



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:15 AM UTC

PDB ID : 8CGN / pdb\_00008cgn  
EMDB ID : EMD-16648  
Title : Non-rotated 80S *S. cerevisiae* ribosome with ligands  
Authors : Milicevic, N.; Jenner, L.; Myasnikov, A.; Yusupov, M.; Yusupova, G.  
Deposited on : 2023-02-06  
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

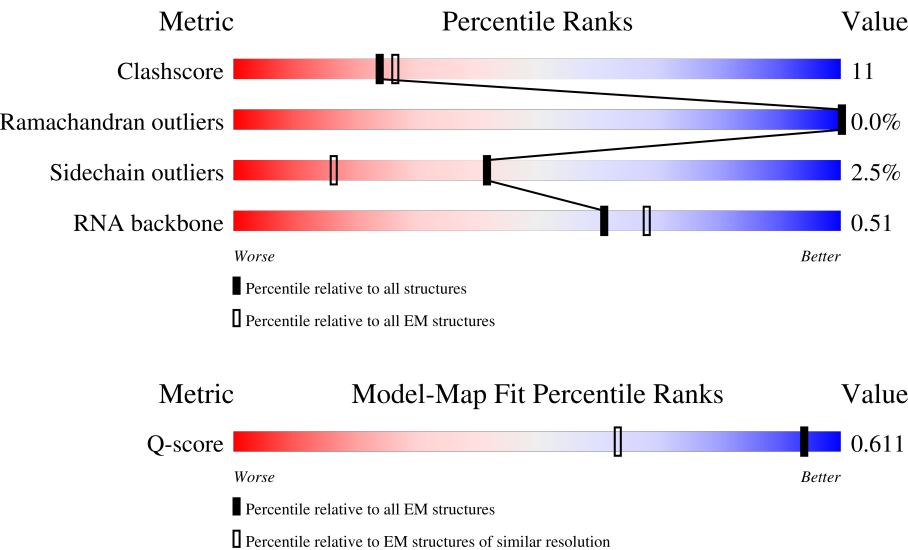
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.28 Å.

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



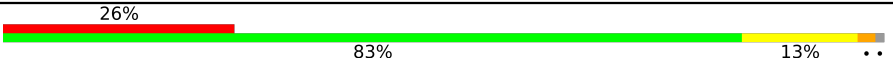
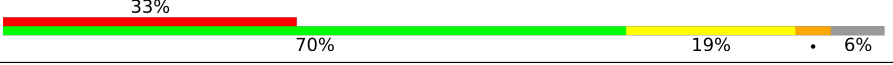
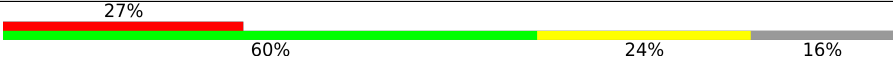
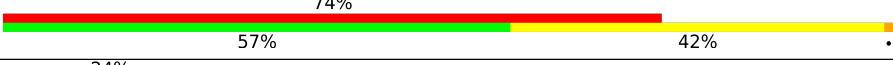
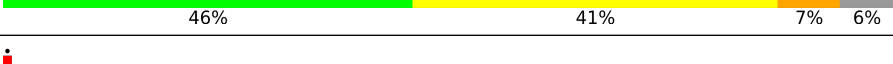
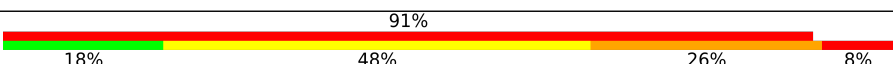
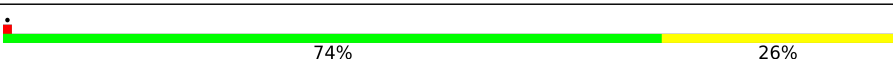
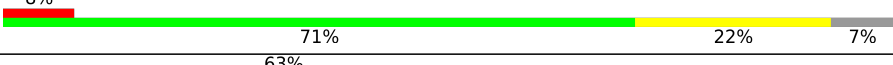
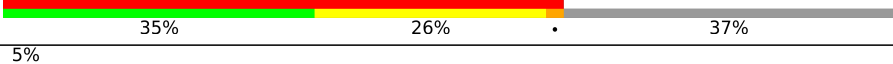
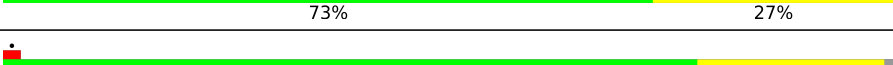
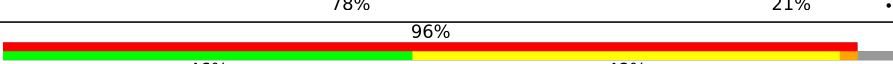
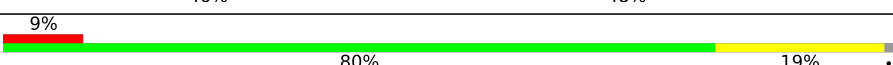
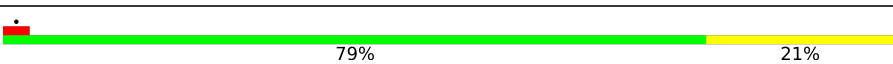
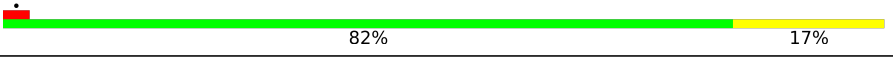
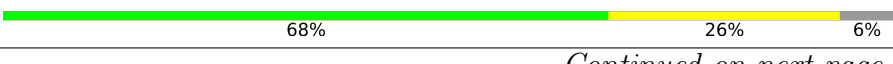
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 3643 ( 1.78 - 2.78 )                                     |

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   | 0     | 135    |                  |
| 2   | 1     | 108    |                  |
| 3   | 2     | 119    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 82     |    |
| 5   | 4     | 67     |    |
| 6   | 5     | 56     |    |
| 7   | 6     | 63     |    |
| 8   | 7     | 319    |    |
| 9   | 8     | 152    |    |
| 10  | A     | 199    |    |
| 11  | AA    | 3396   |    |
| 12  | B     | 338    |    |
| 13  | BB    | 121    |    |
| 14  | Bb    | 77     |   |
| 14  | Cc    | 77     |  |
| 15  | C     | 186    |  |
| 16  | CC    | 158    |  |
| 17  | D     | 189    |  |
| 18  | DD    | 312    |  |
| 19  | Dd    | 39     |  |
| 20  | E     | 172    |  |
| 21  | EE    | 254    |  |
| 22  | Ee    | 165    |  |
| 23  | F     | 160    |  |
| 24  | FF    | 387    |  |
| 25  | G     | 121    |  |
| 26  | GG    | 362    |  |
| 27  | H     | 137    |  |

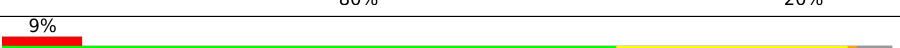
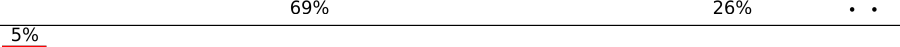
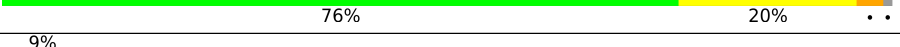
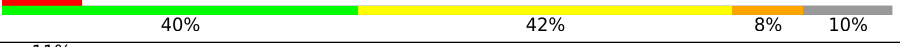
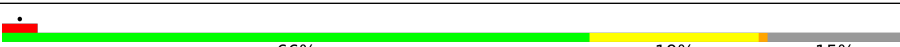
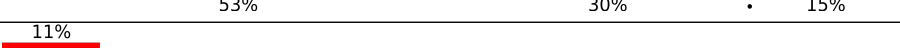
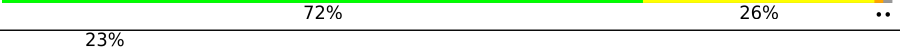
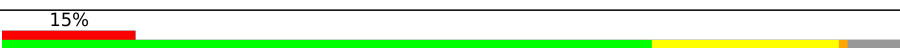
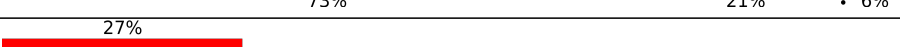
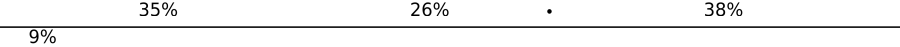
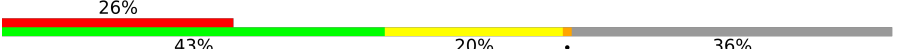
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | HH    | 297    |                  |
| 29  | I     | 155    |                  |
| 30  | II    | 176    |                  |
| 31  | J     | 142    |                  |
| 32  | JJ    | 244    |                  |
| 33  | K     | 127    |                  |
| 34  | KK    | 256    |                  |
| 35  | L     | 136    |                  |
| 36  | LL    | 191    |                  |
| 37  | M     | 149    |                  |
| 38  | MM    | 221    |                  |
| 39  | N     | 59     |                  |
| 40  | NN    | 174    |                  |
| 41  | O     | 105    |                  |
| 42  | OO    | 199    |                  |
| 43  | P     | 113    |                  |
| 44  | PP    | 138    |                  |
| 45  | Q     | 130    |                  |
| 46  | QQ    | 204    |                  |
| 47  | R     | 107    |                  |
| 48  | S     | 121    |                  |
| 49  | T     | 120    |                  |
| 50  | U     | 100    |                  |
| 51  | V     | 88     |                  |
| 52  | W     | 78     |                  |

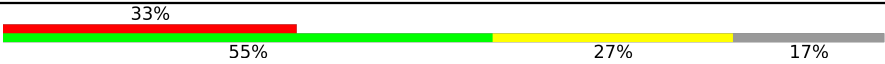
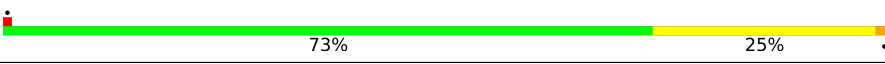
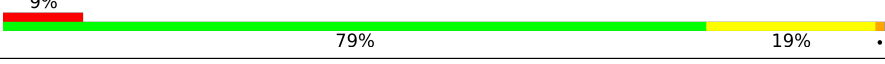
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 53  | X     | 51     |    |
| 54  | Y     | 128    |    |
| 55  | Z     | 25     |    |
| 56  | a     | 106    |    |
| 57  | b     | 92     |    |
| 58  | c     | 1800   |    |
| 59  | d     | 252    |    |
| 60  | e     | 255    |    |
| 61  | f     | 254    |    |
| 62  | g     | 240    |    |
| 63  | h     | 261    |    |
| 64  | i     | 225    |    |
| 65  | j     | 236    |    |
| 66  | k     | 190    |   |
| 67  | l     | 200    |  |
| 68  | m     | 197    |  |
| 69  | n     | 105    |  |
| 70  | o     | 156    |  |
| 71  | p     | 151    |  |
| 72  | q     | 137    |  |
| 73  | r     | 142    |  |
| 74  | s     | 143    |  |
| 75  | t     | 136    |  |
| 76  | u     | 146    |  |
| 77  | v     | 144    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 78  | w     | 121    |  |
| 79  | x     | 87     |  |
| 80  | y     | 130    |  |
| 81  | z     | 145    |  |

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 201528 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 protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | 0     | 134      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 2   | 1     | 70       | Total | C   | N   | O  | 0       | 0     |
|     |       |          | 563   | 360 | 104 | 99 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | 2     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 3     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 63       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |       |

- Molecule 6 is a protein called HLJ1\_G0030400.mRNA.1.CDS.1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 6   | 5     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 404   | 249 | 86 | 65 | 4 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | 6     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 427   | 269 | 88 | 69 | 1 |         |       |

- Molecule 8 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | 7     | 318      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2436  | 1541 | 418 | 469 | 8 |         |       |

- Molecule 9 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | 8     | 36       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 276   | 173 | 54 | 45 | 4 |         |       |

- Molecule 10 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | A     | 197      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |       |

- Molecule 11 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 11  | AA    | 3197     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 68429 | 30589 | 12334 | 22309 | 3197 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 12  | B     | 154      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1222  | 761 | 237 | 224 |         |       |

- Molecule 13 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 13  | BB    | 121      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |       |

- Molecule 14 is a RNA chain called Transfer RNA fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | Bb    | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1644  | 732 | 298 | 537 | 77 |         |       |
| 14  | Cc    | 77       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1644  | 732 | 298 | 537 | 77 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| Bb    | 18      | C        | U      | conflict | GB 170517292 |
| Cc    | 18      | C        | U      | conflict | GB 170517292 |

- Molecule 15 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | C     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |       |

- Molecule 16 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 16  | CC    | 158      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 17  | D     | 176      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1423  | 875 | 308 | 240 |  |         |       |

- Molecule 18 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | DD    | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1531  | 980 | 266 | 281 | 4 |         |       |

- Molecule 19 is a RNA chain called Messenger RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 19  | Dd    | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 131   | 59 | 27 | 39 | 6 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | E     | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | EE    | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1914  | 1191 | 388 | 334 | 1 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L12-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | Ee    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1196  | 750 | 216 | 228 | 2 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | F     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | FF    | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 25  | G     | 97       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 770   | 499 | 126 | 145 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | GG    | 361      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | H     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 963   | 607 | 180 | 169 | 7 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | HH    | 296      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2375  | 1501 | 414 | 458 | 2 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 29  | I     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 521   | 336 | 102 | 82 | 1 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | II    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1230  | 795 | 221 | 213 | 1 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | J     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 959   | 617 | 168 | 172 | 2 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | JJ    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 33  | K     | 126      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |  |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | KK    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 35  | L     | 135      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |  |         |       |

- Molecule 36 is a protein called RPL9A isoform 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | LL    | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | M     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | MM    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1743  | 1102 | 331 | 303 | 7 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|-------|
| 39  | N     | 58       | Total | C   | N   | O  |  | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |  |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | NN    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | O     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 479 | 124 | 138 | 1 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | OO    | 193      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |   |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | P     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 883   | 559 | 167 | 156 | 1 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | PP    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Q     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | QQ    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | R     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | S     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 861   | 533 | 175 | 149 | 4 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | T     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | U     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | V     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 665   | 405 | 145 | 110 | 5 |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 52  | W     | 77       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53  | X     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |       |

- Molecule 54 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | Y     | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 55  | Z     | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | a     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 514 | 166 | 134 | 5 |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | b     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |       |

- Molecule 58 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 58  | c     | 1624     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 34663 | 15513 | 6155 | 11371 | 1624 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59  | d     | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1583  | 1017 | 281 | 283 | 2 |         |       |

- Molecule 60 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | e     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1689  | 1073 | 303 | 309 | 4 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 61  | f     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |       |

- Molecule 62 is a protein called RPS3 isoform 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 62  | g     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1593  | 1008 | 293 | 286 | 6 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 63  | h     | 258      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2056  | 1308 | 387 | 358 | 3 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | i     | 199      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1572  | 987 | 290 | 292 | 3 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 65  | j     | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1798  | 1128 | 347 | 320 | 3 |         |       |

- Molecule 66 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | k     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |   |         |       |

- Molecule 67 is a protein called 40S ribosomal protein S8-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | l     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1457  | 906 | 291 | 258 | 2 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | m     | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 69  | n     | 65       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 556   | 361 | 90 | 105 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | o     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 735 | 217 | 191 | 3 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | p     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | q     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 891   | 545 | 182 | 163 | 1 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | r     | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 732   | 469 | 138 | 120 | 5 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 74  | s     | 137      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1080  | 692 | 199 | 189 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | t     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 961   | 599 | 182 | 178 | 2 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | u     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | v     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | w     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 800   | 509 | 144 | 146 | 1 |         |       |

- Molecule 79 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | x     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | y     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |       |

- Molecule 81 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | z     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |       |

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 82  | 2     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | 5     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | 8     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 82  | S     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 82  | V     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 82  | Y     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 82  | a     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 82  | b     | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 83  | AA    | 199      | Total<br>199 | Mg<br>199 | 0       |
| 83  | B     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 83  | BB    | 5        | Total<br>5   | Mg<br>5   | 0       |
| 83  | Bb    | 2        | Total<br>2   | Mg<br>2   | 0       |
| 83  | CC    | 3        | Total<br>3   | Mg<br>3   | 0       |
| 83  | FF    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 83  | H     | 1        | Total<br>1   | Mg<br>1   | 0       |
| 83  | MM    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 83  | QQ    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 83  | c     | 49       | Total<br>49  | Mg<br>49  | 0       |

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

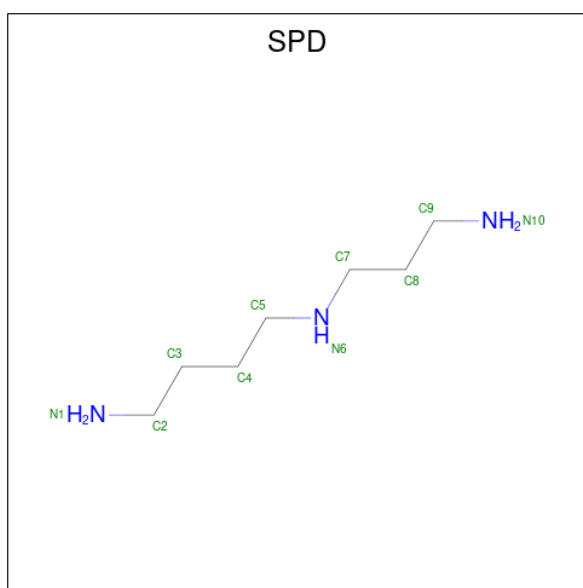
| Mol | Chain | Residues | Atoms       |         | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 84  | AA    | 13       | Total<br>13 | K<br>13 | 0       |
| 84  | EE    | 1        | Total<br>1  | K<br>1  | 0       |

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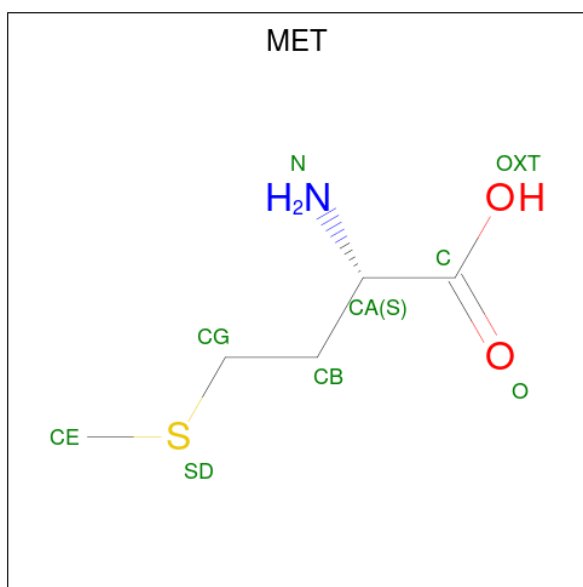
| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 84  | MM    | 1        | Total K<br>1 1 | 0       |
| 84  | Q     | 1        | Total K<br>1 1 | 0       |
| 84  | S     | 1        | Total K<br>1 1 | 0       |
| 84  | c     | 1        | Total K<br>1 1 | 0       |
| 84  | q     | 1        | Total K<br>1 1 | 0       |

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



| Mol | Chain | Residues | Atoms               | AltConf |
|-----|-------|----------|---------------------|---------|
| 85  | AA    | 1        | Total C N<br>10 7 3 | 0       |
| 85  | AA    | 1        | Total C N<br>10 7 3 | 0       |
| 85  | AA    | 1        | Total C N<br>10 7 3 | 0       |
| 85  | c     | 1        | Total C N<br>10 7 3 | 0       |

- Molecule 86 is METHIONINE (CCD ID: MET) (formula:  $C_5H_{11}NO_2S$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 86  | Bb    | 1        | Total | C | N | O | S | 0       |
|     |       |          | 8     | 5 | 1 | 1 | 1 |         |

- Molecule 87 is water.

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 87  | 2     | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |
| 87  | A     | 2        | Total | O   | 0       |
|     |       |          | 2     | 2   |         |
| 87  | AA    | 774      | Total | O   | 0       |
|     |       |          | 774   | 774 |         |
| 87  | B     | 4        | Total | O   | 0       |
|     |       |          | 4     | 4   |         |
| 87  | BB    | 13       | Total | O   | 0       |
|     |       |          | 13    | 13  |         |
| 87  | Bb    | 5        | Total | O   | 0       |
|     |       |          | 5     | 5   |         |
| 87  | CC    | 13       | Total | O   | 0       |
|     |       |          | 13    | 13  |         |
| 87  | Cc    | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |
| 87  | D     | 1        | Total | O   | 0       |
|     |       |          | 1     | 1   |         |
| 87  | Dd    | 3        | Total | O   | 0       |
|     |       |          | 3     | 3   |         |
| 87  | EE    | 11       | Total | O   | 0       |
|     |       |          | 11    | 11  |         |

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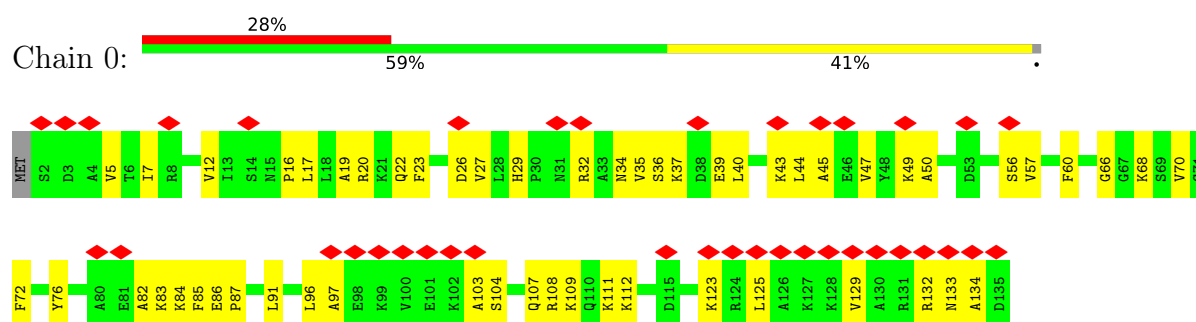
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 87  | F     | 2        | Total<br>2   | O<br>2   | 0       |
| 87  | FF    | 4        | Total<br>4   | O<br>4   | 0       |
| 87  | GG    | 3        | Total<br>3   | O<br>3   | 0       |
| 87  | H     | 3        | Total<br>3   | O<br>3   | 0       |
| 87  | HH    | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | J     | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | JJ    | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | M     | 2        | Total<br>2   | O<br>2   | 0       |
| 87  | MM    | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | N     | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | P     | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | Q     | 4        | Total<br>4   | O<br>4   | 0       |
| 87  | QQ    | 7        | Total<br>7   | O<br>7   | 0       |
| 87  | V     | 4        | Total<br>4   | O<br>4   | 0       |
| 87  | a     | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | c     | 122      | Total<br>122 | O<br>122 | 0       |
| 87  | e     | 1        | Total<br>1   | O<br>1   | 0       |
| 87  | h     | 2        | Total<br>2   | O<br>2   | 0       |
| 87  | o     | 2        | Total<br>2   | O<br>2   | 0       |
| 87  | p     | 1        | Total<br>1   | O<br>1   | 0       |

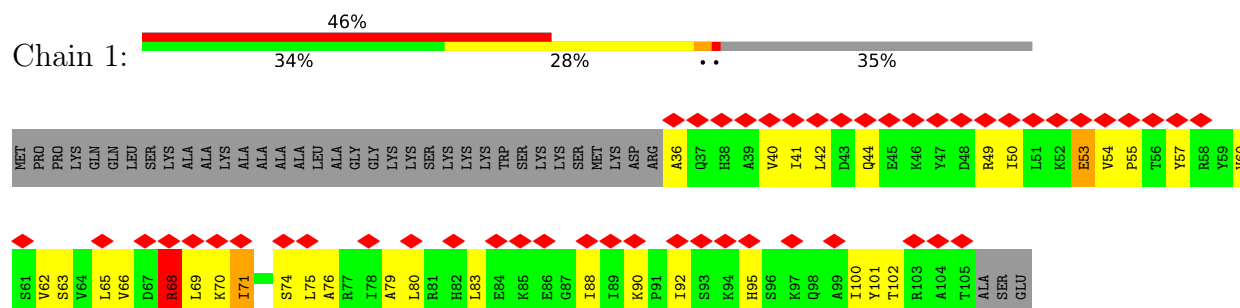
### 3 Residue-property plots [i](#)

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.

