.2.1 Primary map



X Index: 350

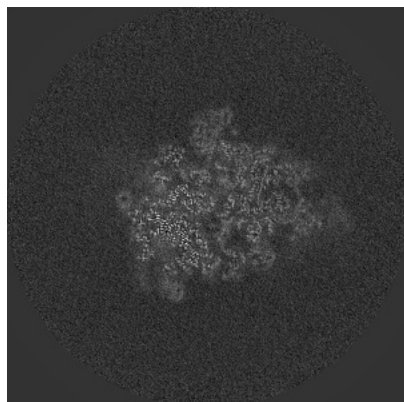


Y Index: 350

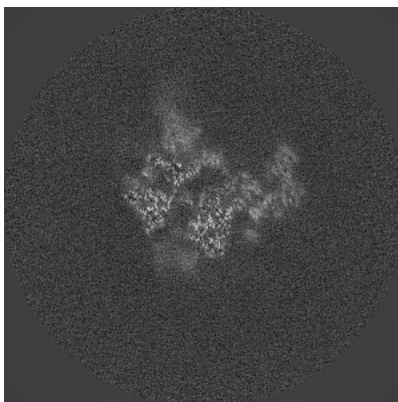


Z Index: 350

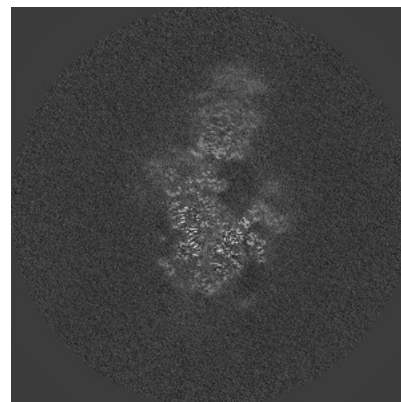
### 6.2.2 Raw map



X Index: 350



Y Index: 350

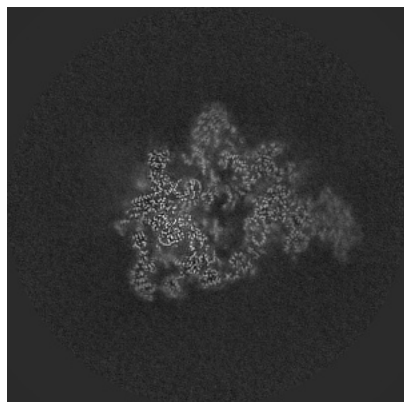


Z Index: 350

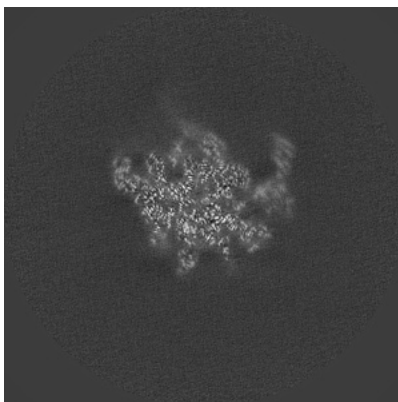
The images above show central slices of the map in three orthogonal directions.

