



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 9N6X / pdb\_00009n6x  
EMDB ID : EMD-49077  
Title : SSU processome maturation and disassembly, State B  
Authors : Buzovetsky, O.; Klinge, S.  
Deposited on : 2025-02-05  
Resolution : 3.71 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:

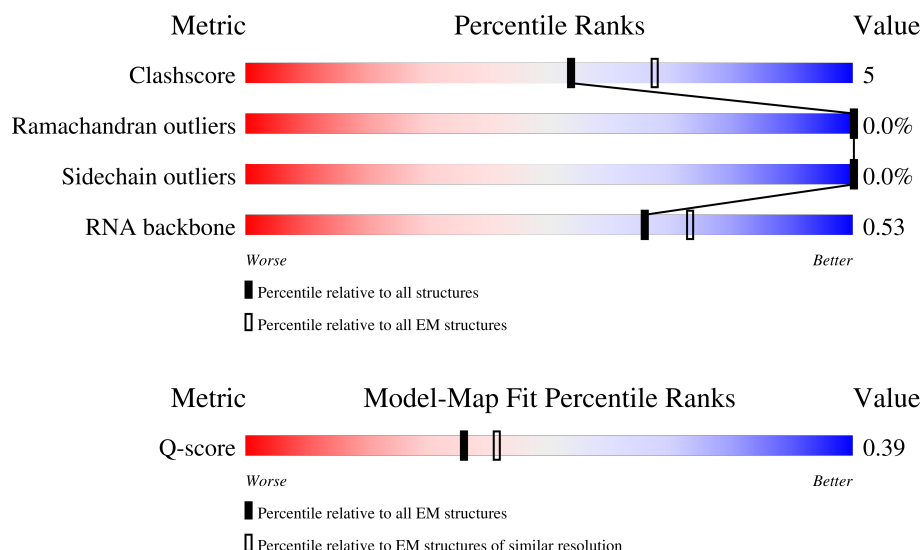
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.71 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                       | 10534 ( 3.21 - 4.21 )                                    |

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   | L0    | 700    | <div> <div>14%</div> <div>47%</div> <div>14%</div> <div>36%</div> </div> |
| 2   | L1    | 1808   | <div> <div>7%</div> <div>49%</div> <div>15%</div> <div>33%</div> </div>  |
| 3   | L2    | 333    | <div> <div>9%</div> <div>40%</div> <div>11%</div> <div>47%</div> </div>  |

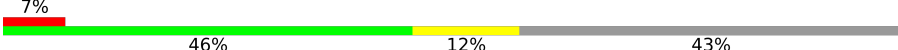
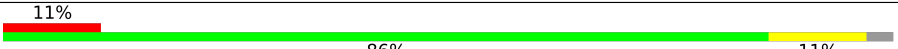
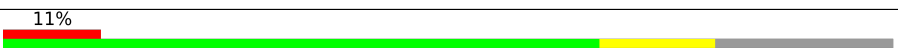
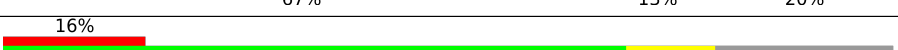
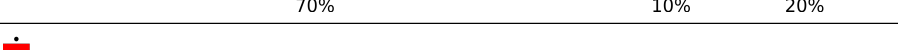
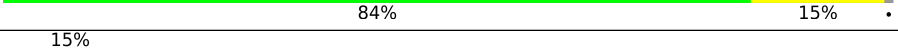
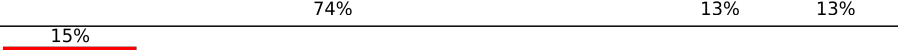
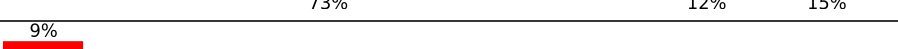
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | L3    | 146    |                  |
| 5   | L4    | 261    |                  |
| 6   | L5    | 225    |                  |
| 7   | L6    | 236    |                  |
| 8   | L7    | 190    |                  |
| 9   | L8    | 200    |                  |
| 10  | L9    | 197    |                  |
| 11  | LC    | 143    |                  |
| 12  | LD    | 156    |                  |
| 13  | LE    | 130    |                  |
| 14  | LF    | 135    |                  |
| 15  | LG    | 67     |                  |
| 16  | LH    | 896    |                  |
| 17  | LI    | 713    |                  |
| 18  | LJ    | 513    |                  |
| 19  | LK    | 575    |                  |
| 20  | LL    | 643    |                  |
| 21  | LM    | 1769   |                  |
| 22  | LN    | 776    |                  |
| 23  | LO    | 923    |                  |
| 24  | LP    | 440    |                  |
| 25  | LQ    | 943    |                  |
| 26  | LR    | 817    |                  |
| 27  | LS    | 594    |                  |
| 28  | LT    | 939    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | LU    | 489    |    |
| 30  | LV    | 707    |    |
| 31  | LW    | 554    |    |
| 32  | LX    | 1056   |    |
| 32  | LY    | 1056   |    |
| 33  | LZ    | 183    |    |
| 34  | NA    | 593    |    |
| 35  | NB    | 610    |    |
| 36  | NC    | 357    |    |
| 37  | ND    | 214    |    |
| 38  | NE    | 346    |    |
| 39  | NF    | 151    |    |
| 40  | NG    | 137    |   |
| 41  | NH    | 1237   |  |
| 42  | NI    | 297    |  |
| 43  | NK    | 316    |  |
| 44  | NM    | 255    |  |
| 45  | NN    | 534    |  |
| 46  | NQ    | 82     |  |
| 47  | OA    | 1729   |  |
| 48  | SA    | 504    |  |
| 49  | SB    | 511    |  |
| 50  | SC    | 327    |  |
| 50  | SD    | 327    |  |
| 51  | SE    | 126    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 51  | SF    | 126    |                  |
| 52  | SG    | 573    |                  |
| 53  | SH    | 367    |                  |
| 54  | SI    | 1183   |                  |
| 55  | SJ    | 252    |                  |
| 55  | SK    | 252    |                  |
| 56  | SL    | 189    |                  |
| 57  | SM    | 290    |                  |
| 58  | SN    | 274    |                  |
| 59  | SP    | 2493   |                  |
| 60  | SQ    | 217    |                  |
| 61  | SR    | 145    |                  |
| 62  | SS    | 899    |                  |
| 63  | ST    | 810    |                  |
| 64  | SU    | 552    |                  |
| 65  | SV    | 206    |                  |
| 66  | SW    | 274    |                  |
| 67  | SY    | 250    |                  |
| 68  | SZ    | 483    |                  |

## 2 Entry composition

There are 72 unique types of molecules in this entry. The entry contains 244461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5'ETS rRNA.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 1   | L0    | 445      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 9483  | 4239 | 1674 | 3125 | 445 |         |       |

- Molecule 2 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
| 2   | L1    | 1205     | Total | C     | N    | O    | P    | 0       | 0     |
|     |       |          | 25709 | 11494 | 4600 | 8410 | 1205 |         |       |

- Molecule 3 is a RNA chain called TPA: *Saccharomyces cerevisiae* U3a gene for small nucleolar RNA U3a.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 3   | L2    | 175      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3712  | 1661 | 649 | 1227 | 175 |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | L3    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 498 | 144 | 142 | 2 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | L4    | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1936  | 1239 | 359 | 335 | 3 |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | L5    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1635  | 1027 | 300 | 305 | 3 |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | L6    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1043 | 315 | 293 | 2 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | L7    | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1347  | 869 | 230 | 248 |   |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | L8    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1348  | 836 | 269 | 241 | 2 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L9    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1388  | 879 | 268 | 240 | 1 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | LC    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 973   | 625 | 174 | 174 |   |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | LD    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 714 | 212 | 183 | 3 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | LE    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 650 | 188 | 181 | 3 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 14  | LF    | 130      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1046  | 662 | 204 | 180 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 15  | LG    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 490   | 302 | 98 | 89 | 1 |         |       |

- Molecule 16 is a protein called NET1-associated nuclear protein 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 16  | LH    | 808      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6465  | 4123 | 1090 | 1233 | 19 |         |       |

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | LI    | 600      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3792  | 2375 | 679 | 733 | 5 |         |       |

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | LJ    | 493      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3911  | 2462 | 702 | 735 | 12 |         |       |

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | LK    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1068  | 681 | 185 | 199 | 3 |         |       |

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | LL    | 504      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3982  | 2522 | 679 | 768 | 13 |         |       |

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 10.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 21  | LM    | 1613     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9380  | 5798 | 1748 | 1822 | 12 |         |       |

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | LN    | 663      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5263  | 3333 | 913 | 995 | 22 |         |       |

- Molecule 23 is a protein called Periodic tryptophan protein 2.

| Mol | Chain | Residues | Atoms |      |      |      |   |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---|----|---------|-------|
| 23  | LO    | 834      | Total | C    | N    | O    | P | S  | 0       | 0     |
|     |       |          | 6639  | 4223 | 1140 | 1256 | 1 | 19 |         |       |

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | LP    | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3220  | 2081 | 545 | 578 | 16 |         |       |

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 12.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 25  | LQ    | 841      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6707  | 4284 | 1125 | 1271 | 27 |         |       |

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 13.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 26  | LR    | 793      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6207  | 3931 | 1044 | 1203 | 29 |         |       |

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 18.

| Mol | Chain | Residues | Atoms |      |     |     |   |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---|---------|-------|
| 27  | LS    | 480      | Total | C    | N   | O   | P | S | 0       | 0     |
|     |       |          | 3793  | 2402 | 666 | 715 | 1 | 9 |         |       |

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 21.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 28  | LT    | 873      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6876  | 4363 | 1188 | 1303 | 22 |         |       |

- Molecule 29 is a protein called Protein SOF1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | LU    | 460      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3756  | 2349 | 685 | 706 | 16 |         |       |

- Molecule 30 is a protein called Ribosome biogenesis protein ENP2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30  | LV    | 405      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3286  | 2083 | 567 | 626 | 10 |         |       |

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 31  | LW    | 535      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4237  | 2656 | 762 | 807 | 12 |         |       |

- Molecule 32 is a protein called RNA cytidine acetyltransferase.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | LX    | 842      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6720  | 4301 | 1155 | 1238 | 26 |         |       |
| 32  | LY    | 846      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6179  | 3918 | 1079 | 1165 | 17 |         |       |

- Molecule 33 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | LZ    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1524  | 964 | 286 | 267 | 7 |         |       |

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein MPP10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | NA    | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2075  | 1279 | 378 | 414 | 4 |         |       |

- Molecule 35 is a protein called Something about silencing protein 10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35  | NB    | 267      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1873  | 1156 | 360 | 356 | 1 |         |       |

- Molecule 36 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 36  | NC    | 115      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 575   | 345 | 115 | 115 |  |         |       |

- Molecule 37 is a protein called Bud site selection protein 21.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 37  | ND    | 74       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 609   | 380 | 119 | 110 |  |         |       |

- Molecule 38 is a protein called Protein FAF1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 38  | NE    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 1021 | 327 | 298 | 3 |         |       |

- Molecule 39 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | NF    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1135  | 725 | 214 | 194 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | NG    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 541 | 166 | 165 | 3 |         |       |

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein 22.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 41  | NH    | 1077     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8693  | 5650 | 1434 | 1585 | 24 |         |       |

- Molecule 42 is a protein called Ribosomal RNA-processing protein 7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | NI    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1953  | 1248 | 331 | 366 | 8 |         |       |

- Molecule 43 is a protein called KRR1 small subunit processome component.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43  | NK    | 257      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2107  | 1344 | 369 | 381 | 13 |         |       |

- Molecule 44 is a protein called Small ribosomal subunit protein eS1A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44  | NM    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1838  | 1163 | 337 | 334 | 4 |         |       |

- Molecule 45 is a protein called Protein BFR2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | NN    | 267      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1481  | 909 | 280 | 292 |   |         |       |

- Molecule 46 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | NQ    | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 595   | 371 | 108 | 111 | 5 |         |       |

- Molecule 47 is a protein called rRNA biogenesis protein RRP5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | OA    | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 539 | 172 | 177 |   |         |       |

- Molecule 48 is a protein called Nucleolar protein 56.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 48  | SA    | 385      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3035  | 1926 | 521 | 579 | 9 |         |       |

- Molecule 49 is a protein called Nucleolar protein 58.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | SB    | 436      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3357  | 2116 | 574 | 657 | 10 |         |       |

- Molecule 50 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | SC    | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1871  | 1185 | 337 | 339 | 10 |         |       |
| 50  | SD    | 232      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1817  | 1153 | 324 | 330 | 10 |         |       |

- Molecule 51 is a protein called 13 kDa ribonucleoprotein-associated protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | SE    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 583 | 158 | 171 | 4 |         |       |
| 51  | SF    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 583 | 158 | 171 | 4 |         |       |

- Molecule 52 is a protein called Ribosomal RNA-processing protein 9.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | SG    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3672  | 2331 | 645 | 686 | 10 |         |       |

- Molecule 53 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | SH    | 360      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2781  | 1781 | 473 | 516 | 11 |         |       |

- Molecule 54 is a protein called Ribosome biogenesis protein BMS1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 54  | SI    | 811      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6577  | 4219 | 1156 | 1173 | 29 |         |       |

- Molecule 55 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | SJ    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1678  | 1069 | 292 | 306 | 11 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | SK    | 229      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1793  | 1141 | 312 | 329 | 11 |         |       |

- Molecule 56 is a protein called rRNA-processing protein FCF1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 56  | SL    | 173      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1384  | 881 | 254 | 239 | 10 |         |       |

- Molecule 57 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | SM    | 282      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2296  | 1441 | 430 | 418 | 7 |         |       |

- Molecule 58 is a protein called Ribosome biogenesis protein UTP30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 58  | SN    | 253      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2053  | 1313 | 364 | 368 | 8 |         |       |

- Molecule 59 is a protein called U3 small nucleolar RNA-associated protein 20.

| Mol | Chain | Residues | Atoms |       |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|---------|-------|
| 59  | SP    | 2356     | Total | C     | N    | O    | S  | 0       | 0     |
|     |       |          | 18367 | 11791 | 3084 | 3434 | 58 |         |       |

- Molecule 60 is a protein called rRNA-processing protein FCF2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | SQ    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1280  | 807 | 240 | 228 | 5 |         |       |

- Molecule 61 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SR    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 506 | 145 | 139 | 2 |         |       |

- Molecule 62 is a protein called U3 small nucleolar RNA-associated protein 14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 62  | SS    | 272      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2267  | 1415 | 427 | 415 | 10 |         |       |

- Molecule 63 is a protein called Nucleolar complex protein 14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 63  | ST    | 582      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4448  | 2823 | 802 | 811 | 12 |         |       |

- Molecule 64 is a protein called Nucleolar complex protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 64  | SU    | 534      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4370  | 2845 | 709 | 802 | 14 |         |       |

- Molecule 65 is a protein called Regulator of rDNA transcription protein 14.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 65  | SV    | 147      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 869   | 529 | 160 | 180 |  |         |       |

- Molecule 66 is a protein called Pre-rRNA-processing protein PNO1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | SW    | 199      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1565  | 998 | 284 | 279 | 4 |         |       |

- Molecule 67 is a protein called U3 small nucleolar RNA-associated protein 11.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 67  | SY    | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1953  | 1218 | 379 | 349 | 7 |         |       |

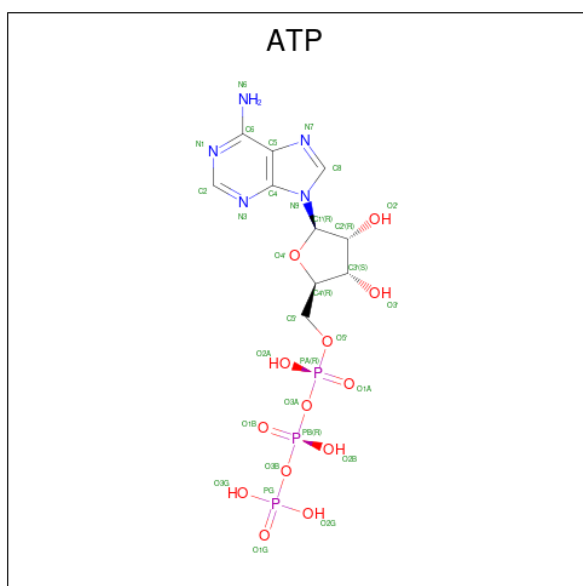
- Molecule 68 is a protein called Essential nuclear protein 1.

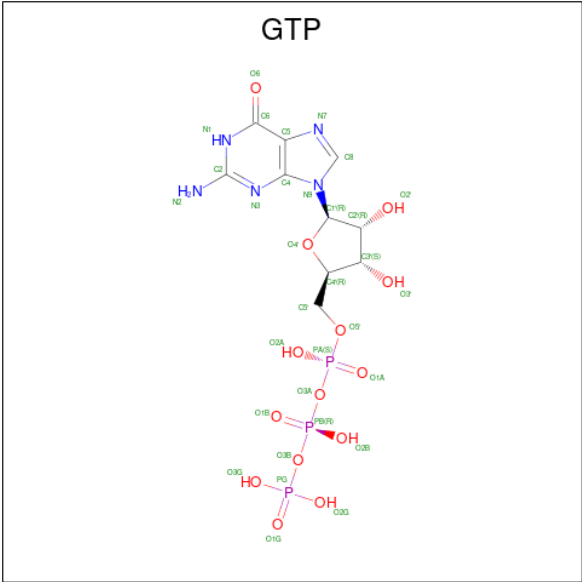
| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 68  | SZ    | 259      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1314  | 796 | 259 | 259 |  |         |       |

- Molecule 69 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 69  | L0    | 3        | Total | Mg | 0       |
|     |       |          | 3     | 3  |         |
| 69  | L1    | 27       | Total | Mg | 0       |
|     |       |          | 27    | 27 |         |
| 69  | L2    | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 69  | NH    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 69  | SI    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 70 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



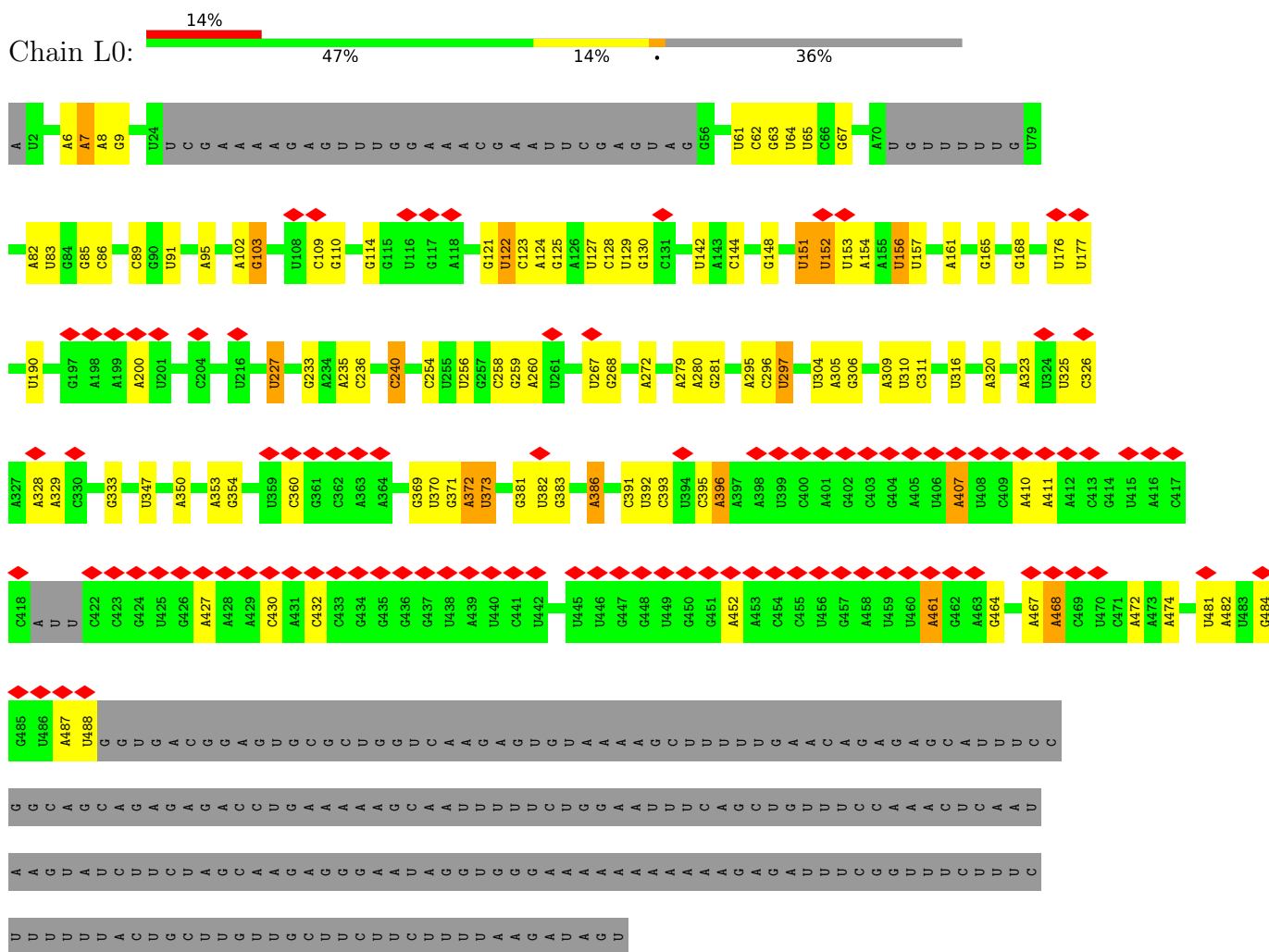


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 72  | SI    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

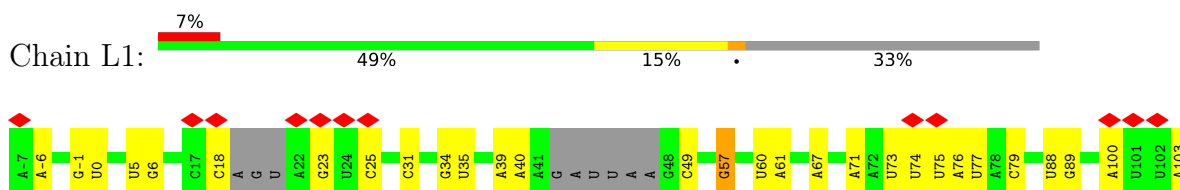
### 3 Residue-property plots

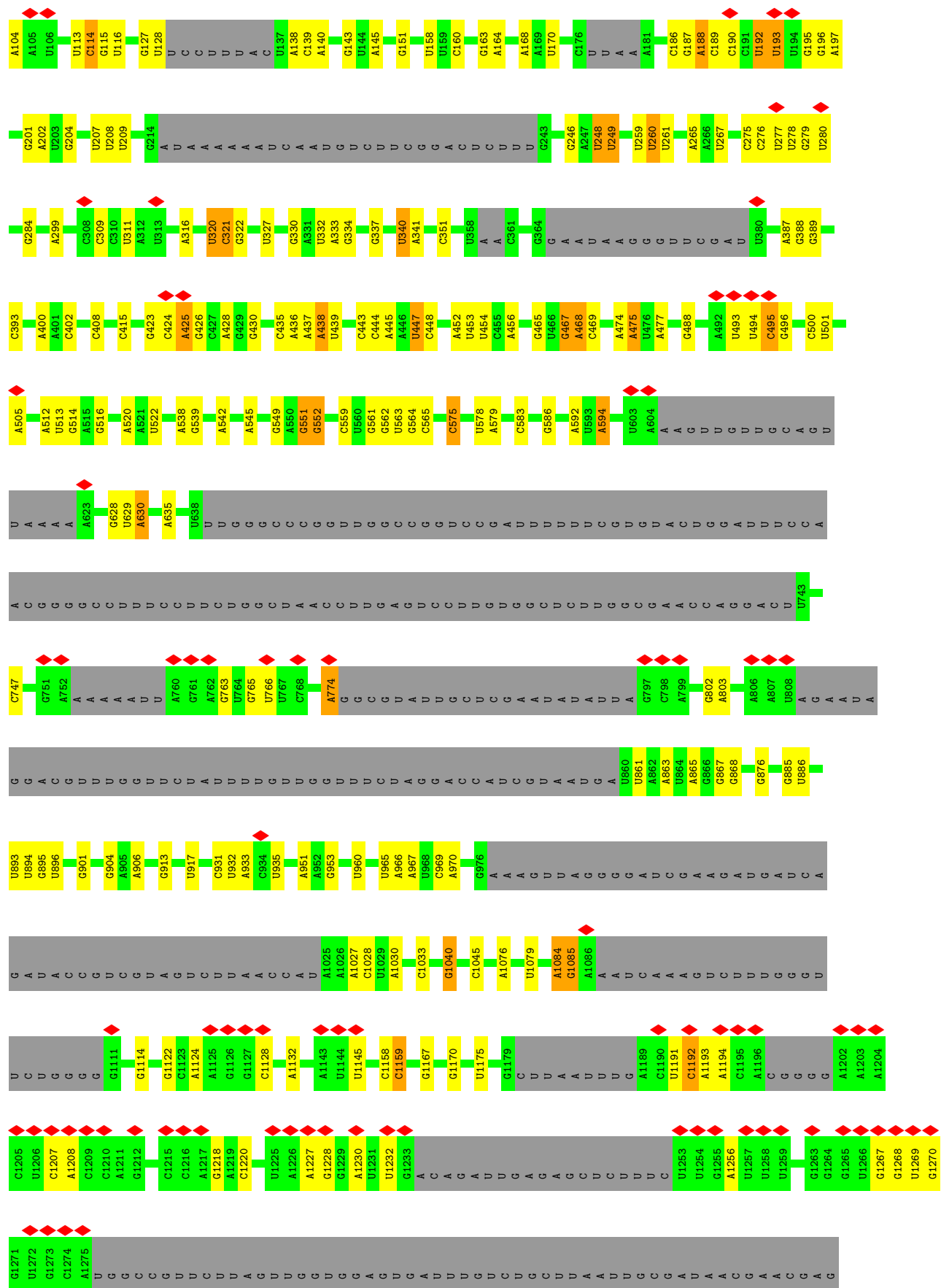
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