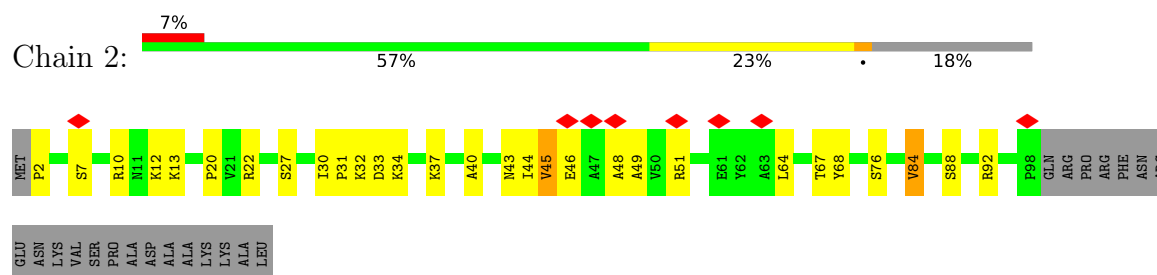
#### • Molecule 1: 40S ribosomal protein S24-A



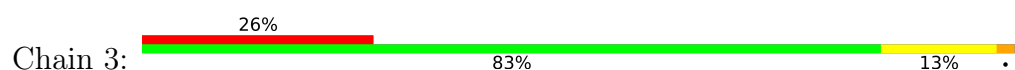
#### • Molecule 2: 40S ribosomal protein S25-A

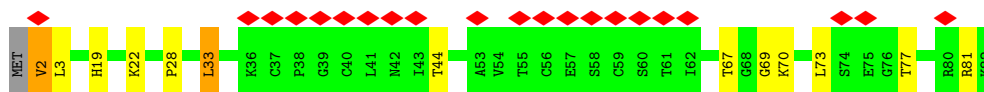


#### • Molecule 3: 40S ribosomal protein S26



#### • Molecule 4: 40S ribosomal protein S27-A





- Molecule 5: 40S ribosomal protein S28-A



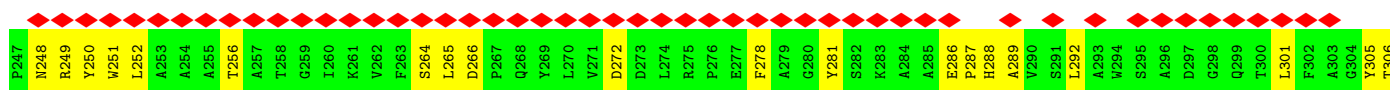
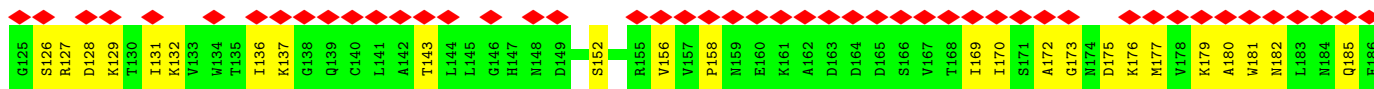
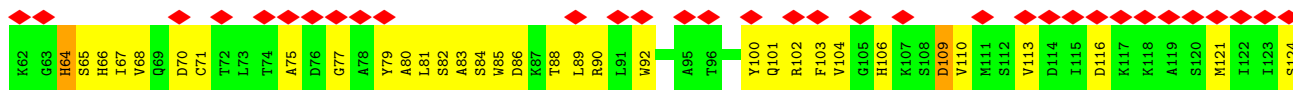
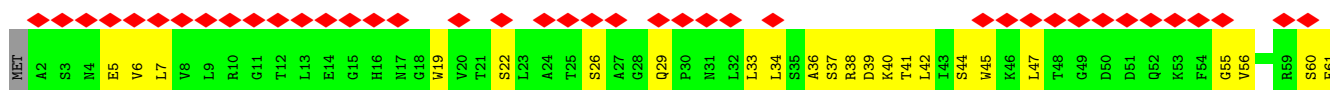
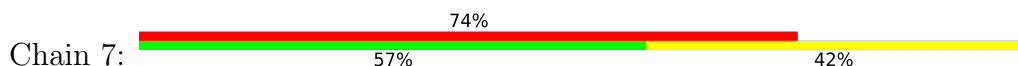
- Molecule 6: HLJ1\_G0030400.mRNA.1.CDS.1

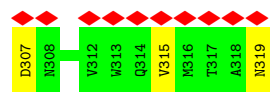


- Molecule 7: 40S ribosomal protein S30-A

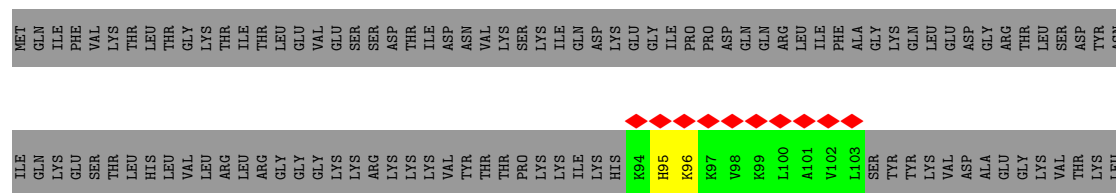


- Molecule 8: Guanine nucleotide-binding protein subunit beta-like protein

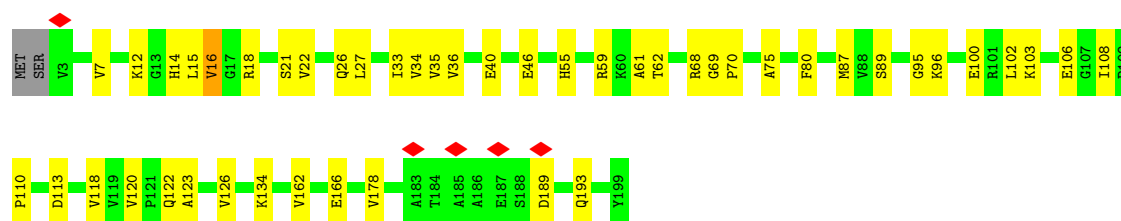
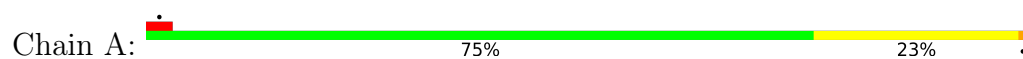




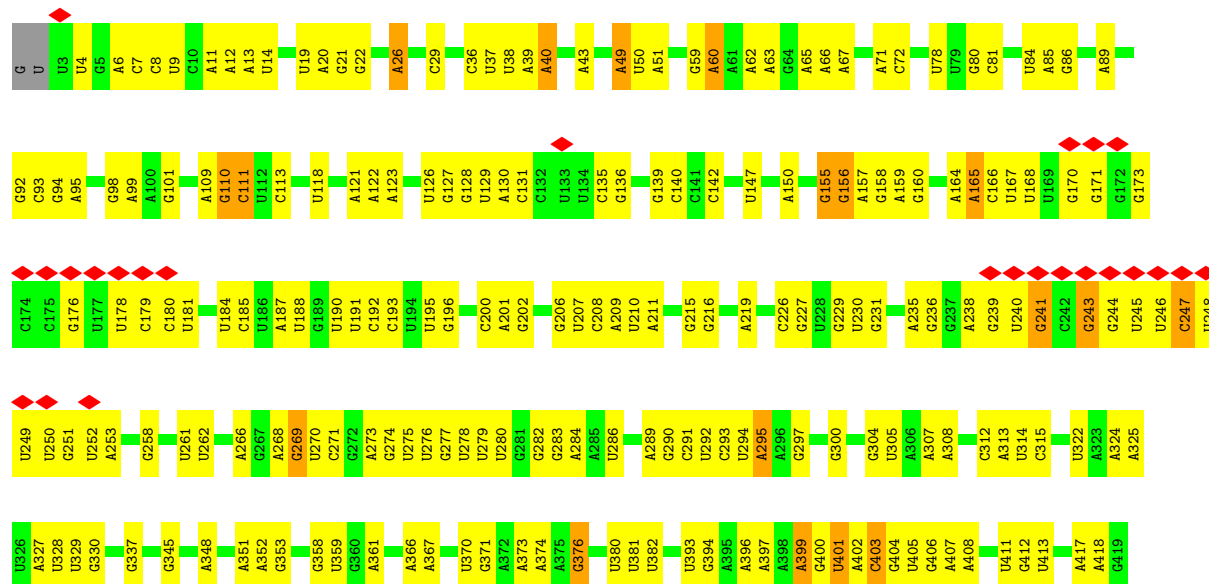
• Molecule 9: Ubiquitin-40S ribosomal protein S31



• Molecule 10: 60S ribosomal protein L16-A

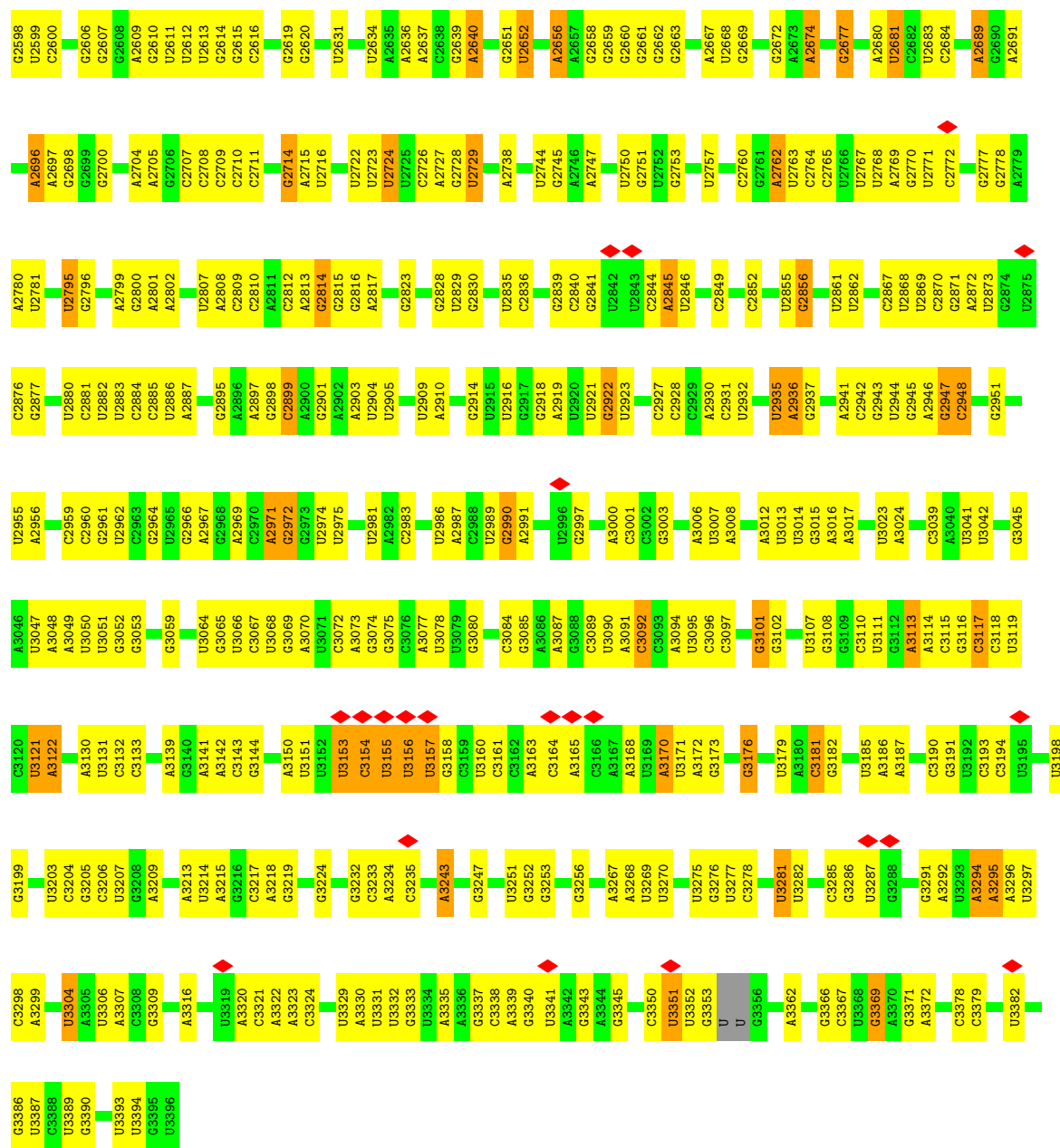


• Molecule 11: 25S ribosomal RNA

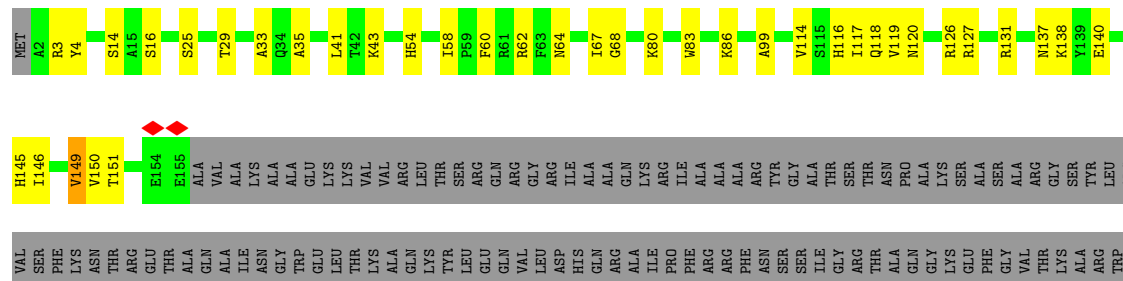
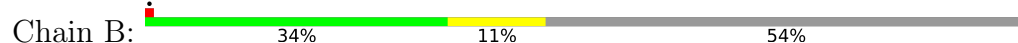


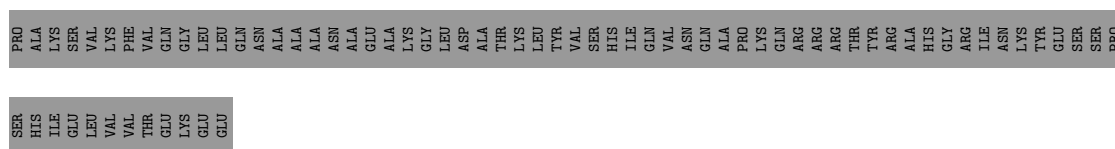




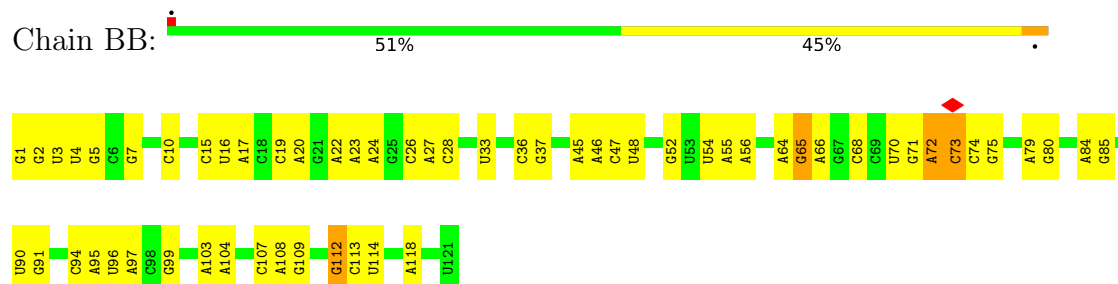


• Molecule 12: 60S ribosomal protein L17-A

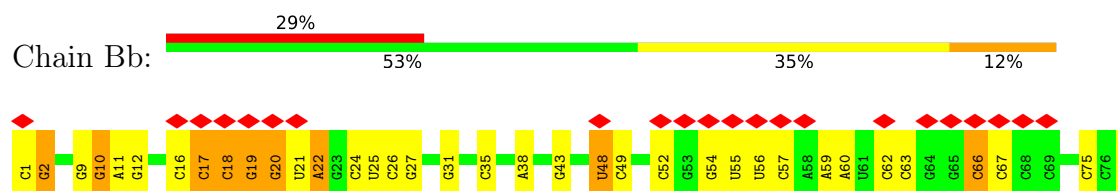




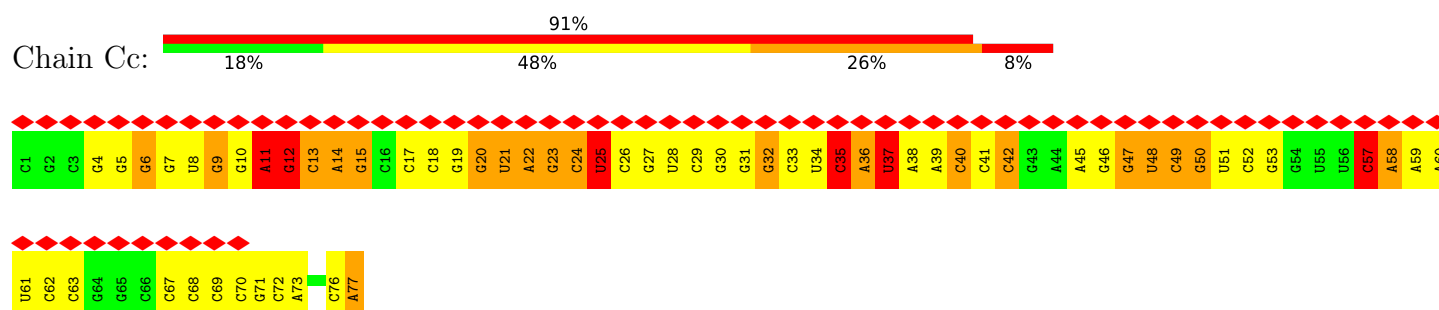
- Molecule 13: 5S ribosomal RNA



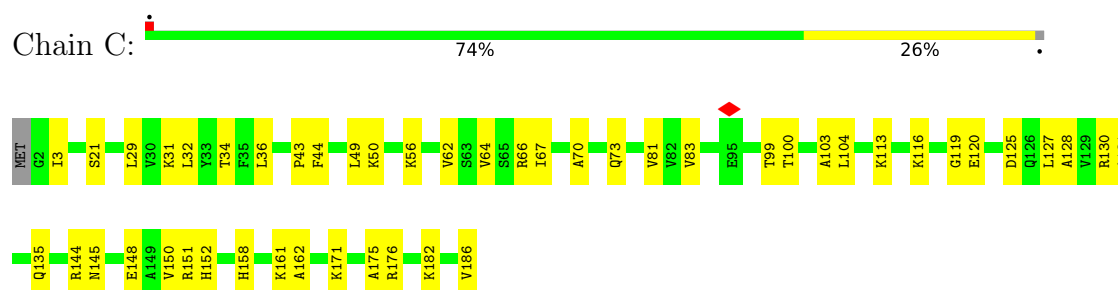
- Molecule 14: Transfer RNA fMet



- Molecule 14: Transfer RNA fMet

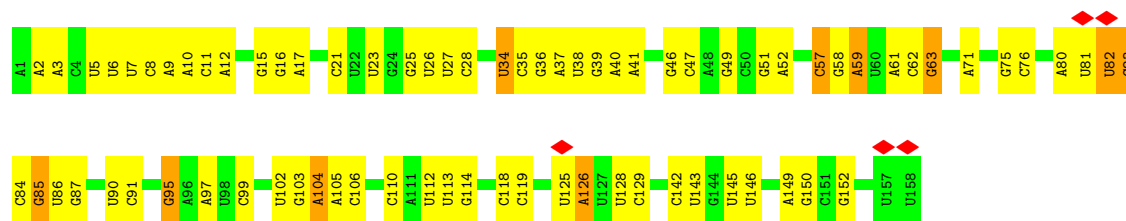


- Molecule 15: 60S ribosomal protein L18-A

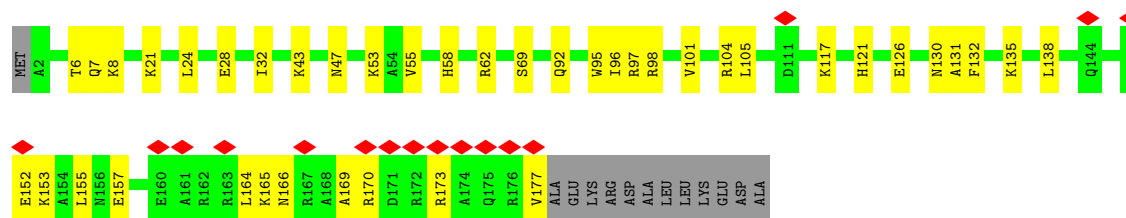


- Molecule 16: 5.8S ribosomal RNA

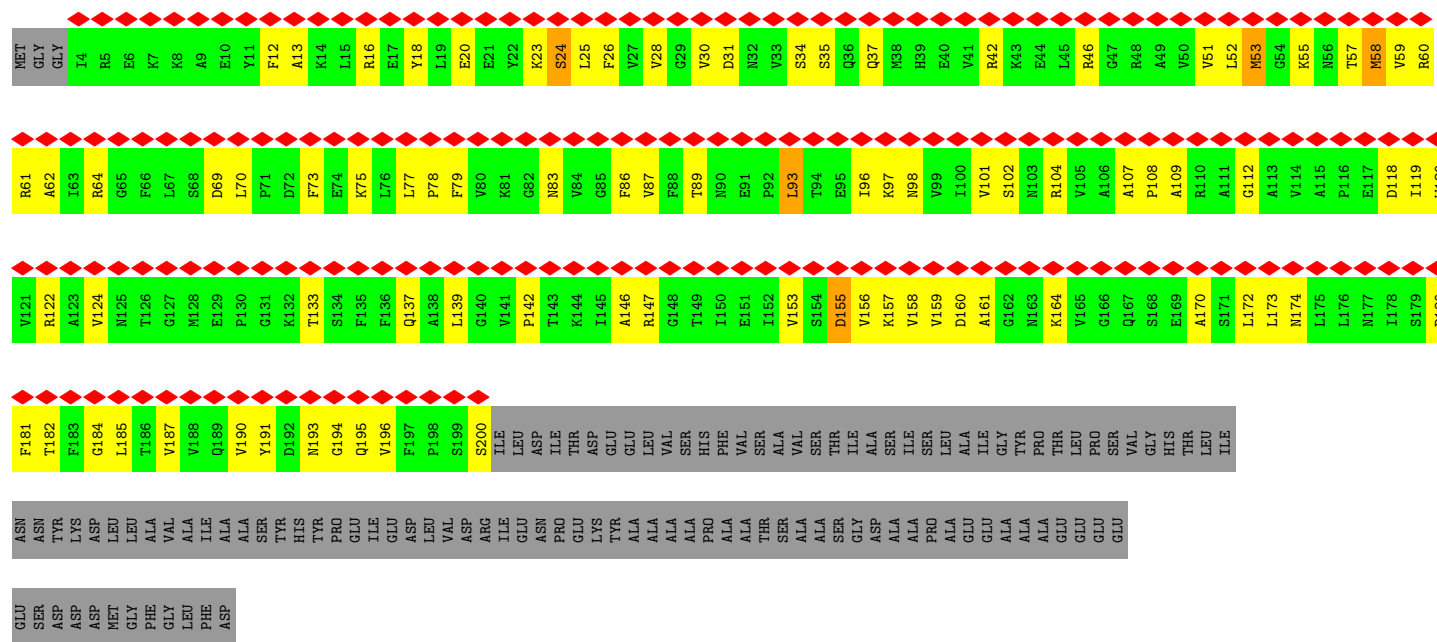




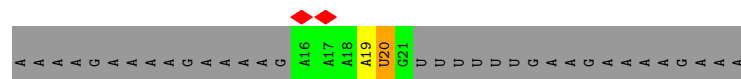
• Molecule 17: 60S ribosomal protein L19-A



• Molecule 18: 60S acidic ribosomal protein P0

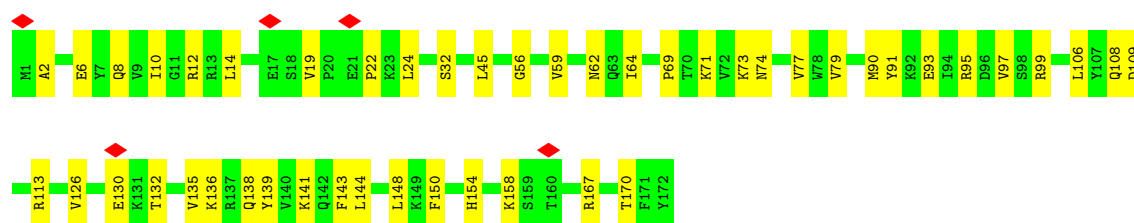


• Molecule 19: Messenger RNA



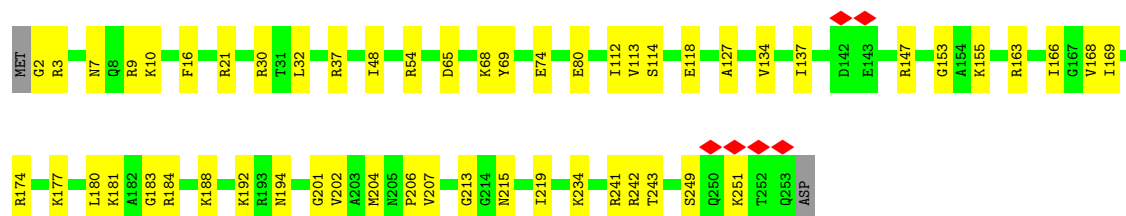
• Molecule 20: 60S ribosomal protein L20-A

Chain E:  73% 27%

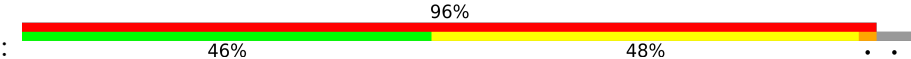


• Molecule 21: 60S ribosomal protein L2-A

Chain EE:  78% 21%



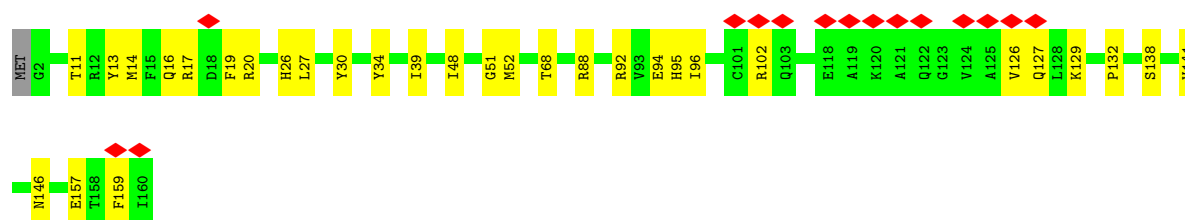
• Molecule 22: 60S ribosomal protein L12-A

Chain Ee:  46% 96% 48%



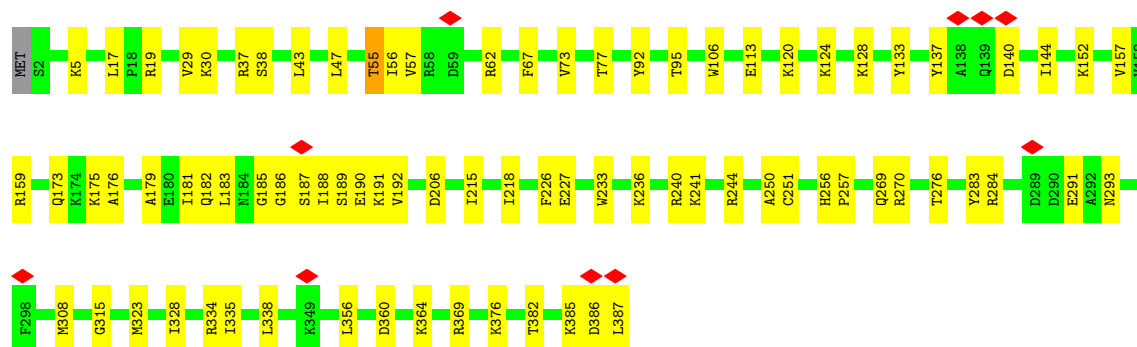
• Molecule 23: 60S ribosomal protein L21-A