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

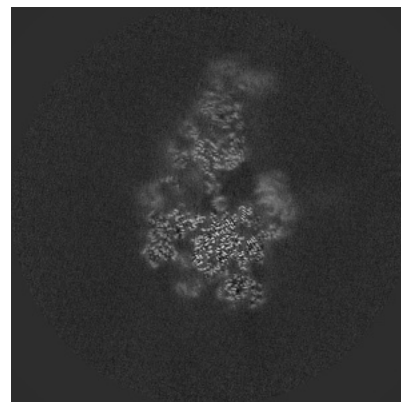
### 6.3.1 Primary map



X Index: 369

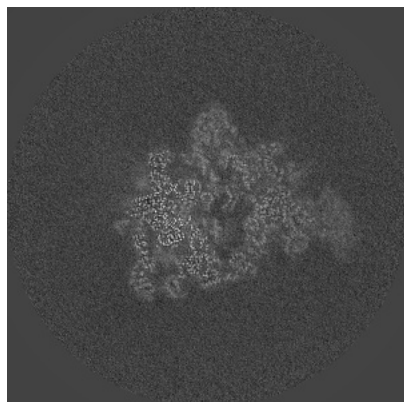


Y Index: 326

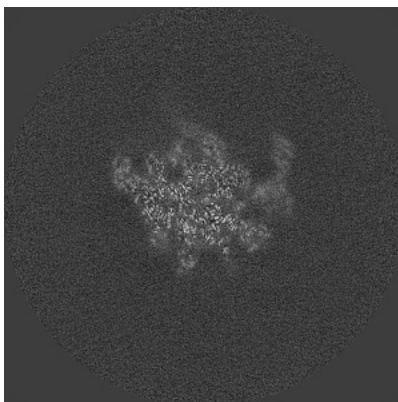


Z Index: 320

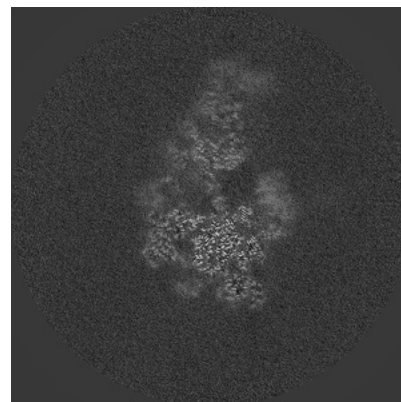
### 6.3.2 Raw map



X Index: 368



Y Index: 326

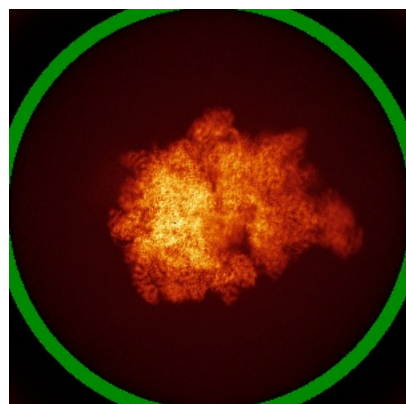


Z Index: 320

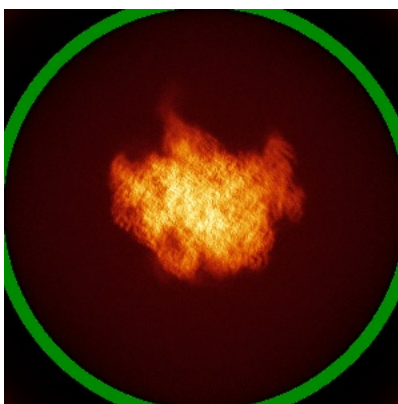
The images above show the largest variance slices of the map in three orthogonal directions.

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

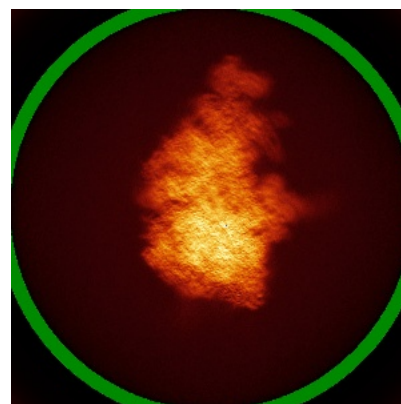
### 6.4.1 Primary map



X

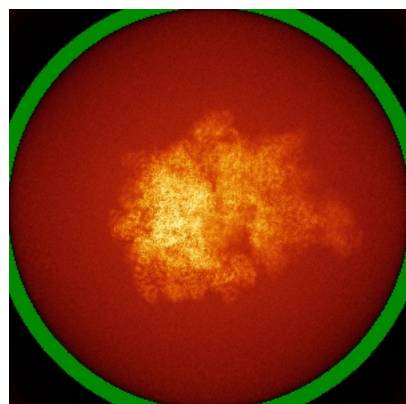


Y

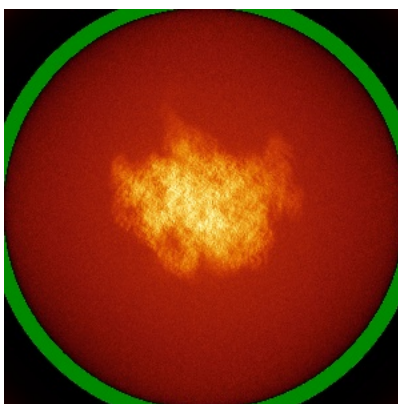


Z

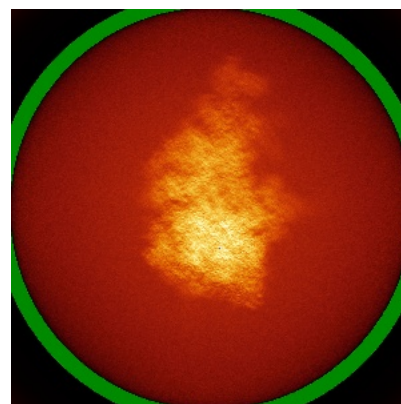
### 6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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



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.

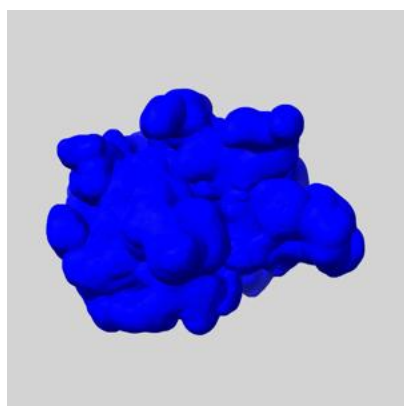
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

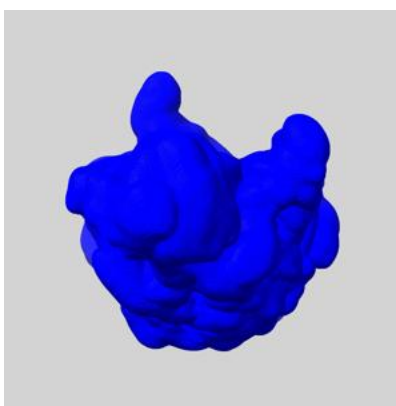
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

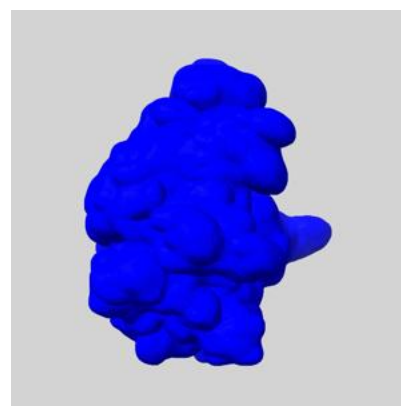
### 6.6.1 emd\_15576\_msk\_1.map [i](#)



