



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:25 AM UTC

PDB ID : 5DGF / pdb\_00005dgf  
Title : Complex of yeast 80S ribosome with hypusine-containing/non-modified eIF5A and/or a peptidyl-tRNA analog  
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.; Dever, T.E.; Yusupov, M.  
Deposited on : 2015-08-27  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

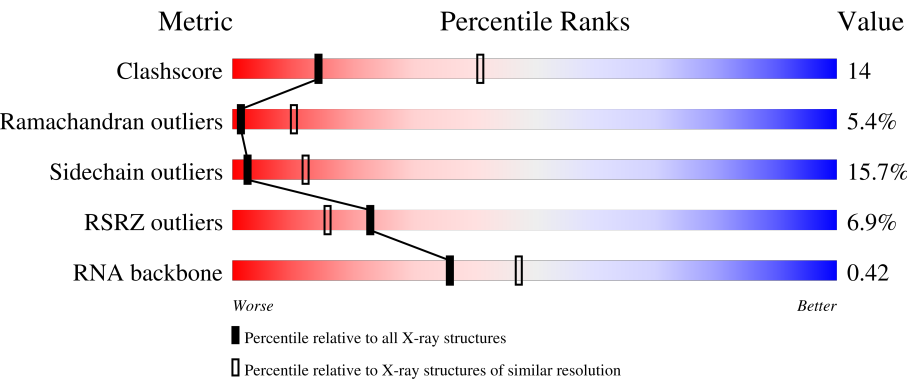
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| 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:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |
| Sidechain outliers    | 187428                      | 1187 (3.32-3.28)                                      |
| RSRZ outliers         | 180081                      | 1169 (3.32-3.28)                                      |
| RNA backbone          | 3983                        | 1048 (3.60-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                            |
|-----|-------|--------|-------------------------------------------------------------|
| 1   | 2     | 1800   | <div><div>3%</div><div>38%47%13%</div><div></div></div>     |
| 1   | 6     | 1800   | <div><div>2%</div><div>41%45%14%</div><div></div></div>     |
| 2   | S0    | 251    | <div><div>12%</div><div>36%35%10%18%</div><div></div></div> |
| 2   | s0    | 251    | <div><div>6%</div><div>41%31%9%18%</div><div></div></div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | S1    | 254    |                  |
| 3   | s1    | 254    |                  |
| 4   | S2    | 253    |                  |
| 4   | s2    | 253    |                  |
| 5   | S3    | 239    |                  |
| 5   | s3    | 239    |                  |
| 6   | S4    | 260    |                  |
| 6   | s4    | 260    |                  |
| 7   | S5    | 224    |                  |
| 7   | s5    | 224    |                  |
| 8   | S6    | 236    |                  |
| 8   | s6    | 236    |                  |
| 9   | S7    | 189    |                  |
| 9   | s7    | 189    |                  |
| 10  | S8    | 200    |                  |
| 10  | s8    | 200    |                  |
| 11  | S9    | 196    |                  |
| 11  | s9    | 196    |                  |
| 12  | C0    | 96     |                  |
| 12  | c0    | 96     |                  |
| 13  | C1    | 155    |                  |
| 13  | c1    | 155    |                  |
| 14  | C2    | 142    |                  |
| 14  | c2    | 142    |                  |
| 15  | C3    | 150    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | c3    | 150    |                  |
| 16  | C4    | 136    |                  |
| 16  | c4    | 136    |                  |
| 17  | C5    | 141    |                  |
| 17  | c5    | 141    |                  |
| 18  | C6    | 142    |                  |
| 18  | c6    | 142    |                  |
| 19  | C7    | 136    |                  |
| 19  | c7    | 136    |                  |
| 20  | C8    | 145    |                  |
| 20  | c8    | 145    |                  |
| 21  | C9    | 143    |                  |
| 21  | c9    | 143    |                  |
| 22  | D0    | 120    |                  |
| 22  | d0    | 120    |                  |
| 23  | D1    | 87     |                  |
| 23  | d1    | 87     |                  |
| 24  | D2    | 129    |                  |
| 24  | d2    | 129    |                  |
| 25  | D3    | 144    |                  |
| 25  | d3    | 144    |                  |
| 26  | D4    | 134    |                  |
| 26  | d4    | 134    |                  |
| 27  | D5    | 107    |                  |
| 27  | d5    | 107    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | D6    | 97     |                  |
| 28  | d6    | 97     |                  |
| 29  | D7    | 81     |                  |
| 29  | d7    | 81     |                  |
| 30  | D8    | 66     |                  |
| 30  | d8    | 66     |                  |
| 31  | D9    | 55     |                  |
| 31  | d9    | 55     |                  |
| 32  | E0    | 62     |                  |
| 32  | e0    | 62     |                  |
| 33  | E1    | 76     |                  |
| 33  | e1    | 76     |                  |
| 34  | SR    | 318    |                  |
| 34  | sR    | 318    |                  |