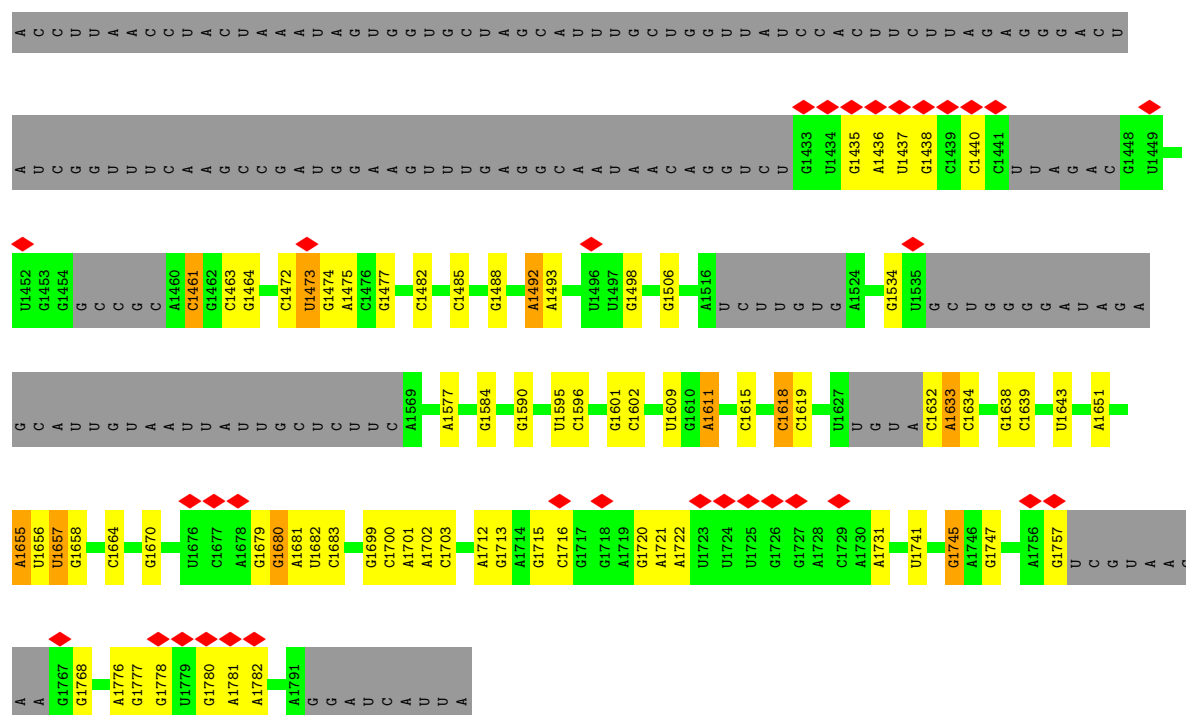
#### • Molecule 1: 5'ETS rRNA



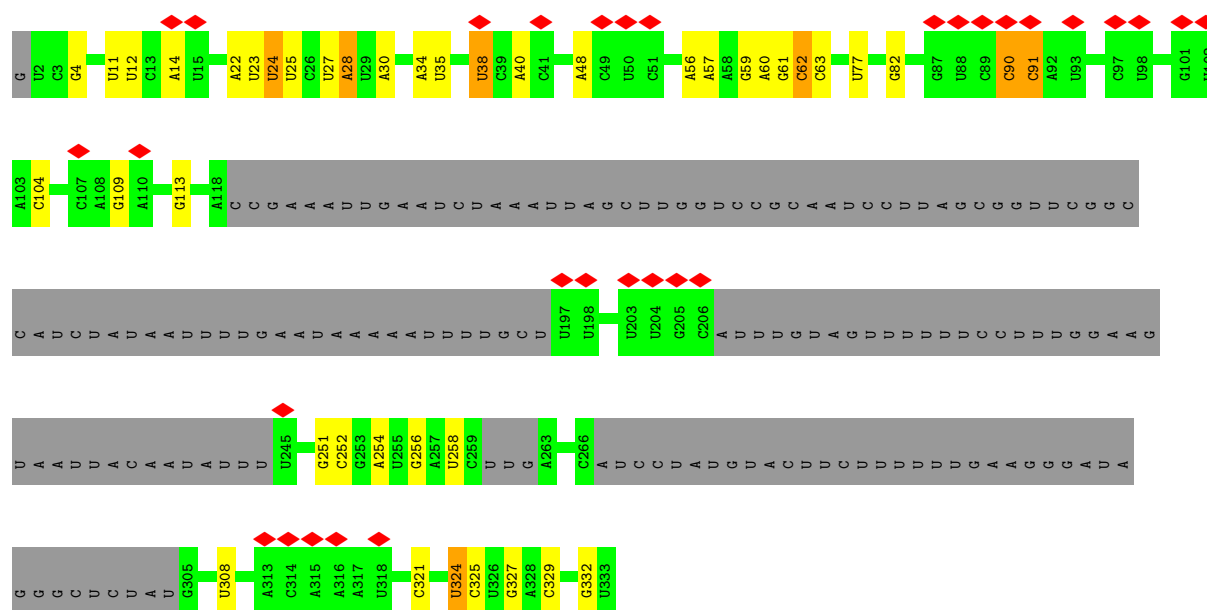
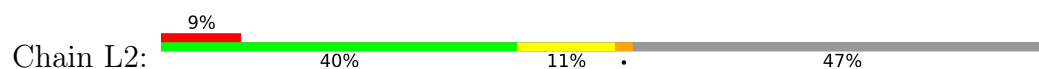
#### • Molecule 2: 18S rRNA





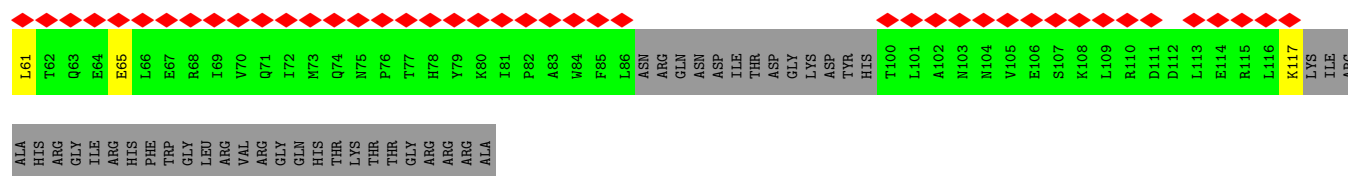


- Molecule 3: TPA: *Saccharomyces cerevisiae* U3a gene for small nucleolar RNA U3a

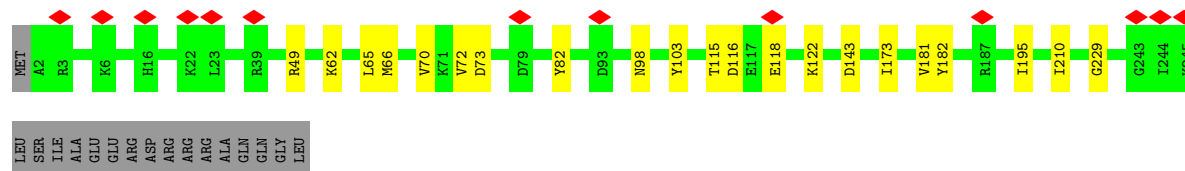
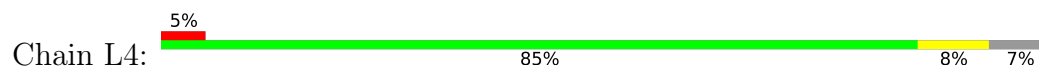


- Molecule 4: 40S ribosomal protein S18-A

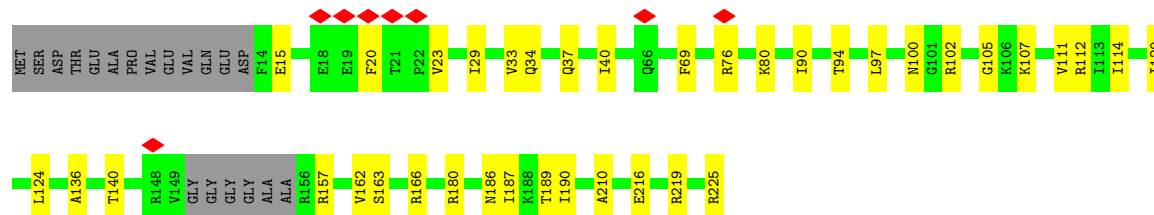
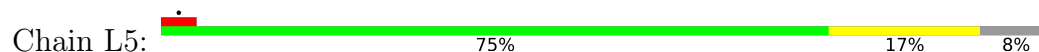




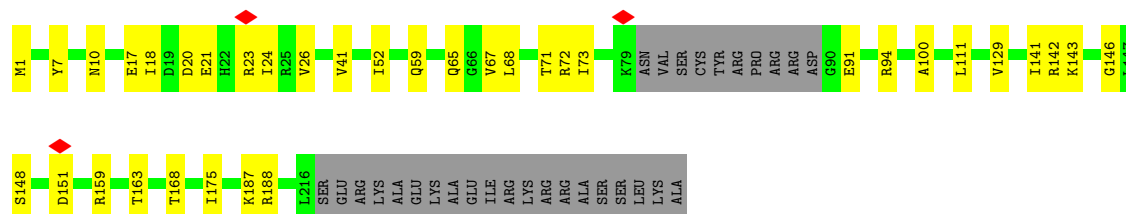
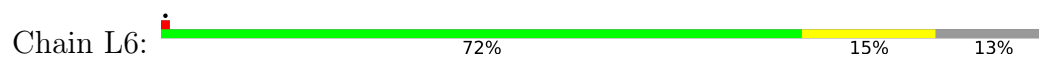
• Molecule 5: 40S ribosomal protein S4-A



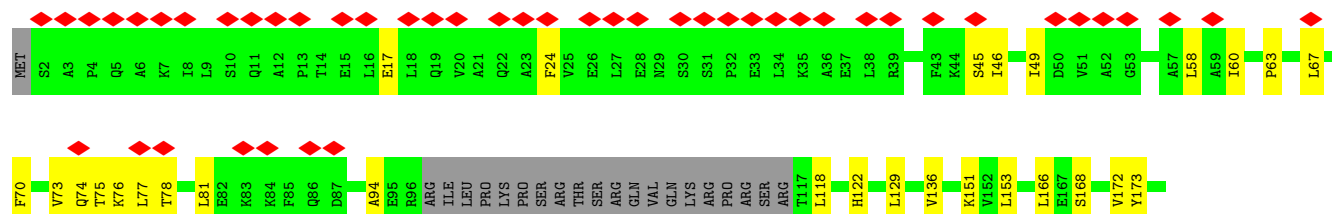
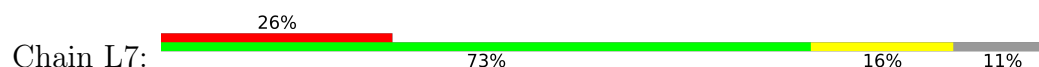
• Molecule 6: 40S ribosomal protein S5

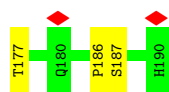


• Molecule 7: 40S ribosomal protein S6-A

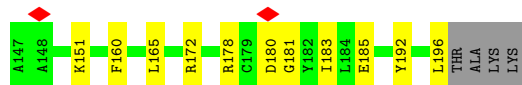
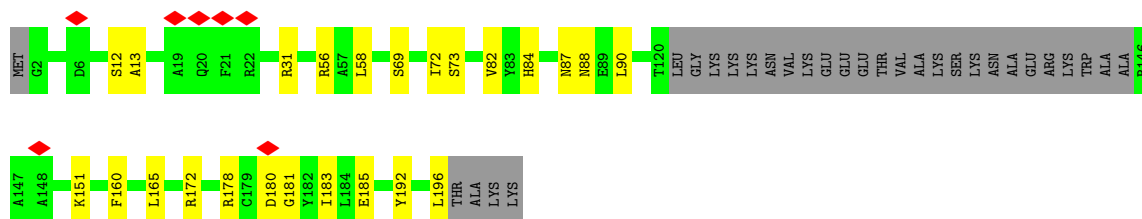
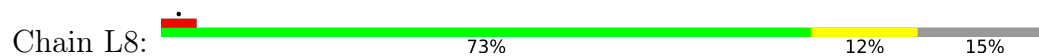


• Molecule 8: 40S ribosomal protein S7-A

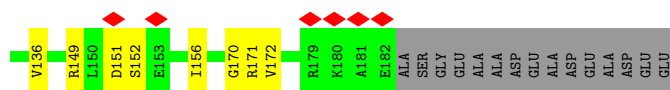
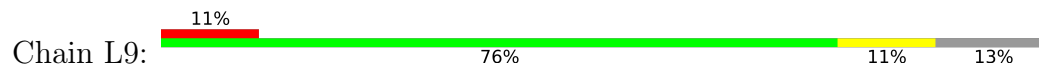




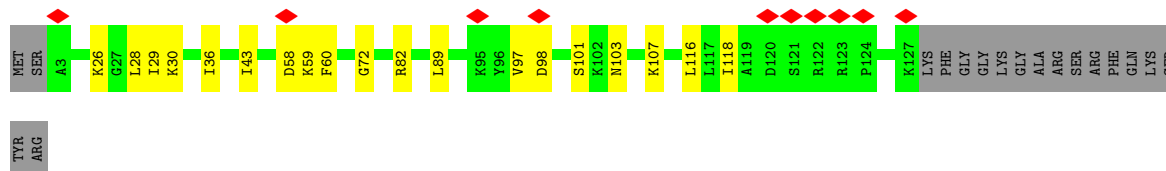
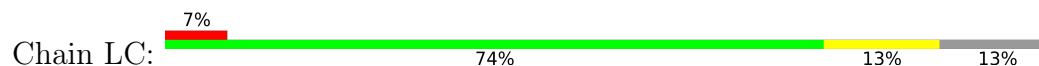
- Molecule 9: 40S ribosomal protein S8-A



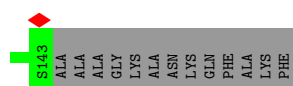
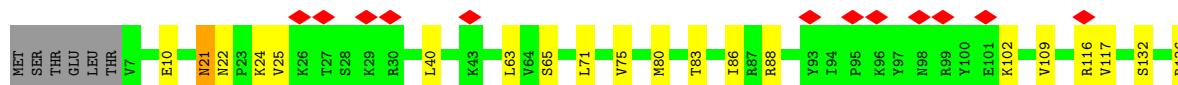
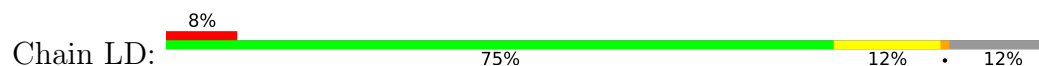
- Molecule 10: 40S ribosomal protein S9-A



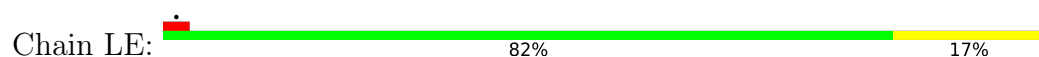
- Molecule 11: 40S ribosomal protein S16-A



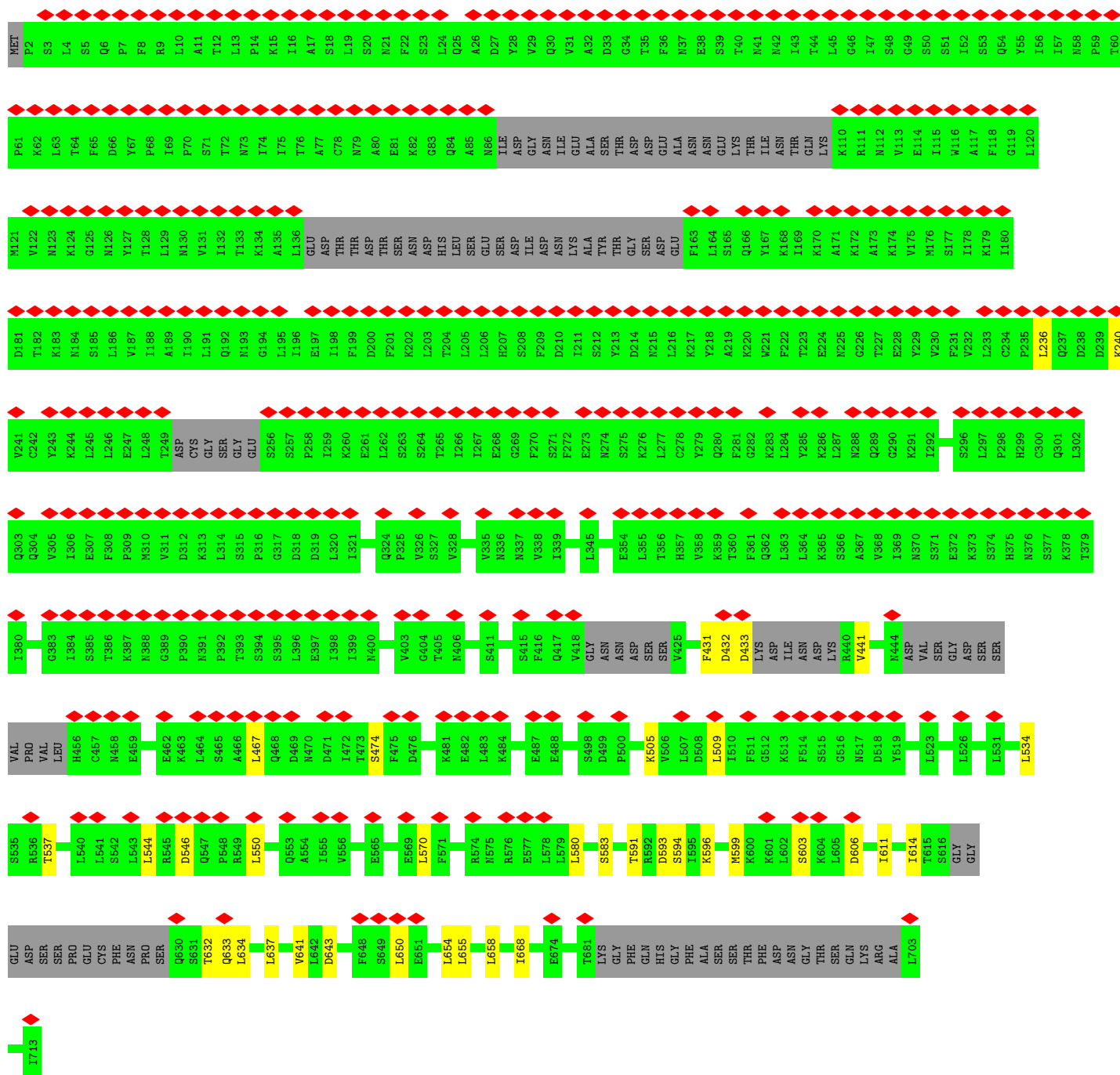
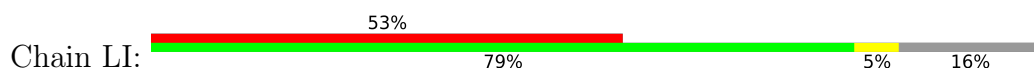
- Molecule 12: 40S ribosomal protein S11-A



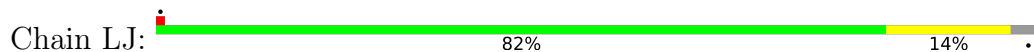
- Molecule 13: 40S ribosomal protein S22-A