X



Y

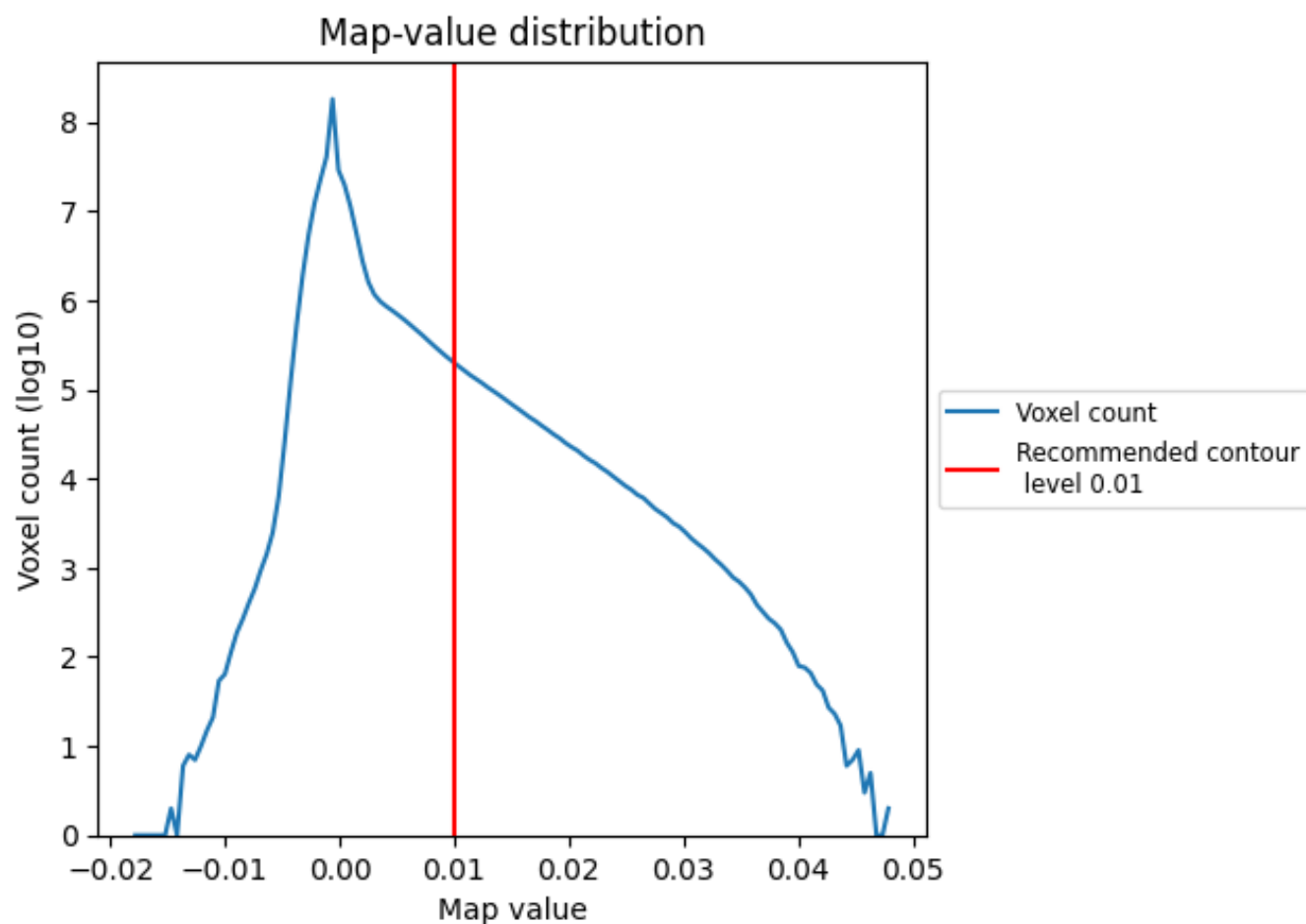


Z

## 7 Map analysis [i](#)

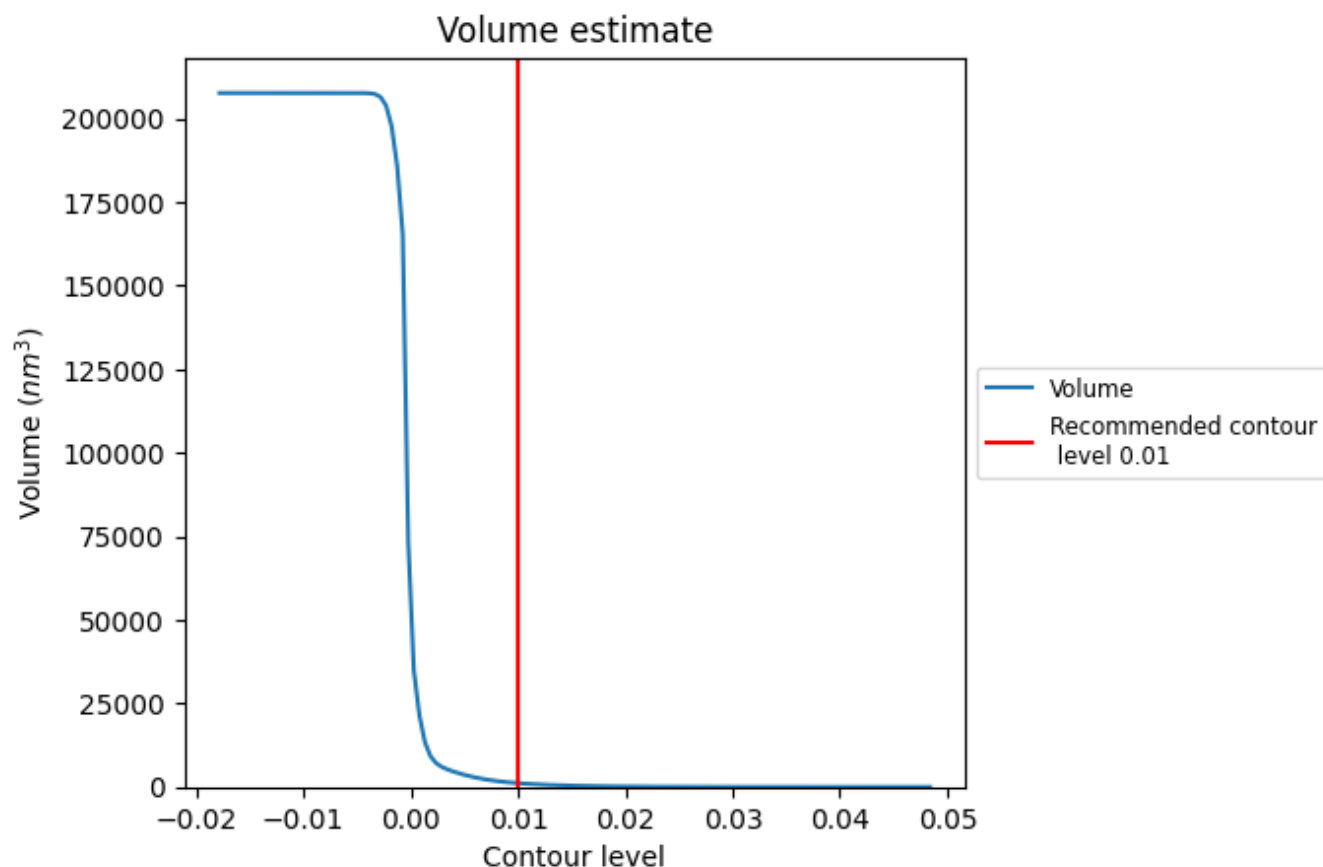
This section contains the results of statistical analysis of the map.

### 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.