Chain F:  9% 80% 19%

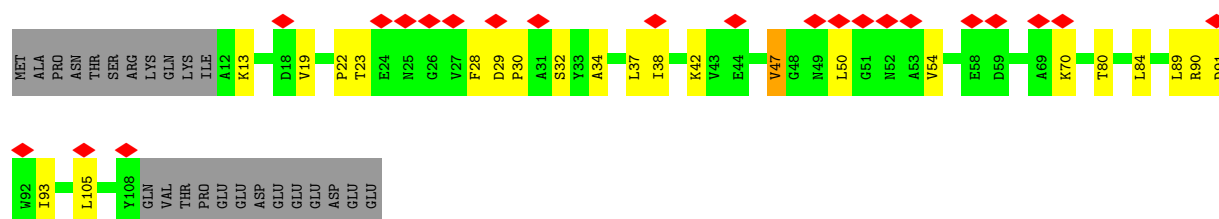


• Molecule 24: 60S ribosomal protein L3

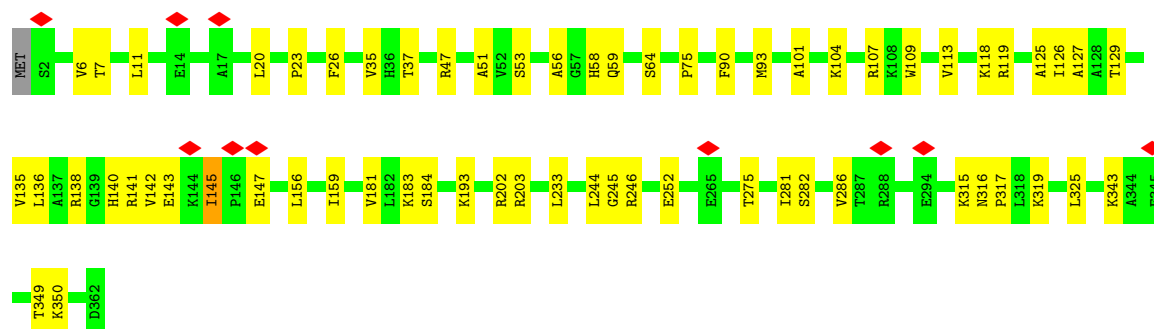
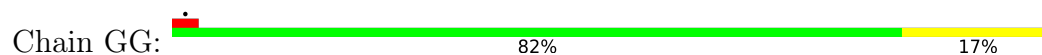
Chain FF:  79% 21%



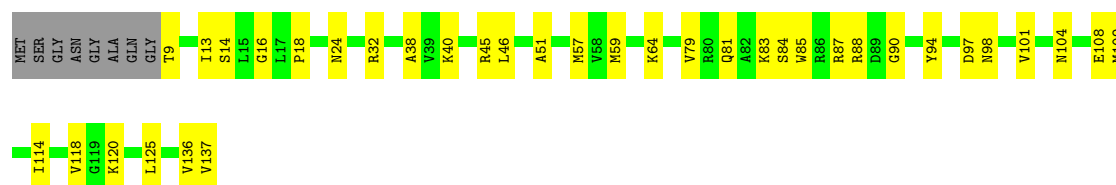
• Molecule 25: 60S ribosomal protein L22-A



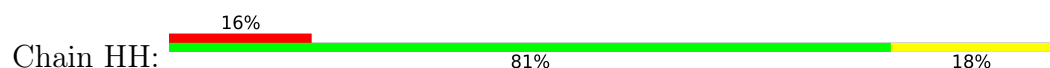
• Molecule 26: 60S ribosomal protein L4-A

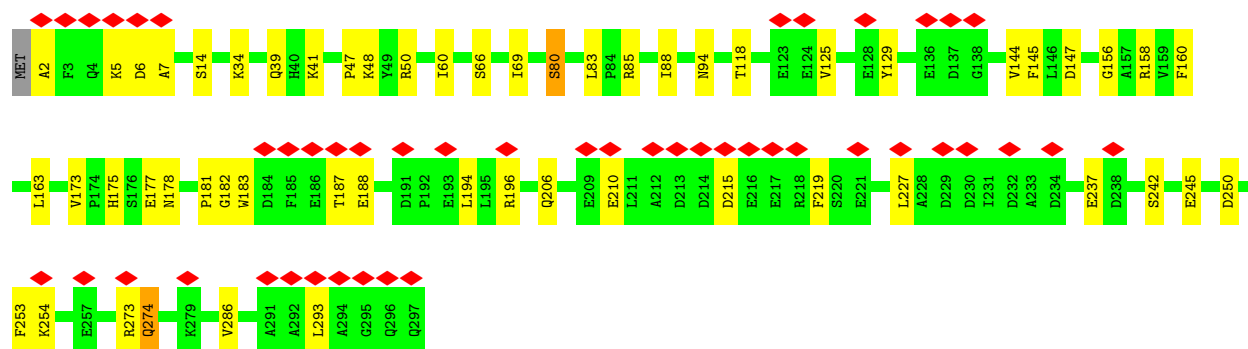


• Molecule 27: 60S ribosomal protein L23-A

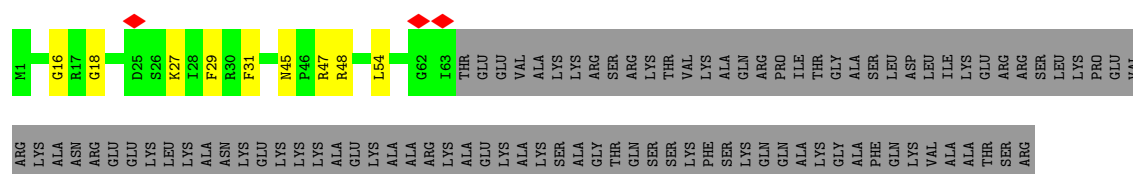
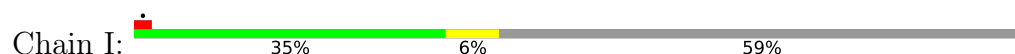


• Molecule 28: 60S ribosomal protein L5

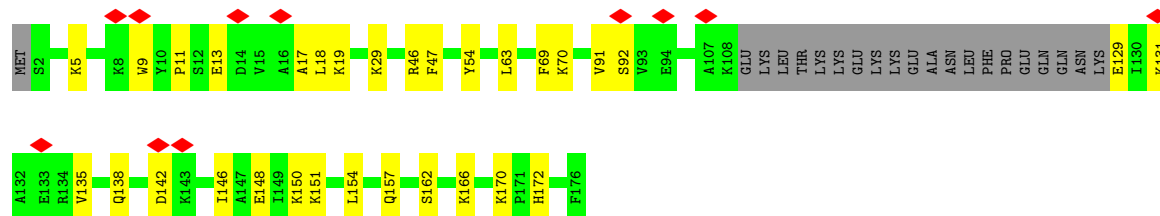




- Molecule 29: 60S ribosomal protein L24-A



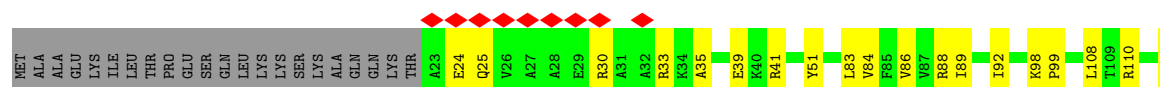
- Molecule 30: 60S ribosomal protein L6-A



- Molecule 31: 60S ribosomal protein L25

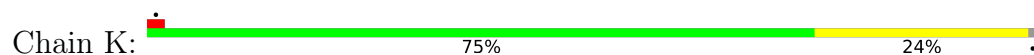


- Molecule 32: 60S ribosomal protein L7-A

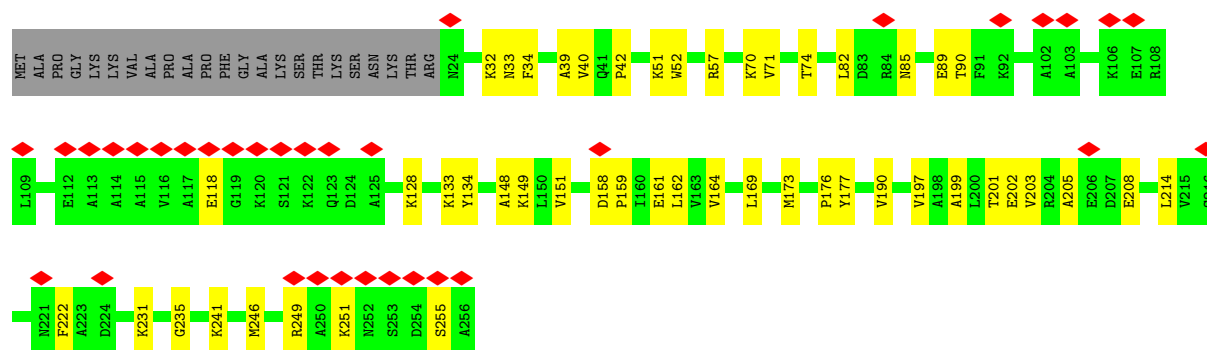
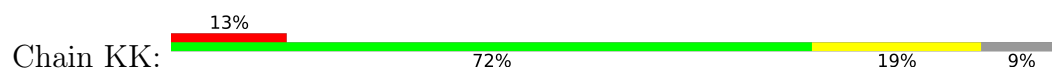




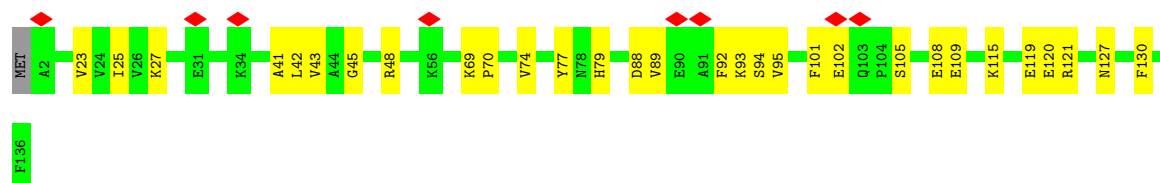
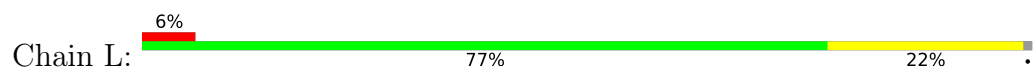
- Molecule 33: 60S ribosomal protein L26-A



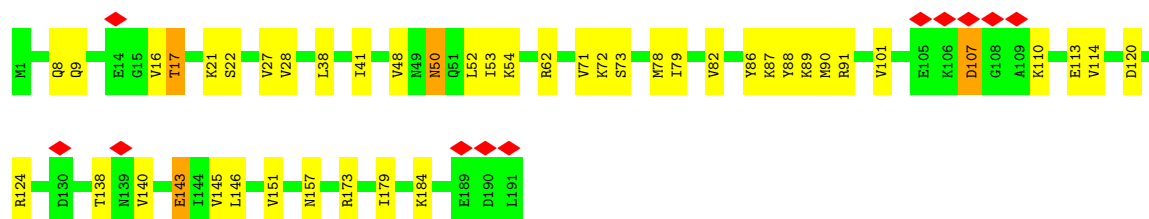
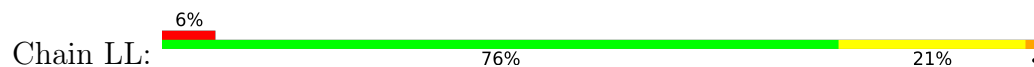
- Molecule 34: 60S ribosomal protein L8-A



- Molecule 35: 60S ribosomal protein L27-A

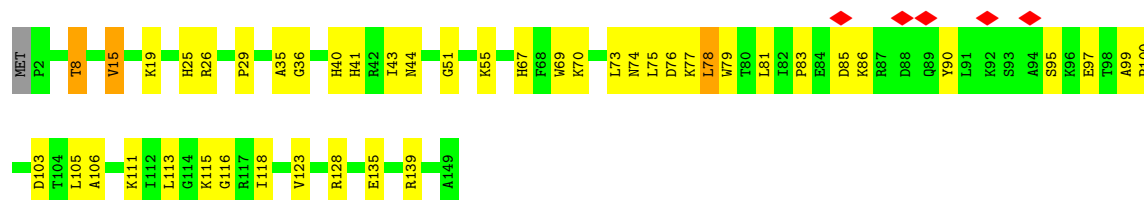


- Molecule 36: RPL9A isoform 1

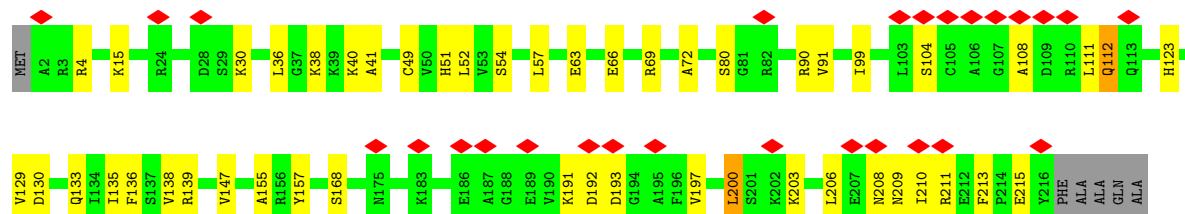
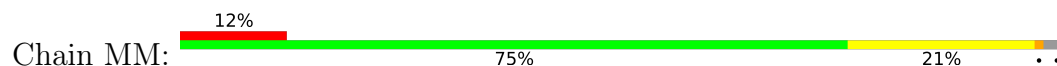


- Molecule 37: 60S ribosomal protein L28

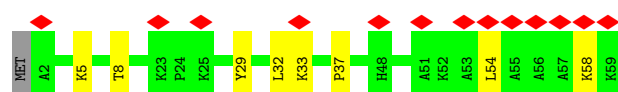
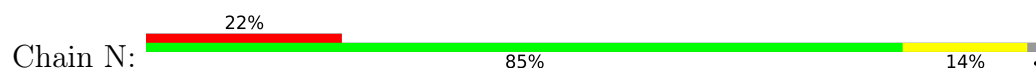




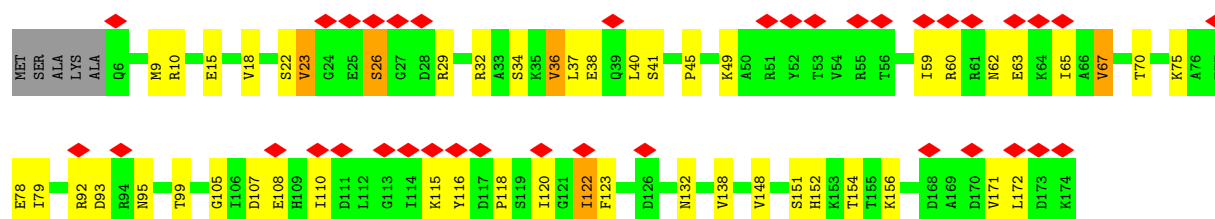
• Molecule 38: 60S ribosomal protein L10



• Molecule 39: 60S ribosomal protein L29



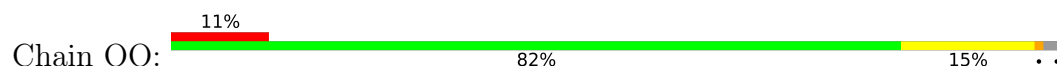
• Molecule 40: 60S ribosomal protein L11-A

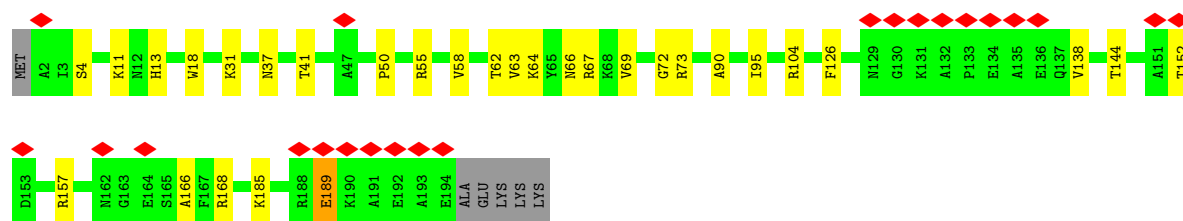


• Molecule 41: 60S ribosomal protein L30

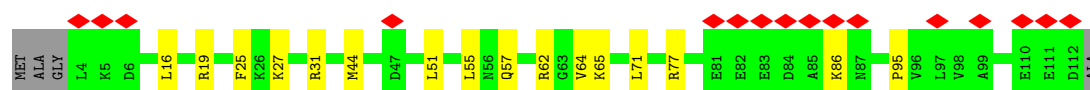
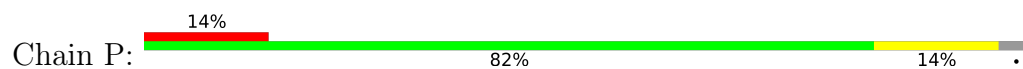


• Molecule 42: 60S ribosomal protein L13-A

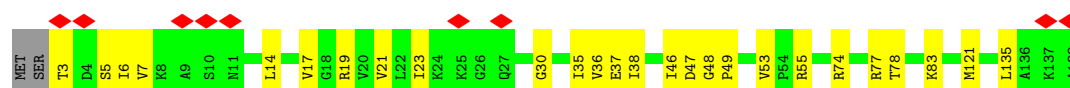
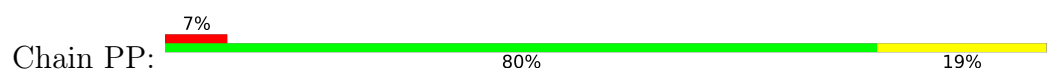




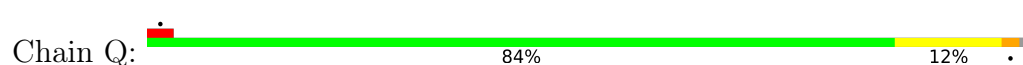
- Molecule 43: 60S ribosomal protein L31-A



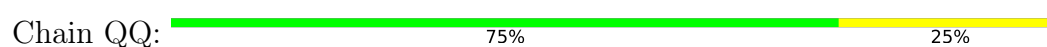
- Molecule 44: 60S ribosomal protein L14-A



- Molecule 45: 60S ribosomal protein L32



- Molecule 46: 60S ribosomal protein L15-A



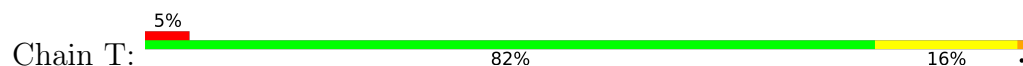
- Molecule 47: 60S ribosomal protein L33-A



- Molecule 48: 60S ribosomal protein L34-A



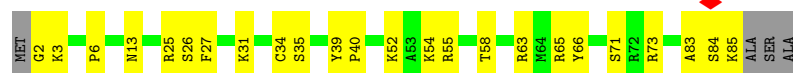
- Molecule 49: 60S ribosomal protein L35-A



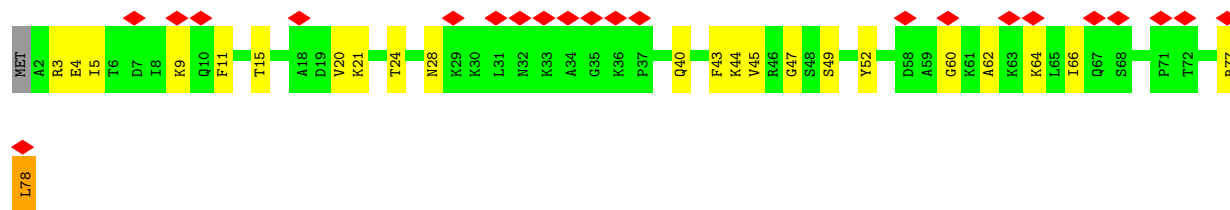
- Molecule 50: 60S ribosomal protein L36-A



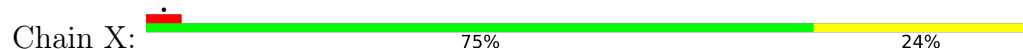
- Molecule 51: 60S ribosomal protein L37-A



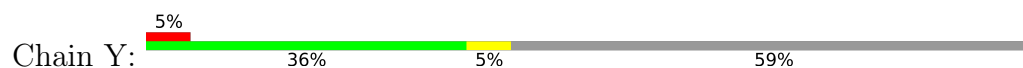
- Molecule 52: 60S ribosomal protein L38

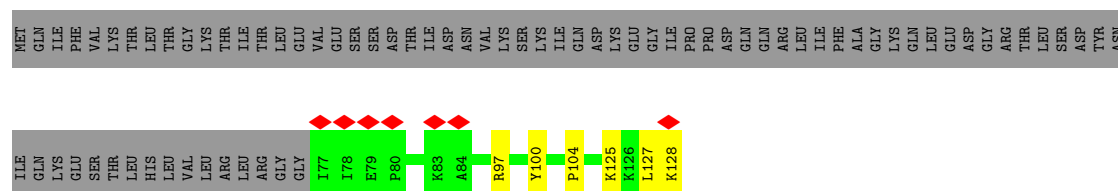


- Molecule 53: 60S ribosomal protein L39

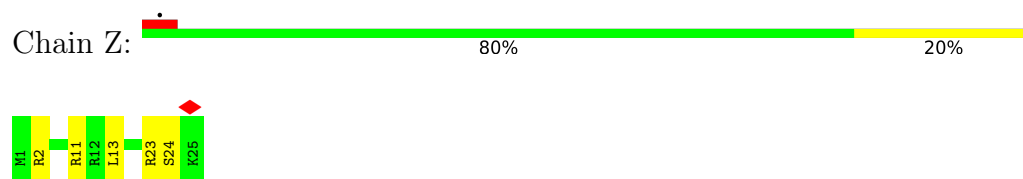


- Molecule 54: Ubiquitin-60S ribosomal protein L40

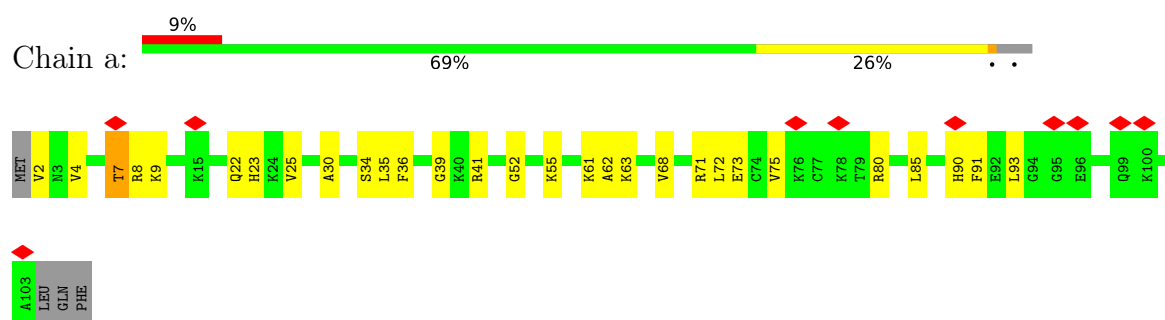




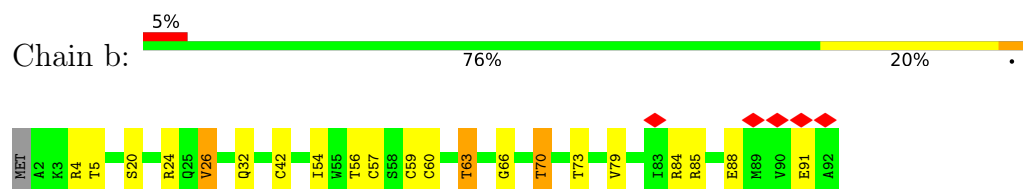
- Molecule 55: 60S ribosomal protein L41



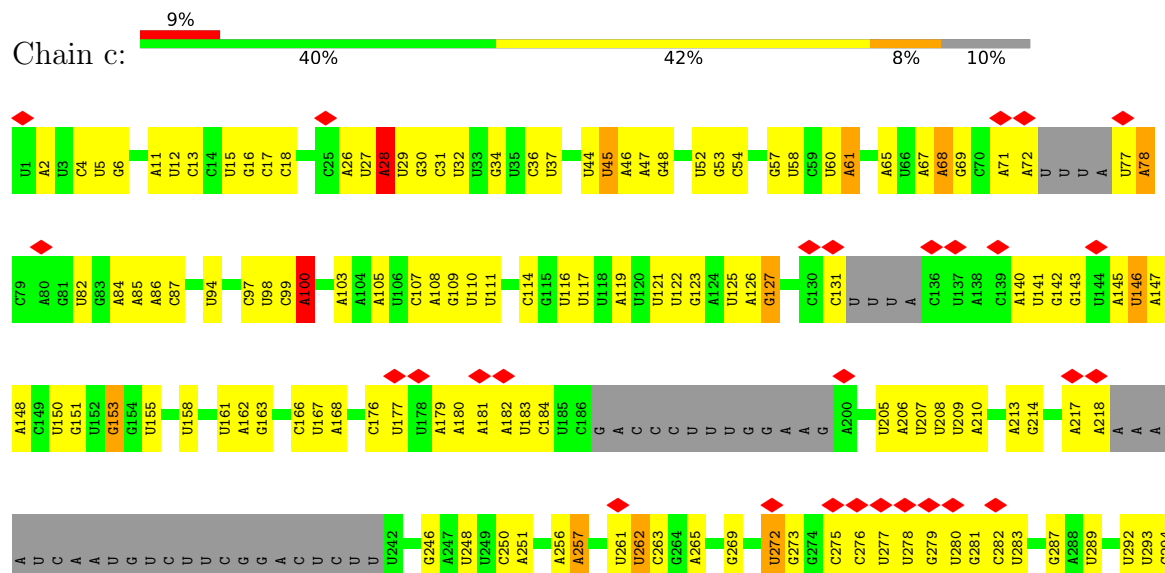
- Molecule 56: 60S ribosomal protein L42-A