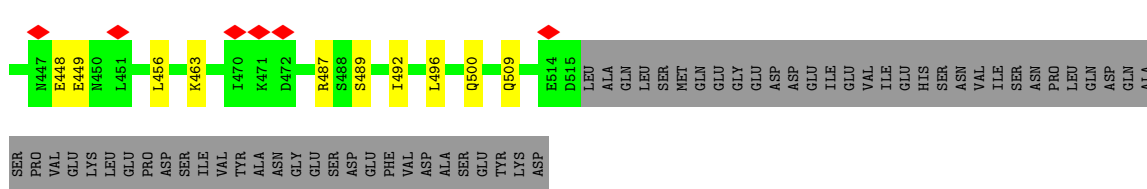




- Molecule 18: U3 small nucleolar RNA-associated protein 15

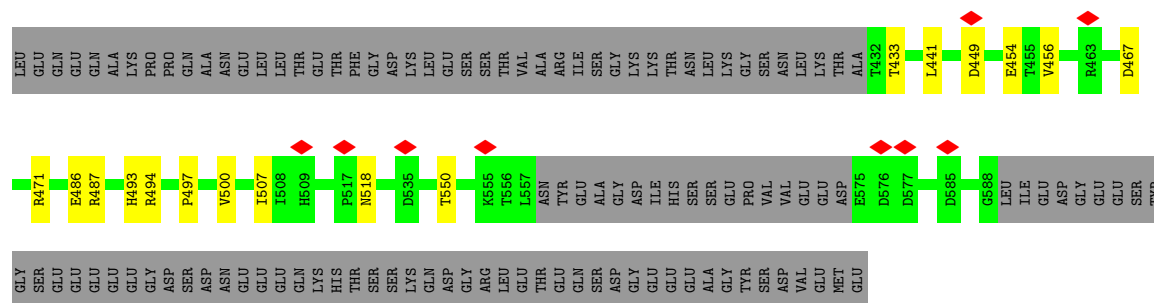


- Molecule 19: U3 small nucleolar RNA-associated protein 9

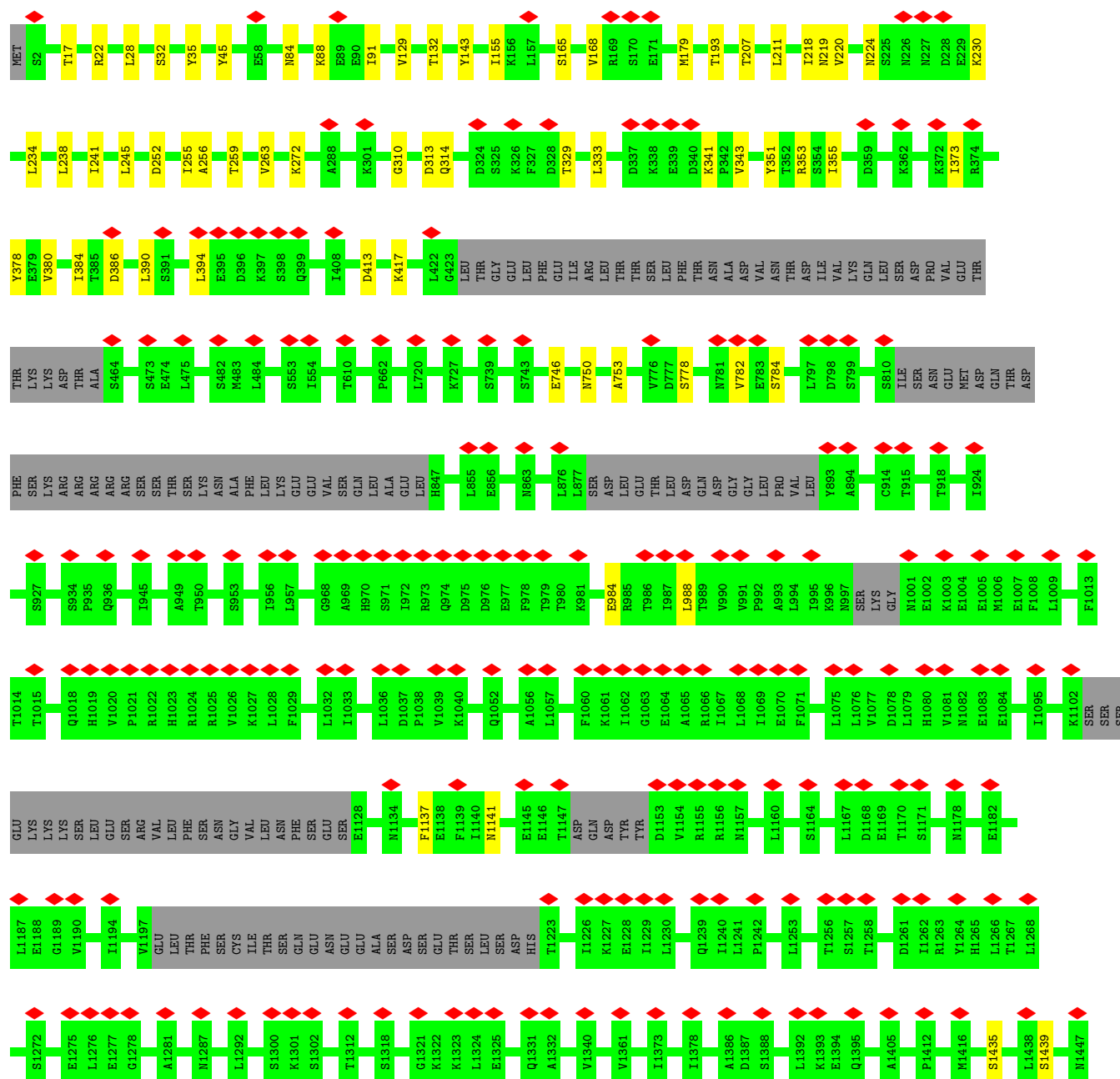


- Molecule 20: U3 small nucleolar RNA-associated protein 5

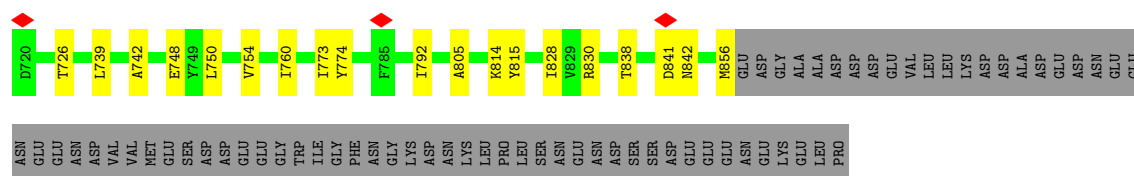




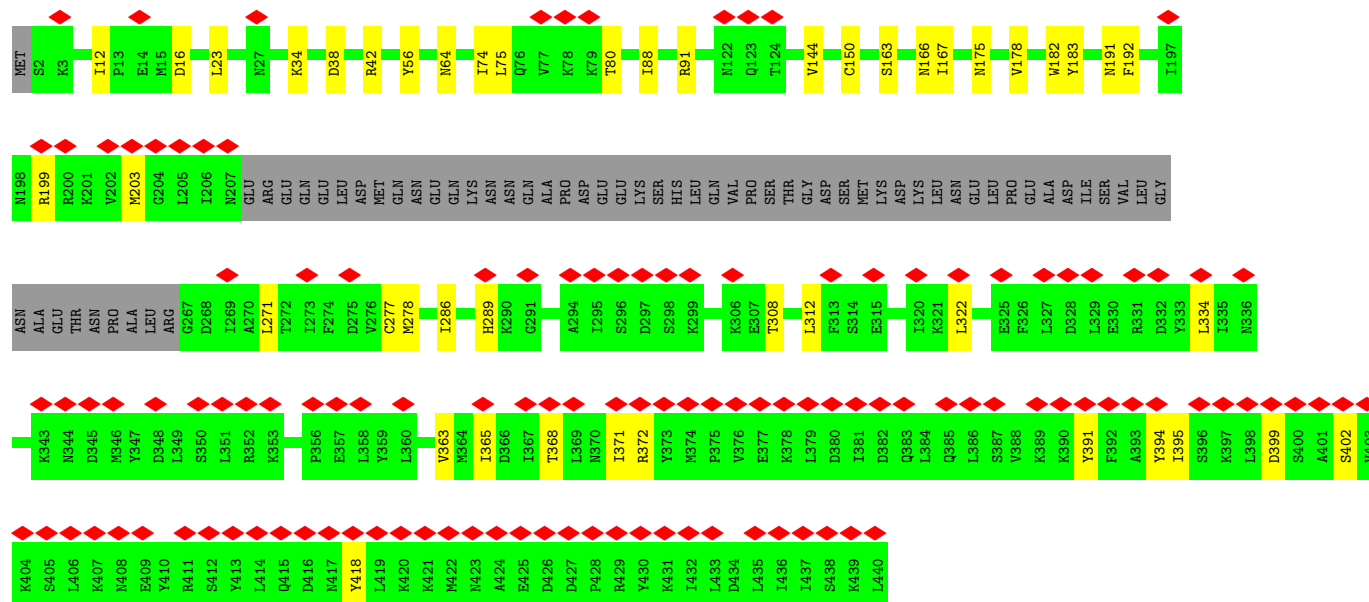
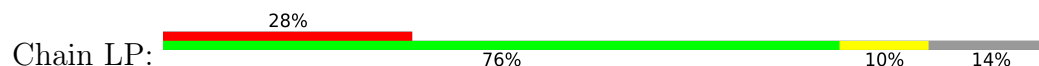
• Molecule 21: U3 small nucleolar RNA-associated protein 10



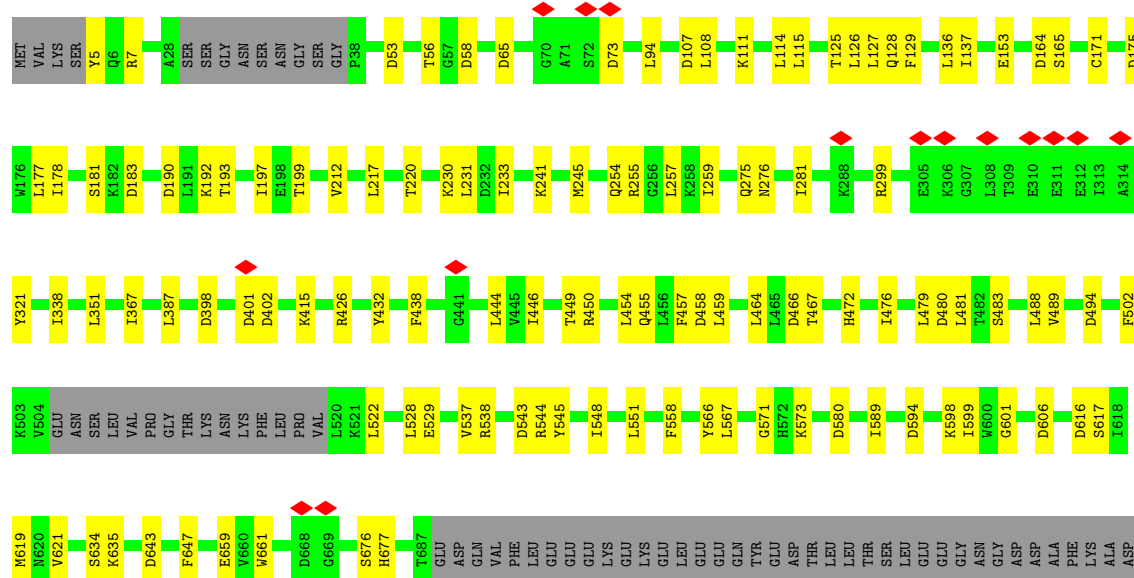


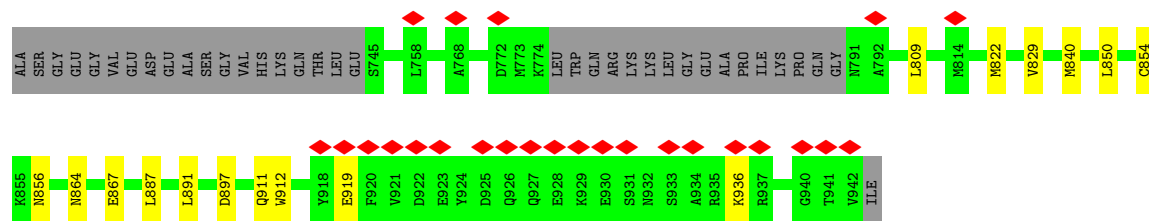


• Molecule 24: U3 small nucleolar RNA-associated protein 6

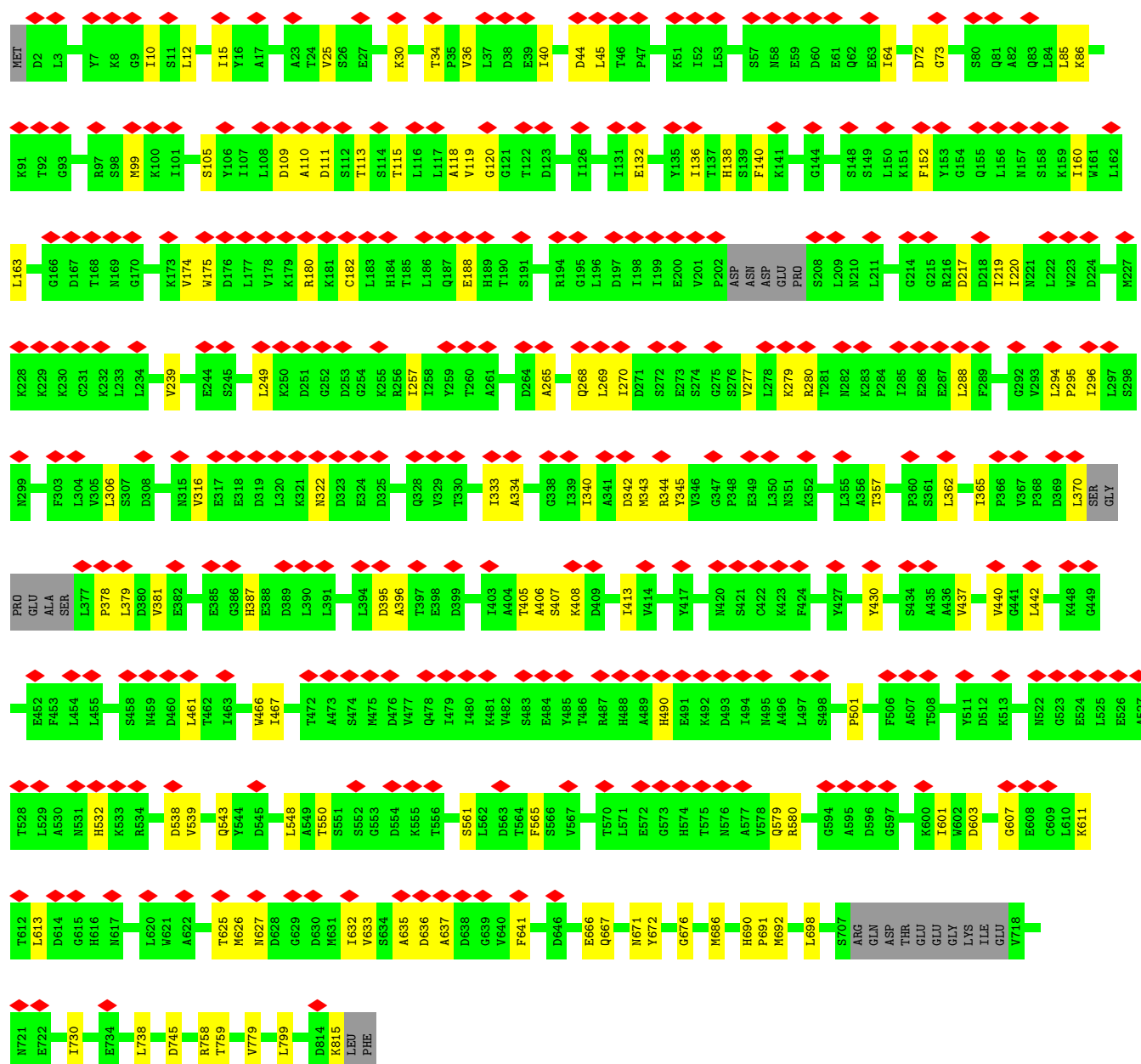
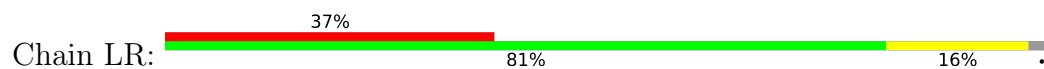


• Molecule 25: U3 small nucleolar RNA-associated protein 12



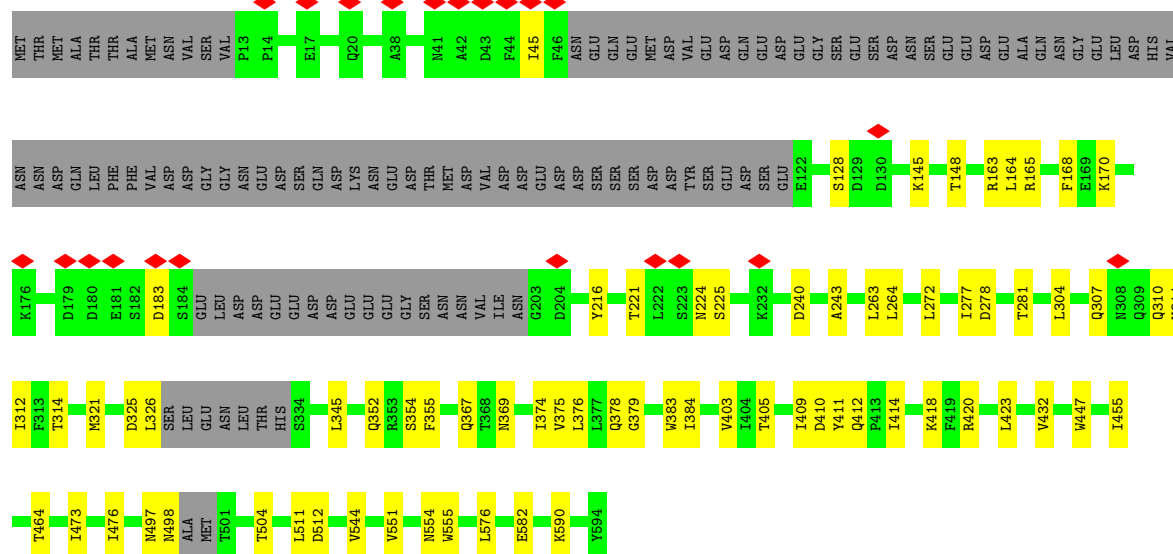


• Molecule 26: U3 small nucleolar RNA-associated protein 13



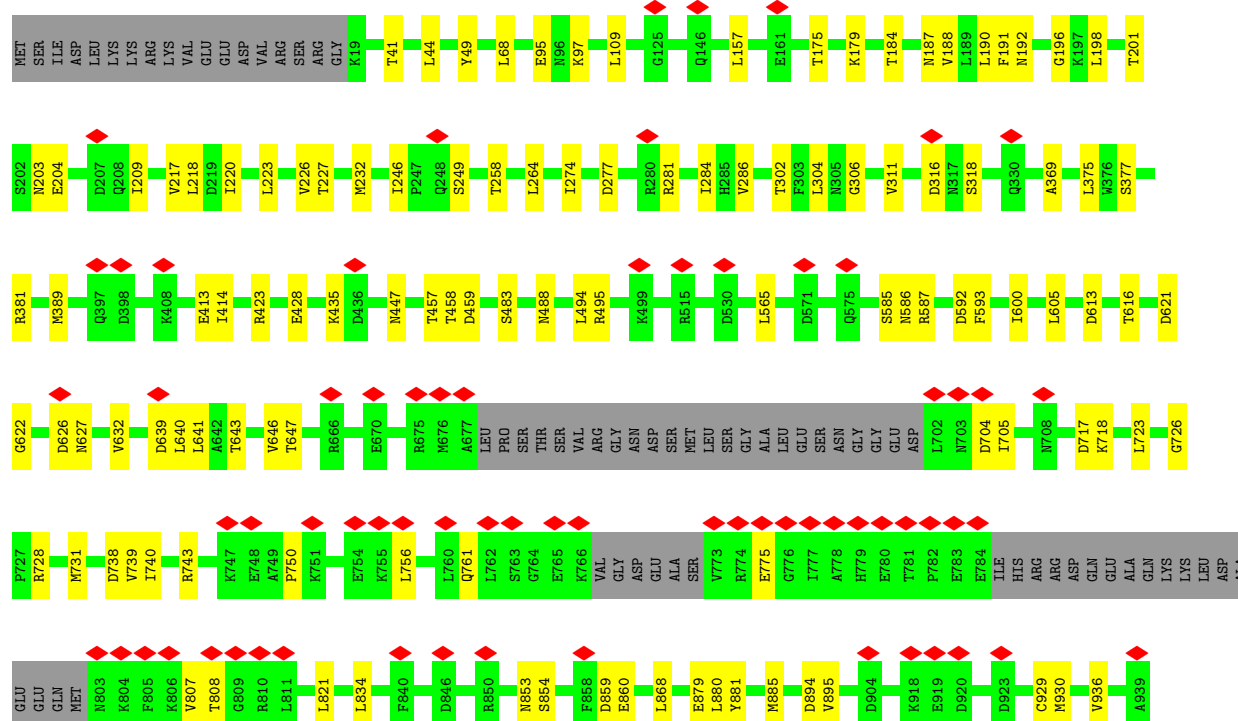
• Molecule 27: U3 small nucleolar RNA-associated protein 18

Chain LS: 



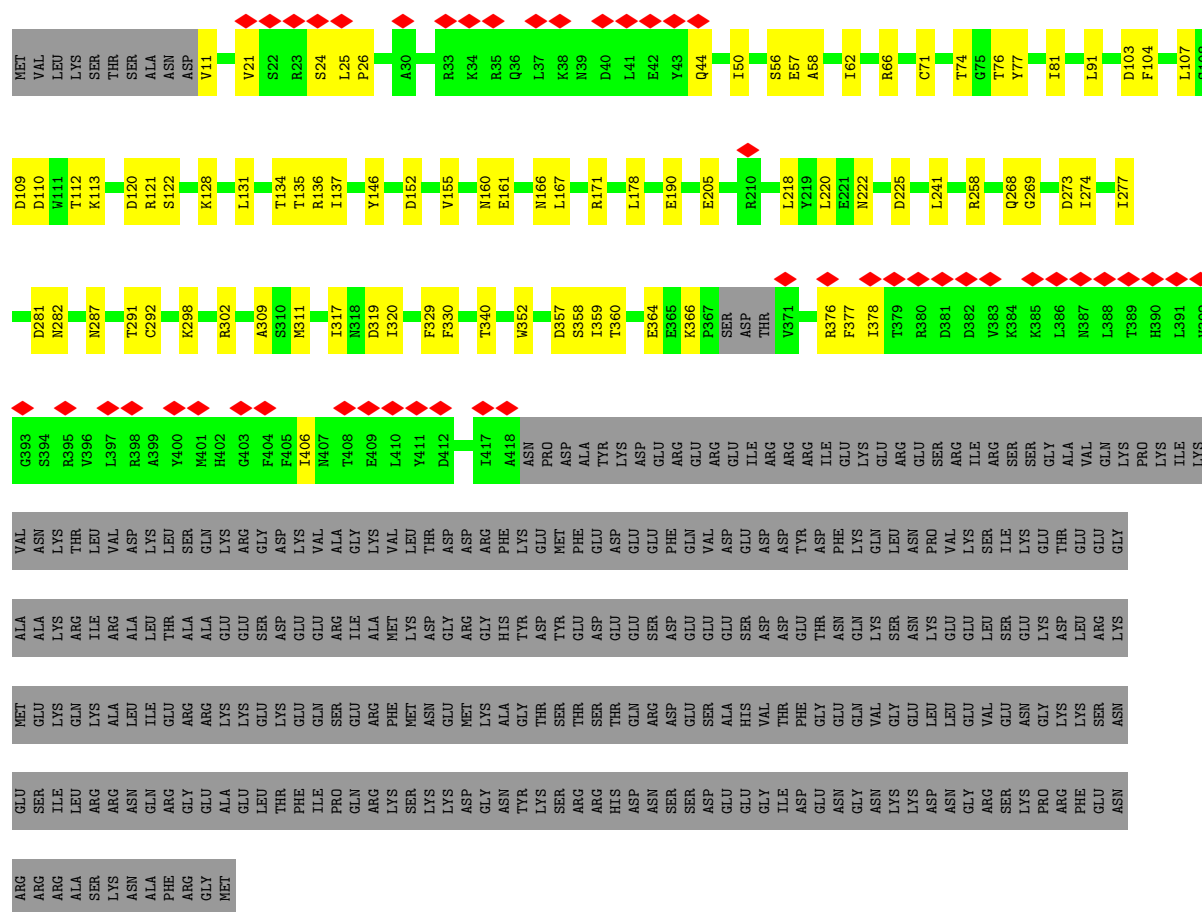
- Molecule 28: U3 small nucleolar RNA-associated protein 21

Chain LT: 

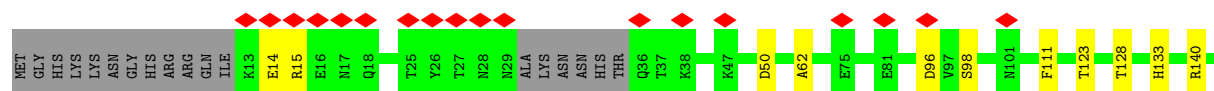


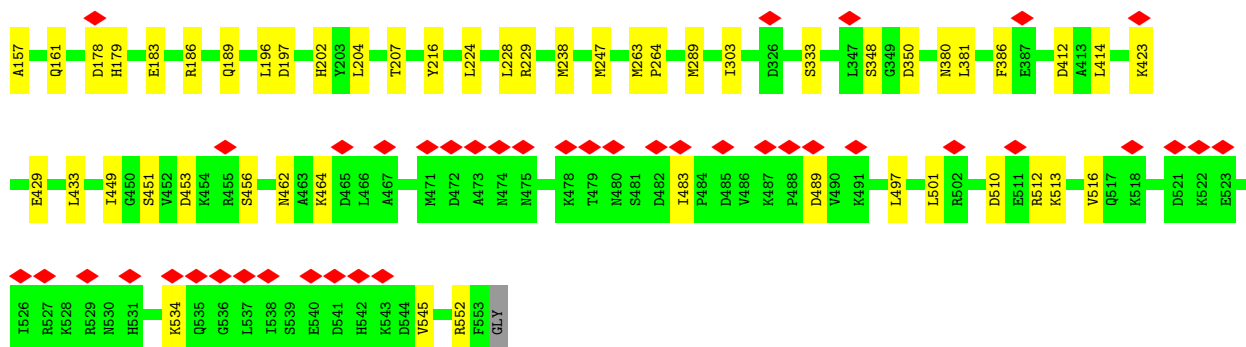
- Molecule 29: Protein SOF1

Chain LU: 