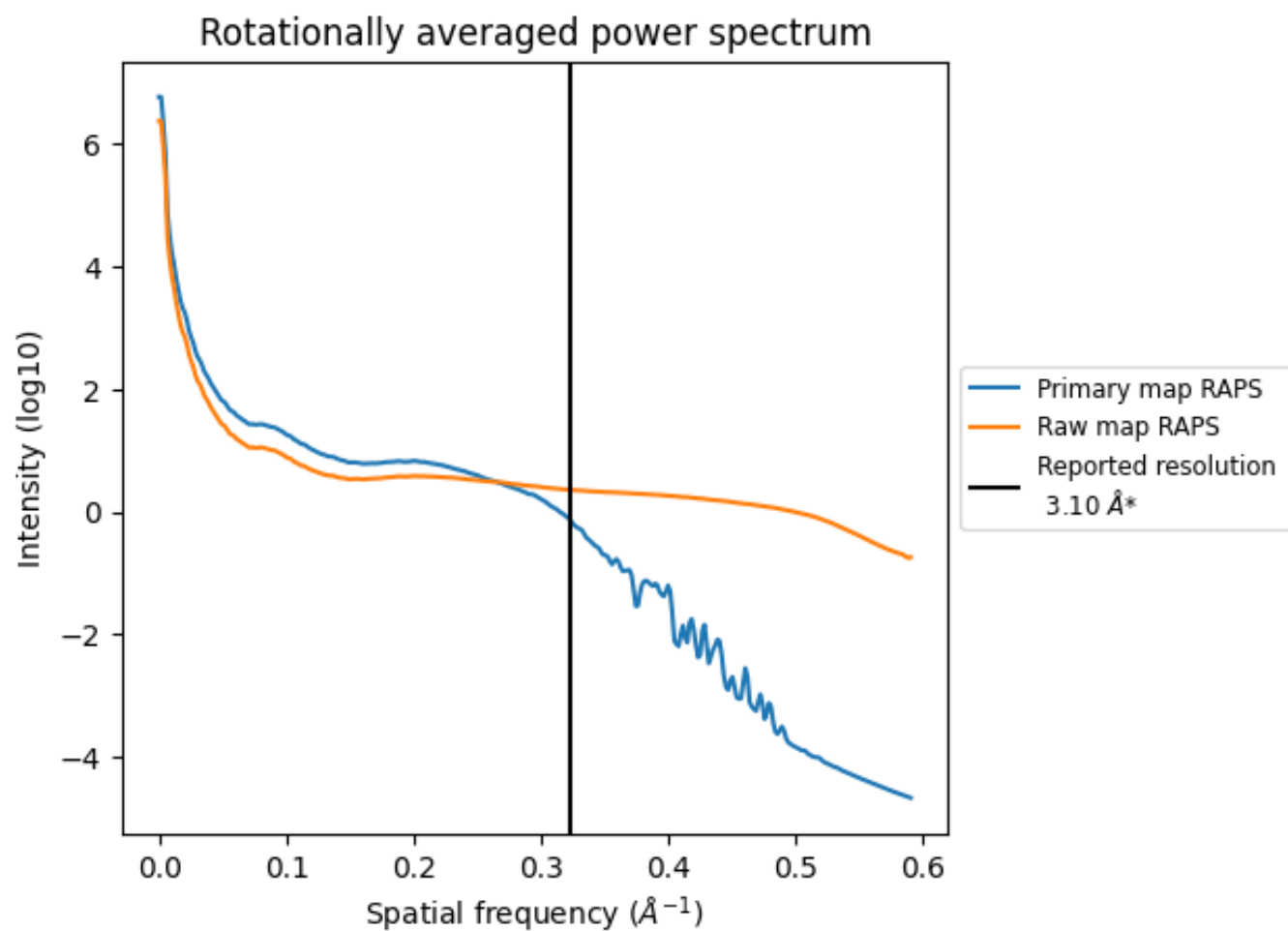
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1137  $\text{nm}^3$ ; this corresponds to an approximate mass of 1027 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 ⓘ