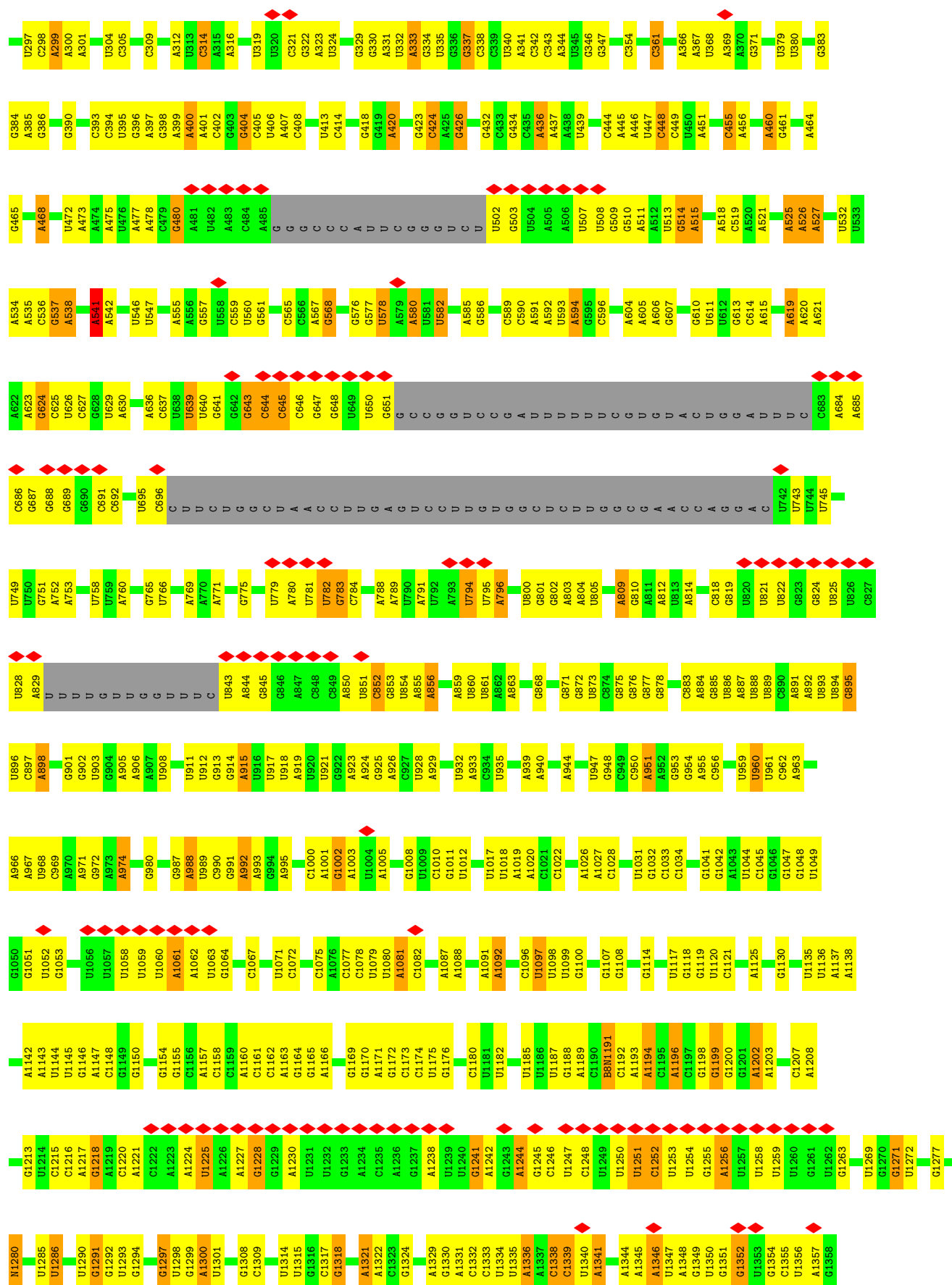


- Molecule 57: 60S ribosomal protein L43-A

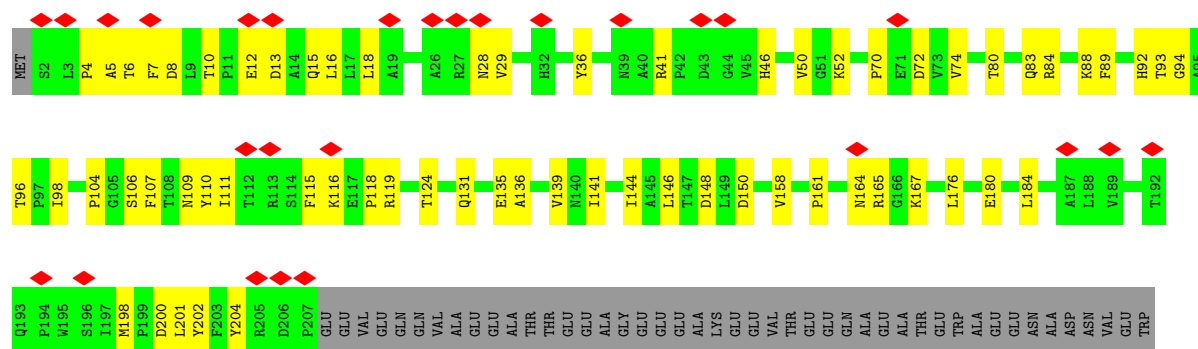


- Molecule 58: 18S ribosomal RNA

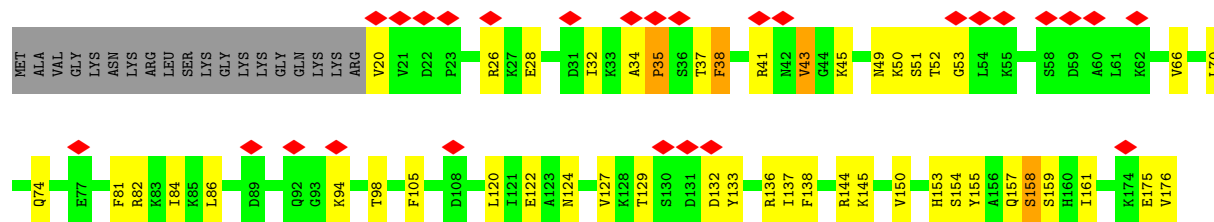


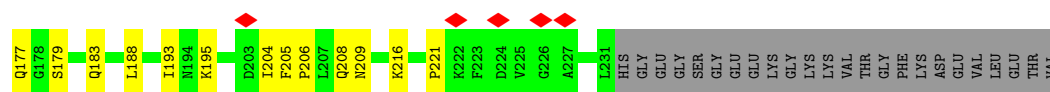


- Molecule 59: 40S ribosomal protein S0-A



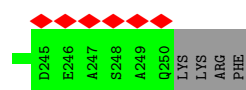
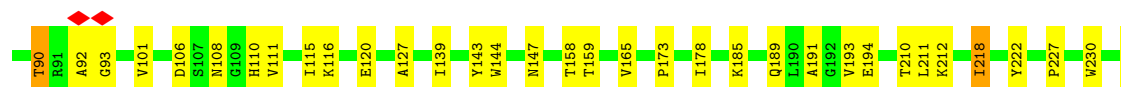
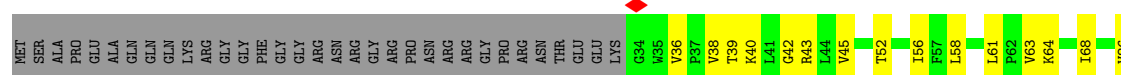
- Molecule 60: 40S ribosomal protein S1-A





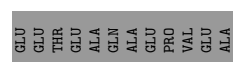
• Molecule 61: 40S ribosomal protein S2

Chain f: 66% 19% 15%



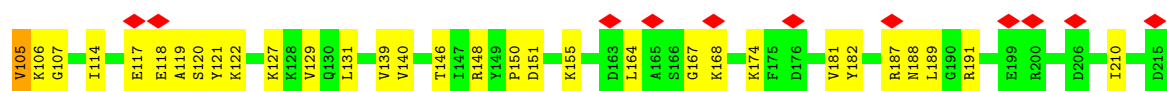
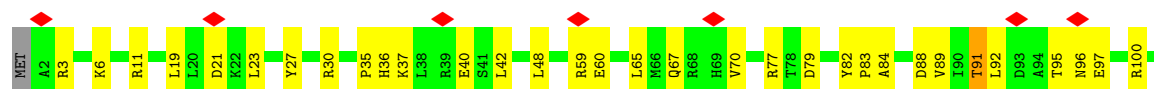
• Molecule 62: RPS3 isoform 1

Chain g: 24% 53% 30% 15%

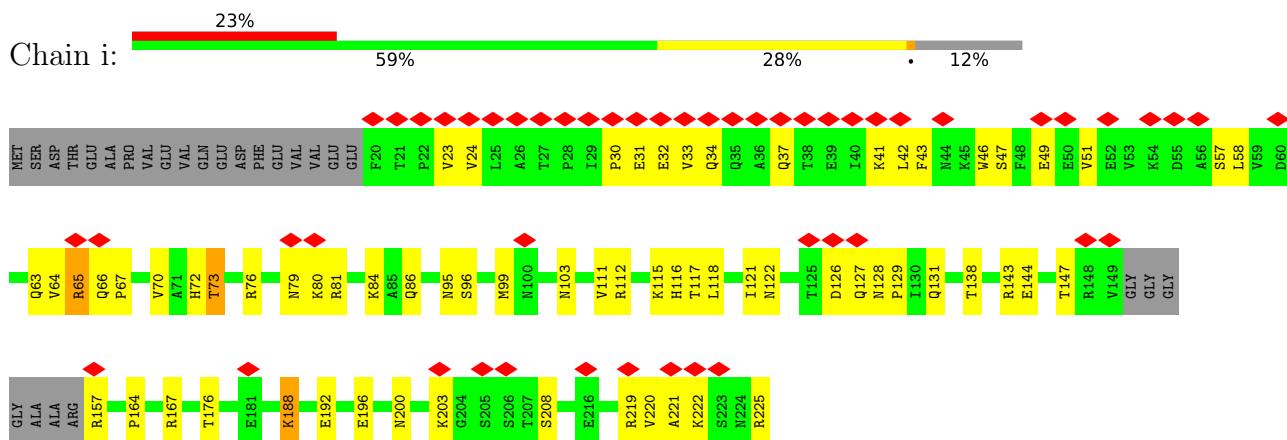


• Molecule 63: 40S ribosomal protein S4-A

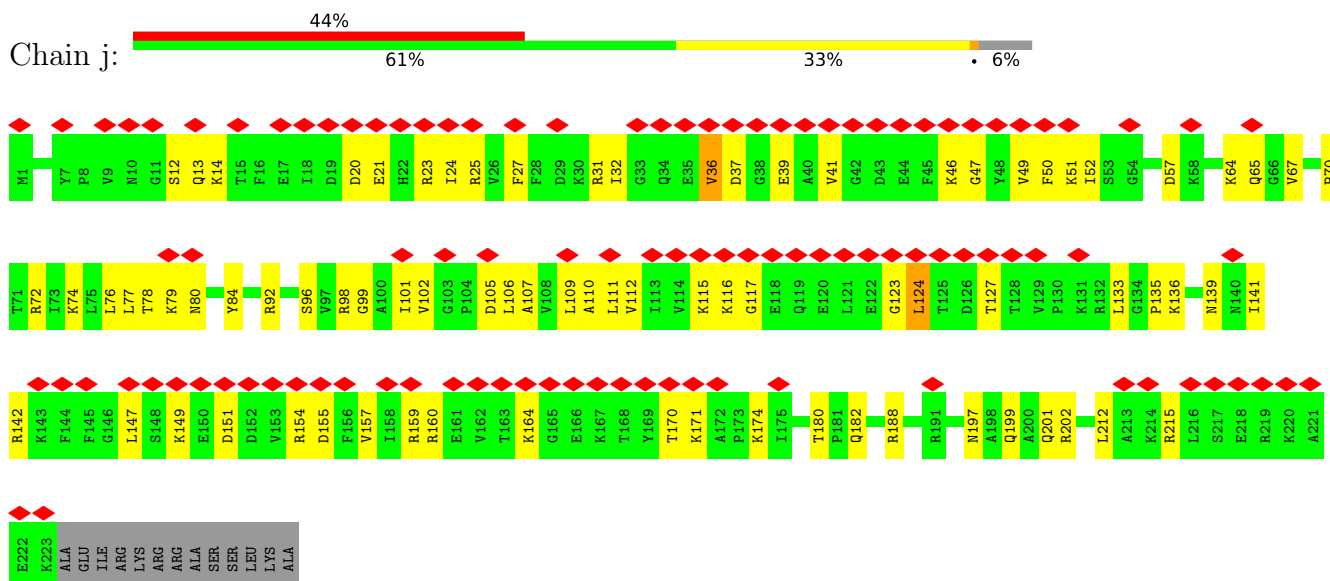
Chain h: 11% 72% 26%



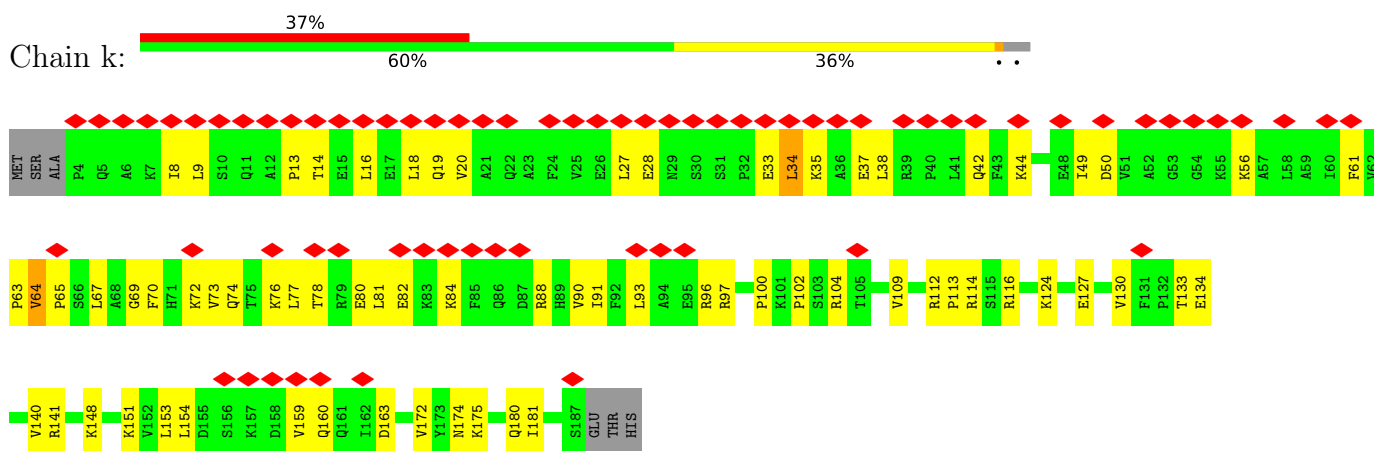
- Molecule 64: 40S ribosomal protein S5



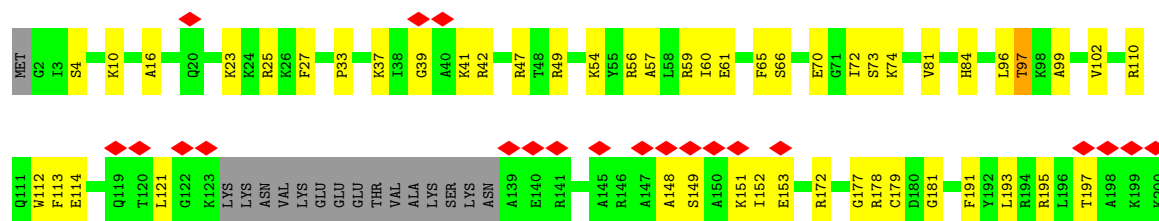
- Molecule 65: 40S ribosomal protein S6-A



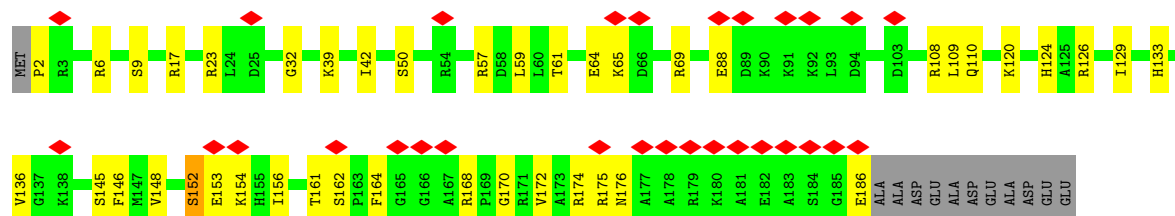
- Molecule 66: 40S ribosomal protein S7-A



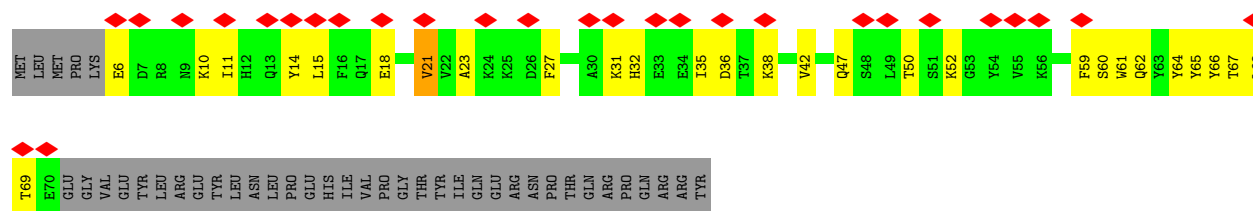
- Molecule 67: 40S ribosomal protein S8-B



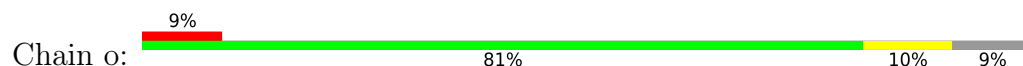
• Molecule 68: 40S ribosomal protein S9-A



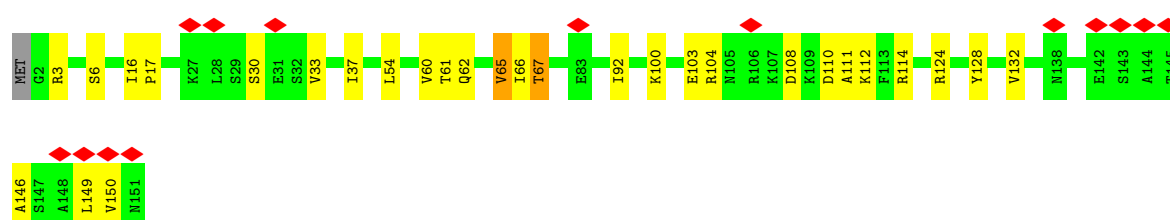
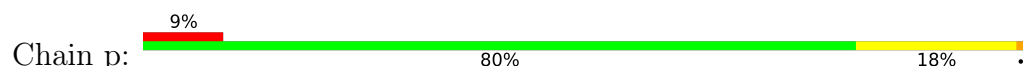
• Molecule 69: 40S ribosomal protein S10-A



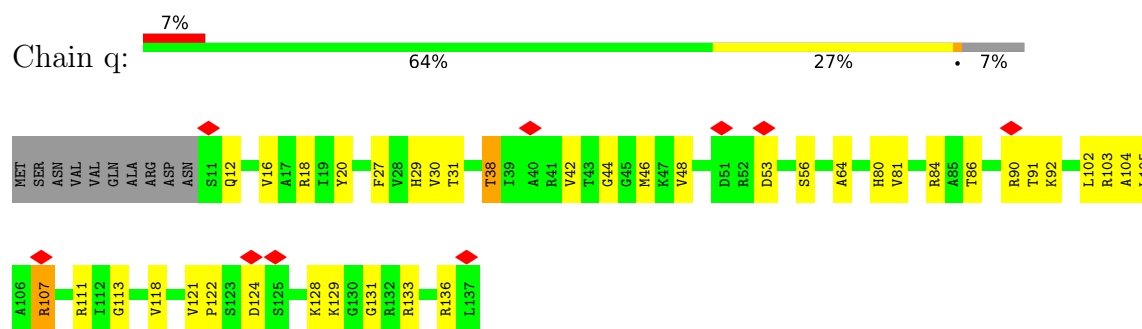
• Molecule 70: 40S ribosomal protein S11-A



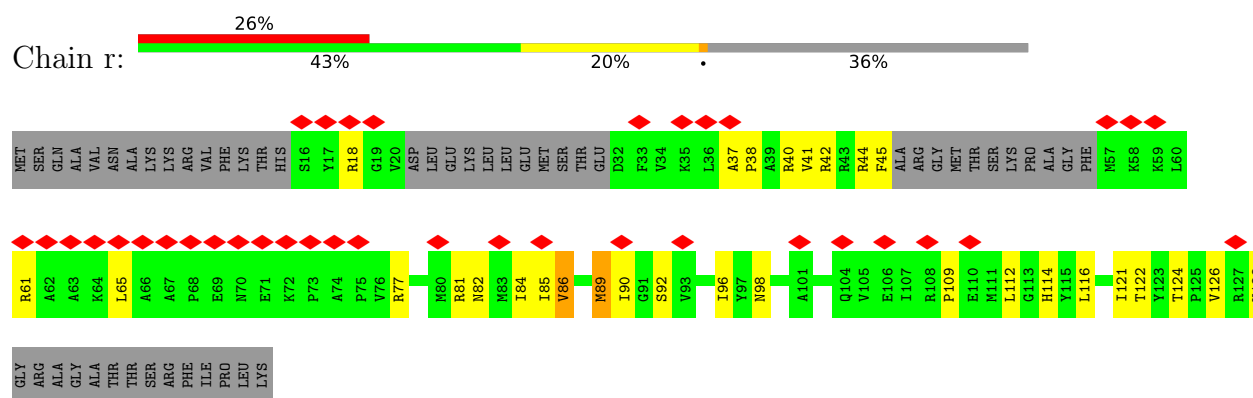
• Molecule 71: 40S ribosomal protein S13



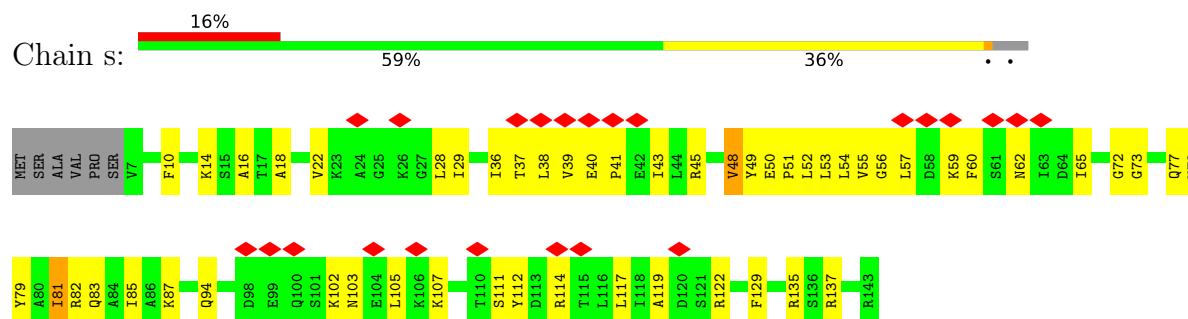
- Molecule 72: 40S ribosomal protein S14-A



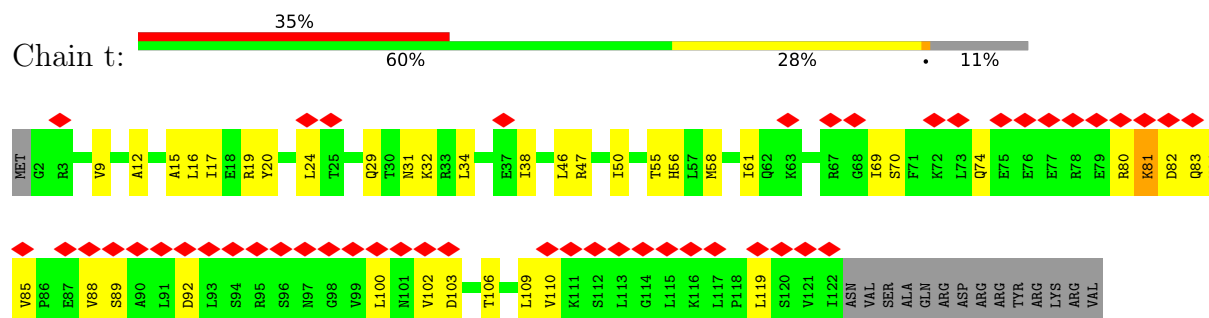
- Molecule 73: 40S ribosomal protein S15