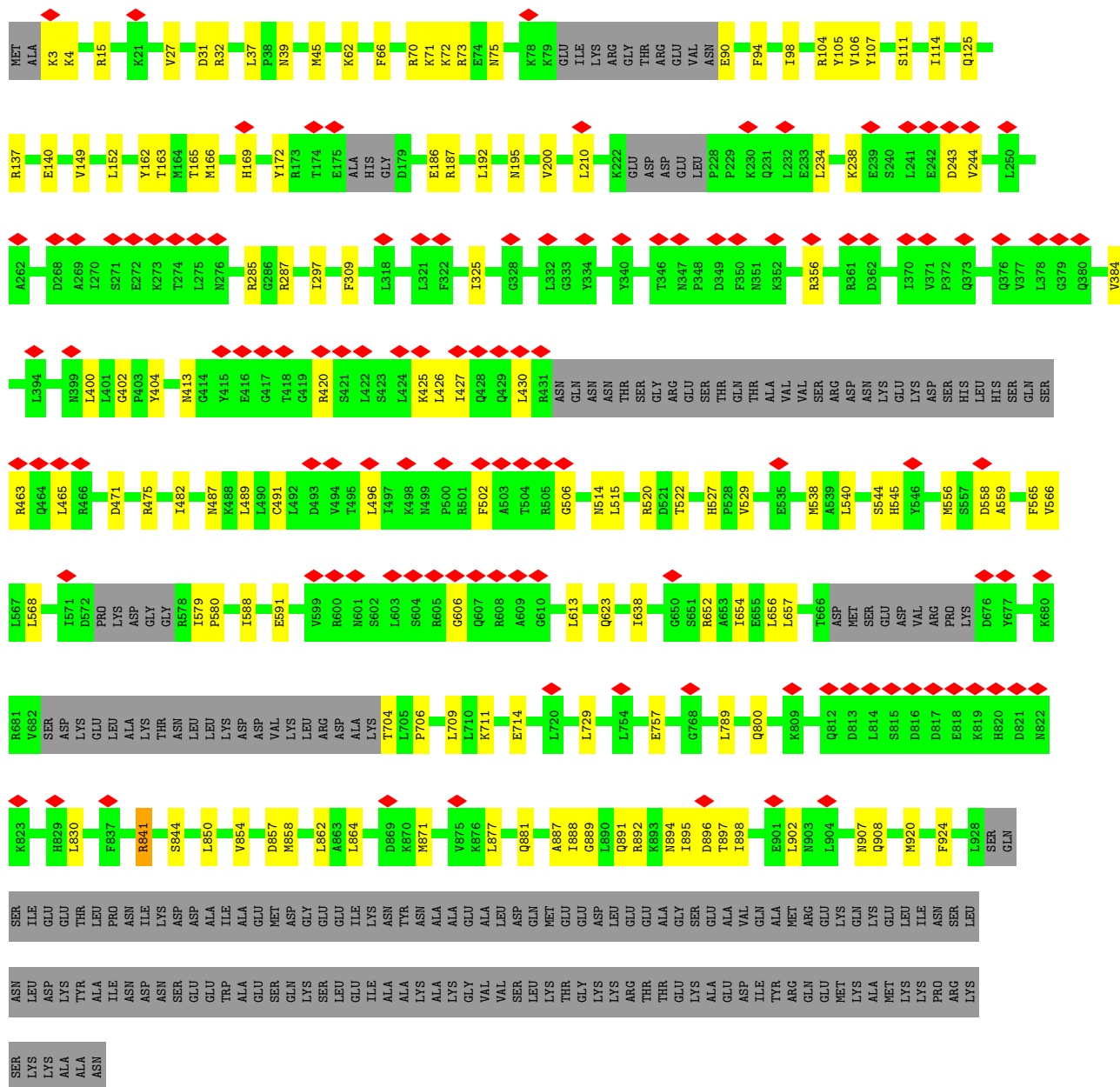


- Molecule 31: U3 small nucleolar RNA-associated protein 7

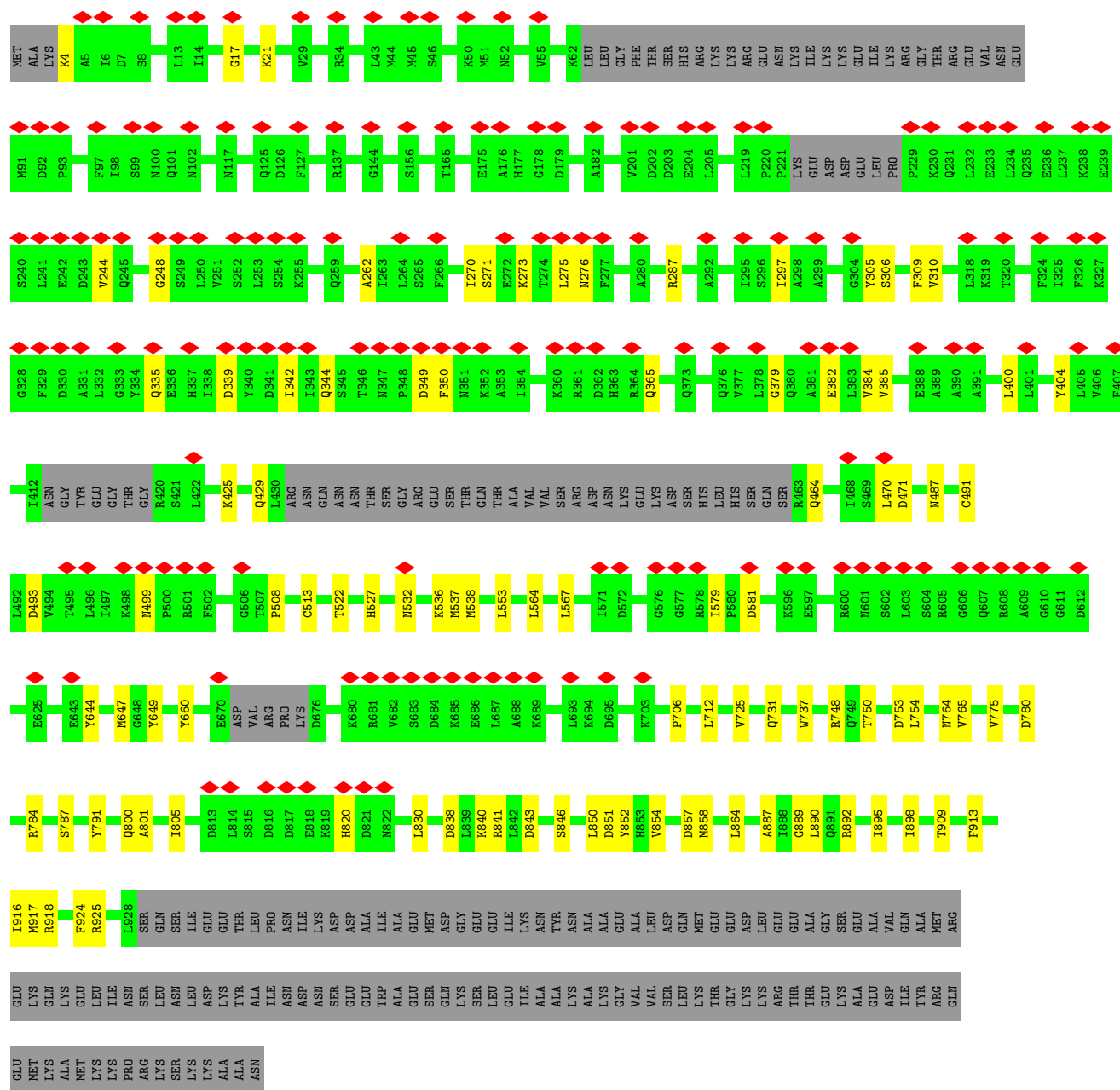




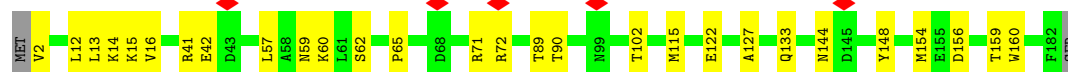
• Molecule 32: RNA cytidine acetyltransferase

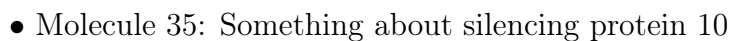


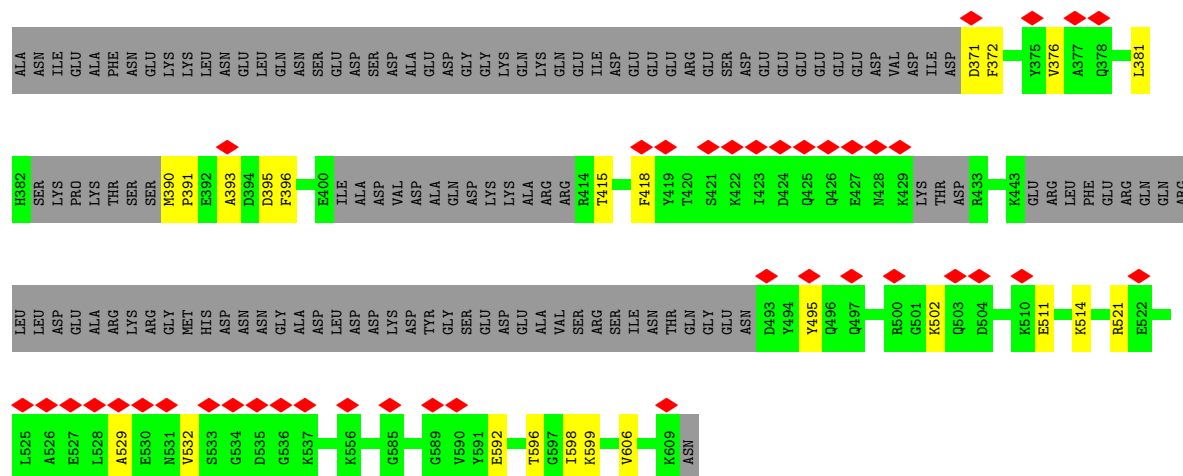
Chain LY: 



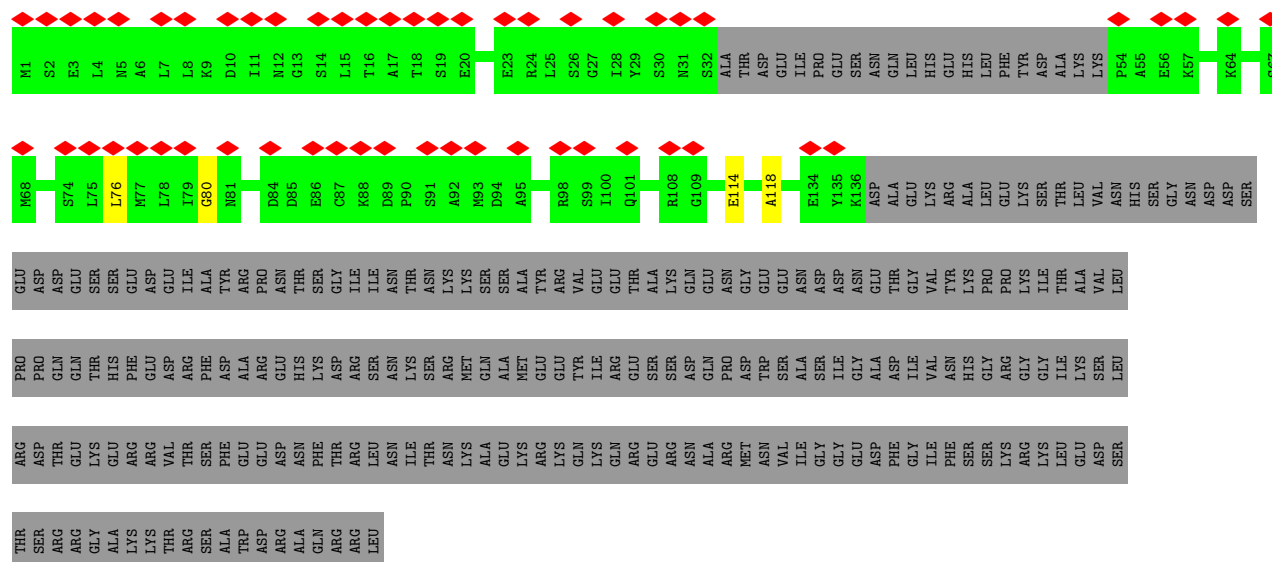
Chain LZ:  84% 15%



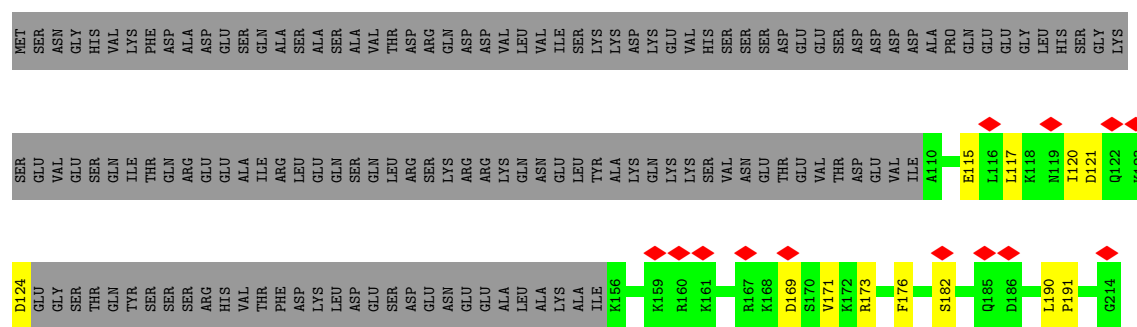




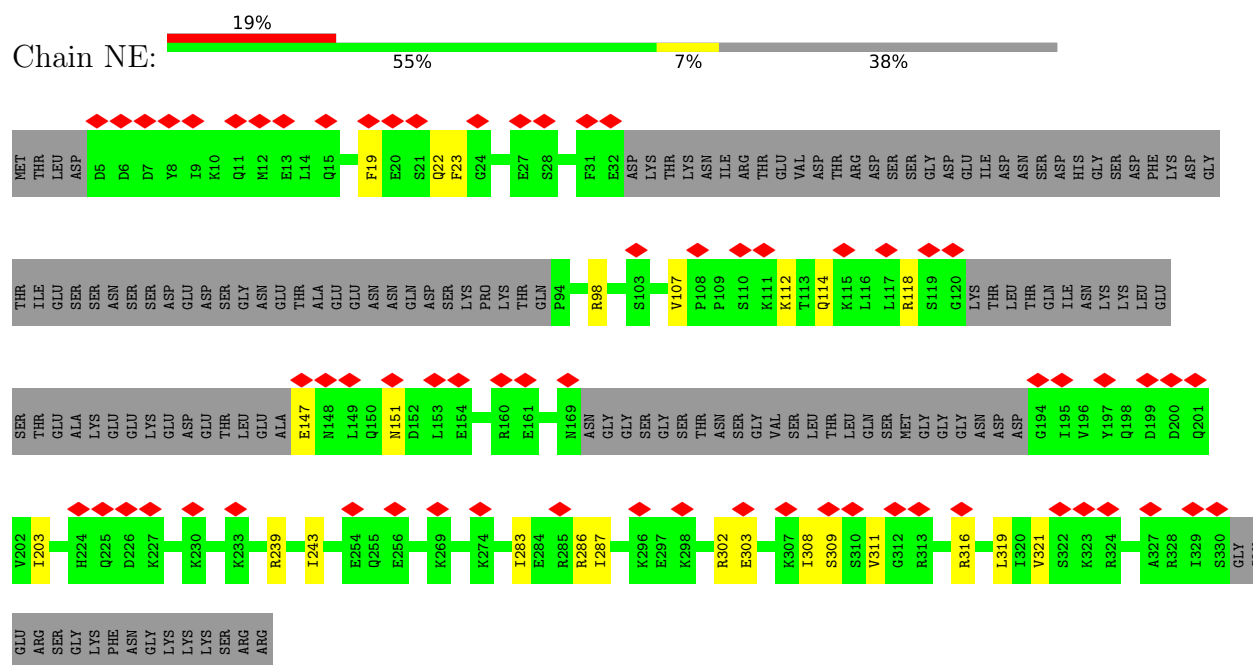
• Molecule 36: U3 small nucleolar ribonucleoprotein protein LCP5



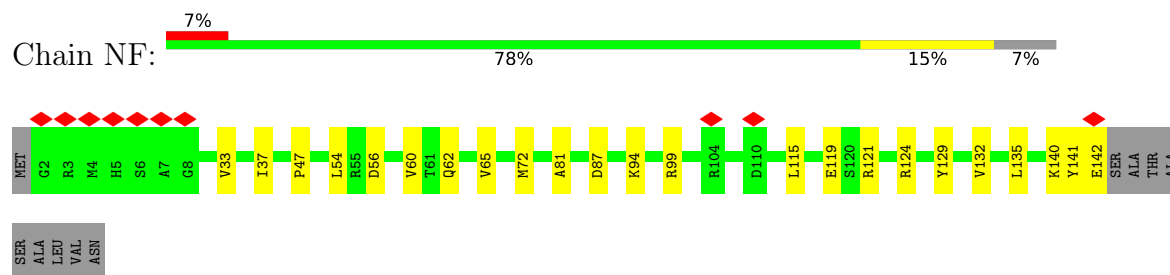
• Molecule 37: Bud site selection protein 21



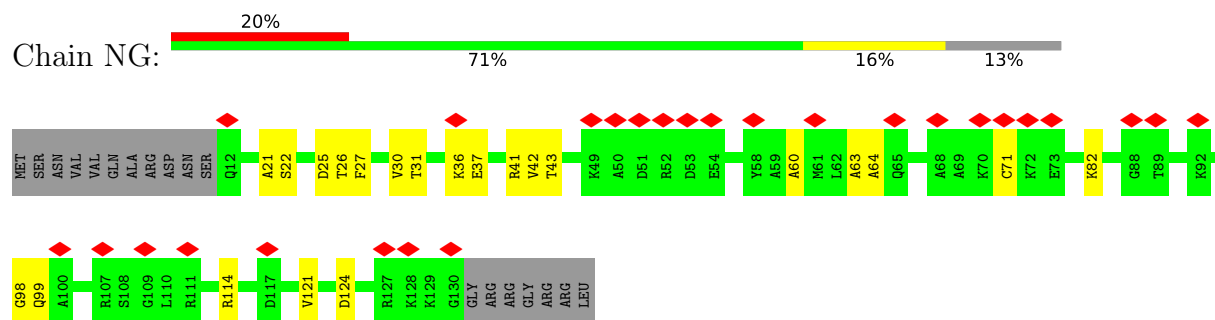
• Molecule 38: Protein FAF1



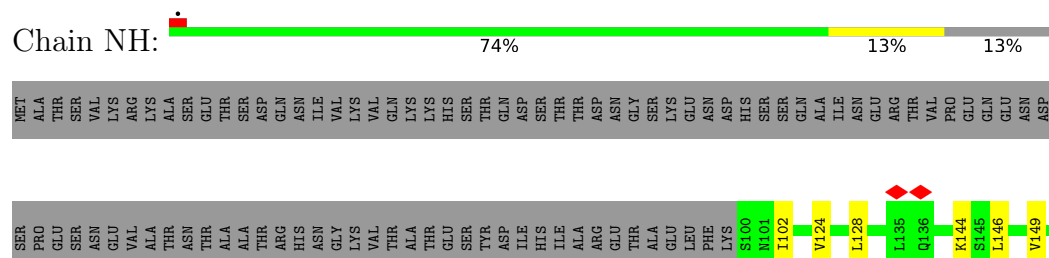
- Molecule 39: 40S ribosomal protein S13

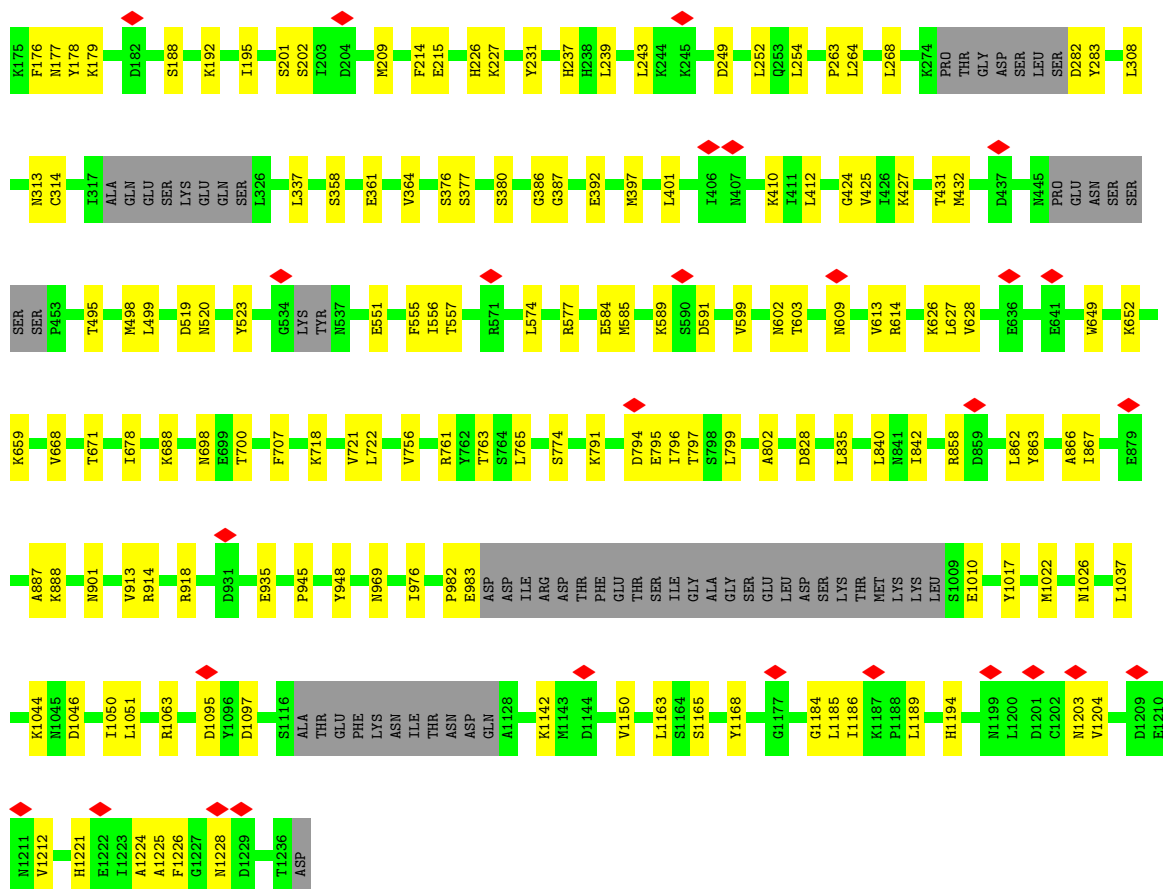


- Molecule 40: 40S ribosomal protein S14-A

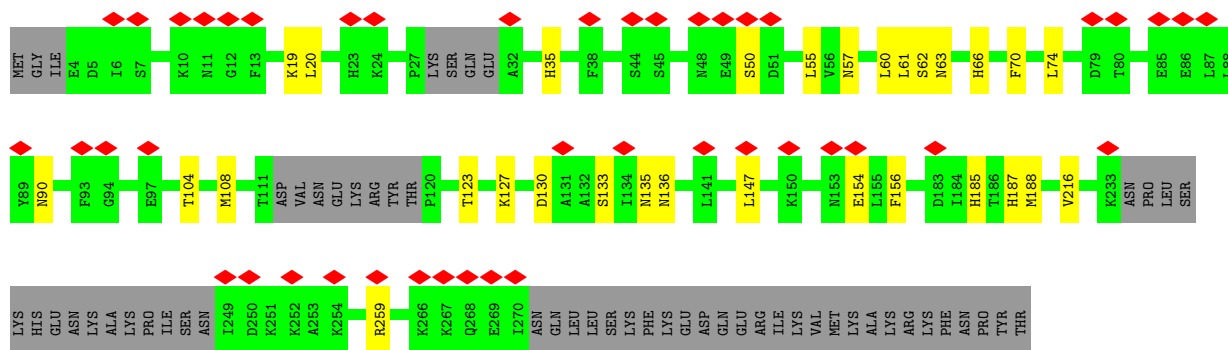
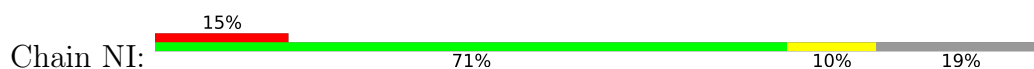


- Molecule 41: U3 small nucleolar RNA-associated protein 22

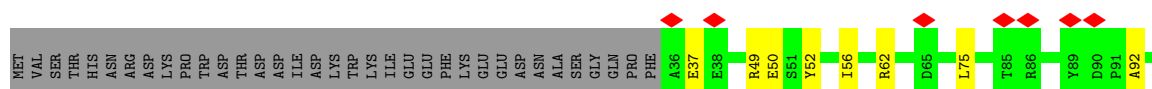
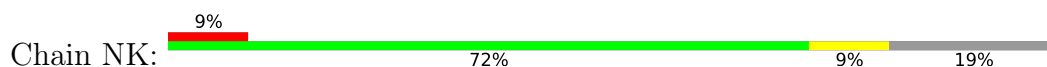




• Molecule 42: Ribosomal RNA-processing protein 7



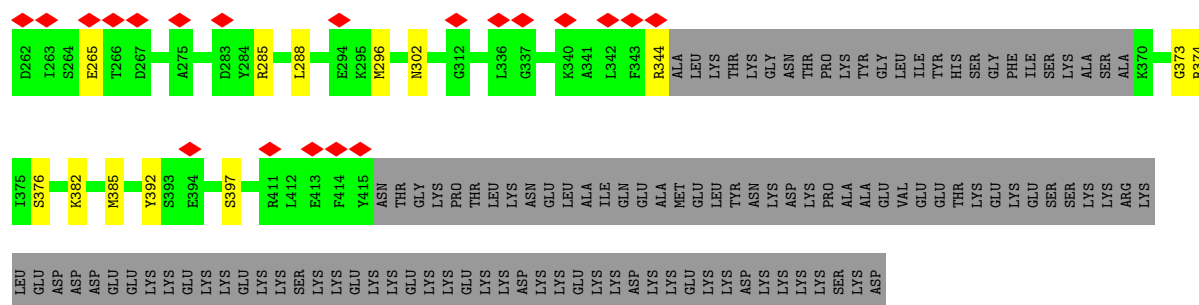
• Molecule 43: KRR1 small subunit processome component