| 35  | SM    | 273    |                  |
| 35  | sM    | 273    |                  |
| 36  | 1     | 3396   |                  |
| 36  | 5     | 3396   |                  |
| 37  | 3     | 121    |                  |
| 37  | 7     | 121    |                  |
| 38  | 4     | 158    |                  |
| 38  | 8     | 158    |                  |
| 39  | L2    | 253    |                  |
| 39  | l2    | 253    |                  |
| 40  | L3    | 386    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | l3    | 386    |                  |
| 41  | L4    | 361    |                  |
| 41  | l4    | 361    |                  |
| 42  | L5    | 296    |                  |
| 42  | l5    | 296    |                  |
| 43  | L6    | 175    |                  |
| 43  | l6    | 175    |                  |
| 44  | L7    | 243    |                  |
| 44  | l7    | 243    |                  |
| 45  | L8    | 255    |                  |
| 45  | l8    | 255    |                  |
| 46  | L9    | 191    |                  |
| 46  | l9    | 191    |                  |
| 47  | M0    | 220    |                  |
| 47  | m0    | 220    |                  |
| 48  | M1    | 173    |                  |
| 48  | m1    | 173    |                  |
| 49  | M3    | 198    |                  |
| 49  | m3    | 198    |                  |
| 50  | M4    | 137    |                  |
| 50  | m4    | 137    |                  |
| 51  | M5    | 203    |                  |
| 51  | m5    | 203    |                  |
| 52  | M6    | 198    |                  |
| 52  | m6    | 198    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | M7    | 183    |                  |
| 53  | m7    | 183    |                  |
| 54  | M8    | 185    |                  |
| 54  | m8    | 185    |                  |
| 55  | M9    | 188    |                  |
| 55  | m9    | 188    |                  |
| 56  | N0    | 172    |                  |
| 56  | n0    | 172    |                  |
| 57  | N1    | 159    |                  |
| 57  | n1    | 159    |                  |
| 58  | N2    | 120    |                  |
| 58  | n2    | 120    |                  |
| 59  | N3    | 136    |                  |
| 59  | n3    | 136    |                  |
| 60  | N4    | 155    |                  |
| 60  | n4    | 155    |                  |
| 61  | N5    | 141    |                  |
| 61  | n5    | 141    |                  |
| 62  | N6    | 126    |                  |
| 62  | n6    | 126    |                  |
| 63  | N7    | 135    |                  |
| 63  | n7    | 135    |                  |
| 64  | N8    | 148    |                  |
| 64  | n8    | 148    |                  |
| 65  | N9    | 58     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 65  | n9    | 58     |                  |
| 66  | O0    | 104    |                  |
| 66  | o0    | 104    |                  |
| 67  | O1    | 112    |                  |
| 67  | o1    | 112    |                  |
| 68  | O2    | 129    |                  |
| 68  | o2    | 129    |                  |
| 69  | O3    | 106    |                  |
| 69  | o3    | 106    |                  |
| 70  | O4    | 120    |                  |
| 70  | o4    | 120    |                  |
| 71  | O5    | 119    |                  |
| 71  | o5    | 119    |                  |
| 72  | O6    | 99     |                  |
| 72  | o6    | 99     |                  |
| 73  | O7    | 87     |                  |
| 73  | o7    | 87     |                  |
| 74  | O8    | 77     |                  |
| 74  | o8    | 77     |                  |
| 75  | O9    | 50     |                  |
| 75  | o9    | 50     |                  |
| 76  | Q0    | 52     |                  |
| 76  | q0    | 52     |                  |
| 77  | Q1    | 25     |                  |
| 77  | q1    | 25     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 78  | Q2    | 105    |                  |
| 78  | q2    | 105    |                  |
| 79  | Q3    | 91     |                  |
| 79  | q3    | 91     |                  |
| 80  | m2    | 165    |                  |
| 81  | p0    | 311    |                  |
| 82  | p1    | 47     |                  |
| 82  | p2    | 47     |                  |
| 83  | f     | 157    |                  |