- Molecule 74: 40S ribosomal protein S16-A

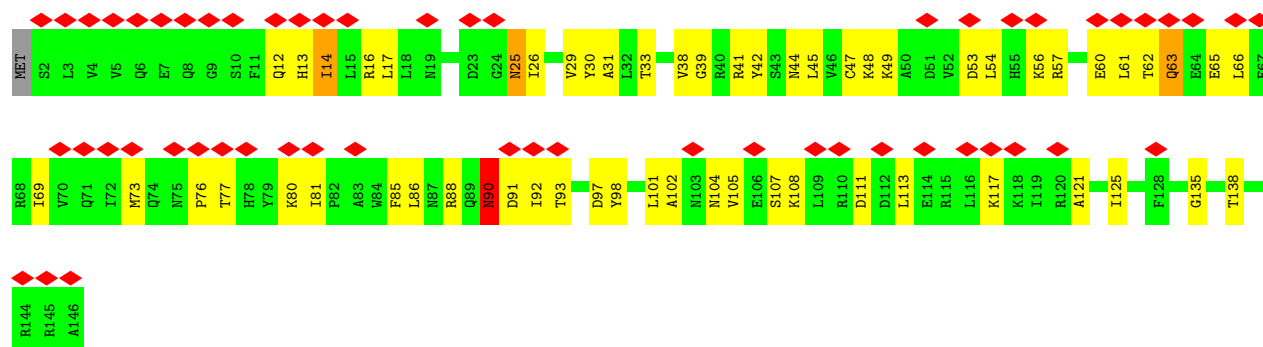


- Molecule 75: 40S ribosomal protein S17-A

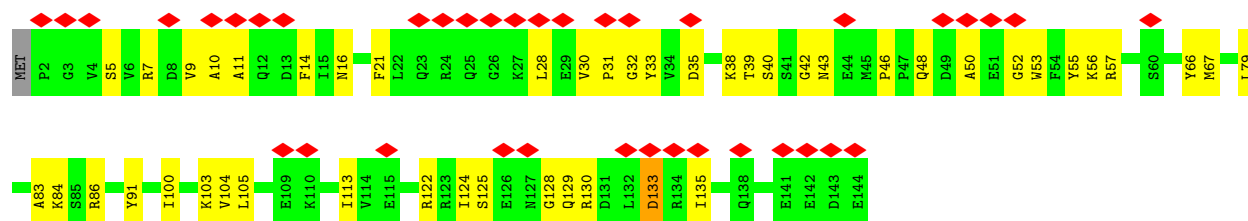


- Molecule 76: 40S ribosomal protein S18-A

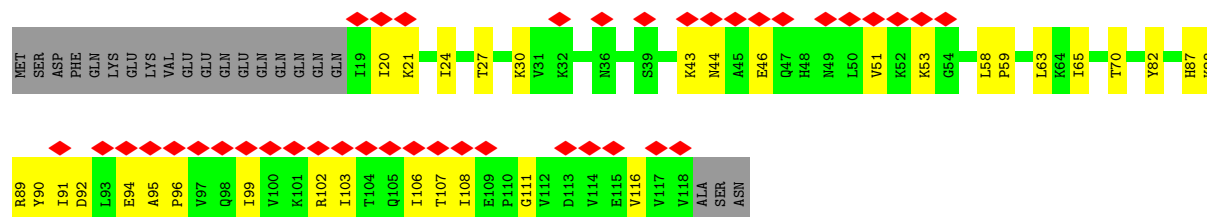




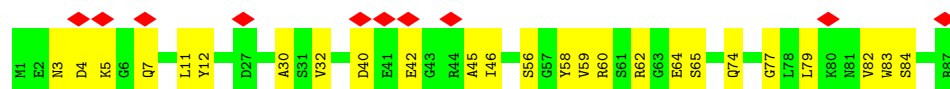
- Molecule 77: 40S ribosomal protein S19-A



- Molecule 78: 40S ribosomal protein S20



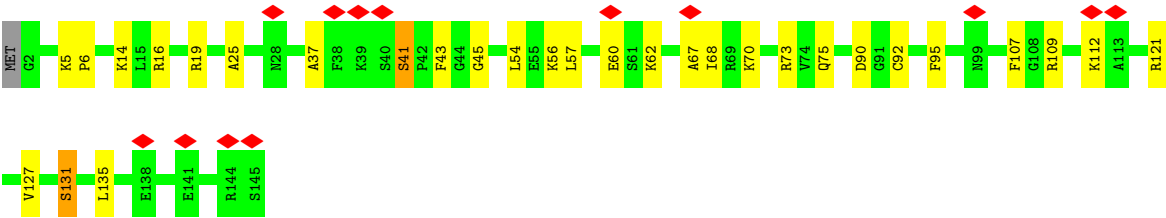
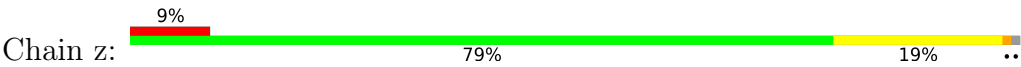
- Molecule 79: 40S ribosomal protein S21-A



- Molecule 80: 40S ribosomal protein S22-A



- Molecule 81: 40S ribosomal protein S23-A



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 21458                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 1000                                    | Depositor |
| Magnification                        | 270000                                  | Depositor |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.688                                   | Depositor |
| Minimum map value                    | -0.693                                  | Depositor |
| Average map value                    | -0.001                                  | Depositor |
| Map value standard deviation         | 0.055                                   | Depositor |
| Recommended contour level            | 0.249                                   | Depositor |
| Map size (Å)                         | 540.0, 540.0, 540.0                     | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.9, 0.9, 0.9                           | 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, A2M, B8N, OMU, K, 1MA, MA6, 5MC, OMG, SPD, G7M, UR3, 4AC, OMC, ZN

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   | 0     | 0.13         | 0/1087        | 0.31        | 0/1449        |
| 2   | 1     | 0.22         | 0/571         | 0.63        | 3/768 (0.4%)  |
| 3   | 2     | 0.11         | 0/782         | 0.36        | 0/1047        |
| 4   | 3     | 0.10         | 0/620         | 0.37        | 0/838         |
| 5   | 4     | 0.15         | 0/499         | 0.39        | 0/670         |
| 6   | 5     | 0.11         | 0/412         | 0.28        | 0/544         |
| 7   | 6     | 0.11         | 0/433         | 0.35        | 0/575         |
| 8   | 7     | 0.15         | 0/2489        | 0.44        | 0/3389        |
| 9   | 8     | 0.12         | 0/279         | 0.44        | 0/369         |
| 10  | A     | 0.14         | 0/1585        | 0.34        | 0/2128        |
| 11  | AA    | 0.14         | 0/75545       | 0.28        | 0/117782      |
| 12  | B     | 0.15         | 0/1245        | 0.31        | 0/1676        |
| 13  | BB    | 0.10         | 0/2883        | 0.23        | 0/4491        |
| 14  | Bb    | 0.11         | 0/1836        | 0.26        | 0/2859        |
| 14  | Cc    | 0.41         | 5/1836 (0.3%) | 0.52        | 3/2859 (0.1%) |
| 15  | C     | 0.11         | 0/1465        | 0.29        | 0/1965        |
| 16  | CC    | 0.11         | 0/3746        | 0.27        | 0/5832        |
| 17  | D     | 0.13         | 0/1440        | 0.31        | 0/1921        |
| 18  | DD    | 0.17         | 0/1558        | 0.50        | 2/2107 (0.1%) |
| 19  | Dd    | 0.17         | 0/147         | 0.46        | 0/227         |
| 20  | E     | 0.12         | 0/1481        | 0.36        | 0/1990        |
| 21  | EE    | 0.11         | 0/1948        | 0.31        | 0/2617        |
| 22  | Ee    | 0.22         | 0/1210        | 0.52        | 0/1627        |
| 23  | F     | 0.12         | 0/1300        | 0.32        | 0/1743        |
| 24  | FF    | 0.12         | 0/3146        | 0.34        | 0/4228        |
| 25  | G     | 0.11         | 0/786         | 0.33        | 0/1065        |
| 26  | GG    | 0.11         | 0/2800        | 0.32        | 0/3790        |
| 27  | H     | 0.11         | 0/978         | 0.31        | 0/1316        |
| 28  | HH    | 0.10         | 0/2425        | 0.29        | 0/3271        |
| 29  | I     | 0.11         | 0/533         | 0.28        | 0/707         |
| 30  | II    | 0.12         | 0/1251        | 0.31        | 0/1682        |
| 31  | J     | 0.11         | 0/974         | 0.31        | 0/1314        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 32  | JJ    | 0.13         | 0/1821  | 0.33        | 0/2451        |
| 33  | K     | 0.11         | 0/1004  | 0.27        | 0/1341        |
| 34  | KK    | 0.12         | 0/1836  | 0.31        | 0/2481        |
| 35  | L     | 0.12         | 0/1118  | 0.31        | 0/1497        |
| 36  | LL    | 0.13         | 0/1539  | 0.35        | 0/2073        |
| 37  | M     | 0.12         | 0/1204  | 0.35        | 0/1612        |
| 38  | MM    | 0.11         | 0/1779  | 0.30        | 0/2386        |
| 39  | N     | 0.11         | 0/473   | 0.29        | 0/629         |
| 40  | NN    | 0.13         | 0/1374  | 0.35        | 0/1842        |
| 41  | O     | 0.09         | 0/750   | 0.25        | 0/1008        |
| 42  | OO    | 0.13         | 0/1568  | 0.36        | 0/2106        |
| 43  | P     | 0.12         | 0/897   | 0.31        | 0/1205        |
| 44  | PP    | 0.10         | 0/1068  | 0.27        | 0/1438        |
| 45  | Q     | 0.11         | 0/1041  | 0.28        | 0/1394        |
| 46  | QQ    | 0.12         | 0/1757  | 0.34        | 0/2354        |
| 47  | R     | 0.13         | 0/868   | 0.32        | 0/1168        |
| 48  | S     | 0.12         | 0/871   | 0.29        | 0/1164        |
| 49  | T     | 0.11         | 0/978   | 0.29        | 0/1301        |
| 50  | U     | 0.13         | 0/778   | 0.35        | 0/1034        |
| 51  | V     | 0.14         | 0/680   | 0.36        | 0/901         |
| 52  | W     | 0.13         | 0/618   | 0.35        | 0/826         |
| 53  | X     | 0.13         | 0/443   | 0.40        | 0/588         |
| 54  | Y     | 0.08         | 0/423   | 0.27        | 0/562         |
| 55  | Z     | 0.13         | 0/234   | 0.24        | 0/300         |
| 56  | a     | 0.13         | 0/831   | 0.40        | 0/1097        |
| 57  | b     | 0.12         | 0/701   | 0.36        | 0/934         |
| 58  | c     | 0.14         | 0/38143 | 0.28        | 0/59408       |
| 59  | d     | 0.12         | 0/1623  | 0.35        | 0/2222        |
| 60  | e     | 0.14         | 0/1714  | 0.39        | 0/2308        |
| 61  | f     | 0.13         | 0/1665  | 0.38        | 0/2263        |
| 62  | g     | 0.15         | 0/1614  | 0.37        | 0/2169        |
| 63  | h     | 0.12         | 0/2097  | 0.32        | 0/2823        |
| 64  | i     | 0.14         | 0/1591  | 0.41        | 2/2151 (0.1%) |
| 65  | j     | 0.11         | 0/1822  | 0.31        | 0/2434        |
| 66  | k     | 0.13         | 0/1506  | 0.39        | 0/2028        |
| 67  | l     | 0.15         | 0/1482  | 0.37        | 0/1980        |
| 68  | m     | 0.11         | 0/1519  | 0.32        | 0/2035        |
| 69  | n     | 0.14         | 0/569   | 0.44        | 0/767         |
| 70  | o     | 0.10         | 0/1172  | 0.29        | 0/1580        |
| 71  | p     | 0.11         | 0/1215  | 0.30        | 0/1638        |
| 72  | q     | 0.15         | 0/901   | 0.44        | 1/1217 (0.1%) |
| 73  | r     | 0.14         | 0/747   | 0.38        | 0/1002        |
| 74  | s     | 0.17         | 0/1099  | 0.49        | 0/1473        |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 75  | t     | 0.14         | 0/971           | 0.44        | 0/1303           |
| 76  | u     | 0.15         | 0/1211          | 0.41        | 0/1628           |
| 77  | v     | 0.13         | 0/1130          | 0.34        | 0/1517           |
| 78  | w     | 0.15         | 0/810           | 0.40        | 0/1095           |
| 79  | x     | 0.13         | 0/693           | 0.41        | 0/935            |
| 80  | y     | 0.15         | 0/1038          | 0.37        | 0/1395           |
| 81  | z     | 0.11         | 0/1139          | 0.35        | 0/1518           |
| All | All   | 0.14         | 5/213415 (0.0%) | 0.31        | 11/313427 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | 1     | 0                   | 1                   |
| 18  | DD    | 0                   | 1                   |
| 32  | JJ    | 0                   | 1                   |
| 35  | L     | 0                   | 1                   |
| 56  | a     | 0                   | 1                   |
| 60  | e     | 0                   | 2                   |
| 64  | i     | 0                   | 1                   |
| 66  | k     | 0                   | 1                   |
| 72  | q     | 0                   | 1                   |
| 74  | s     | 0                   | 1                   |
| 76  | u     | 0                   | 1                   |
| All | All   | 0                   | 12                  |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 14  | Cc    | 37  | U    | C1'-N1 | 6.19  | 1.57        | 1.48     |
| 14  | Cc    | 25  | U    | C1'-N1 | 5.98  | 1.57        | 1.48     |
| 14  | Cc    | 24  | C    | C1'-N1 | 5.73  | 1.57        | 1.48     |
| 14  | Cc    | 35  | C    | C1'-N1 | 5.63  | 1.56        | 1.48     |
| 14  | Cc    | 11  | A    | C1'-N9 | -5.07 | 1.40        | 1.48     |

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

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | Cc    | 57  | C    | O4'-C1'-C2' | -6.43 | 99.37       | 105.80   |
| 2   | 1     | 53  | GLU  | CA-C-N      | 6.29  | 124.20      | 120.24   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | 1     | 53  | GLU  | C-N-CA | 6.29  | 124.20      | 120.24   |
| 64  | i     | 219 | ARG  | CA-C-N | -5.67 | 116.32      | 121.65   |
| 64  | i     | 219 | ARG  | C-N-CA | -5.67 | 116.32      | 121.65   |

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | 1     | 68  | ARG  | Sidechain |
| 18  | DD    | 20  | GLU  | Peptide   |
| 32  | JJ    | 232 | ARG  | Peptide   |
| 35  | L     | 102 | GLU  | Peptide   |
| 56  | a     | 7   | THR  | Peptide   |

## 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   | 0     | 1073  | 0        | 1132     | 39      | 0            |
| 2   | 1     | 563   | 0        | 603      | 25      | 0            |
| 3   | 2     | 769   | 0        | 814      | 23      | 0            |
| 4   | 3     | 610   | 0        | 633      | 9       | 0            |
| 5   | 4     | 497   | 0        | 535      | 11      | 0            |
| 6   | 5     | 404   | 0        | 398      | 7       | 0            |
| 7   | 6     | 427   | 0        | 476      | 11      | 0            |
| 8   | 7     | 2436  | 0        | 2386     | 99      | 0            |
| 9   | 8     | 276   | 0        | 289      | 5       | 0            |
| 10  | A     | 1555  | 0        | 1659     | 31      | 0            |
| 11  | AA    | 68429 | 0        | 34441    | 1215    | 0            |
| 12  | B     | 1222  | 0        | 1231     | 25      | 0            |
| 13  | BB    | 2579  | 0        | 1304     | 48      | 0            |
| 14  | Bb    | 1644  | 0        | 836      | 17      | 0            |
| 14  | Cc    | 1644  | 0        | 837      | 95      | 0            |
| 15  | C     | 1441  | 0        | 1543     | 32      | 0            |
| 16  | CC    | 3353  | 0        | 1695     | 57      | 0            |
| 17  | D     | 1423  | 0        | 1510     | 29      | 0            |
| 18  | DD    | 1531  | 0        | 1571     | 66      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | Dd    | 131   | 0        | 66       | 4       | 0            |
| 20  | E     | 1445  | 0        | 1487     | 37      | 0            |
| 21  | EE    | 1914  | 0        | 1981     | 42      | 0            |
| 22  | Ee    | 1196  | 0        | 1257     | 66      | 0            |
| 23  | F     | 1276  | 0        | 1323     | 22      | 0            |
| 24  | FF    | 3075  | 0        | 3142     | 60      | 0            |
| 25  | G     | 770   | 0        | 780      | 15      | 0            |
| 26  | GG    | 2748  | 0        | 2859     | 46      | 0            |
| 27  | H     | 963   | 0        | 1015     | 24      | 0            |
| 28  | HH    | 2375  | 0        | 2325     | 38      | 0            |
| 29  | I     | 521   | 0        | 551      | 6       | 0            |
| 30  | II    | 1230  | 0        | 1320     | 20      | 0            |
| 31  | J     | 959   | 0        | 1023     | 17      | 0            |
| 32  | JJ    | 1784  | 0        | 1862     | 28      | 0            |
| 33  | K     | 993   | 0        | 1081     | 21      | 0            |
| 34  | KK    | 1804  | 0        | 1877     | 29      | 0            |
| 35  | L     | 1092  | 0        | 1155     | 17      | 0            |
| 36  | LL    | 1518  | 0        | 1587     | 30      | 0            |
| 37  | M     | 1173  | 0        | 1215     | 38      | 0            |
| 38  | MM    | 1743  | 0        | 1785     | 34      | 0            |
| 39  | N     | 462   | 0        | 491      | 8       | 0            |
| 40  | NN    | 1353  | 0        | 1383     | 41      | 0            |
| 41  | O     | 742   | 0        | 797      | 14      | 0            |
| 42  | OO    | 1543  | 0        | 1608     | 22      | 0            |
| 43  | P     | 883   | 0        | 918      | 13      | 0            |
| 44  | PP    | 1053  | 0        | 1149     | 19      | 0            |
| 45  | Q     | 1020  | 0        | 1090     | 15      | 0            |
| 46  | QQ    | 1720  | 0        | 1779     | 42      | 0            |
| 47  | R     | 850   | 0        | 880      | 12      | 0            |
| 48  | S     | 861   | 0        | 918      | 15      | 0            |
| 49  | T     | 969   | 0        | 1078     | 24      | 0            |
| 50  | U     | 771   | 0        | 849      | 15      | 0            |
| 51  | V     | 665   | 0        | 668      | 20      | 0            |
| 52  | W     | 612   | 0        | 682      | 20      | 0            |
| 53  | X     | 436   | 0        | 475      | 11      | 0            |
| 54  | Y     | 417   | 0        | 455      | 5       | 0            |
| 55  | Z     | 233   | 0        | 284      | 7       | 0            |
| 56  | a     | 819   | 0        | 886      | 30      | 0            |
| 57  | b     | 694   | 0        | 734      | 15      | 0            |
| 58  | c     | 34663 | 0        | 17463    | 704     | 0            |
| 59  | d     | 1583  | 0        | 1578     | 46      | 0            |
| 60  | e     | 1689  | 0        | 1763     | 49      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61  | f     | 1635  | 0        | 1723     | 37      | 0            |
| 62  | g     | 1593  | 0        | 1671     | 51      | 0            |
| 63  | h     | 2056  | 0        | 2140     | 50      | 0            |
| 64  | i     | 1572  | 0        | 1639     | 57      | 0            |
| 65  | j     | 1798  | 0        | 1896     | 66      | 0            |
| 66  | k     | 1481  | 0        | 1572     | 53      | 0            |
| 67  | l     | 1457  | 0        | 1488     | 42      | 0            |
| 68  | m     | 1494  | 0        | 1573     | 33      | 0            |
| 69  | n     | 556   | 0        | 542      | 23      | 0            |
| 70  | o     | 1146  | 0        | 1213     | 12      | 0            |
| 71  | p     | 1192  | 0        | 1255     | 19      | 0            |
| 72  | q     | 891   | 0        | 883      | 31      | 0            |
| 73  | r     | 732   | 0        | 760      | 22      | 0            |
| 74  | s     | 1080  | 0        | 1140     | 42      | 0            |
| 75  | t     | 961   | 0        | 999      | 33      | 0            |
| 76  | u     | 1192  | 0        | 1222     | 51      | 0            |
| 77  | v     | 1112  | 0        | 1124     | 40      | 0            |
| 78  | w     | 800   | 0        | 869      | 31      | 0            |
| 79  | x     | 684   | 0        | 672      | 19      | 0            |
| 80  | y     | 1021  | 0        | 1060     | 29      | 0            |
| 81  | z     | 1121  | 0        | 1196     | 22      | 0            |
| 82  | 2     | 1     | 0        | 0        | 0       | 0            |
| 82  | 5     | 1     | 0        | 0        | 0       | 0            |
| 82  | 8     | 1     | 0        | 0        | 0       | 0            |
| 82  | S     | 1     | 0        | 0        | 0       | 0            |
| 82  | V     | 1     | 0        | 0        | 0       | 0            |
| 82  | Y     | 1     | 0        | 0        | 0       | 0            |
| 82  | a     | 1     | 0        | 0        | 0       | 0            |
| 82  | b     | 1     | 0        | 0        | 0       | 0            |
| 83  | AA    | 199   | 0        | 0        | 0       | 0            |
| 83  | B     | 1     | 0        | 0        | 0       | 0            |
| 83  | BB    | 5     | 0        | 0        | 0       | 0            |
| 83  | Bb    | 2     | 0        | 0        | 0       | 0            |
| 83  | CC    | 3     | 0        | 0        | 0       | 0            |
| 83  | FF    | 1     | 0        | 0        | 0       | 0            |
| 83  | H     | 1     | 0        | 0        | 0       | 0            |
| 83  | MM    | 1     | 0        | 0        | 0       | 0            |
| 83  | QQ    | 1     | 0        | 0        | 0       | 0            |
| 83  | c     | 49    | 0        | 0        | 0       | 0            |
| 84  | AA    | 13    | 0        | 0        | 0       | 0            |
| 84  | EE    | 1     | 0        | 0        | 0       | 0            |
| 84  | MM    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 84  | Q     | 1      | 0        | 0        | 0       | 0            |
| 84  | S     | 1      | 0        | 0        | 0       | 0            |
| 84  | c     | 1      | 0        | 0        | 0       | 0            |
| 84  | q     | 1      | 0        | 0        | 0       | 0            |
| 85  | AA    | 30     | 0        | 57       | 3       | 0            |
| 85  | c     | 10     | 0        | 19       | 0       | 0            |
| 86  | Bb    | 8      | 0        | 8        | 2       | 0            |
| 87  | 2     | 1      | 0        | 0        | 0       | 0            |
| 87  | A     | 2      | 0        | 0        | 0       | 0            |
| 87  | AA    | 774    | 0        | 0        | 14      | 0            |
| 87  | B     | 4      | 0        | 0        | 0       | 0            |
| 87  | BB    | 13     | 0        | 0        | 0       | 0            |
| 87  | Bb    | 5      | 0        | 0        | 2       | 0            |
| 87  | CC    | 13     | 0        | 0        | 0       | 0            |
| 87  | Cc    | 1      | 0        | 0        | 0       | 0            |
| 87  | D     | 1      | 0        | 0        | 0       | 0            |
| 87  | Dd    | 3      | 0        | 0        | 0       | 0            |
| 87  | EE    | 11     | 0        | 0        | 0       | 0            |
| 87  | F     | 2      | 0        | 0        | 0       | 0            |
| 87  | FF    | 4      | 0        | 0        | 0       | 0            |
| 87  | GG    | 3      | 0        | 0        | 0       | 0            |
| 87  | H     | 3      | 0        | 0        | 0       | 0            |
| 87  | HH    | 1      | 0        | 0        | 0       | 0            |
| 87  | J     | 1      | 0        | 0        | 0       | 0            |
| 87  | JJ    | 1      | 0        | 0        | 0       | 0            |
| 87  | M     | 2      | 0        | 0        | 0       | 0            |
| 87  | MM    | 1      | 0        | 0        | 0       | 0            |
| 87  | N     | 1      | 0        | 0        | 0       | 0            |
| 87  | P     | 1      | 0        | 0        | 0       | 0            |
| 87  | Q     | 4      | 0        | 0        | 0       | 0            |
| 87  | QQ    | 7      | 0        | 0        | 0       | 0            |
| 87  | V     | 4      | 0        | 0        | 1       | 0            |
| 87  | a     | 1      | 0        | 0        | 0       | 0            |
| 87  | c     | 122    | 0        | 0        | 2       | 0            |
| 87  | e     | 1      | 0        | 0        | 0       | 0            |
| 87  | h     | 2      | 0        | 0        | 0       | 0            |
| 87  | o     | 2      | 0        | 0        | 0       | 0            |
| 87  | p     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 201528 | 0        | 148233   | 3721    | 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 11.