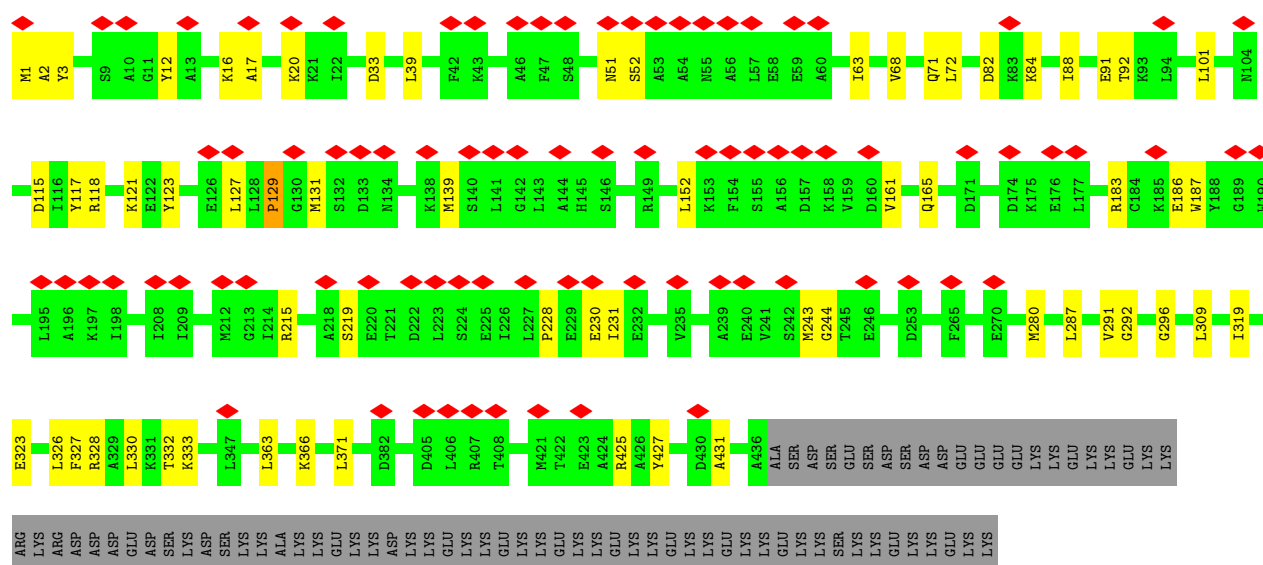
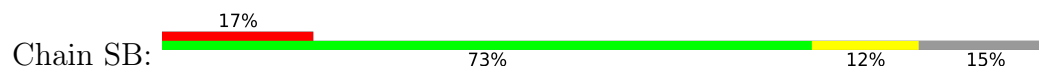


[illegible]

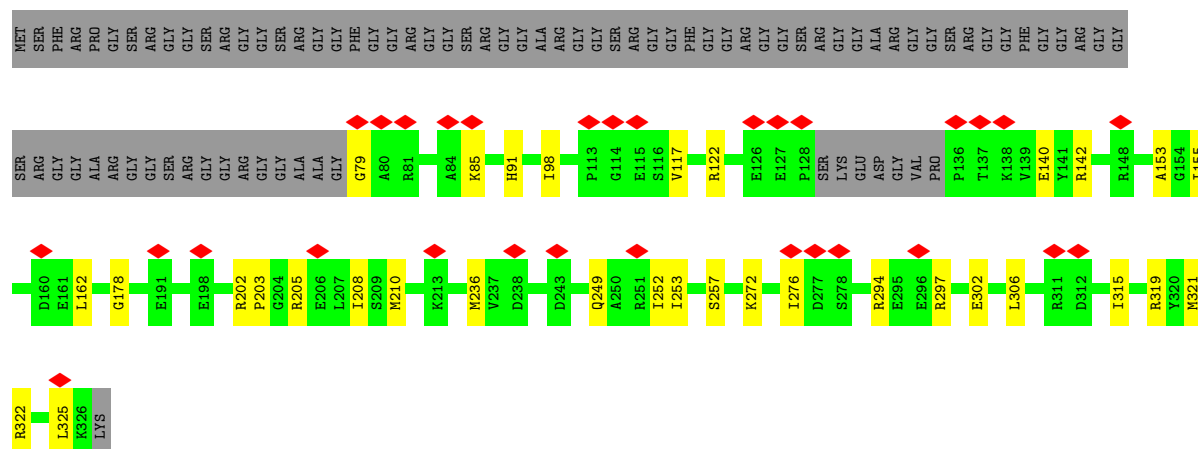




• Molecule 49: Nucleolar protein 58



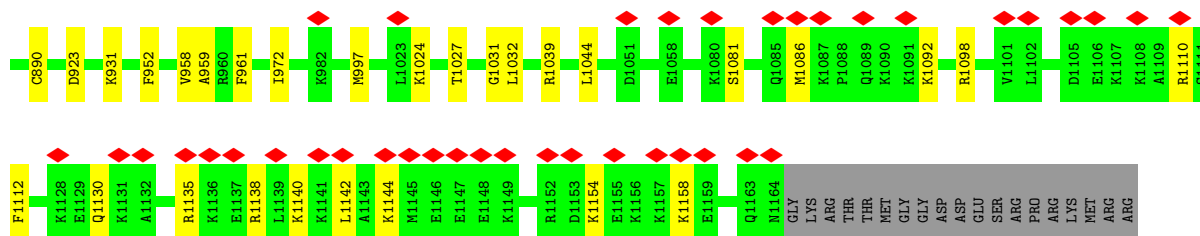
• Molecule 50: rRNA 2'-O-methyltransferase fibrillar



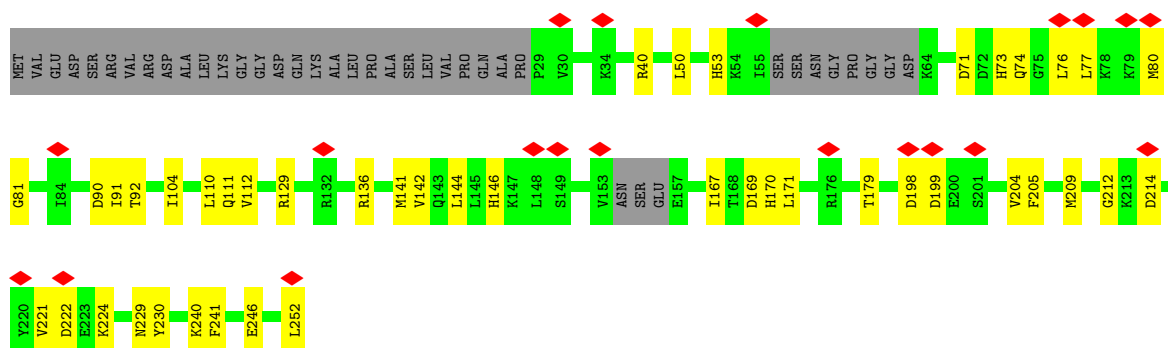
• Molecule 50: rRNA 2'-O-methyltransferase fibrillar



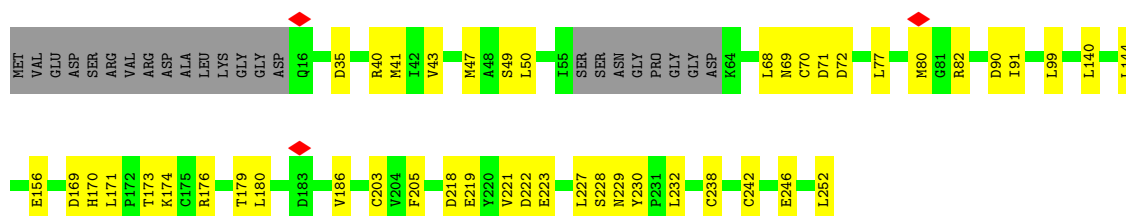
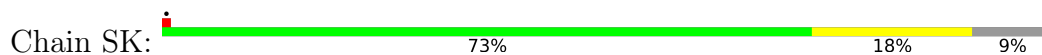




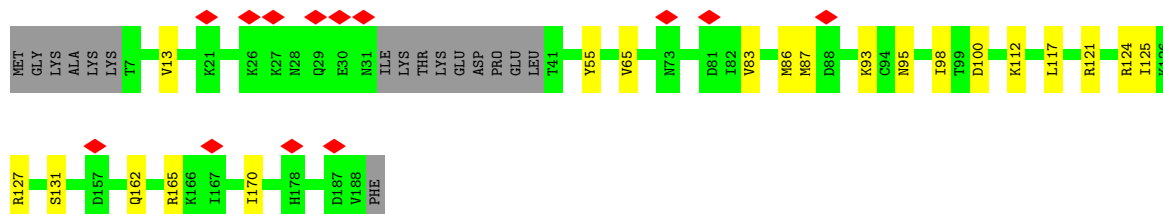
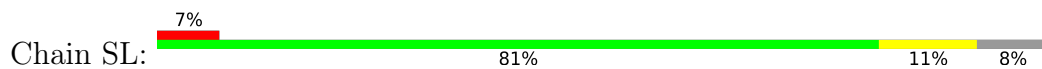
• Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1



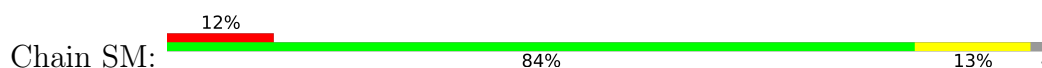
• Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

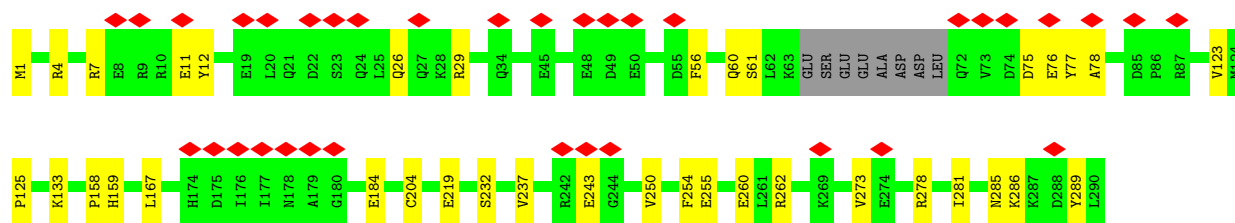


• Molecule 56: rRNA-processing protein FCF1

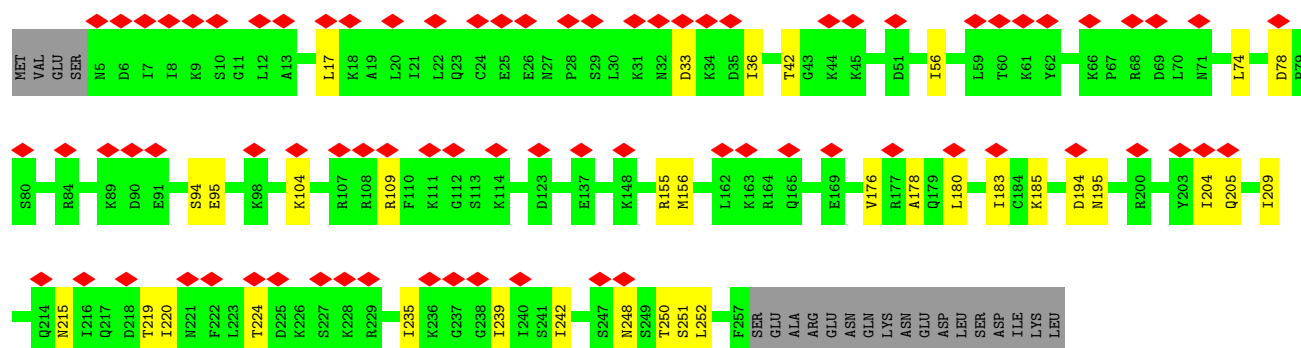
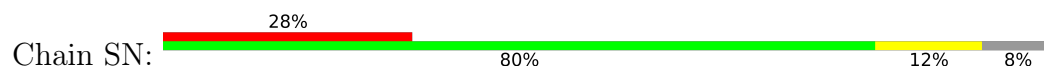


• Molecule 57: U3 small nucleolar ribonucleoprotein protein IMP4

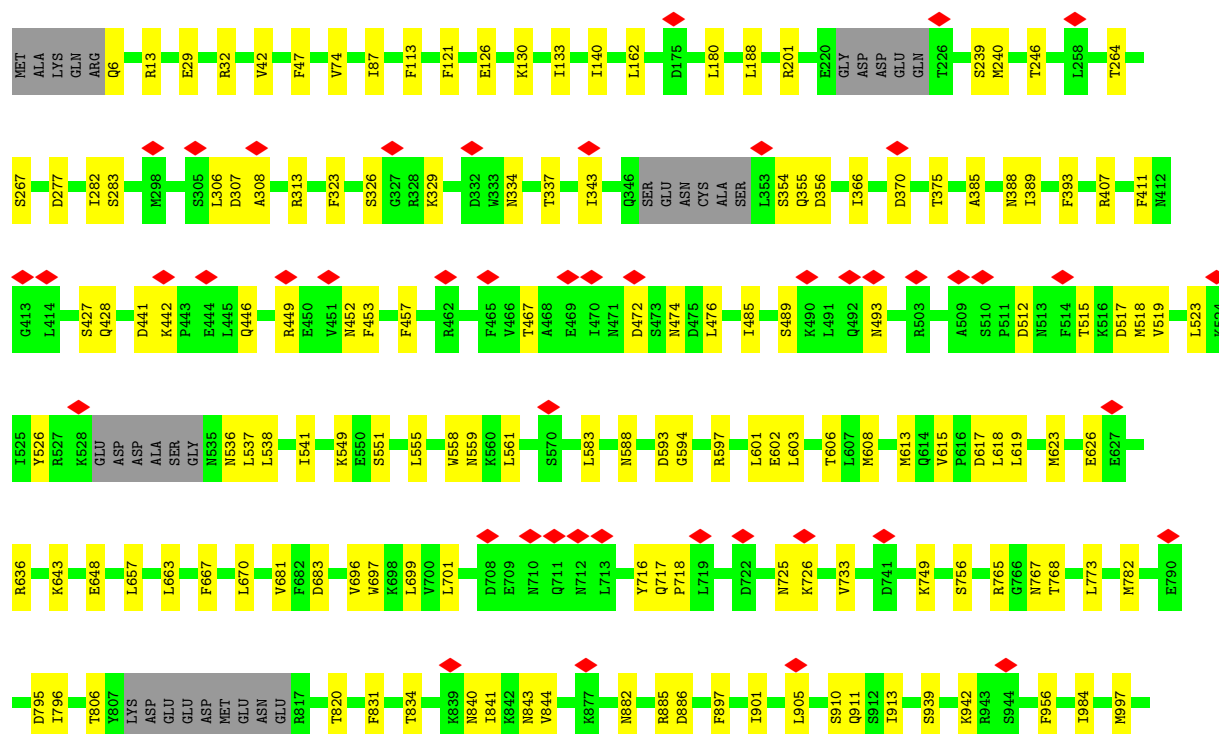
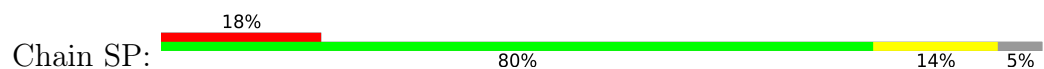




• Molecule 58: Ribosome biogenesis protein UTP30



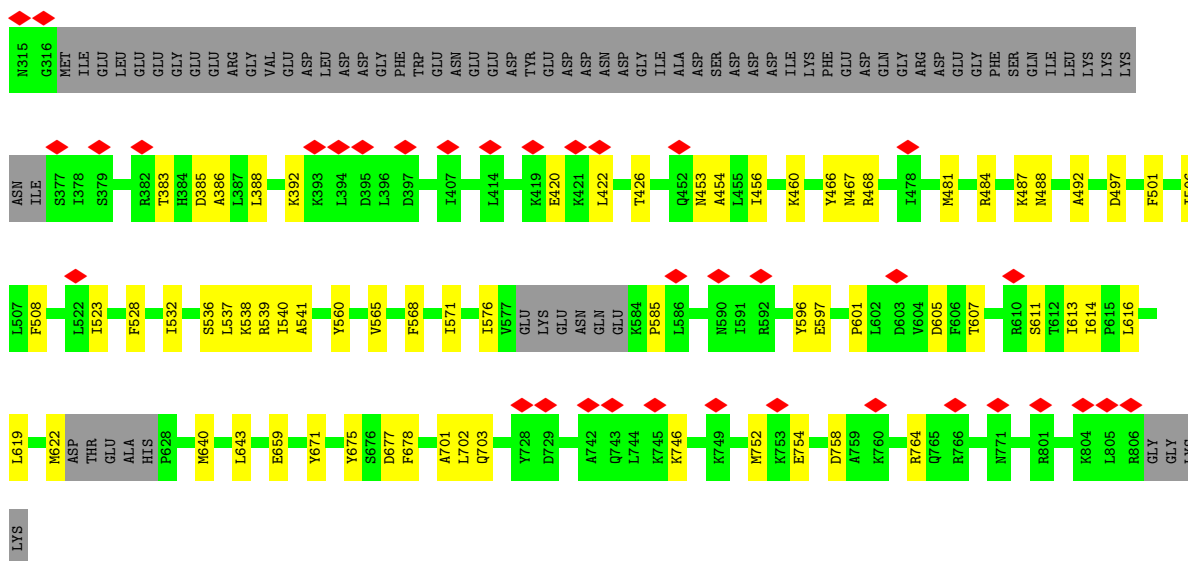
• Molecule 59: U3 small nucleolar RNA-associated protein 20



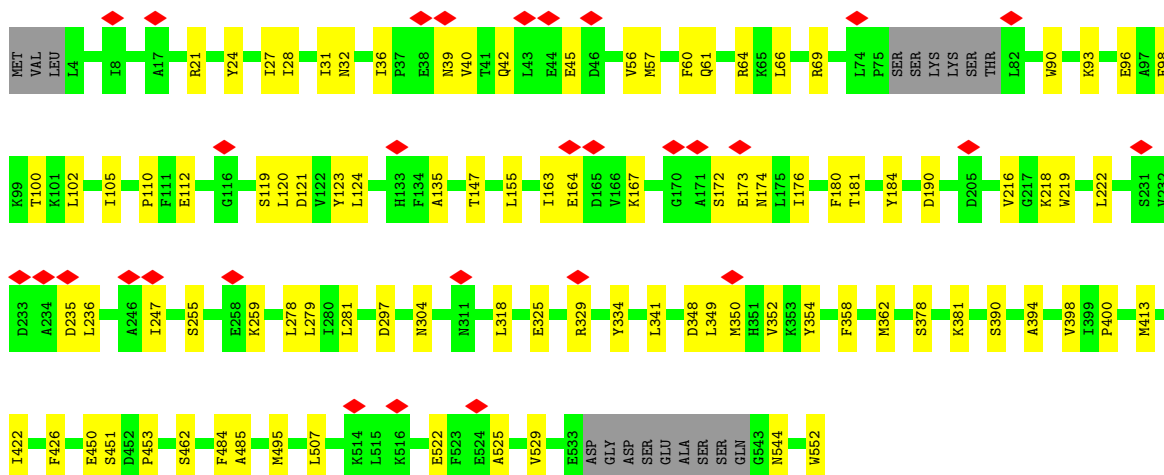
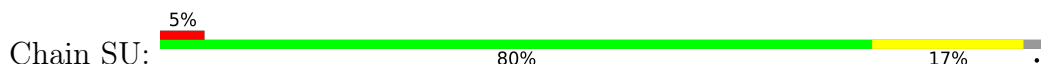




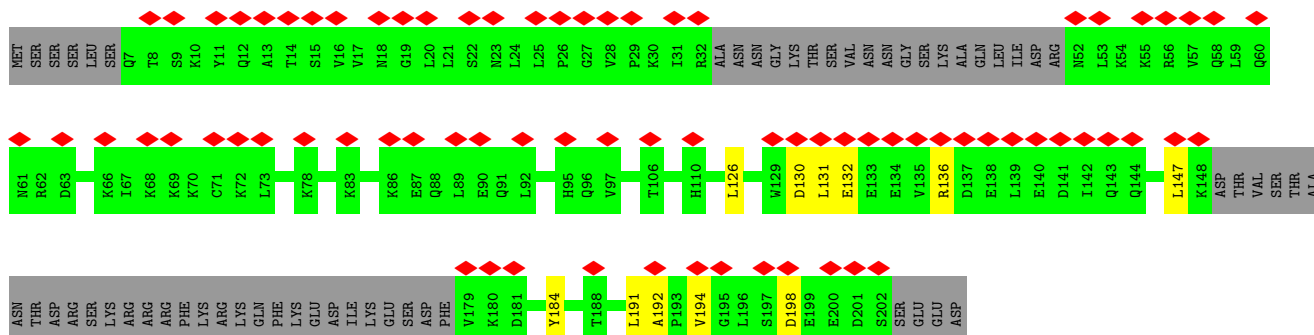
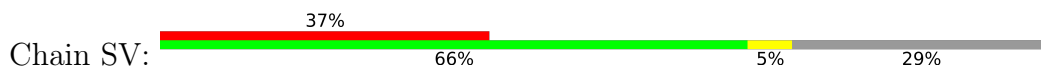




- Molecule 64: Nucleolar complex protein 4



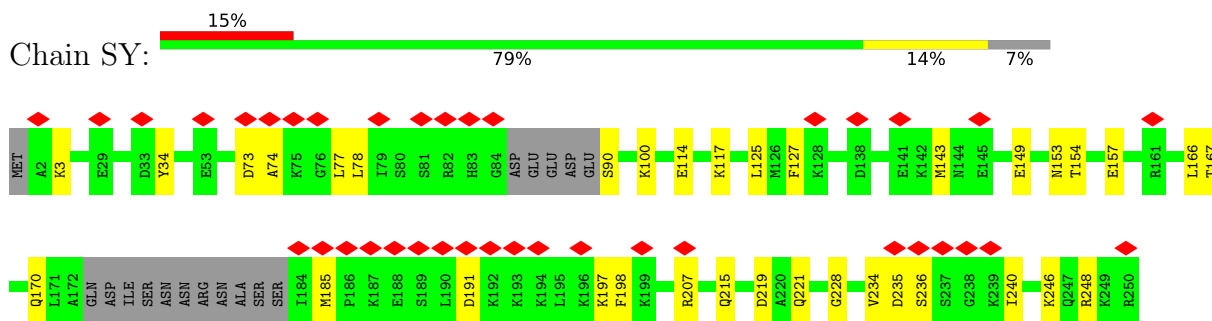
- Molecule 65: Regulator of rDNA transcription protein 14