## 2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 404292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | 2     | 1781     | Total | C     | N    | O     | P    | 0       | 1       | 0     |
|     |       |          | 37970 | 16975 | 6720 | 12493 | 1782 |         |         |       |
| 1   | 6     | 1795     | Total | C     | N    | O     | P    | 0       | 1       | 0     |
|     |       |          | 38260 | 17105 | 6763 | 12596 | 1796 |         |         |       |

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | S0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1577  | 1014 | 278 | 283 | 2 |         |         |       |
| 2   | s0    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1583  | 1017 | 281 | 283 | 2 |         |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | S1    | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1709  | 1084 | 310 | 311 | 4 |         |         |       |
| 3   | s1    | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1091 | 312 | 315 | 4 |         |         |       |

- Molecule 4 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | S2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |
| 4   | s2    | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1635  | 1047 | 289 | 297 | 2 |         |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | S3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |
| 5   | s3    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1734  | 1101 | 313 | 314 | 6 |         |         |       |

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | S4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |
| 6   | s4    | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2068  | 1316 | 389 | 360 | 3 |         |         |       |

- Molecule 7 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | S5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |
| 7   | s5    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1609  | 1007 | 300 | 299 | 3 |         |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | S6    | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1799  | 1129 | 346 | 321 | 3 |         |         |       |
| 8   | s6    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1102 | 337 | 313 | 3 |         |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 9   | S7    | 184      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1481  | 951 | 265 | 265 |  |         |         |       |
| 9   | s7    | 186      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1491  | 957 | 267 | 267 |  |         |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | S8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | s8    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1489  | 925 | 298 | 264 | 2 |         |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | S9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |
| 11  | s9    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1494  | 943 | 289 | 261 | 1 |         |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | C0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 773   | 500 | 126 | 145 | 2 |         |         |       |
| 12  | c0    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 762   | 491 | 125 | 144 | 2 |         |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | C1    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1214  | 775 | 230 | 206 | 3 |         |         |       |
| 13  | c1    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1168  | 747 | 221 | 197 | 3 |         |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | C2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 892   | 562 | 156 | 172 | 2 |         |         |       |
| 14  | c2    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 892   | 562 | 156 | 172 | 2 |         |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | C3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |
| 15  | c3    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 759 | 224 | 207 | 2 |         |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | C4    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 891   | 545 | 182 | 163 | 1 |         |         |       |
| 16  | c4    | 128      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 949   | 582 | 188 | 176 | 3 |         |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S15 (uS19).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | C5    | 124      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 977   | 622 | 182 | 166 | 7 |         |         |       |
| 17  | c5    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1039  | 658 | 196 | 178 | 7 |         |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 18  | C6    | 141      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1105  | 708 | 203 | 194 |  |         |         |       |
| 18  | c6    | 142      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1111  | 711 | 204 | 196 |  |         |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | C7    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 926   | 577 | 177 | 170 | 2 |         |         |       |
| 19  | c7    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 906   | 563 | 174 | 167 | 2 |         |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | C8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |
| 20  | c8    | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 743 | 237 | 210 | 2 |         |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | C9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |
| 21  | c9    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1112  | 694 | 208 | 208 | 2 |         |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | D0    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 855   | 539 | 156 | 159 | 1 |         |         |       |
| 22  | d0    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 882   | 554 | 161 | 166 | 1 |         |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | D1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |
| 23  | d1    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 684   | 420 | 125 | 137 | 2 |         |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | D2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |
| 24  | d2    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 650 | 188 | 180 | 3 |         |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | D3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |
| 25  | d3    | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 708 | 220 | 191 | 2 |         |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | D4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 26  | d4    | 134      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1073  | 676 | 208 | 189 |         |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 27  | D5    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 563   | 360 | 104 | 99 |         |         |       |
| 27  | d5    | 69       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 558   | 357 | 103 | 98 |         |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | D6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |
| 28  | d6    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 769   | 475 | 160 | 129 | 5 |         |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | D7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |
| 29  | d7    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 610   | 382 | 110 | 113 | 5 |         |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30  | D8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |
| 30  | d8    | 63       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 497   | 306 | 99 | 91 | 1 |         |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | D9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |
| 31  | d9    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 442   | 274 | 92 | 72 | 4 |         |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32  | E0    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 475   | 299 | 98  | 77 | 1 |         |         |       |
| 32  | e0    | 62       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 491   | 309 | 101 | 80 | 1 |         |         |       |