The worst 5 of 3721 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) |
|------------------|-------------------|--------------------------|-------------------|
| 11:AA:1018:G:OP1 | 11:AA:1035:G:N2   | 1.72                     | 1.21              |
| 14:Cc:32:G:H21   | 64:i:157:ARG:NH1  | 1.44                     | 1.14              |
| 11:AA:1257:C:H42 | 11:AA:1261:G:N2   | 1.45                     | 1.14              |
| 14:Cc:32:G:N2    | 64:i:157:ARG:HH12 | 1.47                     | 1.11              |
| 11:AA:1257:C:N4  | 11:AA:1261:G:H22  | 1.48                     | 1.11              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | 0     | 132/135 (98%) | 127 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 2   | 1     | 68/108 (63%)  | 62 (91%)   | 6 (9%)  | 0        | 100         | 100 |
| 3   | 2     | 95/119 (80%)  | 89 (94%)   | 6 (6%)  | 0        | 100         | 100 |
| 4   | 3     | 79/82 (96%)   | 74 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 5   | 4     | 61/67 (91%)   | 60 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 6   | 5     | 47/56 (84%)   | 47 (100%)  | 0       | 0        | 100         | 100 |
| 7   | 6     | 51/63 (81%)   | 49 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 8   | 7     | 316/319 (99%) | 297 (94%)  | 19 (6%) | 0        | 100         | 100 |
| 9   | 8     | 32/152 (21%)  | 25 (78%)   | 7 (22%) | 0        | 100         | 100 |
| 10  | A     | 195/199 (98%) | 193 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 12  | B     | 152/338 (45%) | 150 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 15  | C     | 183/186 (98%) | 182 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 17  | D     | 174/189 (92%) | 170 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 18  | DD    | 195/312 (62%) | 189 (97%)  | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 20  | E     | 170/172 (99%) | 163 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 21  | EE    | 250/254 (98%) | 247 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 22  | Ee    | 156/165 (94%) | 150 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 23  | F     | 157/160 (98%) | 154 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 24  | FF    | 384/387 (99%) | 373 (97%)  | 11 (3%) | 0        | 100         | 100 |
| 25  | G     | 95/121 (78%)  | 92 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 26  | GG    | 359/362 (99%) | 345 (96%)  | 14 (4%) | 0        | 100         | 100 |
| 27  | H     | 127/137 (93%) | 126 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 28  | HH    | 294/297 (99%) | 288 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 29  | I     | 61/155 (39%)  | 61 (100%)  | 0       | 0        | 100         | 100 |
| 30  | II    | 151/176 (86%) | 148 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 31  | J     | 118/142 (83%) | 115 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 32  | JJ    | 220/244 (90%) | 217 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 33  | K     | 124/127 (98%) | 123 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 34  | KK    | 231/256 (90%) | 227 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 35  | L     | 133/136 (98%) | 128 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 36  | LL    | 189/191 (99%) | 181 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 37  | M     | 146/149 (98%) | 141 (97%)  | 4 (3%)  | 1 (1%)   | 18          | 21  |
| 38  | MM    | 213/221 (96%) | 208 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 39  | N     | 56/59 (95%)   | 54 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 40  | NN    | 167/174 (96%) | 161 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 41  | O     | 95/105 (90%)  | 95 (100%)  | 0       | 0        | 100         | 100 |
| 42  | OO    | 191/199 (96%) | 178 (93%)  | 12 (6%) | 1 (0%)   | 24          | 29  |
| 43  | P     | 107/113 (95%) | 103 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 44  | PP    | 134/138 (97%) | 133 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 45  | Q     | 125/130 (96%) | 125 (100%) | 0       | 0        | 100         | 100 |
| 46  | QQ    | 201/204 (98%) | 194 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 47  | R     | 104/107 (97%) | 103 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 48  | S     | 107/121 (88%) | 107 (100%) | 0       | 0        | 100         | 100 |
| 49  | T     | 117/120 (98%) | 115 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 50  | U     | 97/100 (97%)  | 90 (93%)   | 7 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 51  | V     | 82/88 (93%)       | 81 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 52  | W     | 75/78 (96%)       | 71 (95%)    | 4 (5%)   | 0        | 100         | 100 |
| 53  | X     | 48/51 (94%)       | 46 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 54  | Y     | 50/128 (39%)      | 50 (100%)   | 0        | 0        | 100         | 100 |
| 55  | Z     | 23/25 (92%)       | 23 (100%)   | 0        | 0        | 100         | 100 |
| 56  | a     | 100/106 (94%)     | 96 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 57  | b     | 89/92 (97%)       | 89 (100%)   | 0        | 0        | 100         | 100 |
| 59  | d     | 204/252 (81%)     | 194 (95%)   | 10 (5%)  | 0        | 100         | 100 |
| 60  | e     | 210/255 (82%)     | 195 (93%)   | 15 (7%)  | 0        | 100         | 100 |
| 61  | f     | 215/254 (85%)     | 203 (94%)   | 12 (6%)  | 0        | 100         | 100 |
| 62  | g     | 203/240 (85%)     | 196 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 63  | h     | 256/261 (98%)     | 248 (97%)   | 8 (3%)   | 0        | 100         | 100 |
| 64  | i     | 195/225 (87%)     | 186 (95%)   | 9 (5%)   | 0        | 100         | 100 |
| 65  | j     | 221/236 (94%)     | 215 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 66  | k     | 182/190 (96%)     | 175 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 67  | l     | 180/200 (90%)     | 164 (91%)   | 16 (9%)  | 0        | 100         | 100 |
| 68  | m     | 183/197 (93%)     | 178 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 69  | n     | 63/105 (60%)      | 58 (92%)    | 5 (8%)   | 0        | 100         | 100 |
| 70  | o     | 140/156 (90%)     | 132 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 71  | p     | 148/151 (98%)     | 145 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 72  | q     | 125/137 (91%)     | 118 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 73  | r     | 85/142 (60%)      | 82 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 74  | s     | 135/143 (94%)     | 125 (93%)   | 10 (7%)  | 0        | 100         | 100 |
| 75  | t     | 119/136 (88%)     | 111 (93%)   | 8 (7%)   | 0        | 100         | 100 |
| 76  | u     | 143/146 (98%)     | 132 (92%)   | 11 (8%)  | 0        | 100         | 100 |
| 77  | v     | 141/144 (98%)     | 137 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 78  | w     | 98/121 (81%)      | 98 (100%)   | 0        | 0        | 100         | 100 |
| 79  | x     | 85/87 (98%)       | 78 (92%)    | 7 (8%)   | 0        | 100         | 100 |
| 80  | y     | 127/130 (98%)     | 125 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 81  | z     | 142/145 (98%)     | 129 (91%)   | 13 (9%)  | 0        | 100         | 100 |
| All | All   | 10926/12368 (88%) | 10539 (96%) | 385 (4%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | OO    | 63  | VAL  |
| 37  | M     | 78  | LEU  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | 0     | 112/113 (99%)  | 110 (98%) | 2 (2%)   | 51          | 68  |
| 2   | 1     | 61/89 (68%)    | 58 (95%)  | 3 (5%)   | 22          | 31  |
| 3   | 2     | 83/101 (82%)   | 80 (96%)  | 3 (4%)   | 31          | 44  |
| 4   | 3     | 70/71 (99%)    | 67 (96%)  | 3 (4%)   | 26          | 36  |
| 5   | 4     | 56/60 (93%)    | 51 (91%)  | 5 (9%)   | 9           | 10  |
| 6   | 5     | 43/49 (88%)    | 42 (98%)  | 1 (2%)   | 44          | 60  |
| 7   | 6     | 46/54 (85%)    | 45 (98%)  | 1 (2%)   | 45          | 62  |
| 8   | 7     | 259/262 (99%)  | 250 (96%) | 9 (4%)   | 32          | 45  |
| 9   | 8     | 30/135 (22%)   | 30 (100%) | 0        | 100         | 100 |
| 10  | A     | 160/162 (99%)  | 157 (98%) | 3 (2%)   | 50          | 66  |
| 12  | B     | 125/271 (46%)  | 122 (98%) | 3 (2%)   | 43          | 59  |
| 15  | C     | 150/151 (99%)  | 147 (98%) | 3 (2%)   | 48          | 65  |
| 17  | D     | 143/154 (93%)  | 139 (97%) | 4 (3%)   | 38          | 53  |
| 18  | DD    | 167/254 (66%)  | 162 (97%) | 5 (3%)   | 36          | 51  |
| 20  | E     | 156/156 (100%) | 154 (99%) | 2 (1%)   | 61          | 76  |
| 21  | EE    | 193/196 (98%)  | 190 (98%) | 3 (2%)   | 55          | 71  |
| 22  | Ee    | 129/136 (95%)  | 122 (95%) | 7 (5%)   | 20          | 27  |
| 23  | F     | 136/137 (99%)  | 135 (99%) | 1 (1%)   | 76          | 86  |
| 24  | FF    | 320/323 (99%)  | 316 (99%) | 4 (1%)   | 61          | 76  |
| 25  | G     | 84/107 (78%)   | 83 (99%)  | 1 (1%)   | 63          | 77  |
| 26  | GG    | 288/289 (100%) | 283 (98%) | 5 (2%)   | 53          | 70  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 27  | H     | 101/105 (96%)  | 101 (100%) | 0        | 100         | 100 |
| 28  | HH    | 244/245 (100%) | 239 (98%)  | 5 (2%)   | 48          | 65  |
| 29  | I     | 55/129 (43%)   | 55 (100%)  | 0        | 100         | 100 |
| 30  | II    | 133/153 (87%)  | 127 (96%)  | 6 (4%)   | 24          | 35  |
| 31  | J     | 104/118 (88%)  | 102 (98%)  | 2 (2%)   | 50          | 66  |
| 32  | JJ    | 186/205 (91%)  | 184 (99%)  | 2 (1%)   | 65          | 79  |
| 33  | K     | 109/110 (99%)  | 107 (98%)  | 2 (2%)   | 51          | 68  |
| 34  | KK    | 187/208 (90%)  | 183 (98%)  | 4 (2%)   | 47          | 63  |
| 35  | L     | 115/116 (99%)  | 113 (98%)  | 2 (2%)   | 53          | 70  |
| 36  | LL    | 171/171 (100%) | 164 (96%)  | 7 (4%)   | 27          | 38  |
| 37  | M     | 118/119 (99%)  | 115 (98%)  | 3 (2%)   | 42          | 58  |
| 38  | MM    | 184/187 (98%)  | 178 (97%)  | 6 (3%)   | 33          | 47  |
| 39  | N     | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 40  | NN    | 147/150 (98%)  | 140 (95%)  | 7 (5%)   | 23          | 32  |
| 41  | O     | 81/88 (92%)    | 76 (94%)   | 5 (6%)   | 16          | 21  |
| 42  | OO    | 154/159 (97%)  | 149 (97%)  | 5 (3%)   | 34          | 49  |
| 43  | P     | 94/97 (97%)    | 94 (100%)  | 0        | 100         | 100 |
| 44  | PP    | 107/109 (98%)  | 106 (99%)  | 1 (1%)   | 70          | 82  |
| 45  | Q     | 109/111 (98%)  | 107 (98%)  | 2 (2%)   | 51          | 68  |
| 46  | QQ    | 175/176 (99%)  | 174 (99%)  | 1 (1%)   | 78          | 87  |
| 47  | R     | 90/91 (99%)    | 90 (100%)  | 0        | 100         | 100 |
| 48  | S     | 94/103 (91%)   | 91 (97%)   | 3 (3%)   | 34          | 49  |
| 49  | T     | 104/105 (99%)  | 102 (98%)  | 2 (2%)   | 50          | 66  |
| 50  | U     | 81/82 (99%)    | 78 (96%)   | 3 (4%)   | 30          | 43  |
| 51  | V     | 69/71 (97%)    | 68 (99%)   | 1 (1%)   | 59          | 74  |
| 52  | W     | 68/69 (99%)    | 65 (96%)   | 3 (4%)   | 25          | 35  |
| 53  | X     | 45/46 (98%)    | 44 (98%)   | 1 (2%)   | 45          | 62  |
| 54  | Y     | 47/116 (40%)   | 47 (100%)  | 0        | 100         | 100 |
| 55  | Z     | 23/23 (100%)   | 22 (96%)   | 1 (4%)   | 26          | 36  |
| 56  | a     | 87/91 (96%)    | 87 (100%)  | 0        | 100         | 100 |
| 57  | b     | 71/72 (99%)    | 68 (96%)   | 3 (4%)   | 26          | 37  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 59  | d     | 165/210 (79%)    | 165 (100%) | 0        | 100         | 100 |
| 60  | e     | 189/224 (84%)    | 184 (97%)  | 5 (3%)   | 40          | 56  |
| 61  | f     | 176/205 (86%)    | 170 (97%)  | 6 (3%)   | 32          | 46  |
| 62  | g     | 166/195 (85%)    | 154 (93%)  | 12 (7%)  | 13          | 16  |
| 63  | h     | 220/222 (99%)    | 216 (98%)  | 4 (2%)   | 51          | 68  |
| 64  | i     | 172/191 (90%)    | 164 (95%)  | 8 (5%)   | 23          | 33  |
| 65  | j     | 191/201 (95%)    | 186 (97%)  | 5 (3%)   | 40          | 56  |
| 66  | k     | 165/170 (97%)    | 161 (98%)  | 4 (2%)   | 43          | 59  |
| 67  | l     | 146/161 (91%)    | 144 (99%)  | 2 (1%)   | 59          | 74  |
| 68  | m     | 158/166 (95%)    | 156 (99%)  | 2 (1%)   | 61          | 76  |
| 69  | n     | 60/98 (61%)      | 58 (97%)   | 2 (3%)   | 33          | 47  |
| 70  | o     | 127/137 (93%)    | 124 (98%)  | 3 (2%)   | 43          | 59  |
| 71  | p     | 127/128 (99%)    | 123 (97%)  | 4 (3%)   | 35          | 50  |
| 72  | q     | 81/105 (77%)     | 80 (99%)   | 1 (1%)   | 63          | 77  |
| 73  | r     | 77/118 (65%)     | 75 (97%)   | 2 (3%)   | 40          | 56  |
| 74  | s     | 114/119 (96%)    | 109 (96%)  | 5 (4%)   | 25          | 35  |
| 75  | t     | 105/124 (85%)    | 101 (96%)  | 4 (4%)   | 29          | 42  |
| 76  | u     | 128/129 (99%)    | 121 (94%)  | 7 (6%)   | 19          | 26  |
| 77  | v     | 115/116 (99%)    | 114 (99%)  | 1 (1%)   | 70          | 82  |
| 78  | w     | 94/114 (82%)     | 90 (96%)   | 4 (4%)   | 26          | 36  |
| 79  | x     | 74/74 (100%)     | 72 (97%)   | 2 (3%)   | 39          | 55  |
| 80  | y     | 110/111 (99%)    | 107 (97%)  | 3 (3%)   | 39          | 55  |
| 81  | z     | 119/120 (99%)    | 115 (97%)  | 4 (3%)   | 32          | 46  |
| All | All   | 9289/10380 (90%) | 9054 (98%) | 235 (2%) | 42          | 58  |

5 of 235 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | O     | 24  | THR  |
| 77  | v     | 133 | ASP  |
| 57  | b     | 63  | THR  |
| 76  | u     | 107 | SER  |
| 71  | p     | 60  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 63  | h     | 96  | ASN  |
| 70  | o     | 92  | HIS  |
| 64  | i     | 79  | ASN  |
| 66  | k     | 19  | GLN  |
| 73  | r     | 114 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | AA    | 3193/3396 (94%) | 478 (14%)         | 16 (0%)         |
| 13  | BB    | 120/121 (99%)   | 8 (6%)            | 1 (0%)          |
| 14  | Bb    | 76/77 (98%)     | 21 (27%)          | 0               |
| 14  | Cc    | 76/77 (98%)     | 34 (44%)          | 0               |
| 16  | CC    | 157/158 (99%)   | 22 (14%)          | 1 (0%)          |
| 19  | Dd    | 5/39 (12%)      | 1 (20%)           | 0               |
| 58  | c     | 1614/1800 (89%) | 287 (17%)         | 0               |
| All | All   | 5241/5668 (92%) | 851 (16%)         | 18 (0%)         |

5 of 851 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | AA    | 4   | U    |
| 11  | AA    | 6   | A    |
| 11  | AA    | 14  | U    |
| 11  | AA    | 26  | A    |
| 11  | AA    | 40  | A    |

5 of 18 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | AA    | 3121 | U    |
| 16  | CC    | 57   | C    |
| 13  | BB    | 72   | A    |
| 11  | AA    | 2458 | A    |
| 11  | AA    | 2971 | A    |

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

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

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |       | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 11  | A2M  | AA    | 2640 | 11    | 22,25,26     | 3.20 | 9 (40%)     | 30,36,39    | 2.93 | 10 (33%)    |
| 58  | A2M  | c     | 100  | 58,83 | 22,25,26     | 3.20 | 9 (40%)     | 30,36,39    | 2.92 | 10 (33%)    |
| 11  | OMU  | AA    | 2421 | 11    | 19,22,23     | 3.12 | 8 (42%)     | 25,31,34    | 1.80 | 4 (16%)     |
| 58  | A2M  | c     | 541  | 58    | 22,25,26     | 3.20 | 9 (40%)     | 30,36,39    | 2.99 | 13 (43%)    |
| 58  | MA6  | c     | 1781 | 58    | 23,26,27     | 1.40 | 4 (17%)     | 33,38,41    | 3.19 | 12 (36%)    |
| 11  | 1MA  | AA    | 2142 | 11,83 | 21,25,26     | 0.46 | 0           | 30,37,40    | 0.78 | 1 (3%)      |
| 11  | 1MA  | AA    | 645  | 11,83 | 21,25,26     | 0.46 | 0           | 30,37,40    | 0.77 | 1 (3%)      |
| 58  | A2M  | c     | 796  | 58    | 22,25,26     | 3.22 | 9 (40%)     | 30,36,39    | 2.96 | 12 (40%)    |
| 11  | OMC  | AA    | 1437 | 11,83 | 19,22,23     | 0.51 | 0           | 25,31,34    | 0.81 | 1 (4%)      |
| 11  | A2M  | AA    | 876  | 11    | 22,25,26     | 3.20 | 9 (40%)     | 30,36,39    | 2.90 | 10 (33%)    |
| 11  | A2M  | AA    | 2280 | 11    | 22,25,26     | 3.20 | 9 (40%)     | 30,36,39    | 2.91 | 11 (36%)    |
| 58  | G7M  | c     | 1575 | 58,14 | 23,26,27     | 2.65 | 8 (34%)     | 34,39,42    | 2.40 | 10 (29%)    |
| 58  | MA6  | c     | 1782 | 58    | 23,26,27     | 1.38 | 4 (17%)     | 33,38,41    | 3.26 | 12 (36%)    |
| 11  | OMC  | AA    | 2197 | 84,11 | 19,22,23     | 0.50 | 0           | 25,31,34    | 0.60 | 0           |
| 11  | OMG  | AA    | 2288 | 11    | 23,26,27     | 0.45 | 0           | 32,38,41    | 0.49 | 0           |
| 11  | OMU  | AA    | 2347 | 11    | 19,22,23     | 3.13 | 8 (42%)     | 25,31,34    | 1.79 | 5 (20%)     |
| 11  | OMG  | AA    | 2815 | 11    | 23,26,27     | 0.45 | 0           | 32,38,41    | 0.48 | 0           |
| 58  | OMU  | c     | 1269 | 58    | 19,22,23     | 3.14 | 8 (42%)     | 25,31,34    | 1.83 | 5 (20%)     |
| 11  | OMG  | AA    | 2922 | 11    | 23,26,27     | 0.51 | 0           | 32,38,41    | 0.52 | 0           |
| 11  | OMC  | AA    | 2337 | 11    | 19,22,23     | 0.50 | 0           | 25,31,34    | 0.67 | 0           |
| 11  | A2M  | AA    | 2946 | 11,83 | 22,25,26     | 3.20 | 9 (40%)     | 30,36,39    | 2.95 | 11 (36%)    |
| 11  | OMU  | AA    | 2724 | 11    | 19,22,23     | 3.12 | 8 (42%)     | 25,31,34    | 1.79 | 5 (20%)     |
| 11  | 5MC  | AA    | 2278 | 11,83 | 19,22,23     | 0.51 | 0           | 26,32,35    | 0.63 | 0           |
| 58  | A2M  | c     | 619  | 58,83 | 22,25,26     | 3.20 | 10 (45%)    | 30,36,39    | 2.91 | 10 (33%)    |
| 11  | UR3  | AA    | 2634 | 11    | 19,22,23     | 2.95 | 6 (31%)     | 26,32,35    | 1.63 | 3 (11%)     |
| 58  | OMG  | c     | 1126 | 58    | 23,26,27     | 0.47 | 0           | 32,38,41    | 0.53 | 0           |
| 58  | OMU  | c     | 578  | 58    | 19,22,23     | 3.13 | 8 (42%)     | 25,31,34    | 1.77 | 5 (20%)     |
| 11  | OMU  | AA    | 2417 | 11    | 19,22,23     | 3.10 | 8 (42%)     | 25,31,34    | 1.79 | 5 (20%)     |
| 11  | OMU  | AA    | 2729 | 11    | 19,22,23     | 3.10 | 8 (42%)     | 25,31,34    | 1.78 | 5 (20%)     |
| 11  | OMG  | AA    | 2793 | 11    | 23,26,27     | 0.46 | 0           | 32,38,41    | 0.51 | 0           |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | A2M  | AA    | 649  | 11    | 22,25,26     | 3.18 | 10 (45%) | 30,36,39    | 2.90 | 10 (33%) |
| 11  | OMG  | AA    | 805  | 11    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.56 | 0        |
| 58  | 4AC  | c     | 1280 | 58    | 21,24,25     | 3.51 | 10 (47%) | 28,34,37    | 1.70 | 5 (17%)  |
| 58  | A2M  | c     | 420  | 58    | 22,25,26     | 3.20 | 10 (45%) | 30,36,39    | 2.91 | 11 (36%) |
| 11  | A2M  | AA    | 807  | 11    | 22,25,26     | 3.22 | 10 (45%) | 30,36,39    | 2.95 | 13 (43%) |
| 11  | A2M  | AA    | 2256 | 58,11 | 22,25,26     | 3.18 | 9 (40%)  | 30,36,39    | 2.99 | 13 (43%) |
| 58  | OMG  | c     | 1572 | 58    | 23,26,27     | 0.49 | 0        | 32,38,41    | 0.54 | 0        |
| 58  | OMC  | c     | 1007 | 58    | 19,22,23     | 0.50 | 0        | 25,31,34    | 0.67 | 0        |
| 11  | OMG  | AA    | 2791 | 11    | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.48 | 0        |
| 11  | OMG  | AA    | 908  | 11    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.48 | 0        |
| 58  | A2M  | c     | 28   | 58    | 22,25,26     | 3.23 | 9 (40%)  | 30,36,39    | 2.93 | 11 (36%) |
| 58  | OMC  | c     | 1639 | 58,83 | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.63 | 0        |
| 58  | OMG  | c     | 1428 | 58    | 23,26,27     | 0.49 | 0        | 32,38,41    | 0.48 | 0        |
| 11  | OMG  | AA    | 1450 | 11    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.42 | 0        |
| 58  | A2M  | c     | 436  | 58    | 22,25,26     | 3.22 | 9 (40%)  | 30,36,39    | 2.91 | 11 (36%) |
| 11  | A2M  | AA    | 1133 | 11,83 | 22,25,26     | 3.21 | 10 (45%) | 30,36,39    | 2.99 | 11 (36%) |
| 58  | OMC  | c     | 414  | 58    | 19,22,23     | 0.49 | 0        | 25,31,34    | 0.69 | 0        |
| 58  | A2M  | c     | 974  | 58    | 22,25,26     | 3.20 | 9 (40%)  | 30,36,39    | 2.93 | 11 (36%) |
| 11  | A2M  | AA    | 2281 | 11    | 22,25,26     | 3.20 | 10 (45%) | 30,36,39    | 3.11 | 14 (46%) |
| 11  | OMG  | AA    | 867  | 84,11 | 23,26,27     | 0.49 | 0        | 32,38,41    | 0.50 | 0        |
| 11  | A2M  | AA    | 2220 | 11    | 22,25,26     | 3.20 | 9 (40%)  | 30,36,39    | 2.89 | 10 (33%) |
| 11  | OMC  | AA    | 663  | 11    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.78 | 0        |
| 11  | OMG  | AA    | 2619 | 11,14 | 23,26,27     | 0.46 | 0        | 32,38,41    | 0.44 | 0        |
| 11  | OMC  | AA    | 650  | 11    | 19,22,23     | 0.50 | 0        | 25,31,34    | 0.70 | 0        |
| 11  | A2M  | AA    | 1449 | 11,83 | 22,25,26     | 3.20 | 9 (40%)  | 30,36,39    | 2.91 | 10 (33%) |
| 58  | OMG  | c     | 562  | 58    | 23,26,27     | 0.44 | 0        | 32,38,41    | 0.47 | 0        |
| 11  | OMU  | AA    | 1888 | 11    | 19,22,23     | 3.12 | 8 (42%)  | 25,31,34    | 1.86 | 5 (20%)  |
| 58  | OMG  | c     | 1271 | 58    | 23,26,27     | 0.45 | 0        | 32,38,41    | 0.48 | 0        |
| 11  | OMC  | AA    | 2959 | 11,83 | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.68 | 0        |
| 11  | OMU  | AA    | 2921 | 11,83 | 19,22,23     | 3.12 | 8 (42%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 58  | 4AC  | c     | 1773 | 58    | 21,24,25     | 3.51 | 10 (47%) | 28,34,37    | 1.69 | 5 (17%)  |
| 11  | 5MC  | AA    | 2870 | 84,11 | 19,22,23     | 0.64 | 0        | 26,32,35    | 0.59 | 0        |
| 11  | OMC  | AA    | 2948 | 11    | 19,22,23     | 0.51 | 0        | 25,31,34    | 0.87 | 1 (4%)   |
| 11  | OMU  | AA    | 898  | 11    | 19,22,23     | 3.12 | 8 (42%)  | 25,31,34    | 1.79 | 5 (20%)  |
| 58  | B8N  | c     | 1191 | 58    | 25,29,30     | 3.40 | 7 (28%)  | 28,42,45    | 1.98 | 6 (21%)  |
| 11  | A2M  | AA    | 817  | 11,83 | 22,25,26     | 3.18 | 9 (40%)  | 30,36,39    | 2.92 | 11 (36%) |