## Chain SW:

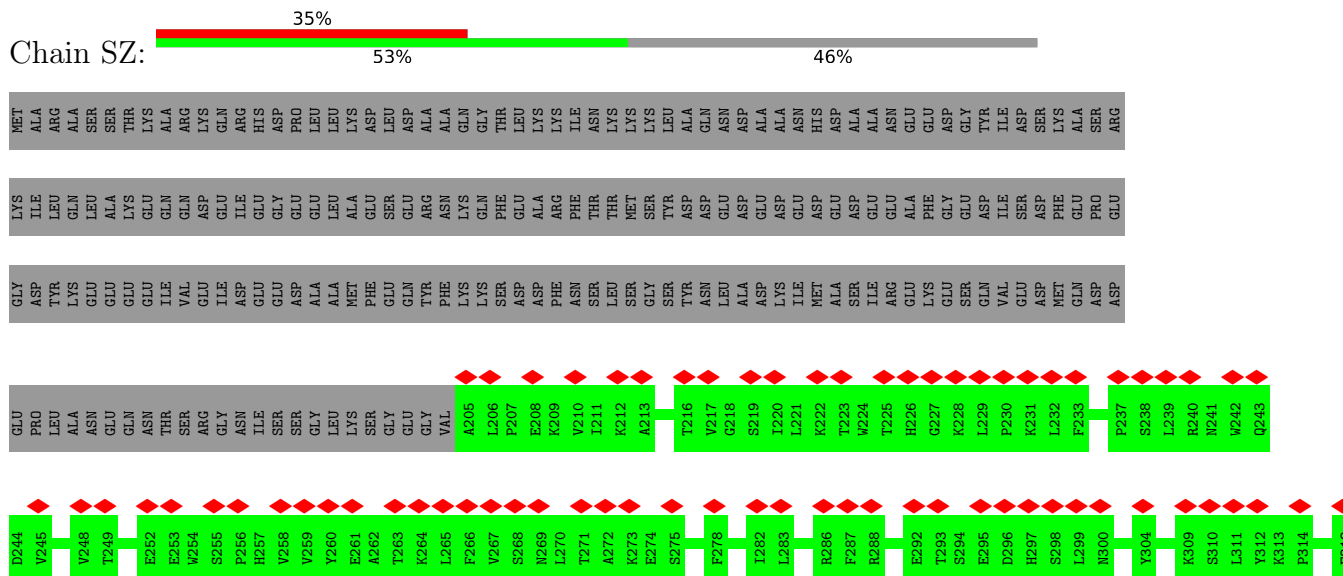


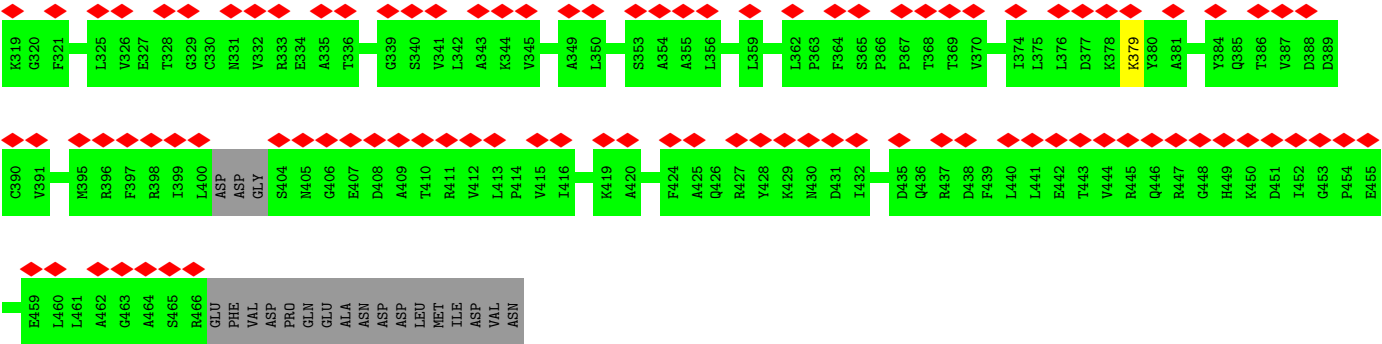
## Chain SY:



- Molecule 68: Essential nuclear protein 1

## Chain SZ:





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 28151                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 25000                                   | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 4.891                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.115                                   | Depositor |
| Map value standard deviation         | 0.183                                   | Depositor |
| Recommended contour level            | 0.77                                    | Depositor |
| Map size (Å)                         | 535.75195, 535.75195, 535.75195         | wwPDB     |
| Map dimensions                       | 504, 504, 504                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.063, 1.063, 1.063                     | 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, SEP, ZN, ATP, GTP

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   | L0    | 0.19         | 0/10603     | 0.28        | 0/16514     |
| 2   | L1    | 0.22         | 0/28743     | 0.30        | 0/44737     |
| 3   | L2    | 0.20         | 0/4143      | 0.27        | 0/6440      |
| 4   | L3    | 0.13         | 0/794       | 0.29        | 0/1069      |
| 5   | L4    | 0.23         | 0/1977      | 0.40        | 0/2664      |
| 6   | L5    | 0.21         | 0/1655      | 0.38        | 0/2237      |
| 7   | L6    | 0.23         | 0/1674      | 0.36        | 0/2236      |
| 8   | L7    | 0.19         | 0/1369      | 0.44        | 0/1846      |
| 9   | L8    | 0.25         | 0/1371      | 0.38        | 0/1833      |
| 10  | L9    | 0.21         | 0/1410      | 0.38        | 0/1888      |
| 11  | LC    | 0.24         | 0/990       | 0.40        | 0/1335      |
| 12  | LD    | 0.21         | 0/1138      | 0.40        | 0/1533      |
| 13  | LE    | 0.24         | 0/1039      | 0.44        | 0/1395      |
| 14  | LF    | 0.26         | 0/1060      | 0.41        | 0/1412      |
| 15  | LG    | 0.18         | 0/492       | 0.34        | 0/659       |
| 16  | LH    | 0.25         | 0/6592      | 0.41        | 0/8924      |
| 17  | LI    | 0.14         | 0/3835      | 0.34        | 0/5263      |
| 18  | LJ    | 0.24         | 0/3993      | 0.36        | 0/5413      |
| 19  | LK    | 0.18         | 0/1085      | 0.34        | 0/1463      |
| 20  | LL    | 0.22         | 0/4052      | 0.37        | 0/5501      |
| 21  | LM    | 0.17         | 0/9462      | 0.35        | 0/13078     |
| 22  | LN    | 0.25         | 0/5359      | 0.34        | 0/7255      |
| 23  | LO    | 0.24         | 0/6773      | 0.38        | 0/9164      |
| 24  | LP    | 0.18         | 0/3288      | 0.32        | 0/4419      |
| 25  | LQ    | 0.20         | 0/6837      | 0.36        | 0/9227      |
| 26  | LR    | 0.17         | 0/6313      | 0.36        | 0/8551      |
| 27  | LS    | 0.28         | 0/3866      | 0.35        | 0/5239      |
| 28  | LT    | 0.22         | 0/7015      | 0.34        | 0/9479      |
| 29  | LU    | 0.26         | 0/3835      | 0.39        | 0/5162      |
| 30  | LV    | 0.27         | 0/3360      | 0.39        | 0/4549      |
| 31  | LW    | 0.23         | 0/4321      | 0.34        | 0/5832      |
| 32  | LX    | 0.21         | 0/6852      | 0.36        | 0/9258      |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 32  | LY    | 0.19         | 0/6292          | 0.35        | 0/8556           |
| 33  | LZ    | 0.24         | 0/1553          | 0.40        | 0/2089           |
| 34  | NA    | 0.25         | 1/2090 (0.0%)   | 0.44        | 3/2817 (0.1%)    |
| 35  | NB    | 0.19         | 0/1891          | 0.38        | 0/2541           |
| 36  | NC    | 0.14         | 0/576           | 0.29        | 0/801            |
| 37  | ND    | 0.20         | 0/613           | 0.38        | 0/811            |
| 38  | NE    | 0.18         | 0/1662          | 0.36        | 0/2212           |
| 39  | NF    | 0.19         | 0/1158          | 0.37        | 0/1559           |
| 40  | NG    | 0.18         | 0/886           | 0.34        | 0/1194           |
| 41  | NH    | 0.22         | 0/8899          | 0.37        | 0/12035          |
| 42  | NI    | 0.18         | 0/1994          | 0.35        | 0/2684           |
| 43  | NK    | 0.19         | 0/2144          | 0.38        | 0/2880           |
| 44  | NM    | 0.21         | 0/1862          | 0.39        | 0/2494           |
| 45  | NN    | 0.17         | 0/1491          | 0.34        | 0/2063           |
| 46  | NQ    | 0.21         | 0/605           | 0.37        | 0/817            |
| 47  | OA    | 0.14         | 0/892           | 0.30        | 0/1241           |
| 48  | SA    | 0.18         | 0/3082          | 0.34        | 0/4151           |
| 49  | SB    | 0.24         | 1/3396 (0.0%)   | 0.41        | 3/4576 (0.1%)    |
| 50  | SC    | 0.21         | 0/1906          | 0.36        | 0/2570           |
| 50  | SD    | 0.18         | 0/1852          | 0.34        | 0/2500           |
| 51  | SE    | 0.26         | 0/928           | 0.37        | 0/1262           |
| 51  | SF    | 0.20         | 0/928           | 0.35        | 0/1262           |
| 52  | SG    | 0.22         | 1/3744 (0.0%)   | 0.39        | 2/5040 (0.0%)    |
| 53  | SH    | 0.19         | 0/2832          | 0.36        | 0/3825           |
| 54  | SI    | 0.21         | 0/6719          | 0.35        | 0/9043           |
| 55  | SJ    | 0.19         | 0/1703          | 0.36        | 0/2295           |
| 55  | SK    | 0.21         | 0/1822          | 0.37        | 0/2462           |
| 56  | SL    | 0.21         | 0/1406          | 0.36        | 0/1890           |
| 57  | SM    | 0.21         | 0/2337          | 0.35        | 0/3148           |
| 58  | SN    | 0.17         | 0/2088          | 0.36        | 0/2808           |
| 59  | SP    | 0.17         | 0/18707         | 0.35        | 1/25354 (0.0%)   |
| 60  | SQ    | 0.18         | 0/1302          | 0.38        | 0/1728           |
| 61  | SR    | 0.21         | 0/804           | 0.38        | 0/1074           |
| 62  | SS    | 0.18         | 0/2307          | 0.41        | 2/3091 (0.1%)    |
| 63  | ST    | 0.26         | 1/4513 (0.0%)   | 0.45        | 4/6075 (0.1%)    |
| 64  | SU    | 0.19         | 0/4480          | 0.34        | 0/6073           |
| 65  | SV    | 0.16         | 0/875           | 0.37        | 0/1206           |
| 66  | SW    | 0.18         | 0/1591          | 0.37        | 0/2143           |
| 67  | SY    | 0.20         | 0/1978          | 0.35        | 0/2616           |
| 68  | SZ    | 0.22         | 0/1326          | 0.35        | 0/1859           |
| All | All   | 0.21         | 4/252530 (0.0%) | 0.35        | 15/350420 (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 |
|-----|-------|---------------------|---------------------|
| 21  | LM    | 0                   | 1                   |
| 32  | LX    | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 63  | ST    | 585 | PRO  | CG-CD | -11.48 | 1.11        | 1.50     |
| 34  | NA    | 458 | PRO  | CG-CD | -7.19  | 1.26        | 1.50     |
| 49  | SB    | 129 | PRO  | CG-CD | -7.00  | 1.26        | 1.50     |
| 52  | SG    | 365 | PRO  | CG-CD | -5.49  | 1.32        | 1.50     |

The worst 5 of 15 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 63  | ST    | 585 | PRO  | N-CD-CG  | -15.73 | 79.60       | 103.20   |
| 49  | SB    | 129 | PRO  | CA-N-CD  | -11.01 | 96.59       | 112.00   |
| 34  | NA    | 458 | PRO  | N-CD-CG  | -10.18 | 87.92       | 103.20   |
| 52  | SG    | 365 | PRO  | CA-N-CD  | -10.05 | 97.92       | 112.00   |
| 63  | ST    | 585 | PRO  | CA-CB-CG | -9.30  | 86.82       | 104.50   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 21  | LM    | 1586 | LEU  | Peptide   |
| 32  | LX    | 841  | ARG  | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | L0    | 9483  | 0        | 4770     | 42      | 0            |
| 2   | L1    | 25709 | 0        | 12967    | 148     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | L2    | 3712  | 0        | 1882     | 29      | 0            |
| 4   | L3    | 786   | 0        | 823      | 8       | 0            |
| 5   | L4    | 1936  | 0        | 2019     | 14      | 0            |
| 6   | L5    | 1635  | 0        | 1697     | 28      | 0            |
| 7   | L6    | 1653  | 0        | 1750     | 27      | 0            |
| 8   | L7    | 1347  | 0        | 1406     | 22      | 0            |
| 9   | L8    | 1348  | 0        | 1366     | 18      | 0            |
| 10  | L9    | 1388  | 0        | 1467     | 14      | 0            |
| 11  | LC    | 973   | 0        | 1029     | 19      | 0            |
| 12  | LD    | 1112  | 0        | 1179     | 16      | 0            |
| 13  | LE    | 1022  | 0        | 1060     | 21      | 0            |
| 14  | LF    | 1046  | 0        | 1114     | 16      | 0            |
| 15  | LG    | 490   | 0        | 529      | 10      | 0            |
| 16  | LH    | 6465  | 0        | 6415     | 102     | 0            |
| 17  | LI    | 3792  | 0        | 2859     | 29      | 0            |
| 18  | LJ    | 3911  | 0        | 3906     | 48      | 0            |
| 19  | LK    | 1068  | 0        | 1120     | 17      | 0            |
| 20  | LL    | 3982  | 0        | 3983     | 70      | 0            |
| 21  | LM    | 9380  | 0        | 6279     | 45      | 0            |
| 22  | LN    | 5263  | 0        | 5270     | 53      | 0            |
| 23  | LO    | 6639  | 0        | 6524     | 86      | 0            |
| 24  | LP    | 3220  | 0        | 3272     | 36      | 0            |
| 25  | LQ    | 6707  | 0        | 6738     | 95      | 0            |
| 26  | LR    | 6207  | 0        | 6247     | 94      | 0            |
| 27  | LS    | 3793  | 0        | 3770     | 53      | 0            |
| 28  | LT    | 6876  | 0        | 6853     | 84      | 0            |
| 29  | LU    | 3756  | 0        | 3708     | 54      | 0            |
| 30  | LV    | 3286  | 0        | 3208     | 57      | 0            |
| 31  | LW    | 4237  | 0        | 4239     | 50      | 0            |
| 32  | LX    | 6720  | 0        | 6840     | 94      | 0            |
| 32  | LY    | 6179  | 0        | 5745     | 62      | 0            |
| 33  | LZ    | 1524  | 0        | 1567     | 25      | 0            |
| 34  | NA    | 2075  | 0        | 1915     | 32      | 0            |
| 35  | NB    | 1873  | 0        | 1638     | 25      | 0            |
| 36  | NC    | 575   | 0        | 274      | 2       | 0            |
| 37  | ND    | 609   | 0        | 671      | 11      | 0            |
| 38  | NE    | 1649  | 0        | 1669     | 20      | 0            |
| 39  | NF    | 1135  | 0        | 1197     | 21      | 0            |
| 40  | NG    | 875   | 0        | 905      | 19      | 0            |
| 41  | NH    | 8693  | 0        | 8806     | 119     | 0            |
| 42  | NI    | 1953  | 0        | 1933     | 21      | 0            |
| 43  | NK    | 2107  | 0        | 2184     | 25      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | NM    | 1838   | 0        | 1933     | 38      | 0            |
| 45  | NN    | 1481   | 0        | 866      | 14      | 0            |
| 46  | NQ    | 595    | 0        | 609      | 6       | 0            |
| 47  | OA    | 888    | 0        | 484      | 5       | 0            |
| 48  | SA    | 3035   | 0        | 3059     | 34      | 0            |
| 49  | SB    | 3357   | 0        | 3471     | 48      | 0            |
| 50  | SC    | 1871   | 0        | 1916     | 27      | 0            |
| 50  | SD    | 1817   | 0        | 1857     | 19      | 0            |
| 51  | SE    | 916    | 0        | 964      | 12      | 0            |
| 51  | SF    | 916    | 0        | 964      | 13      | 0            |
| 52  | SG    | 3672   | 0        | 3690     | 35      | 0            |
| 53  | SH    | 2781   | 0        | 2878     | 18      | 0            |
| 54  | SI    | 6577   | 0        | 6743     | 81      | 0            |
| 55  | SJ    | 1678   | 0        | 1756     | 28      | 0            |
| 55  | SK    | 1793   | 0        | 1874     | 31      | 0            |
| 56  | SL    | 1384   | 0        | 1464     | 15      | 0            |
| 57  | SM    | 2296   | 0        | 2325     | 29      | 0            |
| 58  | SN    | 2053   | 0        | 2168     | 24      | 0            |
| 59  | SP    | 18367  | 0        | 17934    | 238     | 0            |
| 60  | SQ    | 1280   | 0        | 1331     | 15      | 0            |
| 61  | SR    | 792    | 0        | 847      | 6       | 0            |
| 62  | SS    | 2267   | 0        | 2300     | 34      | 0            |
| 63  | ST    | 4448   | 0        | 4337     | 57      | 0            |
| 64  | SU    | 4370   | 0        | 4365     | 74      | 0            |
| 65  | SV    | 869    | 0        | 554      | 12      | 0            |
| 66  | SW    | 1565   | 0        | 1647     | 20      | 0            |
| 67  | SY    | 1953   | 0        | 2050     | 28      | 0            |
| 68  | SZ    | 1314   | 0        | 649      | 1       | 0            |
| 69  | L0    | 3      | 0        | 0        | 0       | 0            |
| 69  | L1    | 27     | 0        | 0        | 0       | 0            |
| 69  | L2    | 2      | 0        | 0        | 0       | 0            |
| 69  | NH    | 1      | 0        | 0        | 0       | 0            |
| 69  | SI    | 1      | 0        | 0        | 0       | 0            |
| 70  | NH    | 31     | 0        | 12       | 1       | 0            |
| 71  | NQ    | 1      | 0        | 0        | 0       | 0            |
| 71  | SL    | 1      | 0        | 0        | 0       | 0            |
| 72  | SI    | 32     | 0        | 12       | 0       | 0            |
| All | All   | 244461 | 0        | 219852   | 2386    | 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 5.

The worst 5 of 2386 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 44:NM:240:LYS:O    | 44:NM:242:LYS:NZ  | 2.01                     | 0.93              |
| 67:SY:114:GLU:OE1  | 67:SY:207:ARG:NH2 | 2.01                     | 0.93              |
| 35:NB:393:ALA:O    | 64:SU:167:LYS:NZ  | 2.03                     | 0.91              |
| 23:LO:828:ILE:HG21 | 28:LT:930:MET:HE3 | 1.52                     | 0.91              |
| 31:LW:433:LEU:HD21 | 33:LZ:16:VAL:HG21 | 1.51                     | 0.91              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 4   | L3    | 91/146 (62%)  | 91 (100%)  | 0       | 0        | 100         | 100 |
| 5   | L4    | 242/261 (93%) | 237 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 6   | L5    | 202/225 (90%) | 197 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 7   | L6    | 202/236 (86%) | 199 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 8   | L7    | 165/190 (87%) | 164 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 9   | L8    | 166/200 (83%) | 163 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 10  | L9    | 169/197 (86%) | 166 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 11  | LC    | 123/143 (86%) | 122 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 12  | LD    | 135/156 (86%) | 132 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 13  | LE    | 127/130 (98%) | 122 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 14  | LF    | 128/135 (95%) | 126 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 15  | LG    | 60/67 (90%)   | 59 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 16  | LH    | 790/896 (88%) | 759 (96%)  | 31 (4%) | 0        | 100         | 100 |
| 17  | LI    | 582/713 (82%) | 570 (98%)  | 12 (2%) | 0        | 100         | 100 |
| 18  | LJ    | 489/513 (95%) | 481 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 19  | LK    | 130/575 (23%) | 130 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 20  | LL    | 496/643 (77%)   | 481 (97%)  | 15 (3%) | 0        | 100         | 100 |
| 21  | LM    | 1597/1769 (90%) | 1565 (98%) | 32 (2%) | 0        | 100         | 100 |
| 22  | LN    | 649/776 (84%)   | 632 (97%)  | 17 (3%) | 0        | 100         | 100 |
| 23  | LO    | 829/923 (90%)   | 816 (98%)  | 13 (2%) | 0        | 100         | 100 |
| 24  | LP    | 376/440 (86%)   | 374 (100%) | 2 (0%)  | 0        | 100         | 100 |
| 25  | LQ    | 831/943 (88%)   | 804 (97%)  | 27 (3%) | 0        | 100         | 100 |
| 26  | LR    | 785/817 (96%)   | 766 (98%)  | 19 (2%) | 0        | 100         | 100 |
| 27  | LS    | 469/594 (79%)   | 452 (96%)  | 17 (4%) | 0        | 100         | 100 |
| 28  | LT    | 865/939 (92%)   | 845 (98%)  | 20 (2%) | 0        | 100         | 100 |
| 29  | LU    | 456/489 (93%)   | 443 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 30  | LV    | 401/707 (57%)   | 388 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 31  | LW    | 531/554 (96%)   | 512 (96%)  | 19 (4%) | 0        | 100         | 100 |
| 32  | LX    | 826/1056 (78%)  | 811 (98%)  | 15 (2%) | 0        | 100         | 100 |
| 32  | LY    | 834/1056 (79%)  | 817 (98%)  | 17 (2%) | 0        | 100         | 100 |
| 33  | LZ    | 179/183 (98%)   | 176 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 34  | NA    | 274/593 (46%)   | 270 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 35  | NB    | 255/610 (42%)   | 251 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 36  | NC    | 111/357 (31%)   | 110 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 37  | ND    | 70/214 (33%)    | 70 (100%)  | 0       | 0        | 100         | 100 |
| 38  | NE    | 207/346 (60%)   | 205 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 39  | NF    | 139/151 (92%)   | 138 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 40  | NG    | 117/137 (85%)   | 113 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 41  | NH    | 1063/1237 (86%) | 1039 (98%) | 24 (2%) | 0        | 100         | 100 |
| 42  | NI    | 232/297 (78%)   | 224 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 43  | NK    | 253/316 (80%)   | 249 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 44  | NM    | 224/255 (88%)   | 219 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 45  | NN    | 257/534 (48%)   | 255 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 46  | NQ    | 77/82 (94%)     | 75 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 47  | OA    | 167/1729 (10%)  | 165 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 48  | SA    | 379/504 (75%)   | 371 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 49  | SB    | 434/511 (85%)   | 426 (98%)  | 8 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 50  | SC    | 237/327 (72%)     | 231 (98%)   | 6 (2%)   | 0        | 100         | 100 |
| 50  | SD    | 228/327 (70%)     | 226 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 51  | SE    | 119/126 (94%)     | 118 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 51  | SF    | 119/126 (94%)     | 114 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 52  | SG    | 453/573 (79%)     | 448 (99%)   | 5 (1%)   | 0        | 100         | 100 |
| 53  | SH    | 358/367 (98%)     | 349 (98%)   | 9 (2%)   | 0        | 100         | 100 |
| 54  | SI    | 799/1183 (68%)    | 788 (99%)   | 11 (1%)  | 0        | 100         | 100 |
| 55  | SJ    | 207/252 (82%)     | 202 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 55  | SK    | 225/252 (89%)     | 220 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 56  | SL    | 169/189 (89%)     | 162 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 57  | SM    | 278/290 (96%)     | 272 (98%)   | 6 (2%)   | 0        | 100         | 100 |
| 58  | SN    | 251/274 (92%)     | 248 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 59  | SP    | 2334/2493 (94%)   | 2287 (98%)  | 46 (2%)  | 1 (0%)   | 100         | 100 |
| 60  | SQ    | 147/217 (68%)     | 140 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 61  | SR    | 102/145 (70%)     | 101 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 62  | SS    | 262/899 (29%)     | 257 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 63  | ST    | 566/810 (70%)     | 559 (99%)   | 7 (1%)   | 0        | 100         | 100 |
| 64  | SU    | 528/552 (96%)     | 522 (99%)   | 6 (1%)   | 0        | 100         | 100 |
| 65  | SV    | 141/206 (68%)     | 139 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 66  | SW    | 193/274 (70%)     | 189 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 67  | SY    | 227/250 (91%)     | 226 (100%)  | 1 (0%)   | 0        | 100         | 100 |
| 68  | SZ    | 255/483 (53%)     | 252 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| All | All   | 26382/35160 (75%) | 25830 (98%) | 551 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 59  | SP    | 1190 | SER  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | L3    | 88/129 (68%)   | 88 (100%)  | 0        | 100         | 100 |
| 5   | L4    | 208/222 (94%)  | 208 (100%) | 0        | 100         | 100 |
| 6   | L5    | 179/191 (94%)  | 179 (100%) | 0        | 100         | 100 |
| 7   | L6    | 175/201 (87%)  | 175 (100%) | 0        | 100         | 100 |
| 8   | L7    | 149/170 (88%)  | 149 (100%) | 0        | 100         | 100 |
| 9   | L8    | 137/161 (85%)  | 137 (100%) | 0        | 100         | 100 |
| 10  | L9    | 147/166 (89%)  | 147 (100%) | 0        | 100         | 100 |
| 11  | LC    | 105/119 (88%)  | 105 (100%) | 0        | 100         | 100 |
| 12  | LD    | 124/137 (90%)  | 123 (99%)  | 1 (1%)   | 73          | 76  |
| 13  | LE    | 110/111 (99%)  | 110 (100%) | 0        | 100         | 100 |
| 14  | LF    | 109/113 (96%)  | 109 (100%) | 0        | 100         | 100 |
| 15  | LG    | 55/60 (92%)    | 55 (100%)  | 0        | 100         | 100 |
| 16  | LH    | 745/826 (90%)  | 745 (100%) | 0        | 100         | 100 |
| 17  | LI    | 244/657 (37%)  | 244 (100%) | 0        | 100         | 100 |
| 18  | LJ    | 437/454 (96%)  | 437 (100%) | 0        | 100         | 100 |
| 19  | LK    | 124/533 (23%)  | 124 (100%) | 0        | 100         | 100 |
| 20  | LL    | 452/574 (79%)  | 452 (100%) | 0        | 100         | 100 |
| 21  | LM    | 421/1633 (26%) | 421 (100%) | 0        | 100         | 100 |
| 22  | LN    | 603/713 (85%)  | 603 (100%) | 0        | 100         | 100 |
| 23  | LO    | 729/811 (90%)  | 729 (100%) | 0        | 100         | 100 |
| 24  | LP    | 360/414 (87%)  | 360 (100%) | 0        | 100         | 100 |
| 25  | LQ    | 746/832 (90%)  | 746 (100%) | 0        | 100         | 100 |
| 26  | LR    | 698/719 (97%)  | 698 (100%) | 0        | 100         | 100 |
| 27  | LS    | 423/528 (80%)  | 423 (100%) | 0        | 100         | 100 |
| 28  | LT    | 763/819 (93%)  | 763 (100%) | 0        | 100         | 100 |
| 29  | LU    | 415/443 (94%)  | 415 (100%) | 0        | 100         | 100 |
| 30  | LV    | 366/636 (58%)  | 366 (100%) | 0        | 100         | 100 |
| 31  | LW    | 465/480 (97%)  | 465 (100%) | 0        | 100         | 100 |
| 32  | LX    | 751/934 (80%)  | 751 (100%) | 0        | 100         | 100 |
| 32  | LY    | 592/934 (63%)  | 592 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 33  | LZ    | 170/172 (99%)   | 170 (100%)  | 0        | 100         | 100 |
| 34  | NA    | 194/535 (36%)   | 194 (100%)  | 0        | 100         | 100 |
| 35  | NB    | 149/538 (28%)   | 149 (100%)  | 0        | 100         | 100 |
| 36  | NC    | 3/315 (1%)      | 3 (100%)    | 0        | 100         | 100 |
| 37  | ND    | 70/196 (36%)    | 70 (100%)   | 0        | 100         | 100 |
| 38  | NE    | 166/304 (55%)   | 166 (100%)  | 0        | 100         | 100 |
| 39  | NF    | 121/128 (94%)   | 121 (100%)  | 0        | 100         | 100 |
| 40  | NG    | 90/105 (86%)    | 90 (100%)   | 0        | 100         | 100 |
| 41  | NH    | 982/1125 (87%)  | 982 (100%)  | 0        | 100         | 100 |
| 42  | NI    | 220/274 (80%)   | 220 (100%)  | 0        | 100         | 100 |
| 43  | NK    | 233/289 (81%)   | 232 (100%)  | 1 (0%)   | 84          | 81  |
| 44  | NM    | 205/224 (92%)   | 205 (100%)  | 0        | 100         | 100 |
| 45  | NN    | 44/482 (9%)     | 44 (100%)   | 0        | 100         | 100 |
| 46  | NQ    | 68/71 (96%)     | 68 (100%)   | 0        | 100         | 100 |
| 47  | OA    | 14/1544 (1%)    | 14 (100%)   | 0        | 100         | 100 |
| 48  | SA    | 328/435 (75%)   | 328 (100%)  | 0        | 100         | 100 |
| 49  | SB    | 360/433 (83%)   | 360 (100%)  | 0        | 100         | 100 |
| 50  | SC    | 200/240 (83%)   | 200 (100%)  | 0        | 100         | 100 |
| 50  | SD    | 197/240 (82%)   | 197 (100%)  | 0        | 100         | 100 |
| 51  | SE    | 100/104 (96%)   | 100 (100%)  | 0        | 100         | 100 |
| 51  | SF    | 100/104 (96%)   | 100 (100%)  | 0        | 100         | 100 |
| 52  | SG    | 399/503 (79%)   | 399 (100%)  | 0        | 100         | 100 |
| 53  | SH    | 307/312 (98%)   | 307 (100%)  | 0        | 100         | 100 |
| 54  | SI    | 718/1039 (69%)  | 718 (100%)  | 0        | 100         | 100 |
| 55  | SJ    | 192/222 (86%)   | 192 (100%)  | 0        | 100         | 100 |
| 55  | SK    | 205/222 (92%)   | 205 (100%)  | 0        | 100         | 100 |
| 56  | SL    | 155/169 (92%)   | 155 (100%)  | 0        | 100         | 100 |
| 57  | SM    | 251/258 (97%)   | 251 (100%)  | 0        | 100         | 100 |
| 58  | SN    | 236/256 (92%)   | 236 (100%)  | 0        | 100         | 100 |
| 59  | SP    | 1956/2307 (85%) | 1956 (100%) | 0        | 100         | 100 |
| 60  | SQ    | 140/200 (70%)   | 139 (99%)   | 1 (1%)   | 76          | 77  |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 61  | SR    | 86/120 (72%)      | 86 (100%)    | 0        | 100         | 100 |
| 62  | SS    | 251/808 (31%)     | 251 (100%)   | 0        | 100         | 100 |
| 63  | ST    | 441/732 (60%)     | 441 (100%)   | 0        | 100         | 100 |
| 64  | SU    | 490/506 (97%)     | 490 (100%)   | 0        | 100         | 100 |
| 65  | SV    | 42/192 (22%)      | 42 (100%)    | 0        | 100         | 100 |
| 66  | SW    | 172/238 (72%)     | 172 (100%)   | 0        | 100         | 100 |
| 67  | SY    | 218/234 (93%)     | 218 (100%)   | 0        | 100         | 100 |
| 68  | SZ    | 14/424 (3%)       | 14 (100%)    | 0        | 100         | 100 |
| All | All   | 21207/31320 (68%) | 21204 (100%) | 3 (0%)   | 100         | 100 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | LD    | 21  | ASN  |
| 43  | NK    | 277 | GLN  |
| 60  | SQ    | 83  | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | SA    | 270 | ASN  |
| 58  | SN    | 217 | GLN  |
| 49  | SB    | 191 | HIS  |
| 53  | SH    | 334 | ASN  |
| 59  | SP    | 428 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | L0    | 442/700 (63%)   | 85 (19%)          | 0               |
| 2   | L1    | 1180/1808 (65%) | 200 (16%)         | 1 (0%)          |
| 3   | L2    | 170/333 (51%)   | 26 (15%)          | 0               |
| All | All   | 1792/2841 (63%) | 311 (17%)         | 1 (0%)          |