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 33  | E1    | 71       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 566   | 362 | 106 | 94 | 4 |         |         |       |
| 33  | e1    | 76       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 117 | 99 | 4 |         |         |       |

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34  | SR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2437  | 1541 | 418 | 470 | 8 |         |         |       |
| 34  | sR    | 318      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2442  | 1544 | 418 | 472 | 8 |         |         |       |

- Molecule 35 is a protein called Suppressor protein STM1.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 35  | SM    | 159      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1105  | 653 | 221 | 231 |  |         |         |       |
| 35  | sM    | 104      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 680   | 403 | 140 | 137 |  |         |         |       |

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 36  | 1     | 3149     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67355 | 30086 | 12142 | 21978 | 3149 |         |         |       |
| 36  | 5     | 3169     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 67780 | 30276 | 12216 | 22120 | 3168 |         |         |       |

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 37  | 3     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |
| 37  | 7     | 121      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2579  | 1152 | 461 | 845 | 121 |         |         |       |

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 38  | 4     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |
| 38  | 8     | 158      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3353  | 1500 | 586 | 1109 | 158 |         |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 39  | L2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1914  | 1191 | 388 | 334 | 1 |         |         |       |
| 39  | l2    | 252      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1912  | 1190 | 388 | 333 | 1 |         |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 40  | L3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |
| 40  | l3    | 386      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3075  | 1950 | 584 | 533 | 8 |         |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 41  | L4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |
| 41  | l4    | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2748  | 1729 | 522 | 494 | 3 |         |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 42  | L5    | 296      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2375  | 1501 | 414 | 458 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 42  | 15    | 294      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2359  | 1489 | 412 | 456 | 2 |         |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | L6    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 800 | 222 | 216 | 1 |         |         |       |
| 43  | 16    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1248  | 806 | 224 | 217 | 1 |         |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 44  | L7    | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1784  | 1151 | 324 | 308 | 1 |         |         |       |
| 44  | 17    | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1791  | 1155 | 325 | 310 | 1 |         |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 45  | L8    | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1804  | 1151 | 323 | 327 | 3 |         |         |       |
| 45  | 18    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1764  | 1131 | 316 | 314 | 3 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L8    | 119     | ALA      | GLY    | conflict | UNP P17076 |
| 18    | 119     | ALA      | GLY    | conflict | UNP P17076 |

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | L9    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |
| 46  | 19    | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 963 | 274 | 277 | 4 |         |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 47  | M0    | 211      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1083 | 322 | 294 | 6 |         |         |       |
| 47  | m0    | 213      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1722  | 1094 | 325 | 297 | 6 |         |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | M1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |
| 48  | m1    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1353  | 847 | 253 | 249 | 4 |         |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 49  | M3    | 193      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1543  | 962 | 315 | 266 |  |         |         |       |
| 49  | m3    | 194      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 1548  | 965 | 316 | 267 |  |         |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | M4    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1053  | 675 | 199 | 177 | 2 |         |         |       |
| 50  | m4    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1059  | 678 | 200 | 179 | 2 |         |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 51  | M5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |
| 51  | m5    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1720  | 1077 | 361 | 281 | 1 |         |         |       |