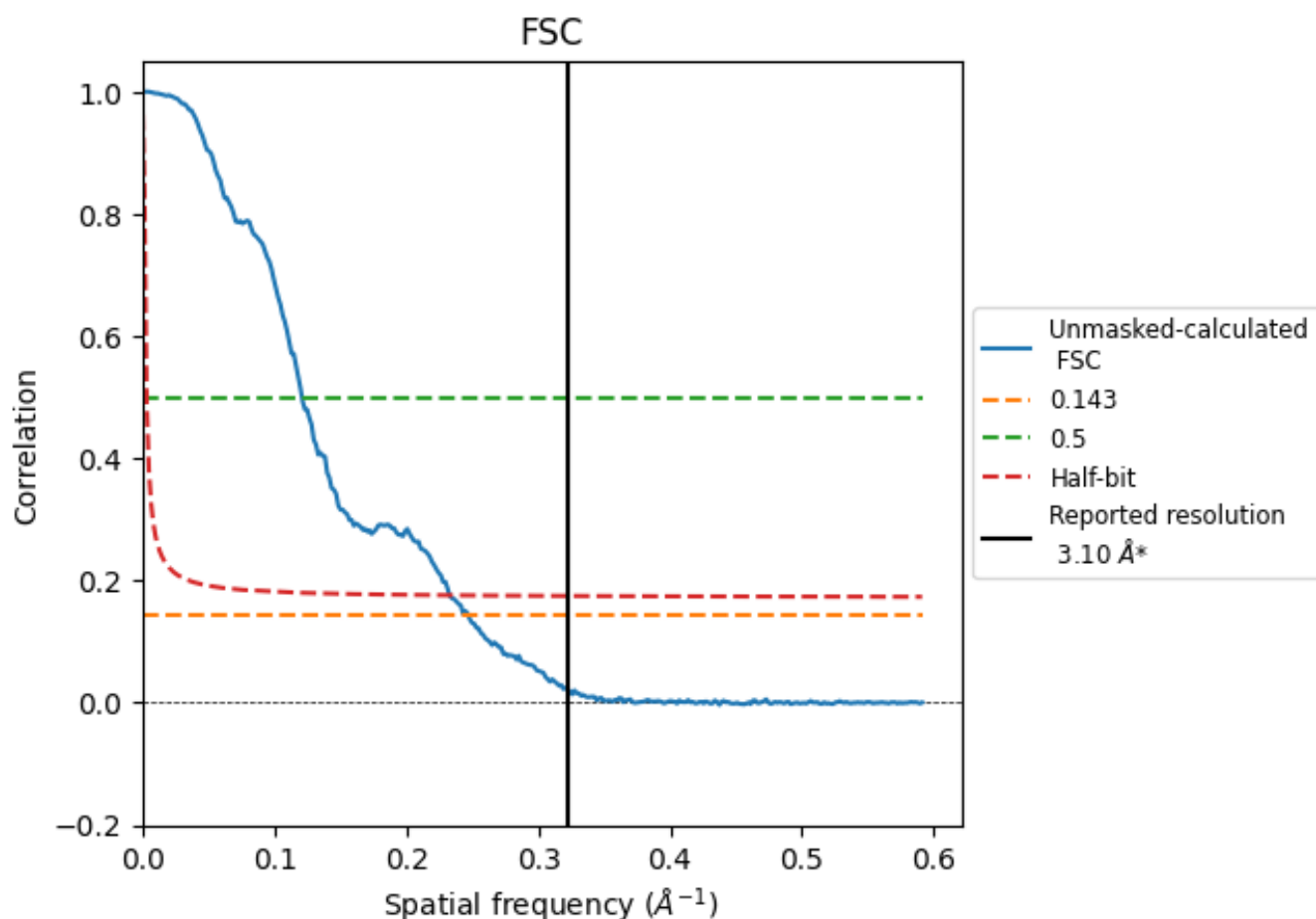


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

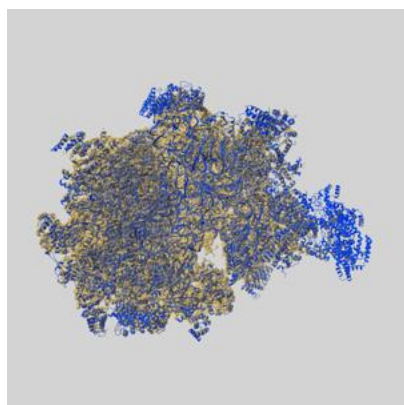
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |       |
|---------------------------|------------------------------------|------|----------|-------|
|                           | 0.143                              | 0.5  | Half-bit | Other |
| Reported by author        | -                                  | -    | -        | 3.10  |
| Author-provided FSC curve | -                                  | -    | -        | -     |