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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 11  | A2M  | AA    | 2640 | 11    | -       | 1/9/27/28  | 0/3/3/3 |
| 58  | A2M  | c     | 100  | 58,83 | -       | 1/9/27/28  | 0/3/3/3 |
| 11  | OMU  | AA    | 2421 | 11    | -       | 1/9/27/28  | 0/2/2/2 |
| 58  | A2M  | c     | 541  | 58    | -       | 2/9/27/28  | 0/3/3/3 |
| 58  | MA6  | c     | 1781 | 58    | -       | 0/11/29/30 | 0/3/3/3 |
| 11  | 1MA  | AA    | 2142 | 11,83 | -       | 0/7/25/26  | 0/3/3/3 |
| 11  | 1MA  | AA    | 645  | 11,83 | -       | 2/7/25/26  | 0/3/3/3 |
| 58  | A2M  | c     | 796  | 58    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | OMC  | AA    | 1437 | 11,83 | -       | 2/9/27/28  | 0/2/2/2 |
| 11  | A2M  | AA    | 876  | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 2280 | 11    | -       | 2/9/27/28  | 0/3/3/3 |
| 58  | G7M  | c     | 1575 | 58,14 | -       | 3/7/25/26  | 0/3/3/3 |
| 58  | MA6  | c     | 1782 | 58    | -       | 1/11/29/30 | 0/3/3/3 |
| 11  | OMC  | AA    | 2197 | 84,11 | -       | 4/9/27/28  | 0/2/2/2 |
| 11  | OMG  | AA    | 2288 | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | OMU  | AA    | 2347 | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | OMG  | AA    | 2815 | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 58  | OMU  | c     | 1269 | 58    | -       | 2/9/27/28  | 0/2/2/2 |
| 11  | OMG  | AA    | 2922 | 11    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | OMC  | AA    | 2337 | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | A2M  | AA    | 2946 | 11,83 | -       | 1/9/27/28  | 0/3/3/3 |
| 11  | OMU  | AA    | 2724 | 11    | -       | 1/9/27/28  | 0/2/2/2 |
| 11  | 5MC  | AA    | 2278 | 11,83 | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | A2M  | c     | 619  | 58,83 | -       | 6/9/27/28  | 0/3/3/3 |
| 11  | UR3  | AA    | 2634 | 11    | -       | 0/7/25/26  | 0/2/2/2 |
| 58  | OMG  | c     | 1126 | 58    | -       | 0/9/27/28  | 0/3/3/3 |
| 58  | OMU  | c     | 578  | 58    | -       | 1/9/27/28  | 0/2/2/2 |
| 11  | OMU  | AA    | 2417 | 11    | -       | 1/9/27/28  | 0/2/2/2 |
| 11  | OMU  | AA    | 2729 | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | OMG  | AA    | 2793 | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 649  | 11    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | OMG  | AA    | 805  | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 58  | 4AC  | c     | 1280 | 58    | -       | 2/11/29/30 | 0/2/2/2 |
| 58  | A2M  | c     | 420  | 58    | -       | 1/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 807  | 11    | -       | 3/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 2256 | 58,11 | -       | 4/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 58  | OMG  | c     | 1572 | 58    | -       | 2/9/27/28  | 0/3/3/3 |
| 58  | OMC  | c     | 1007 | 58    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | OMG  | AA    | 2791 | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | OMG  | AA    | 908  | 11    | -       | 3/9/27/28  | 0/3/3/3 |
| 58  | A2M  | c     | 28   | 58    | -       | 2/9/27/28  | 0/3/3/3 |
| 58  | OMC  | c     | 1639 | 58,83 | -       | 0/9/27/28  | 0/2/2/2 |
| 58  | OMG  | c     | 1428 | 58    | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | OMG  | AA    | 1450 | 11    | -       | 2/9/27/28  | 0/3/3/3 |
| 58  | A2M  | c     | 436  | 58    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 1133 | 11,83 | -       | 0/9/27/28  | 0/3/3/3 |
| 58  | OMC  | c     | 414  | 58    | -       | 1/9/27/28  | 0/2/2/2 |
| 58  | A2M  | c     | 974  | 58    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 2281 | 11    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | OMG  | AA    | 867  | 84,11 | -       | 2/9/27/28  | 0/3/3/3 |
| 11  | A2M  | AA    | 2220 | 11    | -       | 1/9/27/28  | 0/3/3/3 |
| 11  | OMC  | AA    | 663  | 11    | -       | 1/9/27/28  | 0/2/2/2 |
| 11  | OMG  | AA    | 2619 | 11,14 | -       | 1/9/27/28  | 0/3/3/3 |
| 11  | OMC  | AA    | 650  | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | A2M  | AA    | 1449 | 11,83 | -       | 0/9/27/28  | 0/3/3/3 |
| 58  | OMG  | c     | 562  | 58    | -       | 0/9/27/28  | 0/3/3/3 |
| 11  | OMU  | AA    | 1888 | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 58  | OMG  | c     | 1271 | 58    | -       | 4/9/27/28  | 0/3/3/3 |
| 11  | OMC  | AA    | 2959 | 11,83 | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | OMU  | AA    | 2921 | 11,83 | -       | 0/9/27/28  | 0/2/2/2 |
| 58  | 4AC  | c     | 1773 | 58    | -       | 2/11/29/30 | 0/2/2/2 |
| 11  | 5MC  | AA    | 2870 | 84,11 | -       | 4/7/25/26  | 0/2/2/2 |
| 11  | OMC  | AA    | 2948 | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 11  | OMU  | AA    | 898  | 11    | -       | 0/9/27/28  | 0/2/2/2 |
| 58  | B8N  | c     | 1191 | 58    | -       | 4/16/34/35 | 0/2/2/2 |
| 11  | A2M  | AA    | 817  | 11,83 | -       | 1/9/27/28  | 0/3/3/3 |

The worst 5 of 315 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 58  | c     | 28   | A2M  | C3'-C4' | -9.03 | 1.30        | 1.53     |
| 11  | AA    | 807  | A2M  | C3'-C4' | -8.97 | 1.30        | 1.53     |
| 58  | c     | 541  | A2M  | C3'-C4' | -8.90 | 1.30        | 1.53     |
| 11  | AA    | 2220 | A2M  | C3'-C4' | -8.87 | 1.30        | 1.53     |
| 11  | AA    | 1133 | A2M  | C3'-C4' | -8.86 | 1.30        | 1.53     |

The worst 5 of 329 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 58  | c     | 1782 | MA6  | N1-C6-N6 | -11.85 | 102.42      | 116.86   |
| 58  | c     | 1781 | MA6  | N1-C6-N6 | -11.44 | 102.91      | 116.86   |
| 58  | c     | 1782 | MA6  | C5-C6-N6 | 8.01   | 138.01      | 125.33   |
| 58  | c     | 1781 | MA6  | C5-C6-N6 | 7.75   | 137.61      | 125.33   |
| 11  | AA    | 817  | A2M  | N6-C6-N1 | -6.83  | 103.16      | 118.38   |

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | AA    | 649  | A2M  | C1'-C2'-O2'-CM' |
| 11  | AA    | 663  | OMC  | C1'-C2'-O2'-CM2 |
| 11  | AA    | 908  | OMG  | O4'-C4'-C5'-O5' |
| 11  | AA    | 1437 | OMC  | C1'-C2'-O2'-CM2 |
| 11  | AA    | 1450 | OMG  | O4'-C4'-C5'-O5' |

There are no ring outliers.

41 monomers are involved in 61 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | AA    | 2640 | A2M  | 2       | 0            |
| 58  | c     | 100  | A2M  | 1       | 0            |
| 11  | AA    | 2421 | OMU  | 2       | 0            |
| 58  | c     | 541  | A2M  | 1       | 0            |
| 58  | c     | 1781 | MA6  | 1       | 0            |
| 11  | AA    | 1437 | OMC  | 2       | 0            |
| 11  | AA    | 876  | A2M  | 1       | 0            |
| 58  | c     | 1575 | G7M  | 2       | 0            |
| 11  | AA    | 2347 | OMU  | 1       | 0            |
| 11  | AA    | 2815 | OMG  | 1       | 0            |
| 11  | AA    | 2922 | OMG  | 2       | 0            |
| 11  | AA    | 2724 | OMU  | 4       | 0            |
| 11  | AA    | 2278 | 5MC  | 2       | 0            |
| 11  | AA    | 2417 | OMU  | 3       | 0            |
| 11  | AA    | 649  | A2M  | 2       | 0            |
| 58  | c     | 1280 | 4AC  | 1       | 0            |
| 58  | c     | 420  | A2M  | 4       | 0            |
| 11  | AA    | 2256 | A2M  | 1       | 0            |
| 58  | c     | 1572 | OMG  | 1       | 0            |
| 11  | AA    | 908  | OMG  | 1       | 0            |
| 58  | c     | 28   | A2M  | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 58  | c     | 1639 | OMC  | 1       | 0            |
| 58  | c     | 1428 | OMG  | 1       | 0            |
| 58  | c     | 436  | A2M  | 1       | 0            |
| 11  | AA    | 1133 | A2M  | 1       | 0            |
| 58  | c     | 414  | OMC  | 1       | 0            |
| 58  | c     | 974  | A2M  | 1       | 0            |
| 11  | AA    | 2281 | A2M  | 1       | 0            |
| 11  | AA    | 2220 | A2M  | 2       | 0            |
| 11  | AA    | 663  | OMC  | 4       | 0            |
| 11  | AA    | 2619 | OMG  | 1       | 0            |
| 11  | AA    | 650  | OMC  | 2       | 0            |
| 11  | AA    | 1449 | A2M  | 1       | 0            |
| 58  | c     | 1271 | OMG  | 1       | 0            |
| 11  | AA    | 2959 | OMC  | 1       | 0            |
| 58  | c     | 1773 | 4AC  | 3       | 0            |
| 11  | AA    | 2870 | 5MC  | 1       | 0            |
| 11  | AA    | 2948 | OMC  | 1       | 0            |
| 11  | AA    | 898  | OMU  | 1       | 0            |
| 58  | c     | 1191 | B8N  | 1       | 0            |
| 11  | AA    | 817  | A2M  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 295 ligands modelled in this entry, 290 are monoatomic - leaving 5 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 | $\# Z  > 2$ |
| 85  | SPD  | AA    | 3608 | -    | 9,9,9        | 0.34 | 0           | 8,8,8       | 0.79 | 0           |
| 86  | MET  | Bb    | 103  | 14   | 6,7,8        | 0.47 | 0           | 2,7,9       | 0.15 | 0           |
| 85  | SPD  | AA    | 3610 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.82 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 85  | SPD  | AA    | 3611 | -    | 9,9,9        | 0.32 | 0        | 8,8,8       | 0.91 | 0        |
| 85  | SPD  | c     | 1951 | -    | 9,9,9        | 0.32 | 0        | 8,8,8       | 0.83 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 85  | SPD  | AA    | 3608 | -    | -       | 4/7/7/7  | -     |
| 86  | MET  | Bb    | 103  | 14   | -       | 2/5/6/8  | -     |
| 85  | SPD  | AA    | 3610 | -    | -       | 0/7/7/7  | -     |
| 85  | SPD  | AA    | 3611 | -    | -       | 0/7/7/7  | -     |
| 85  | SPD  | c     | 1951 | -    | -       | 1/7/7/7  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 86  | Bb    | 103  | MET  | C-CA-CB-CG   |
| 85  | AA    | 3608 | SPD  | C3-C4-C5-N6  |
| 85  | AA    | 3608 | SPD  | C4-C5-N6-C7  |
| 86  | Bb    | 103  | MET  | CB-CG-SD-CE  |
| 85  | AA    | 3608 | SPD  | C7-C8-C9-N10 |

There are no ring outliers.

4 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 85  | AA    | 3608 | SPD  | 1       | 0            |
| 86  | Bb    | 103  | MET  | 2       | 0            |
| 85  | AA    | 3610 | SPD  | 1       | 0            |
| 85  | AA    | 3611 | SPD  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

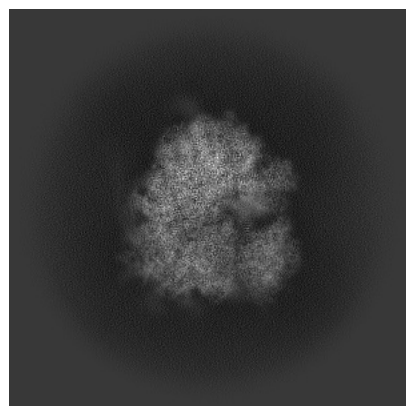
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16648. These allow visual inspection of the internal detail of the map and identification of artifacts.

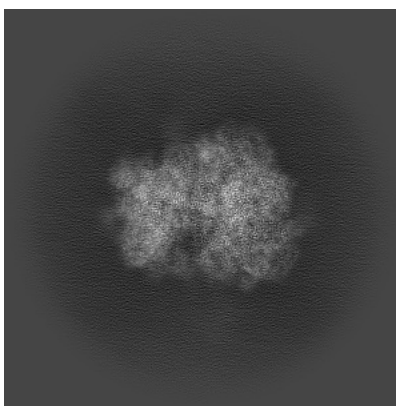
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

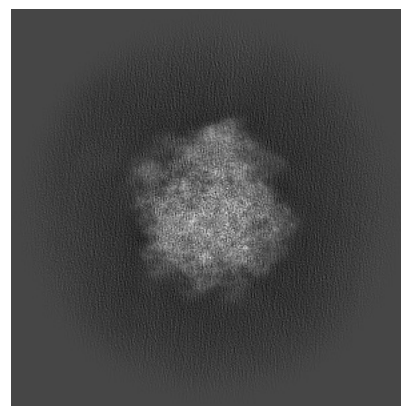
#### 6.1.1 Primary map



X

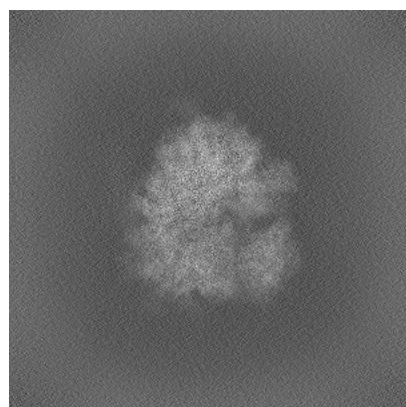


Y

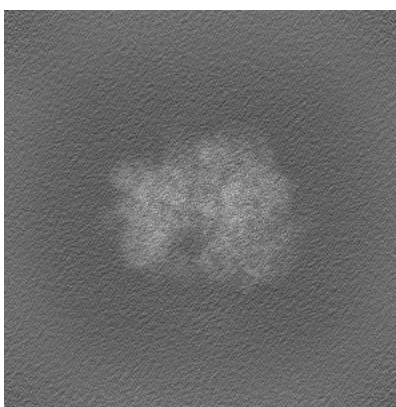


Z

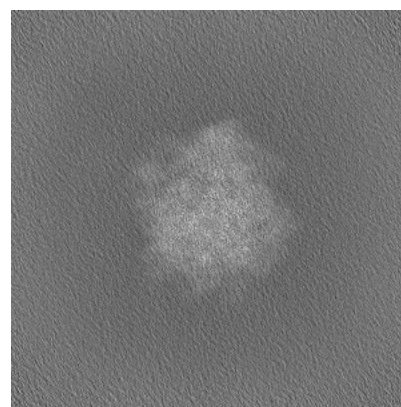
#### 6.1.2 Raw map



X



Y

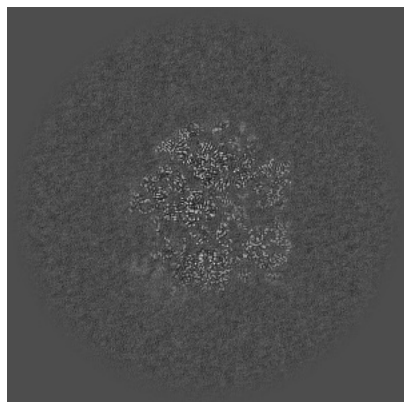


Z

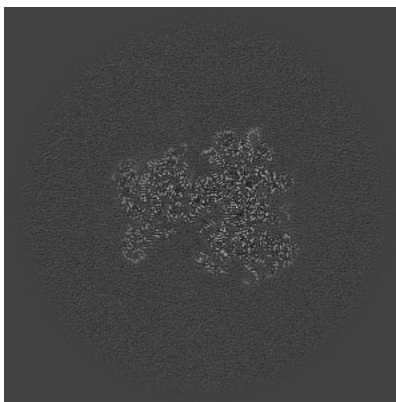
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

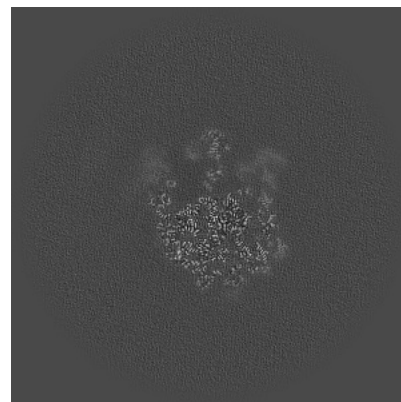
### 6.2.1 Primary map



X Index: 300

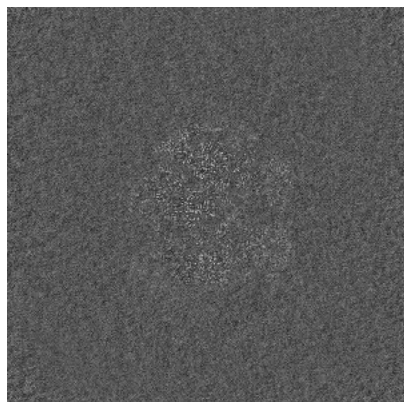


Y Index: 300

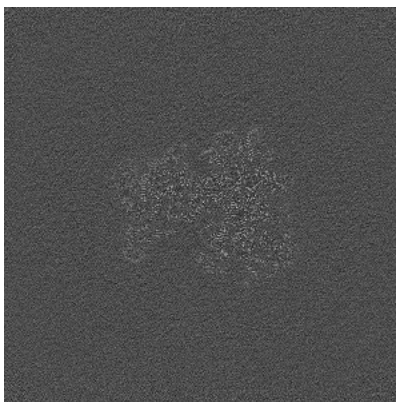


Z Index: 300

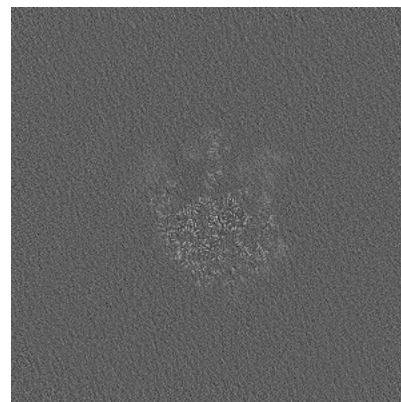
### 6.2.2 Raw map



X Index: 300



Y Index: 300

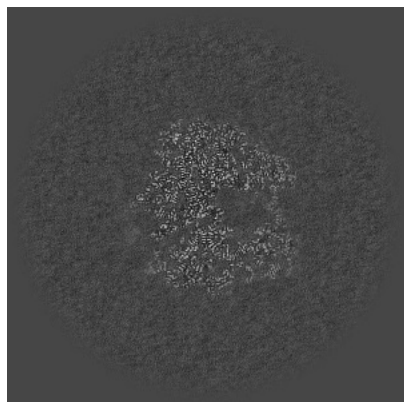


Z Index: 300

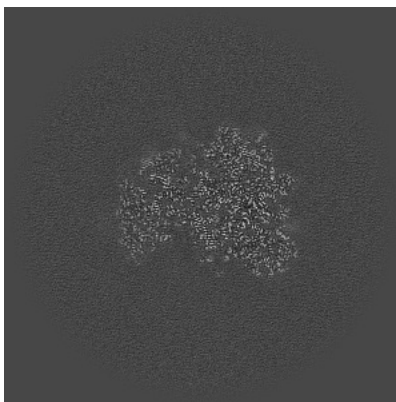
The images above show central slices of the map in three orthogonal directions.

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

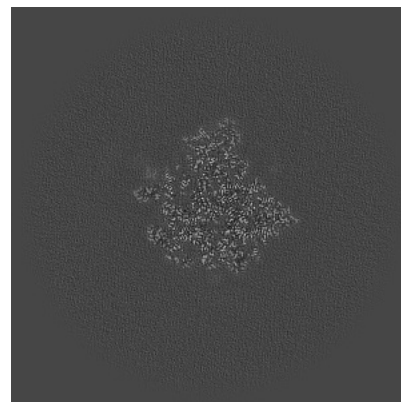
### 6.3.1 Primary map



X Index: 324

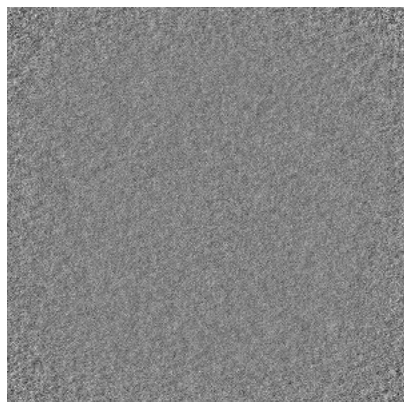


Y Index: 291

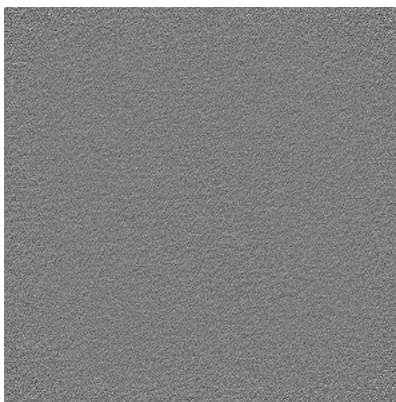


Z Index: 345

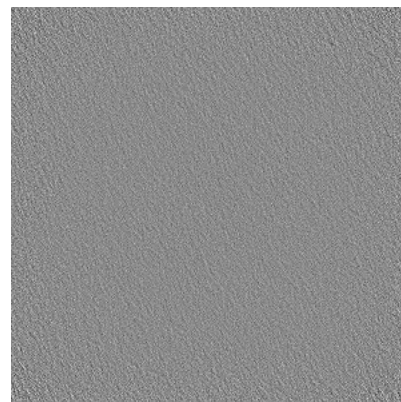
### 6.3.2 Raw map



X Index: 0



Y Index: 0

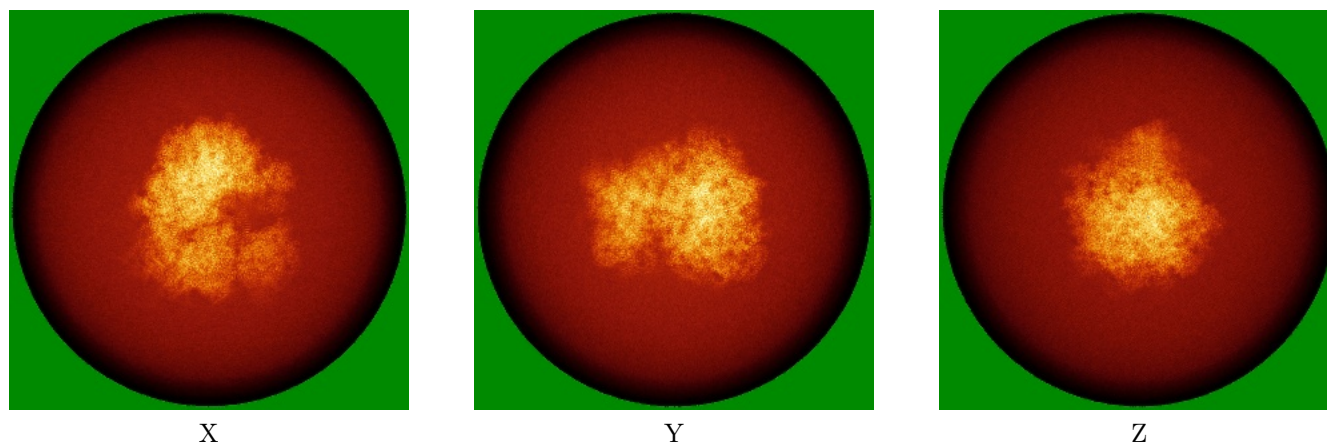


Z Index: 0

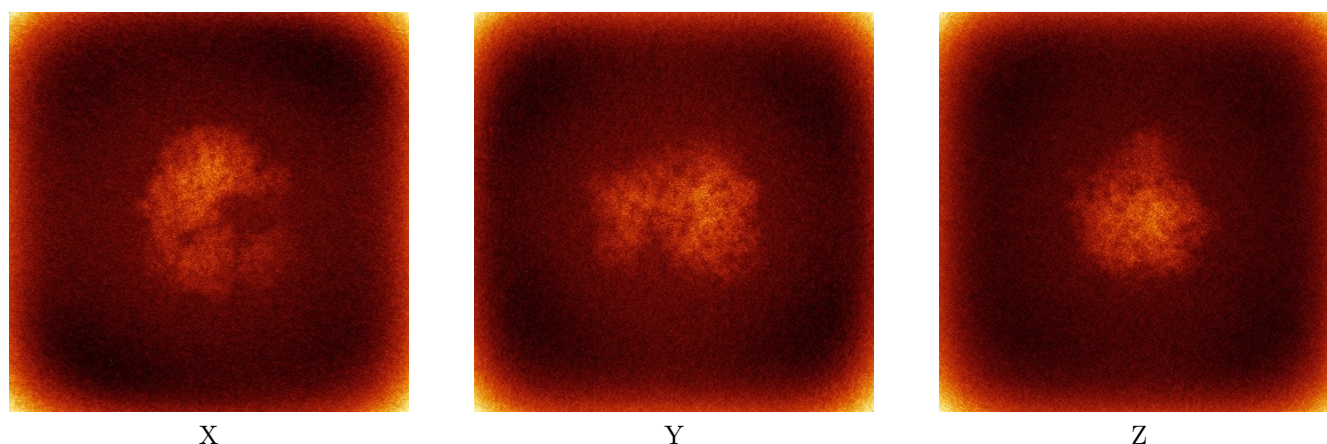
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

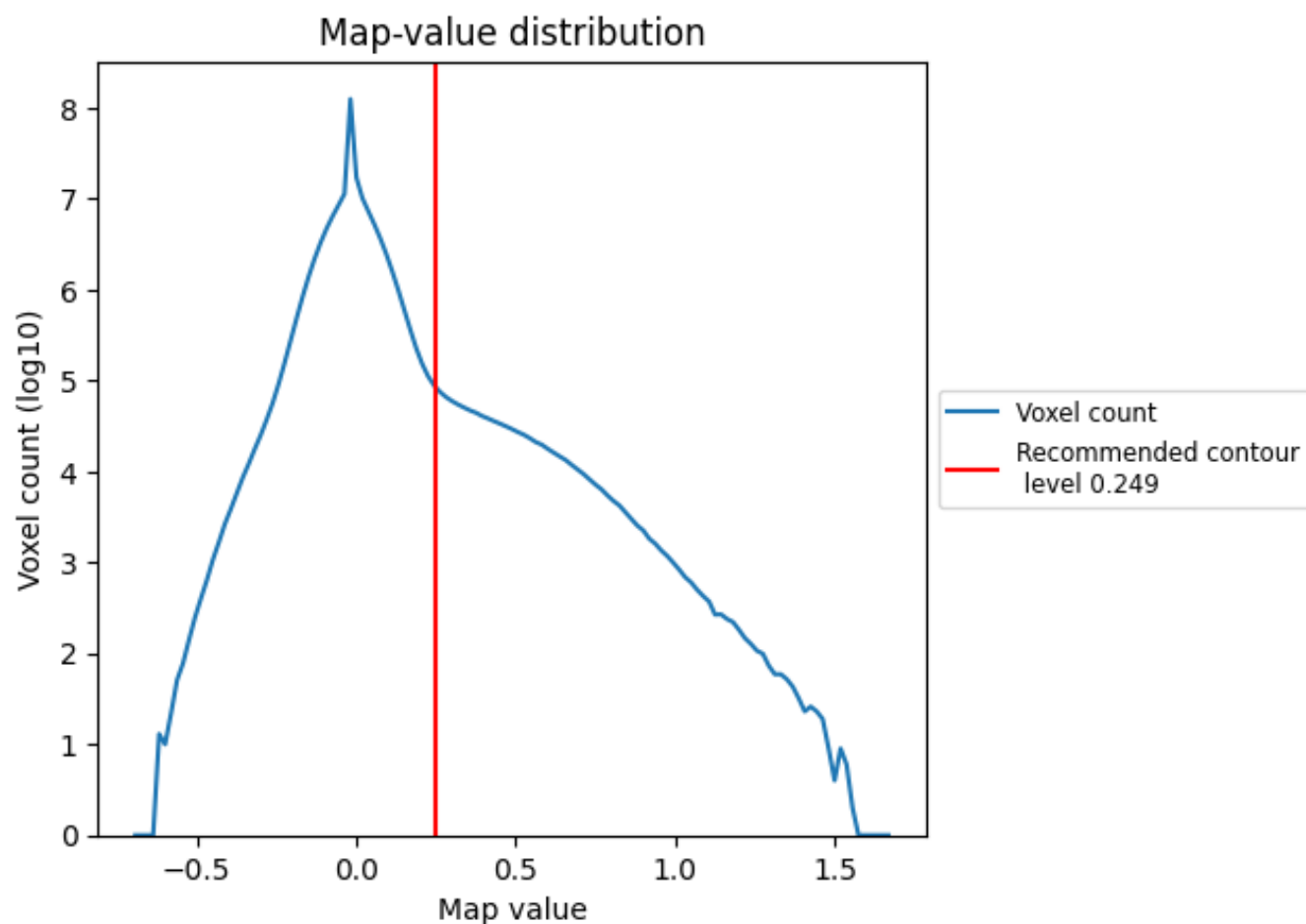
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