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | M6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 52  | m6    | 197      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1555  | 1003 | 289 | 262 | 1 |         |         |       |

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | M7    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1420  | 882 | 281 | 257 |   |         |         |       |
| 53  | m7    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1227  | 764 | 238 | 225 |   |         |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54  | M8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |
| 54  | m8    | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 908 | 290 | 241 | 2 |         |         |       |

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55  | M9    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |   |         |         |       |
| 55  | m9    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1521  | 935 | 326 | 260 |   |         |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 56  | N0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |
| 56  | n0    | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1445  | 930 | 267 | 244 | 4 |         |         |       |

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 57  | N1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |
| 57  | n1    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1276  | 805 | 246 | 221 | 4 |         |         |       |

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 58  | N2    | 100      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 796   | 516 | 131 | 149 |         |         |       |
| 58  | n2    | 98       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 778   | 505 | 127 | 146 |         |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 59  | N3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |
| 59  | n3    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1003  | 628 | 189 | 179 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 60  | N4    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 699   | 443 | 137 | 118 | 1 |         |         |       |
| 60  | n4    | 135      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1038  | 651 | 206 | 180 | 1 |         |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 61  | N5    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 620 | 169 | 173 | 2 |         |         |       |
| 61  | n5    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 617 | 168 | 172 | 2 |         |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 62  | N6    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |         |         |       |
| 62  | n6    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 993   | 625 | 192 | 176 |         |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 63  | N7    | 135      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |         |       |
| 63  | n7    | 135      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1092  | 710 | 202 | 180 |         |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 64  | N8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |
| 64  | n8    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1173  | 749 | 231 | 190 | 3 |         |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 65  | N9    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |         |       |
| 65  | n9    | 58       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 462   | 289 | 100 | 73 |         |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 66  | O0    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 743   | 479 | 124 | 139 | 1 |         |         |       |
| 66  | o0    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 767   | 492 | 128 | 146 | 1 |         |         |       |

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 67  | O1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 876   | 556 | 167 | 152 | 1 |         |         |       |
| 67  | o1    | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 883   | 559 | 167 | 156 | 1 |         |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | O2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |

*Continued on next page...*

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 68  | o2    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1020  | 647 | 205 | 167 | 1 |         |         |       |

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 69  | O3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |
| 69  | o3    | 106      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 165 | 144 | 1 |         |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 70  | O4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |
| 70  | o4    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 880   | 545 | 179 | 152 | 4 |         |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 71  | O5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 969   | 615 | 186 | 167 | 1 |         |         |       |
| 71  | o5    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 612 | 185 | 167 | 1 |         |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 72  | O6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 481 | 156 | 132 | 2 |         |         |       |
| 72  | o6    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 770   | 481 | 156 | 131 | 2 |         |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 73  | O7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |
| 73  | o7    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 414 | 148 | 114 | 5 |         |         |       |

- Molecule 74 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 74  | O8    | 77       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 612   | 391 | 115 | 106 |         |         |       |
| 74  | o8    | 77       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 608   | 388 | 114 | 106 |         |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 75  | O9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |
| 75  | o9    | 50       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 436   | 272 | 97 | 65 | 2 |         |         |       |

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 76  | Q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |
| 76  | q0    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 417   | 259 | 86 | 67 | 5 |         |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 77  | Q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |
| 77  | q1    | 25       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 233   | 142 | 63 | 27 | 1 |         |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 78  | Q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |
| 78  | q2    | 105      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 847   | 534 | 170 | 138 | 5 |         |         |       |

- Molecule 79 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 79  | Q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |
| 79  | q3    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 694   | 429 | 138 | 121 | 6 |         |         |       |

- Molecule 80 is a protein called 60S ribosomal protein L12-A (uL11).

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 80  | m2    | 150      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 750   | 450 | 150 | 150 |  |         |         |       |

- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 81  | p0    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1077  | 687 | 192 | 195 | 3 |         |         |       |

- Molecule 82 is a protein called 60S ribosomal protein P1 alpha/P2 beta.