| Unmasked-calculated*      | 4.05                               | 8.26 | 4.29     | -     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

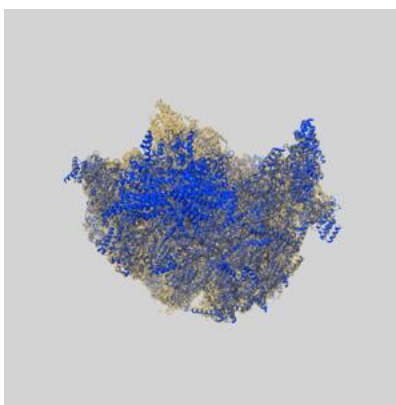
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15576 and PDB model 8APN. Per-residue inclusion information can be found in section [3](#) on page [29](#).

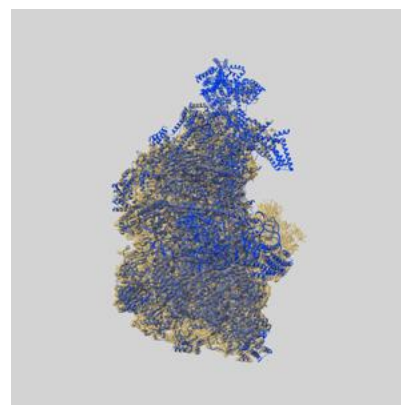
### 9.1 Map-model overlay [i](#)



X



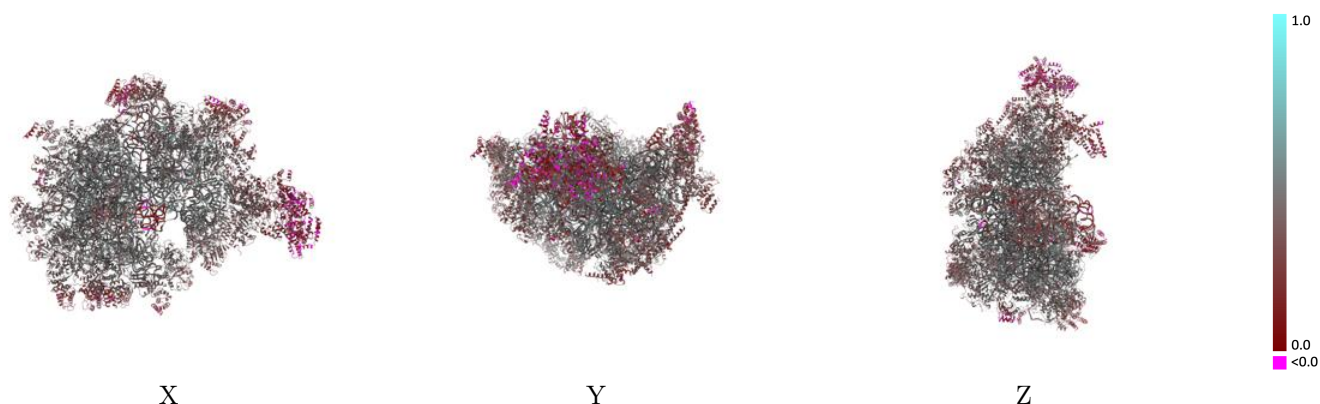
Y



Z

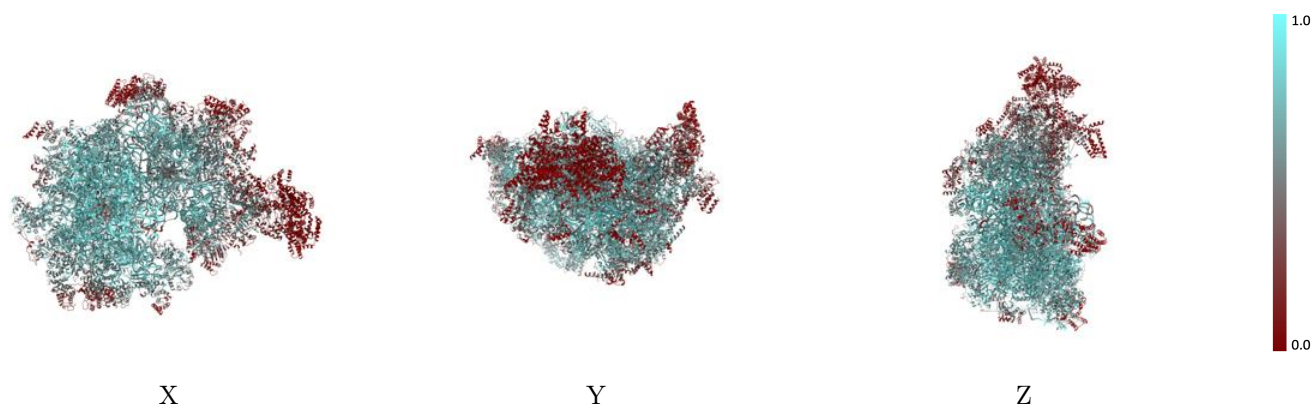
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