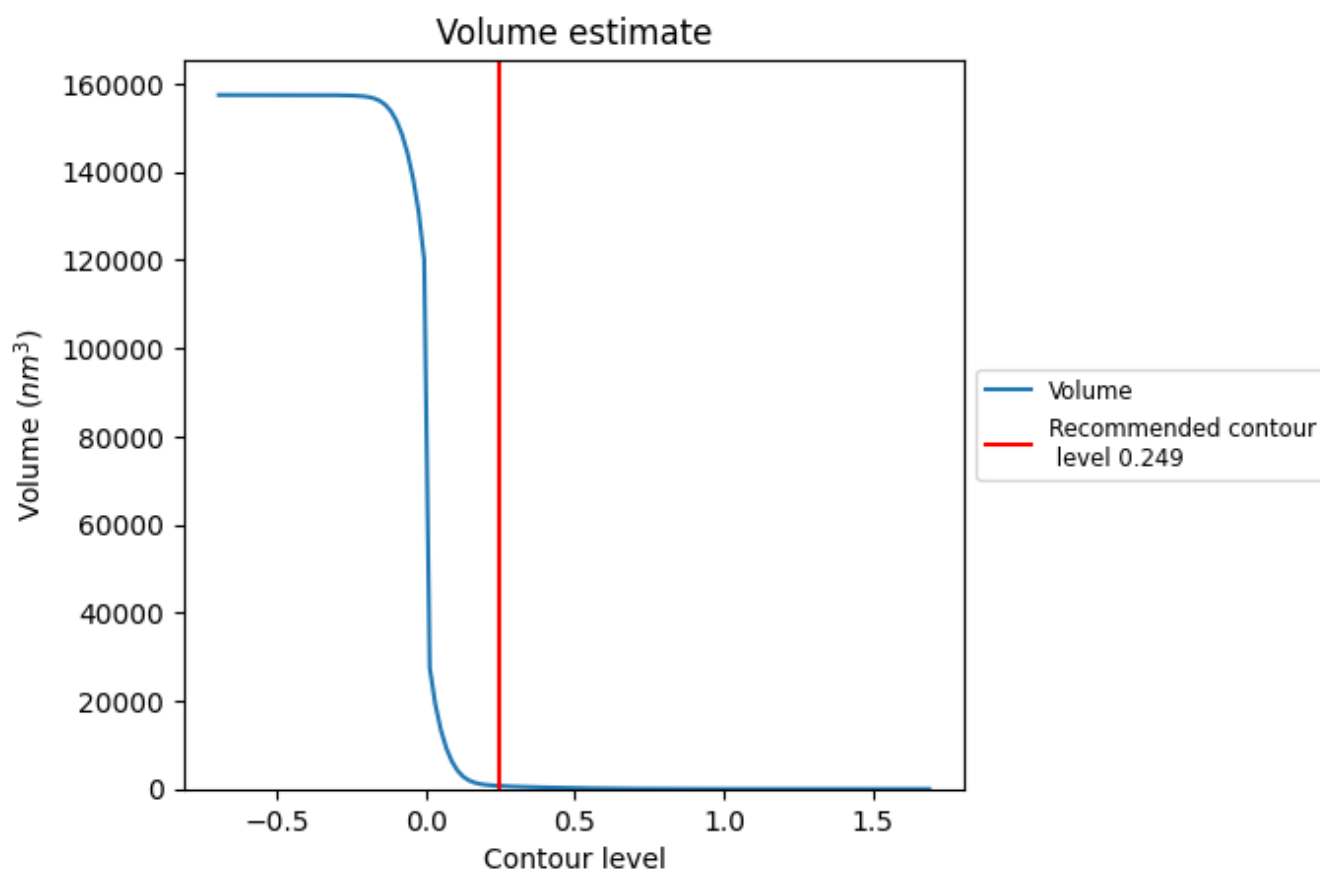
This section contains the results of statistical analysis of the map.

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



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

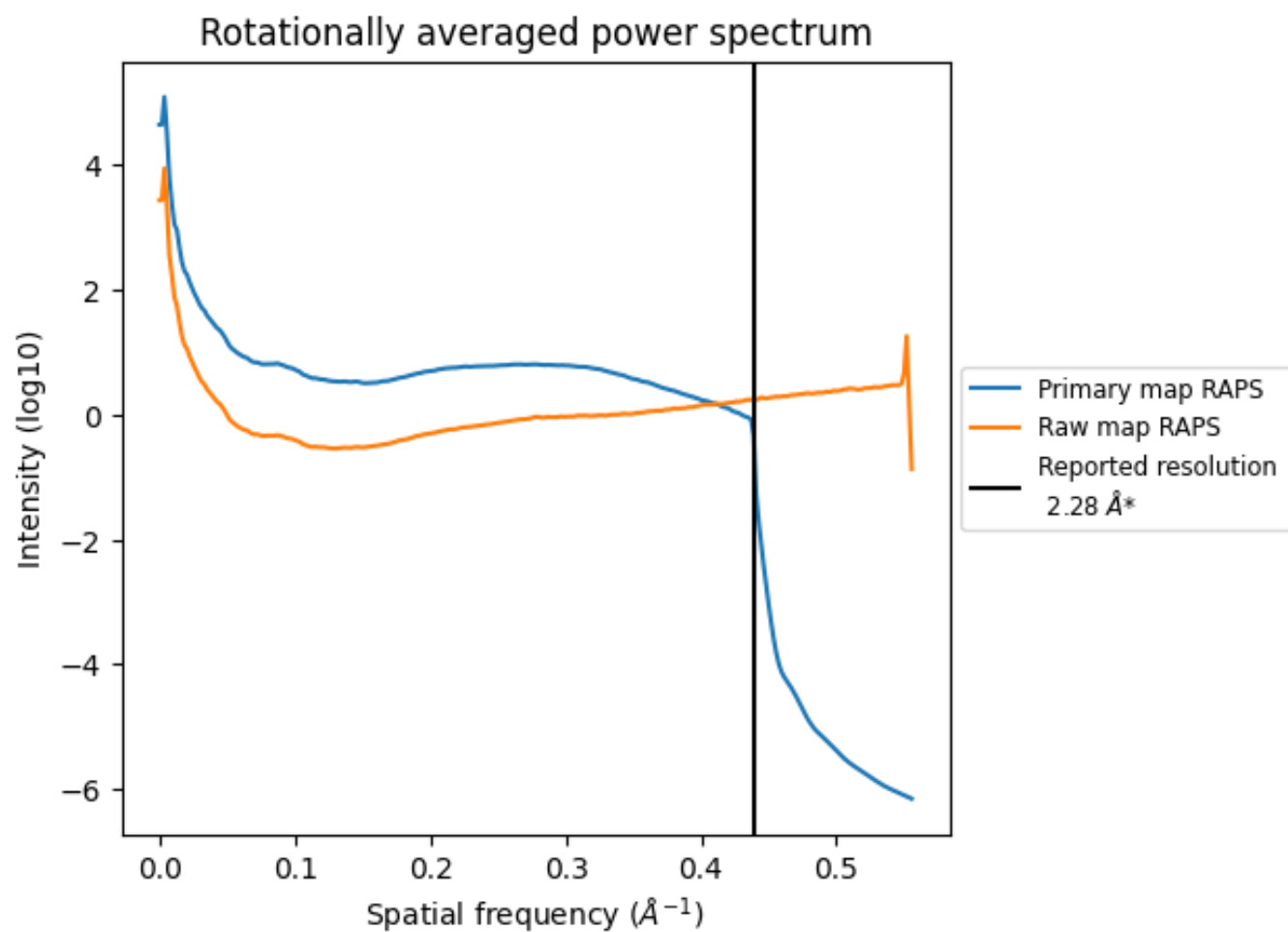
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 688  $\text{nm}^3$ ; this corresponds to an approximate mass of 621 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 ⓘ

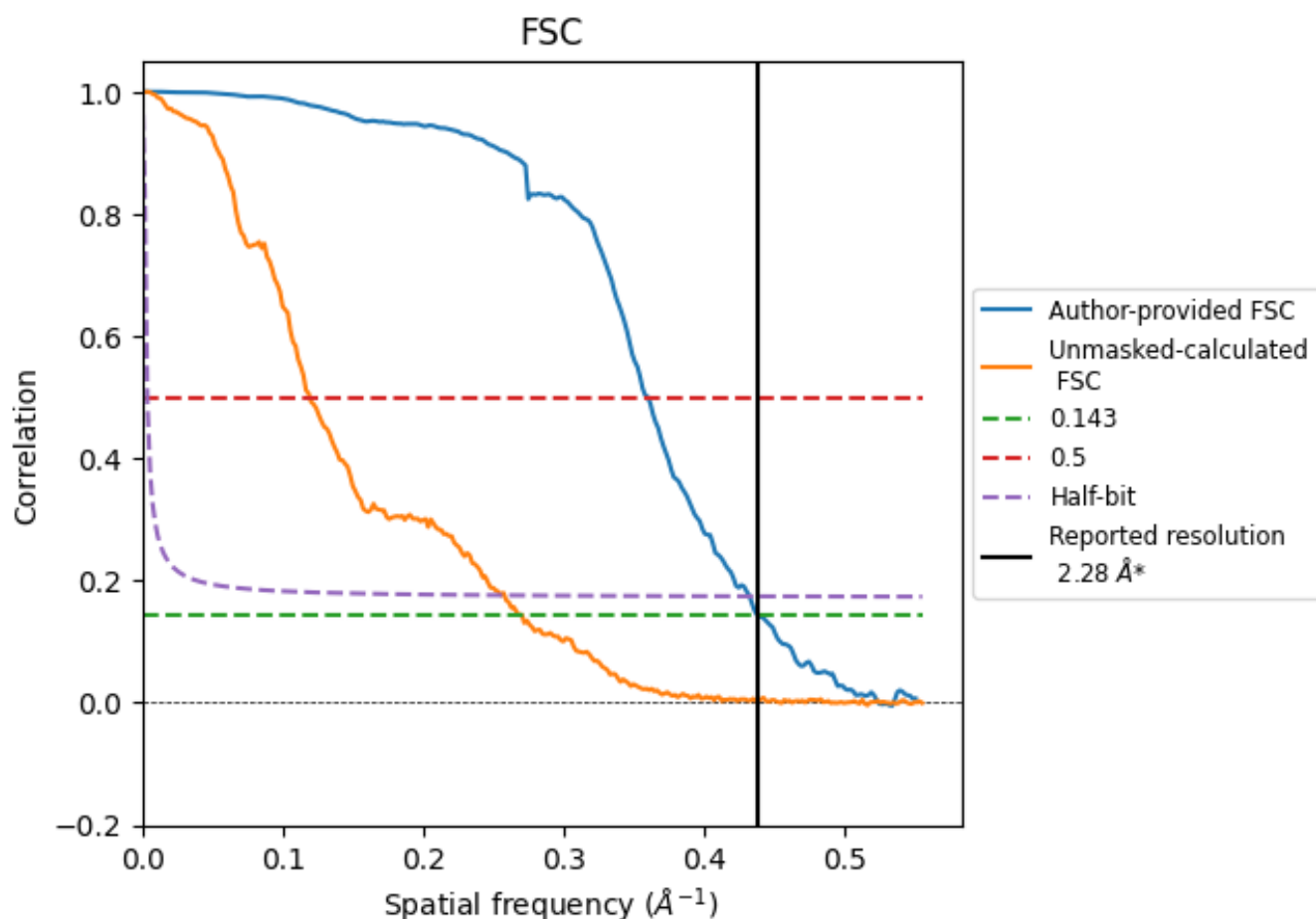


\*Reported resolution corresponds to spatial frequency of 0.439  $\text{\AA}^{-1}$

## 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  $0.439 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

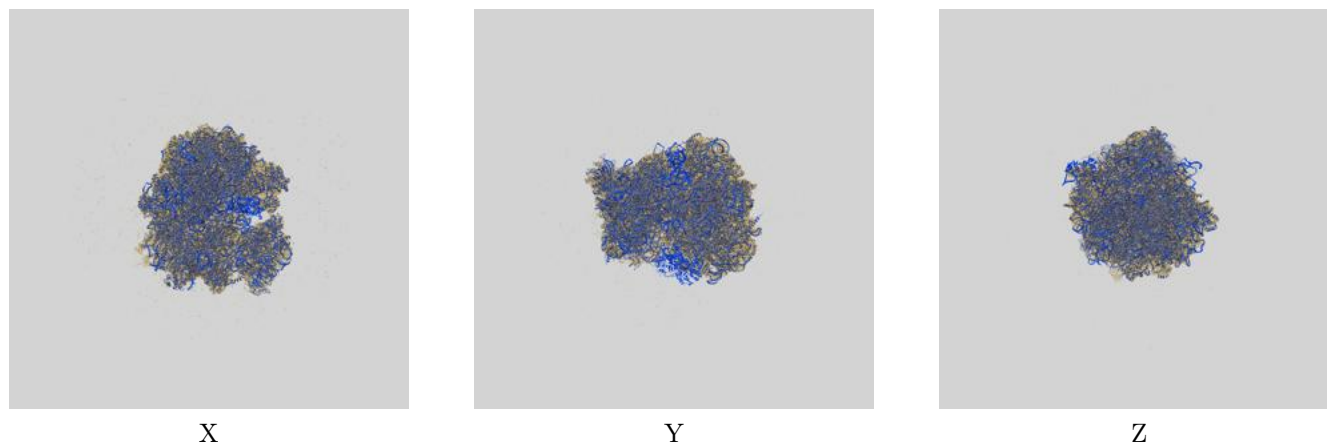
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.28                               | -    | -        |
| Author-provided FSC curve | 2.28                               | 2.78 | 2.31     |
| Unmasked-calculated*      | 3.70                               | 8.38 | 3.88     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 2.28 by more than 10 %

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

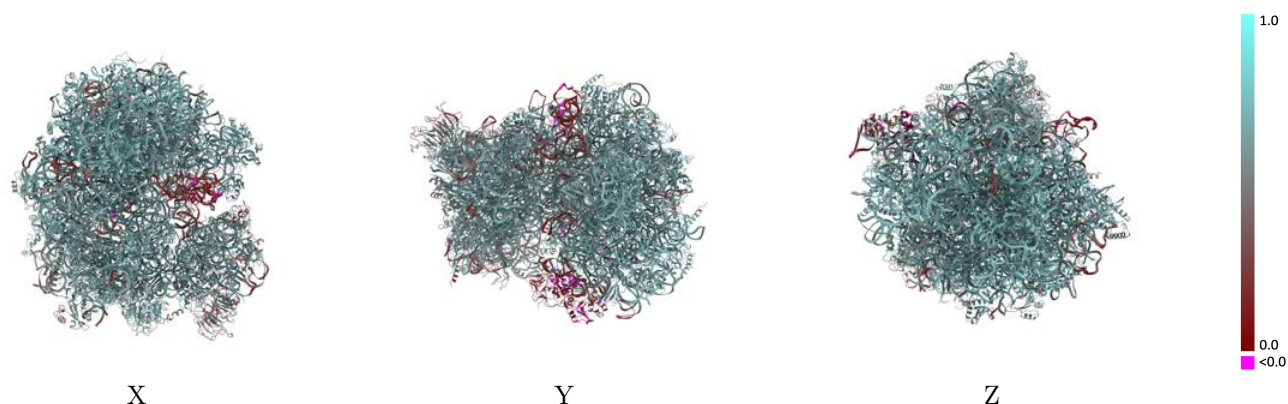
This section contains information regarding the fit between EMDB map EMD-16648 and PDB model 8CGN. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

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



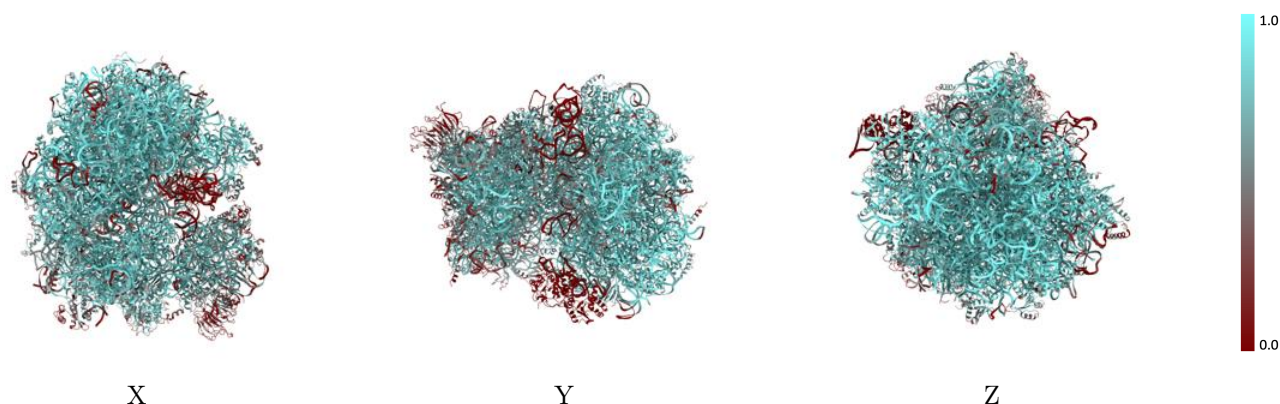
The images above show the 3D surface view of the map at the recommended contour level 0.249 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



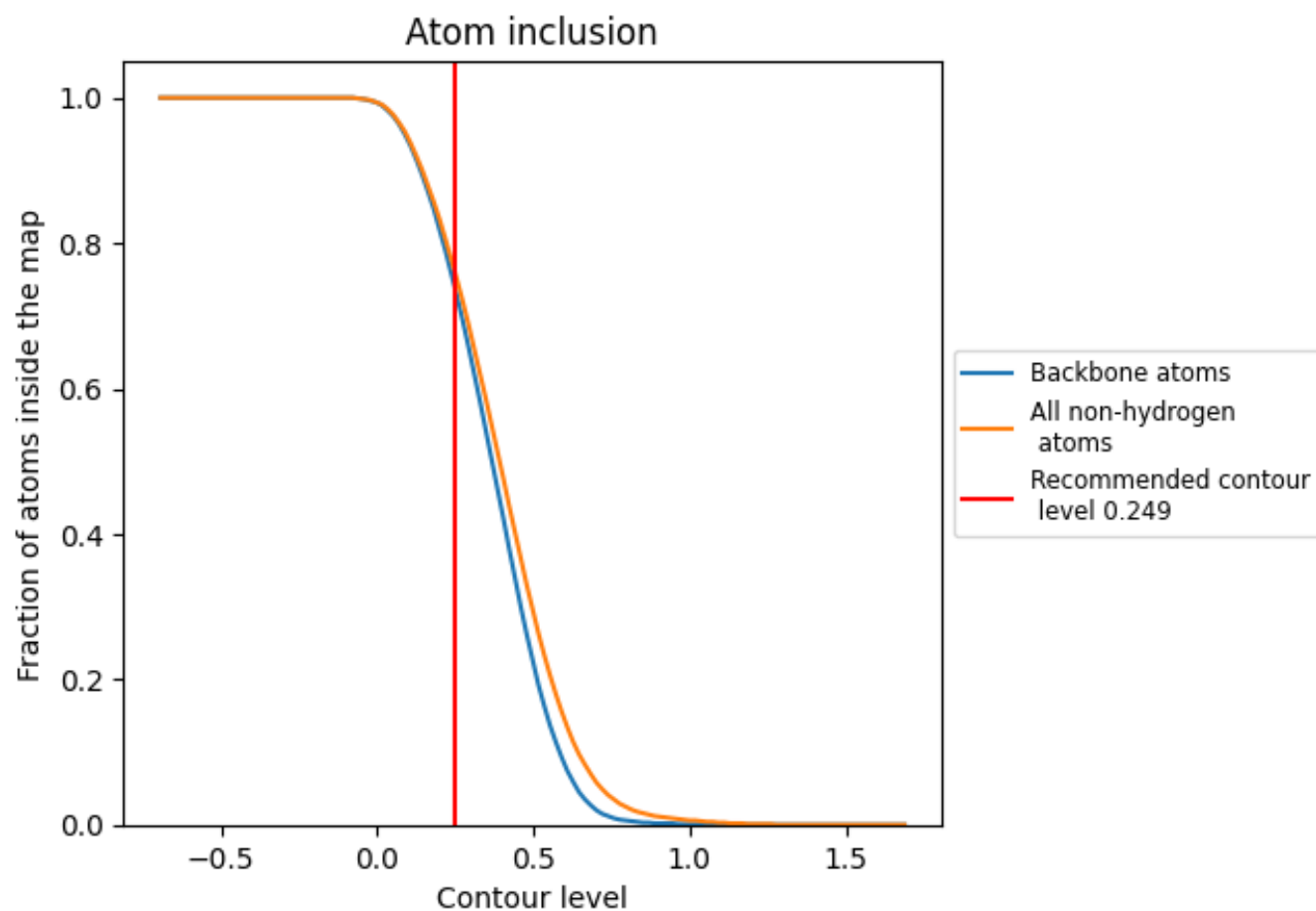
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.249).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.249) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7600   |  0.6110   |
| 0     |  0.5440   |  0.5690   |
| 1     |  0.2650   |  0.3850   |
| 2     |  0.7770   |  0.6370   |
| 3     |  0.6310   |  0.5740   |
| 4     |  0.4950   |  0.5660   |
| 5     |  0.8110   |  0.6460   |
| 6     |  0.5280   |  0.5300   |
| 7     |  0.2620   |  0.4430   |
| 8     |  0.0590   |  0.3080   |
| A     |  0.8640   |  0.6720   |
| AA    |  0.8420   |  0.6230   |
| B     |  0.8950   |  0.6880   |
| BB    |  0.9060   |  0.6450   |
| Bb    |  0.5910  |  0.5460  |
| C     |  0.8840 |  0.6810 |
| CC    |  0.9120 |  0.6520 |
| Cc    |  0.0990 |  0.2980 |
| D     |  0.7890 |  0.6410 |
| DD    |  0.0030 |  0.2590 |
| Dd    |  0.6490 |  0.6000 |
| E     |  0.8560 |  0.6710 |
| EE    |  0.8810 |  0.6860 |
| Ee    |  0.0010 |  0.1550 |
| F     |  0.8070 |  0.6540 |
| FF    |  0.8590 |  0.6710 |
| G     |  0.6090 |  0.5880 |
| GG    |  0.8620 |  0.6730 |
| H     |  0.8610 |  0.6820 |
| HH    |  0.6790 |  0.6110 |
| I     |  0.8240 |  0.6780 |
| II    |  0.7560 |  0.6480 |
| J     |  0.7950 |  0.6540 |
| JJ    |  0.8590 |  0.6760 |
| K     |  0.8280 |  0.6650 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| KK    |  0.6990   |  0.6240   |
| L     |  0.7560   |  0.6330   |
| LL    |  0.7260   |  0.6390   |
| M     |  0.8790   |  0.6770   |
| MM    |  0.7610   |  0.6600   |
| N     |  0.7060   |  0.6130   |
| NN    |  0.6070   |  0.5840   |
| O     |  0.8030   |  0.6630   |
| OO    |  0.7870   |  0.6420   |
| P     |  0.7400   |  0.6310   |
| PP    |  0.7940   |  0.6580   |
| Q     |  0.8760   |  0.6840   |
| QQ    |  0.9240   |  0.6900   |
| R     |  0.9260   |  0.6940   |
| S     |  0.8390   |  0.6620   |
| T     |  0.7930   |  0.6450   |
| U     |  0.7170   |  0.6220   |
| V     |  0.9190  |  0.6880  |
| W     |  0.5930 |  0.5890 |
| X     |  0.8510 |  0.6550 |
| Y     |  0.7050 |  0.6560 |
| Z     |  0.8020 |  0.6610 |
| a     |  0.7780 |  0.6600 |
| b     |  0.7970 |  0.6610 |
| c     |  0.7890 |  0.6040 |
| d     |  0.6830 |  0.6020 |
| e     |  0.6800 |  0.6180 |
| f     |  0.7750 |  0.6430 |
| g     |  0.5330 |  0.5740 |
| h     |  0.6870 |  0.6210 |
| i     |  0.5580 |  0.5640 |
| j     |  0.4070 |  0.5200 |
| k     |  0.4750 |  0.5400 |
| l     |  0.7320 |  0.6200 |
| m     |  0.6670 |  0.6040 |
| n     |  0.4470 |  0.5270 |
| o     |  0.7660 |  0.6360 |
| p     |  0.7610 |  0.6480 |
| q     |  0.7790 |  0.6330 |
| r     |  0.4530 |  0.5400 |
| s     |  0.6280 |  0.5760 |
| t     |  0.4940 |  0.5290 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| u     |  0.5030 |  0.5370 |
| v     |  0.5720 |  0.5600 |
| w     |  0.4590 |  0.5460 |
| x     |  0.7210 |  0.6210 |
| y     |  0.8580 |  0.6750 |
| z     |  0.7050 |  0.6310 |