5 of 311 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L0    | 7   | A    |
| 1   | L0    | 61  | U    |
| 1   | L0    | 62  | C    |
| 1   | L0    | 63  | G    |
| 1   | L0    | 64  | U    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L1    | 248 | U    |

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

2 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$ |
| 27  | SEP  | LS    | 128 | 27   | 8,9,10       | 1.61 | 1 (12%)     | 7,12,14     | 1.27 | 1 (14%)     |
| 23  | SEP  | LO    | 651 | 23   | 8,9,10       | 1.56 | 1 (12%)     | 7,12,14     | 1.20 | 1 (14%)     |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 27  | SEP  | LS    | 128 | 27   | -       | 0/6/8/10 | -     |
| 23  | SEP  | LO    | 651 | 23   | -       | 1/6/8/10 | -     |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 27  | LS    | 128 | SEP  | P-O1P | 3.51 | 1.61        | 1.50     |
| 23  | LO    | 651 | SEP  | P-O1P | 3.44 | 1.61        | 1.50     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 27  | LS    | 128 | SEP  | OG-CB-CA | 2.77 | 110.84      | 108.14   |
| 23  | LO    | 651 | SEP  | OG-CB-CA | 2.42 | 110.50      | 108.14   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 23  | LO    | 651 | SEP  | CA-CB-OG-P |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 36 are monoatomic - leaving 2 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 | $\# Z  > 2$ |
| 70  | ATP  | NH    | 1300 | 69   | 32,33,33     | 0.37 | 0           | 48,52,52    | 0.72 | 1 (2%)      |
| 72  | GTP  | SI    | 2001 | 69   | 33,34,34     | 1.86 | 5 (15%)     | 50,54,54    | 1.47 | 6 (12%)     |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 70  | ATP  | NH    | 1300 | 69   | -       | 6/22/38/38 | 0/3/3/3 |
| 72  | GTP  | SI    | 2001 | 69   | -       | 0/22/38/38 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 72  | SI    | 2001 | GTP  | C5-N7  | 6.51  | 1.52        | 1.39     |
| 72  | SI    | 2001 | GTP  | C8-N9  | -4.39 | 1.27        | 1.37     |
| 72  | SI    | 2001 | GTP  | C4-N9  | -3.95 | 1.28        | 1.38     |
| 72  | SI    | 2001 | GTP  | C4-N3  | 2.11  | 1.39        | 1.34     |
| 72  | SI    | 2001 | GTP  | PB-O2B | -2.08 | 1.45        | 1.55     |

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 72  | SI    | 2001 | GTP  | C8-N9-C4  | 7.26  | 119.63      | 106.03   |
| 72  | SI    | 2001 | GTP  | N9-C4-N3  | 2.69  | 131.32      | 125.95   |
| 72  | SI    | 2001 | GTP  | C1'-N9-C8 | -2.48 | 119.70      | 126.73   |
| 72  | SI    | 2001 | GTP  | C6-C5-N7  | 2.43  | 134.71      | 130.29   |
| 72  | SI    | 2001 | GTP  | C5-C4-N9  | -2.17 | 101.78      | 105.66   |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 70  | NH    | 1300 | ATP  | PB-O3B-PG-O3G   |
| 70  | NH    | 1300 | ATP  | PB-O3B-PG-O2G   |
| 70  | NH    | 1300 | ATP  | O4'-C4'-C5'-O5' |
| 70  | NH    | 1300 | ATP  | PA-O3A-PB-O3B   |
| 70  | NH    | 1300 | ATP  | PA-O3A-PB-O1B   |

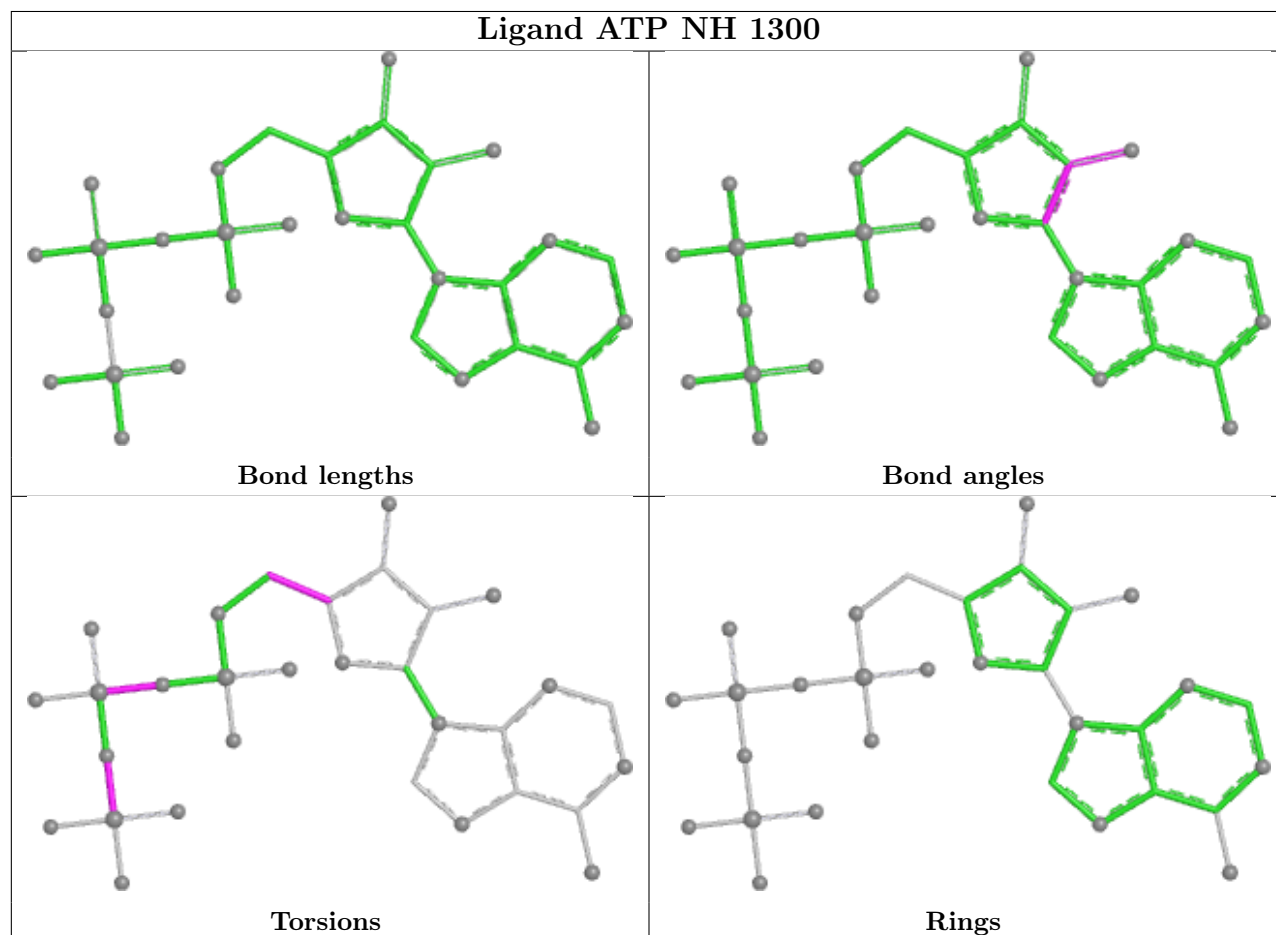
There are no ring outliers.

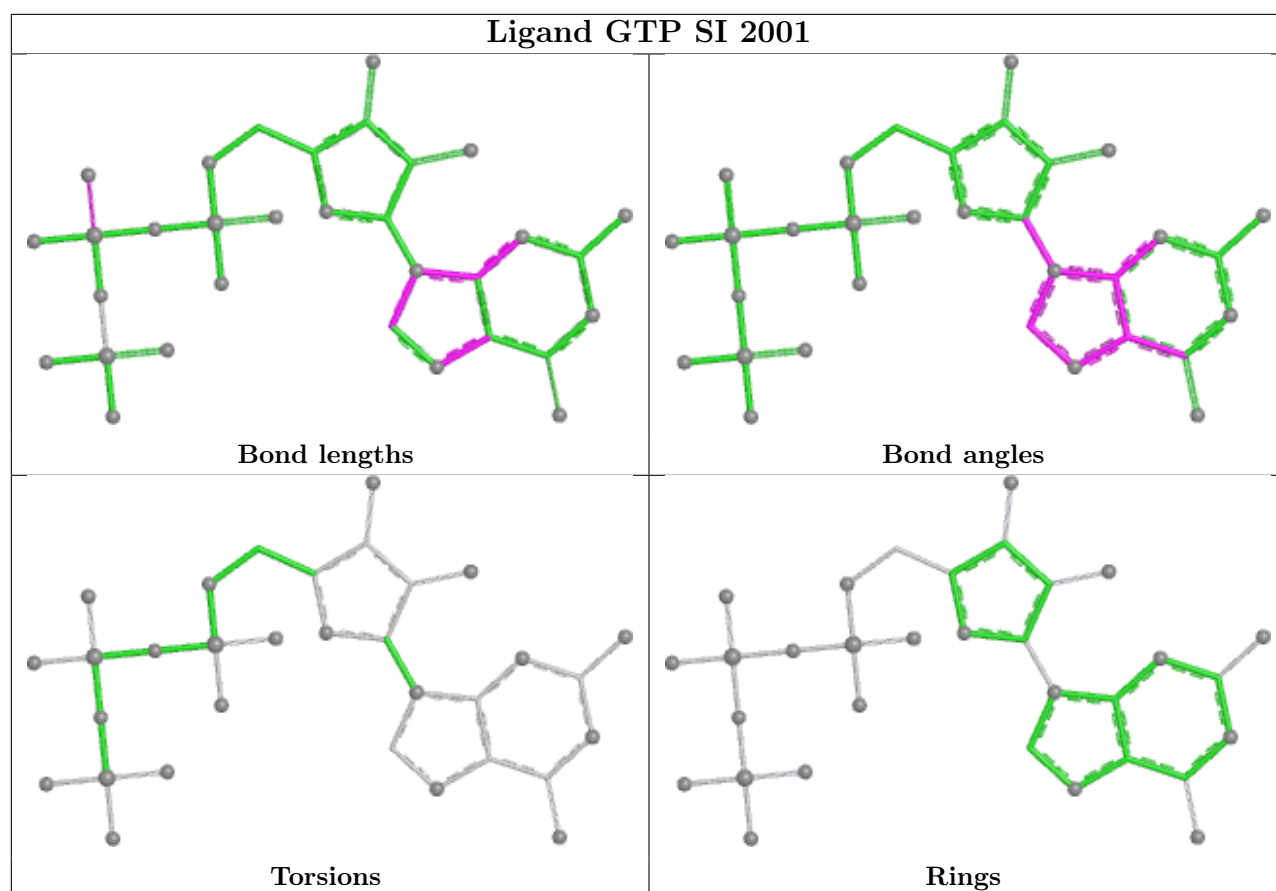
1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 70  | NH    | 1300 | ATP  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

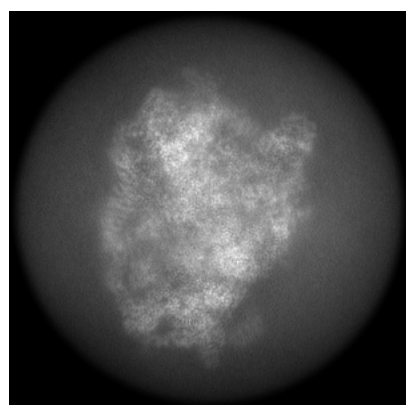
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49077. These allow visual inspection of the internal detail of the map and identification of artifacts.

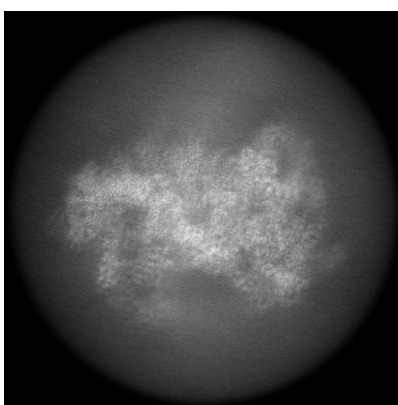
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

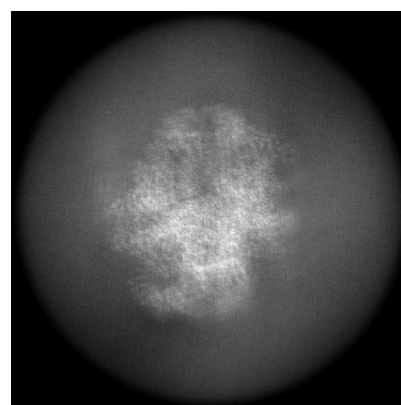
#### 6.1.1 Primary map



X



Y

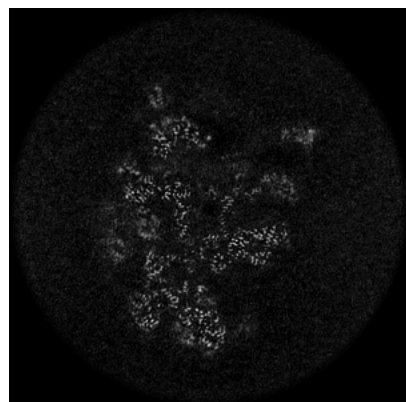


Z

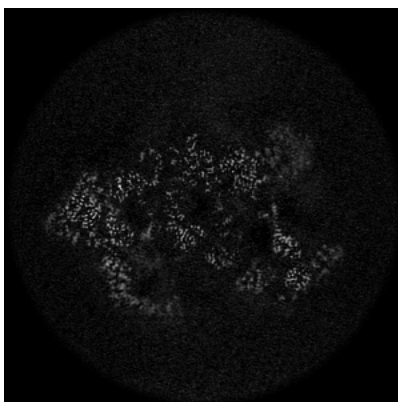
The images above show the map projected in three orthogonal directions.

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

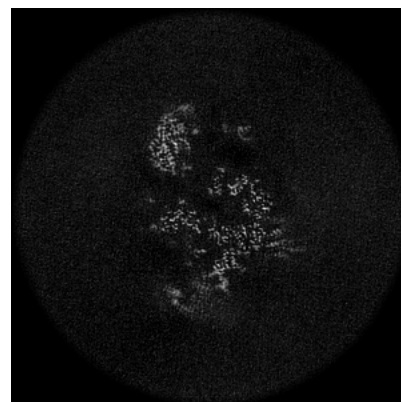
#### 6.2.1 Primary map



X Index: 252



Y Index: 252

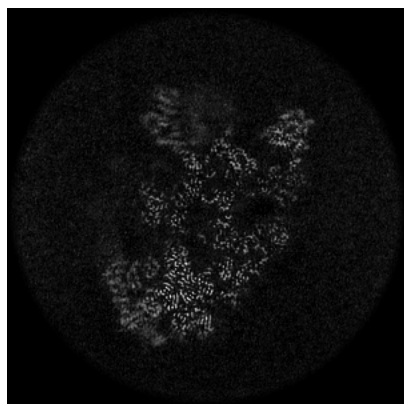


Z Index: 252

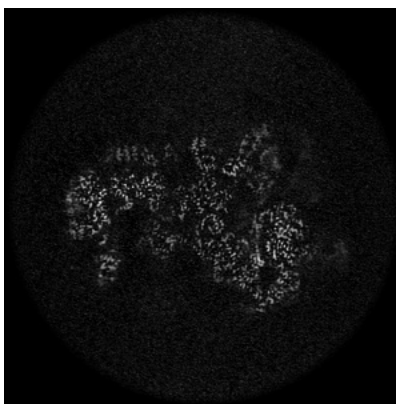
The images above show central slices of the map in three orthogonal directions.

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

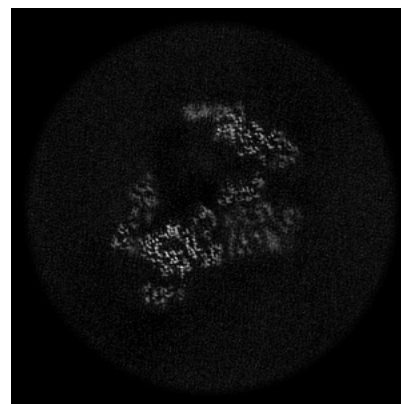
### 6.3.1 Primary map



X Index: 278



Y Index: 222

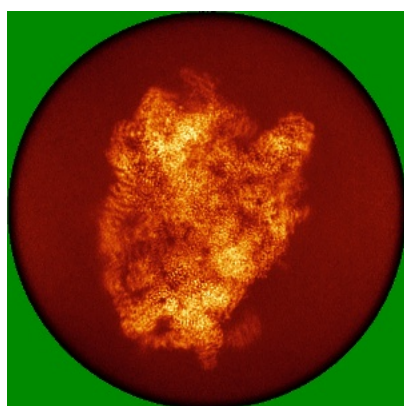


Z Index: 332

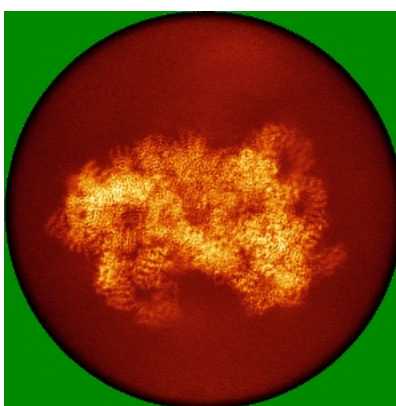
The images above show the largest variance slices of the map in three orthogonal directions.