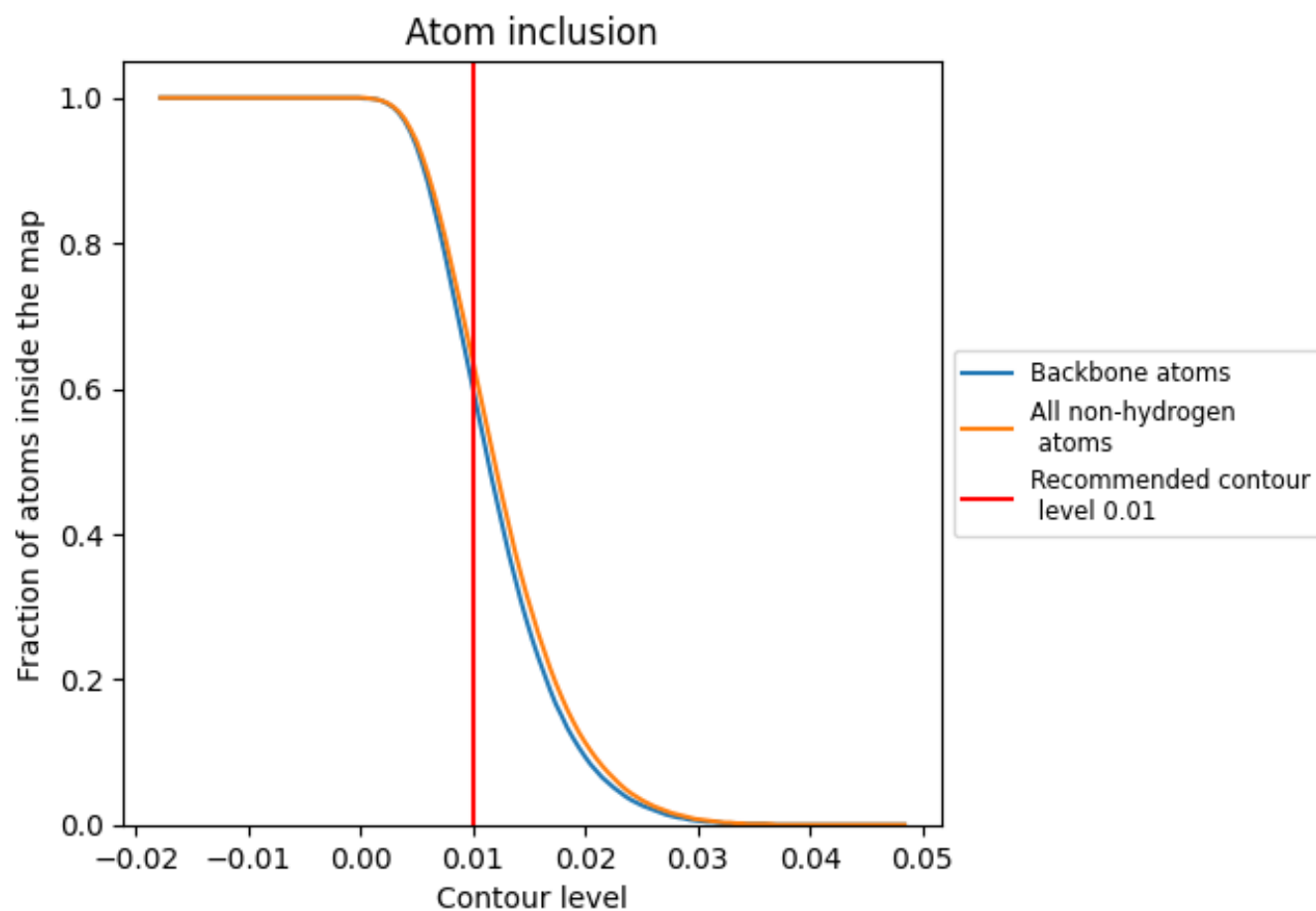
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 64% 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 (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6360   |  0.3990   |
| A1    |  0.8640   |  0.4340   |
| A2    |  0.8850   |  0.4750   |
| A3    |  0.9200   |  0.4480   |
| A4    |  0.9540   |  0.4800   |
| A5    |  0.7900   |  0.2850   |
| A6    |  0.9040   |  0.4510   |
| A7    |  0.9160   |  0.4720   |
| A8    |  0.9040   |  0.4660   |
| A9    |  0.8870   |  0.4630   |
| AA    |  0.8160   |  0.4400   |
| AB    |  0.8620   |  0.4430   |
| AC    |  0.7850   |  0.4460   |
| AD    |  0.6920   |  0.4160   |
| AE    |  0.5960  |  0.3730  |
| AF    |  0.7480 |  0.4170 |
| AG    |  0.7780 |  0.4420 |
| AH    |  0.5490 |  0.3590 |
| AI    |  0.7870 |  0.4530 |
| AJ    |  0.5990 |  0.3790 |
| AK    |  0.8000 |  0.4430 |
| AL    |  0.4760 |  0.3130 |
| AM    |  0.4820 |  0.3360 |
| AN    |  0.5310 |  0.3460 |
| AO    |  0.4930 |  0.3570 |
| Aa    |  0.8250 |  0.4740 |
| Ab    |  0.7780 |  0.4690 |
| Ac    |  0.7460 |  0.4130 |
| Ad    |  0.6050 |  0.4130 |
| Ae    |  0.6260 |  0.3740 |
| Af    |  0.5680 |  0.3680 |
| Ah    |  0.7890 |  0.4520 |
| Ai    |  0.7510 |  0.4810 |
| Aj    |  0.8030 |  0.4390 |
| Ak    |  0.8000 |  0.4770 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Al    |  0.7830   |  0.4390   |
| Am    |  0.6840   |  0.4160   |
| An    |  0.6860   |  0.4520   |
| Ao    |  0.7700   |  0.4420   |
| Ap    |  0.7560   |  0.4460   |
| Aq    |  0.8050   |  0.4520   |
| Ar    |  0.7420   |  0.4260   |
| As    |  0.5620   |  0.3300   |
| At    |  0.7060   |  0.4470   |
| Au    |  0.8080   |  0.4560   |
| Av    |  0.7130   |  0.4380   |
| Aw    |  0.7040   |  0.4150   |
| Ax    |  0.7470   |  0.4380   |
| Ay    |  0.4880   |  0.3800   |
| Az    |  0.7380   |  0.4470   |
| B1    |  0.7020   |  0.4240   |
| B2    |  0.7660   |  0.4270   |
| B3    |  0.8870   |  0.4720   |
| B4    |  0.8460   |  0.4590   |
| BA    |  0.3990  |  0.3750  |
| BB    |  0.4810 |  0.3790 |
| BC    |  0.3370 |  0.3570 |
| BD    |  0.6770 |  0.4280 |