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 82  | p1    | 47       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 235   | 141 | 47 | 47 |  |         |         |       |
| 82  | p2    | 46       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 230   | 138 | 46 | 46 |  |         |         |       |

- Molecule 83 is a protein called Eukaryotic translation initiation factor 5A-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 83  | f     | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1116  | 692 | 188 | 227 | 9 |         |         |       |

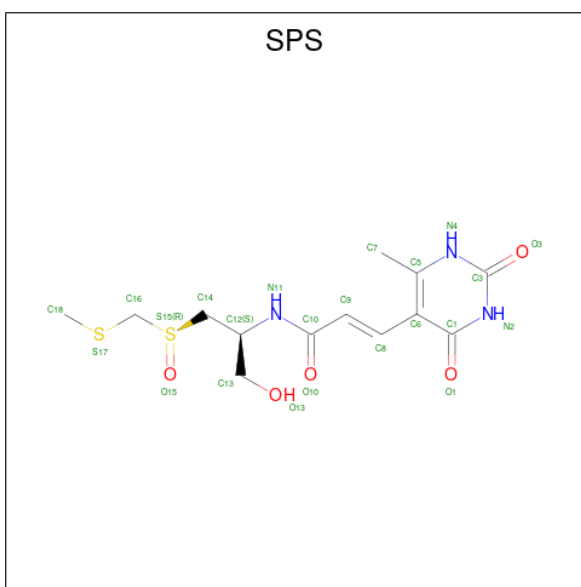
- Molecule 84 is an unknown type called CH-CH-8AN-PRO-PRO.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 84  | B     | 5        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 76    | 38 | 14 | 21 | 3 |         |         |
| 84  | C     | 5        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 73    | 38 | 14 | 19 | 2 |         |         |

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 85  | D6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | D7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | D9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | E1    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | O7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | Q0    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | Q2    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | Q3    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | d6    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | d7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | d9    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | e1    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | o7    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | q0    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | q2    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 85  | q3    | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

- Molecule 86 is SPARSOMYCIN (CCD ID: SPS) (formula:  $C_{13}H_{19}N_3O_5S_2$ ).

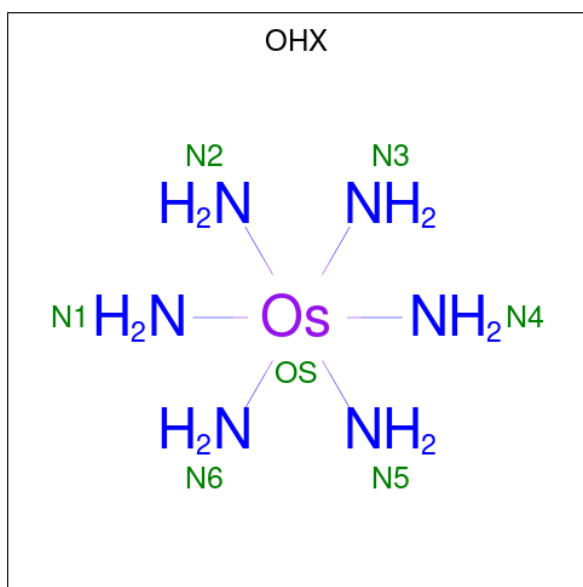


| Mol | Chain | Residues | Atoms       |         |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|---------|
| 86  | 1     | 1        | Total<br>23 | C<br>13 | N<br>3 | O<br>5 | S<br>2 | 0       | 0       |
| 86  | B     | 1        | Total<br>23 | C<br>13 | N<br>3 | O<br>5 | S<br>2 | 0       | 0       |

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 87  | 1     | 3        | Total Mg<br>3 3 | 0       | 0       |
| 87  | 5     | 5        | Total Mg<br>5 5 | 0       | 0       |
| 87  | f     | 2        | Total Mg<br>2 2 | 0       | 0       |
| 87  | B     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 87  | C     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 88 is osmium (III) hexammine (CCD ID: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



| Mol | Chain | Residues | Atoms |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---------|---------|
| 88  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 88  | 1     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |
| 88  | 5     | 1        | Total | N | Os | 0       | 0       |
|     |       |          | 7     | 6 | 1  |         |         |