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

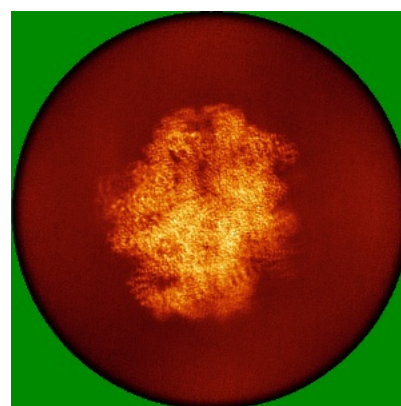
### 6.4.1 Primary map



X



Y

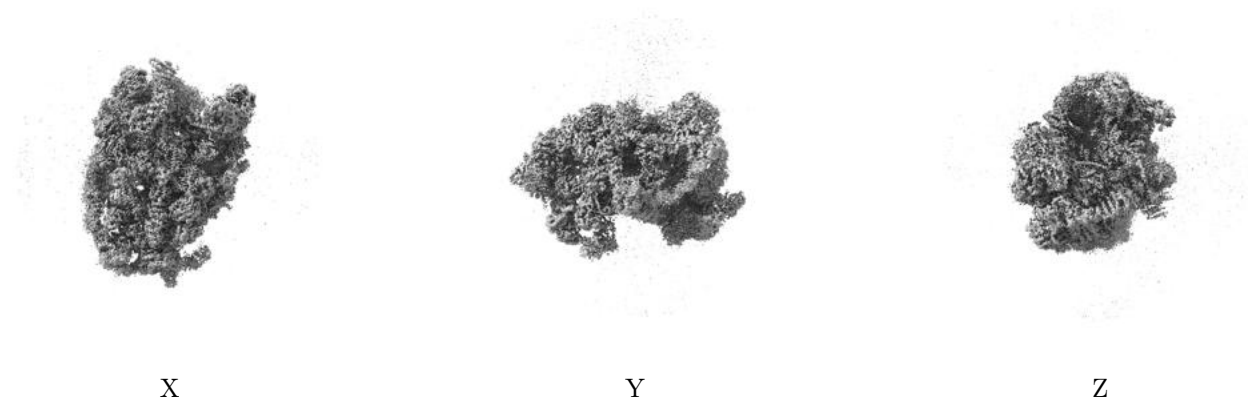


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.77. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

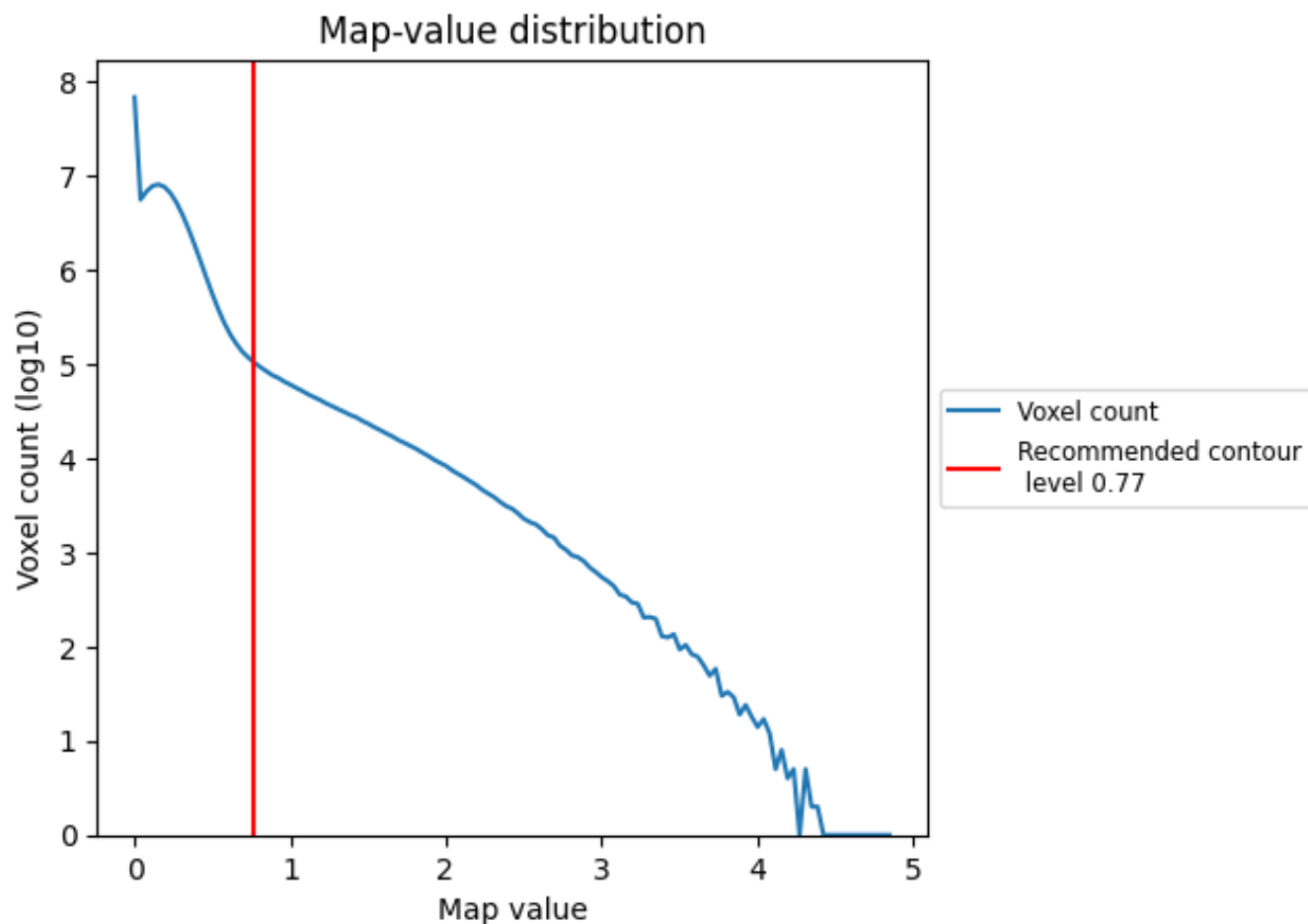
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

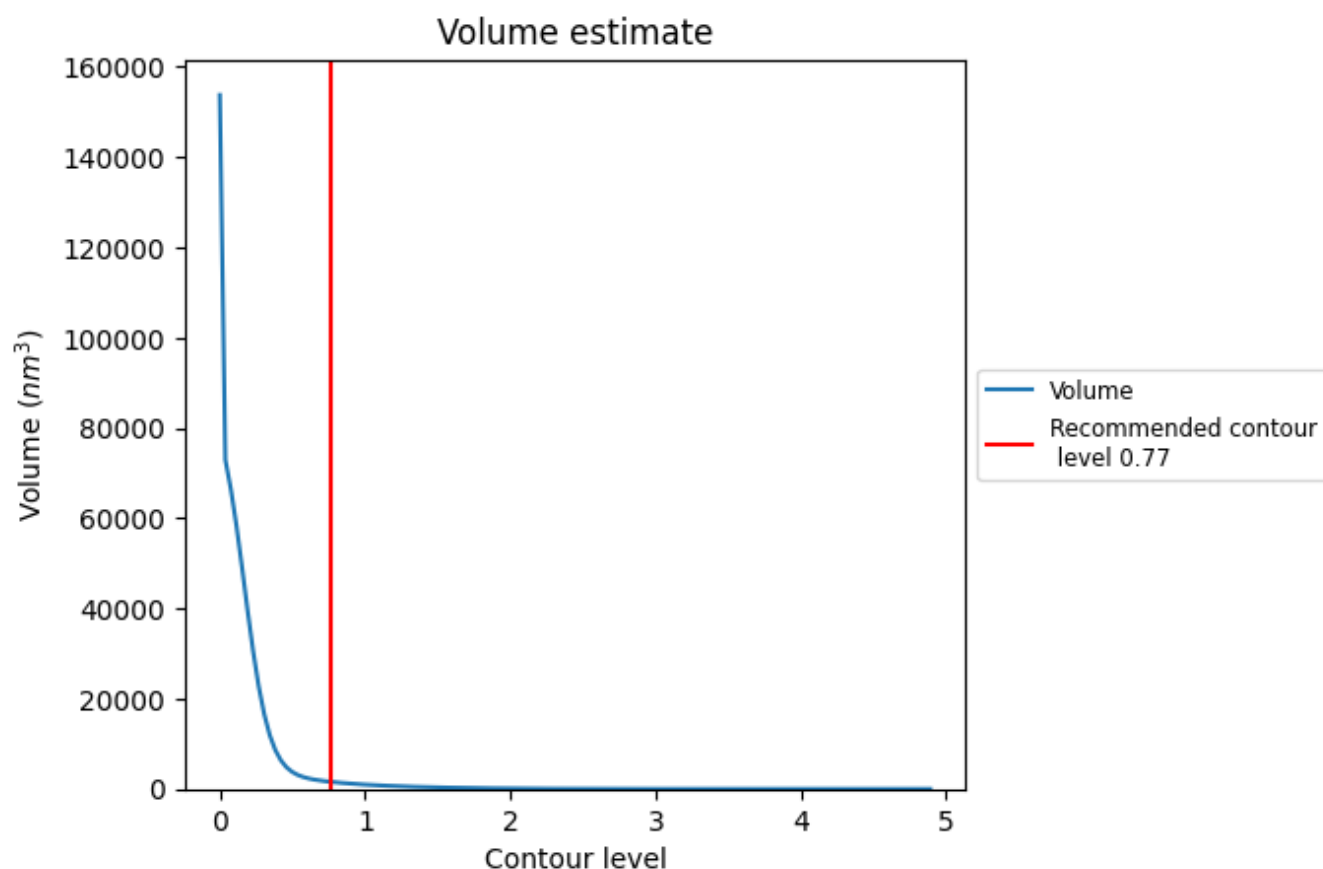
This section contains the results of statistical analysis of the map.

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



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

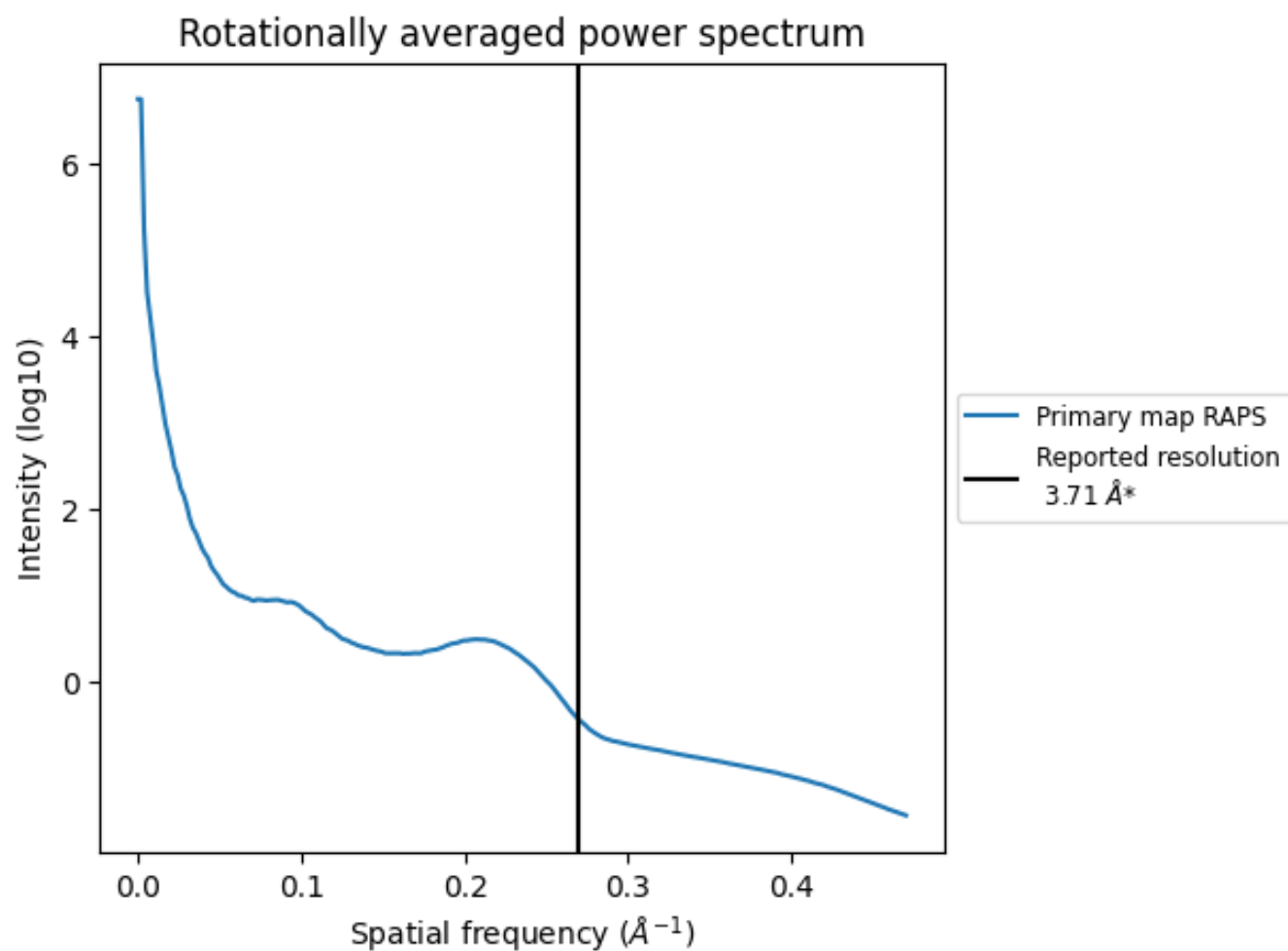
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1552  $\text{nm}^3$ ; this corresponds to an approximate mass of 1402 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 0.270  $\text{\AA}^{-1}$

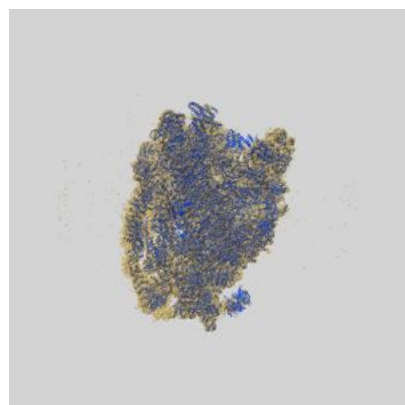
## 8 Fourier-Shell correlation

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

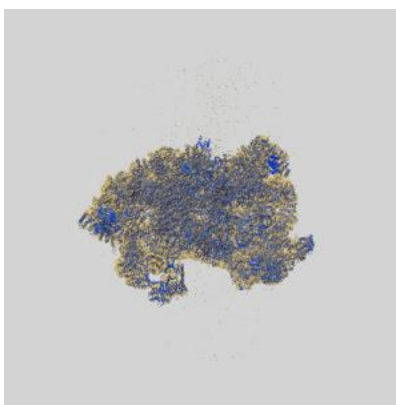
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49077 and PDB model 9N6X. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

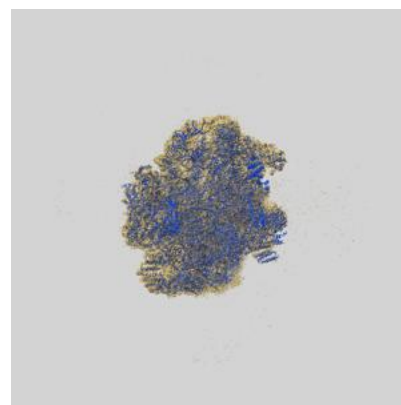
### 9.1 Map-model overlay [i](#)



X



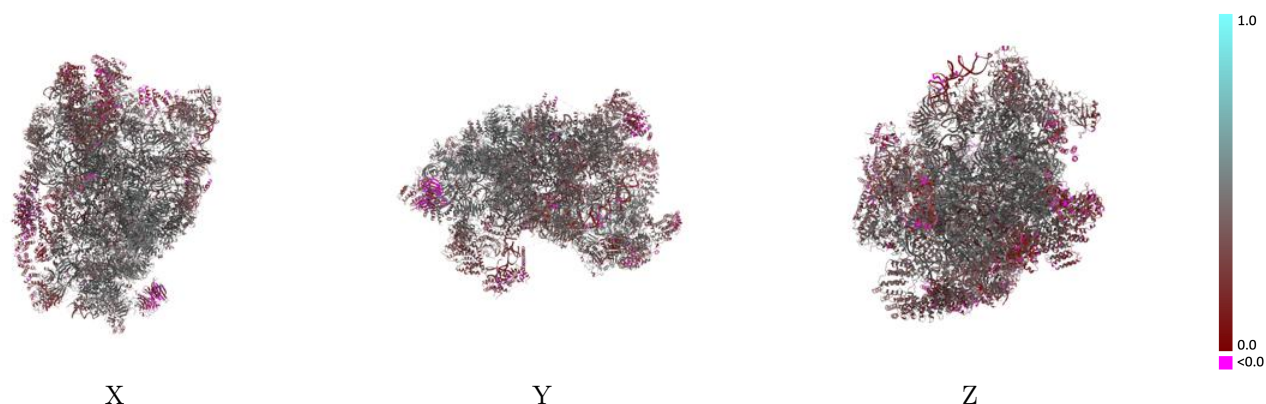
Y



Z

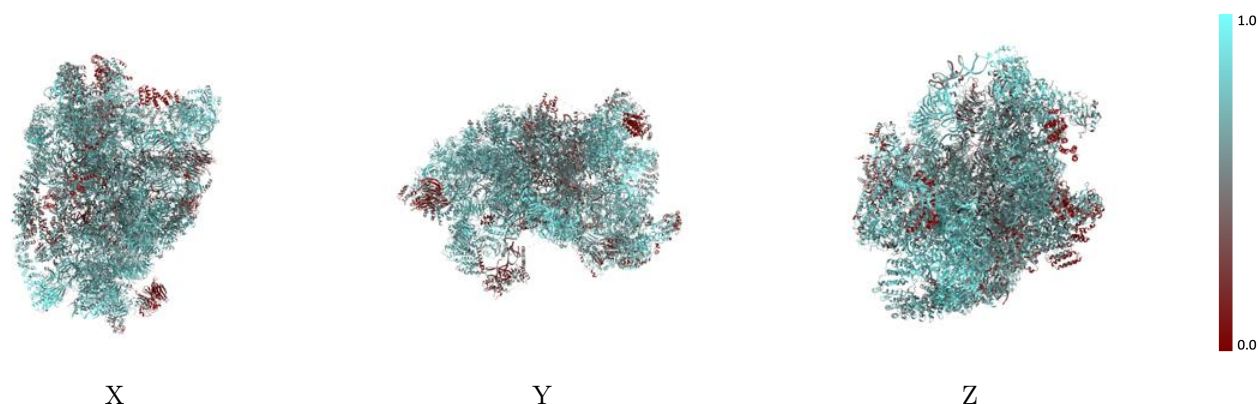
The images above show the 3D surface view of the map at the recommended contour level 0.77 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



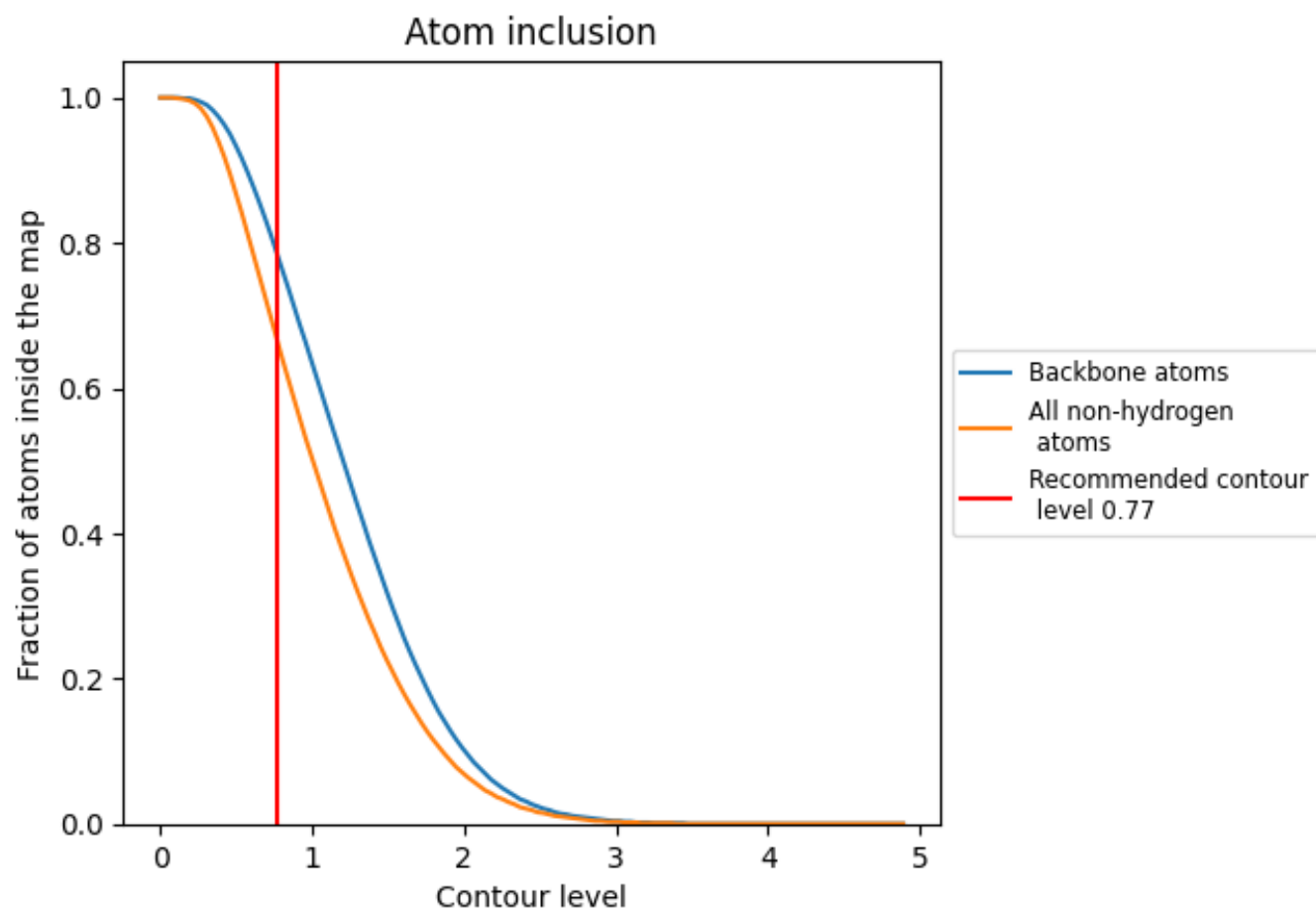
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.77).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 66% 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 (0.77) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6650   |  0.3900   |
| L0    |  0.6560   |  0.3770   |
| L1    |  0.7620   |  0.3790   |
| L2    |  0.6870   |  0.3830   |
| L3    |  0.0750   |  0.2530   |
| L4    |  0.7570   |  0.4600   |
| L5    |  0.7160   |  0.4490   |
| L6    |  0.8110   |  0.4420   |
| L7    |  0.5490   |  0.3020   |
| L8    |  0.8070   |  0.4620   |
| L9    |  0.6380   |  0.4510   |
| LC    |  0.6700   |  0.4650   |
| LD    |  0.7070   |  0.4230   |
| LE    |  0.7060   |  0.4550   |
| LF    |  0.8190  |  0.4520  |
| LG    |  0.6680 |  0.4710 |
| LH    |  0.7780 |  0.4550 |
| LI    |  0.3590 |  0.2430 |
| LJ    |  0.7880 |  0.4590 |
| LK    |  0.5930 |  0.3460 |
| LL    |  0.7480 |  0.4490 |
| LM    |  0.7110 |  0.3070 |
| LN    |  0.8060 |  0.4420 |
| LO    |  0.7130 |  0.4710 |
| LP    |  0.5020 |  0.3520 |
| LQ    |  0.7720 |  0.3880 |
| LR    |  0.4890 |  0.3500 |
| LS    |  0.7540 |  0.4700 |
| LT    |  0.6900 |  0.4660 |
| LU    |  0.7480 |  0.4650 |
| LV    |  0.7540 |  0.4310 |
| LW    |  0.6530 |  0.4700 |
| LX    |  0.6590 |  0.3810 |
| LY    |  0.6460 |  0.3540 |
| LZ    |  0.7000 |  0.4870 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| NA    |  0.5550   |  0.3730   |
| NB    |  0.5280   |  0.3150   |
| NC    |  0.5200   |  0.3090   |
| ND    |  0.6110   |  0.3640   |
| NE    |  0.5130   |  0.4070   |
| NF    |  0.7130   |  0.4420   |
| NG    |  0.5370   |  0.4340   |
| NH    |  0.7830   |  0.3910   |
| NI    |  0.5910   |  0.3370   |
| NK    |  0.5990   |  0.4360   |
| NM    |  0.6200   |  0.4420   |
| NN    |  0.5320   |  0.2800   |
| NQ    |  0.7780   |  0.4560   |
| OA    |  0.0560   |  0.1540   |
| SA    |  0.5630   |  0.3950   |
| SB    |  0.5790   |  0.3660   |
| SC    |  0.6290   |  0.4620   |
| SD    |  0.5940   |  0.4090   |
| SE    |  0.7780   |  0.4680   |
| SF    |  0.6300  |  0.4700  |
| SG    |  0.6400 |  0.4130 |
| SH    |  0.6320 |  0.4380 |
| SI    |  0.6740 |  0.4410 |
| SJ    |  0.6640 |  0.3330 |
| SK    |  0.7960 |  0.3800 |
| SL    |  0.6470 |  0.4670 |
| SM    |  0.6210 |  0.4610 |
| SN    |  0.5080 |  0.4080 |
| SP    |  0.6300 |  0.3270 |
| SQ    |  0.4470 |  0.4060 |
| SR    |  0.6770 |  0.4720 |
| SS    |  0.4030 |  0.3380 |
| ST    |  0.5720 |  0.3110 |
| SU    |  0.7230 |  0.3380 |
| SV    |  0.4580 |  0.2670 |
| SW    |  0.4190 |  0.3720 |
| SY    |  0.6240 |  0.4300 |
| SZ    |  0.3770 |  0.2020 |