| BE    |  0.0500 |  0.1750 |
| BF    |  0.3220 |  0.3130 |
| Ba    |  0.4310 |  0.3250 |
| Bb    |  0.5880 |  0.3980 |
| Bc    |  0.4000 |  0.3980 |
| Bd    |  0.5090 |  0.4360 |
| Be    |  0.6530 |  0.4510 |
| Bf    |  0.6650 |  0.4220 |
| Bg    |  0.6600 |  0.4540 |
| Bh    |  0.6010 |  0.3950 |
| Bi    |  0.5250 |  0.3970 |
| Bj    |  0.2380 |  0.2710 |
| Bk    |  0.7350 |  0.4670 |
| Bl    |  0.4350 |  0.4220 |
| Bm    |  0.5400 |  0.4120 |
| Bn    |  0.6950 |  0.4650 |
| Bo    |  0.7810 |  0.4240 |
| Bp    |  0.4290 |  0.3740 |
| Bq    |  0.6960 |  0.3960 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Br    |  0.6570   |  0.3970   |
| Bs    |  0.4090   |  0.3820   |
| Bt    |  0.6900   |  0.4240   |
| Bu    |  0.4510   |  0.3430   |
| Bv    |  0.5030   |  0.3350   |
| Bw    |  0.4000   |  0.3570   |
| Bx    |  0.1650   |  0.2390   |
| By    |  0.4690   |  0.3930   |
| Bz    |  0.1710   |  0.2490   |
| C1    |  0.6720   |  0.3880   |
| C3    |  0.8740   |  0.5100   |
| Ua    |  0.4270   |  0.4340   |
| Ub    |  0.4020   |  0.2340   |
| Ud    |  0.1910   |  0.2400   |
| Ue    |  0.0130   |  0.2430   |
| Uf    |  0.0800   |  0.1570   |
| Ug    |  0.3110   |  0.3790   |
| Uh    |  0.0000   |  0.1200   |
| Ui    |  0.6080   |  0.4120   |
| Uj    |  0.1560   |  0.3870   |
| Uk    |  0.2000  |  0.2990  |
| Ul    |  0.0500 |  0.2060 |
| Um    |  0.5270 |  0.3200 |
| Xa    |  0.4790 |  0.3520 |
| Xb    |  0.5900 |  0.3960 |
| Xc    |  0.6910 |  0.4040 |
| Xd    |  0.6080 |  0.3930 |
| Xe    |  0.6950 |  0.4140 |
| Xf    |  0.7190 |  0.4420 |
| Xg    |  0.6170 |  0.4010 |
| Xh    |  0.5750 |  0.3860 |
| Xi    |  0.7540 |  0.4040 |
| Xj    |  0.5850 |  0.3830 |
| Ya    |  0.3350 |  0.3640 |
| Yb    |  0.2130 |  0.2880 |
| Yc    |  0.4180 |  0.3790 |
| Yd    |  0.2610 |  0.3300 |
| Ye    |  0.6440 |  0.4740 |
| Yf    |  0.4770 |  0.4040 |
| Yg    |  0.2870 |  0.3360 |
| Yh    |  0.4670 |  0.3920 |
| Yi    |  0.0750 |  0.2610 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Yj    |  0.1020 |  0.1840 |
| Yk    |  0.0630 |  0.2030 |
| Yl    |  0.4830 |  0.3880 |