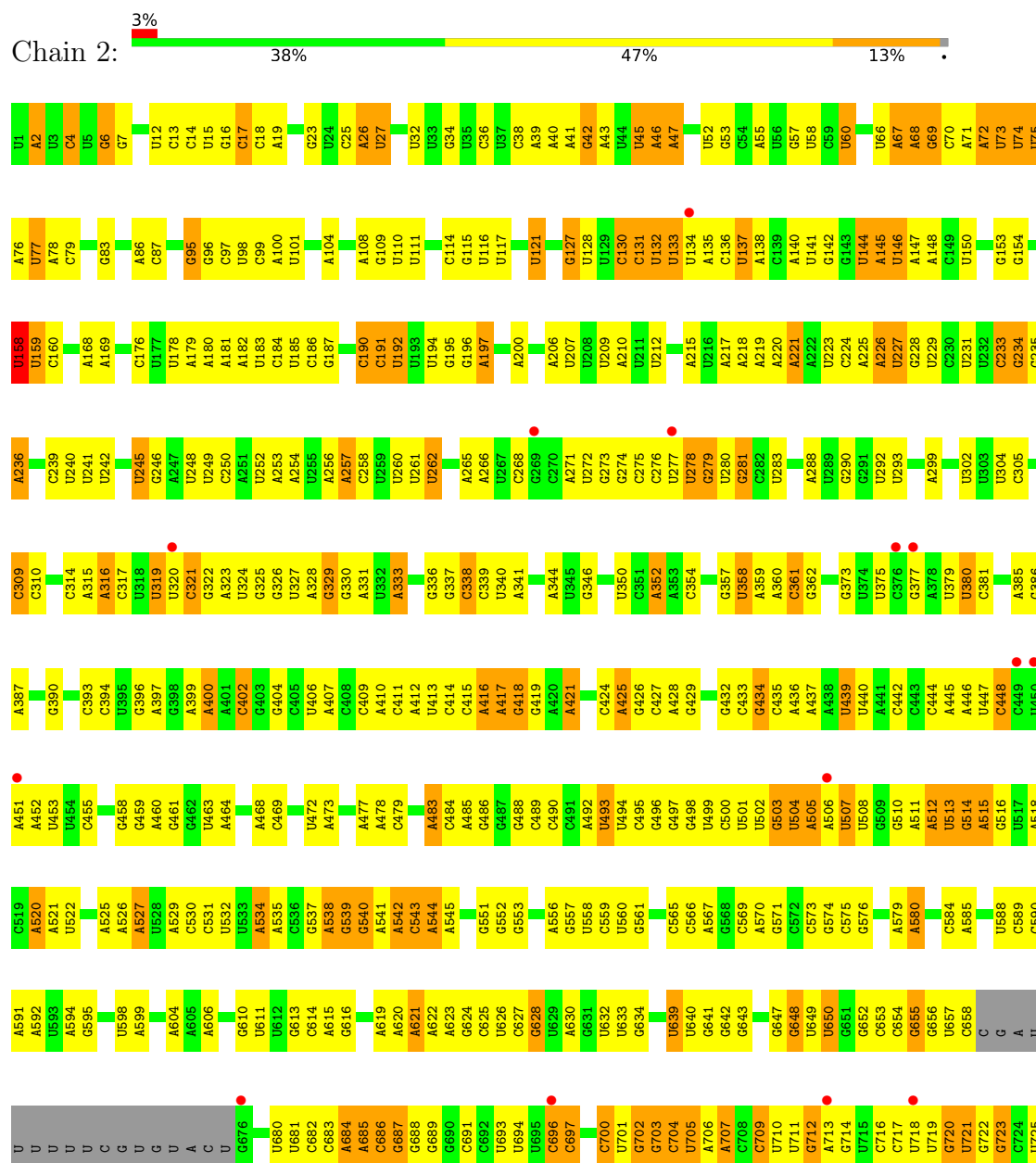
- Molecule 89 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 89  | 5     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 89  | f     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |

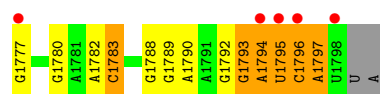
### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

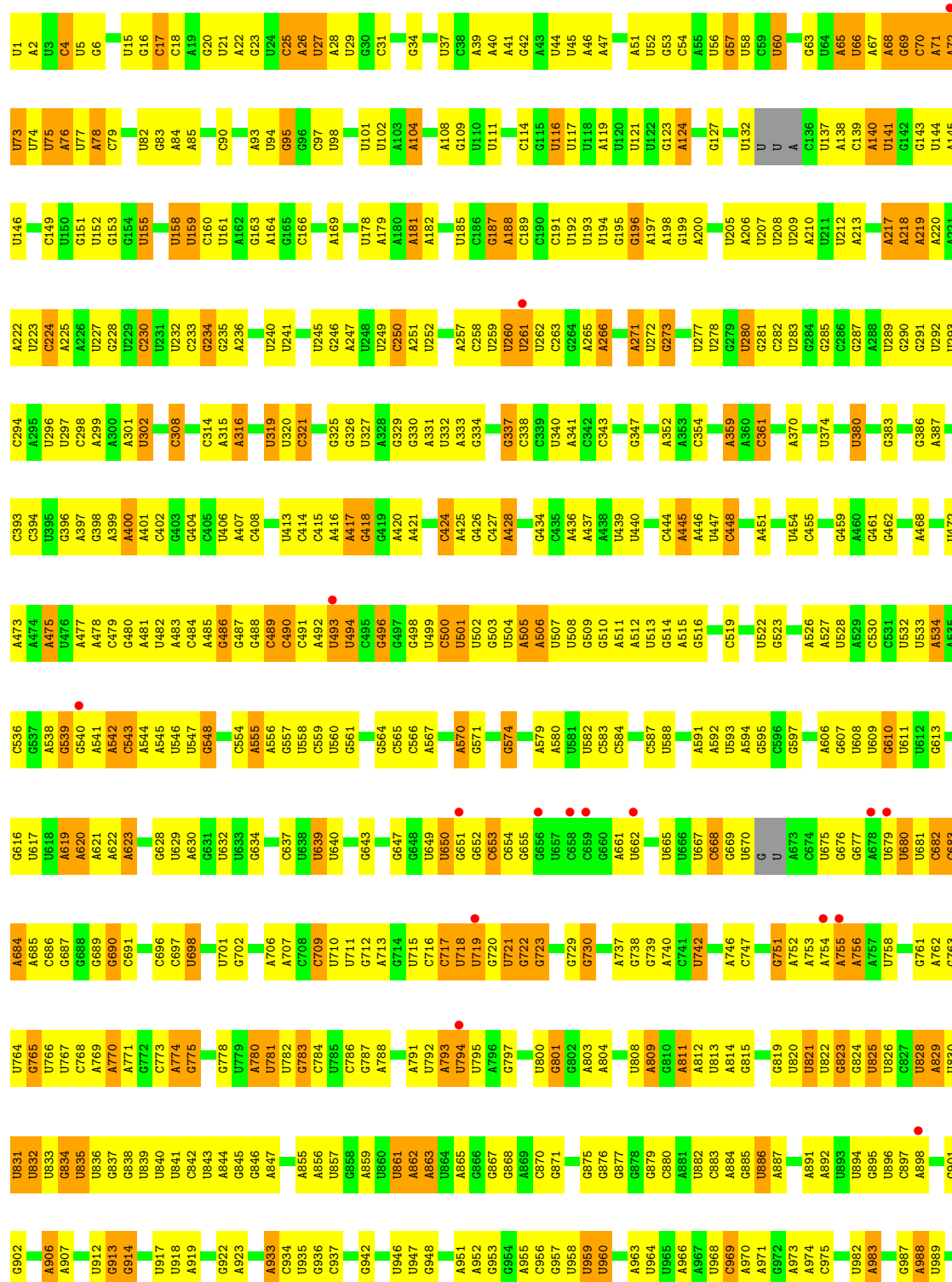
#### • Molecule 1: 18S ribosomal RNA

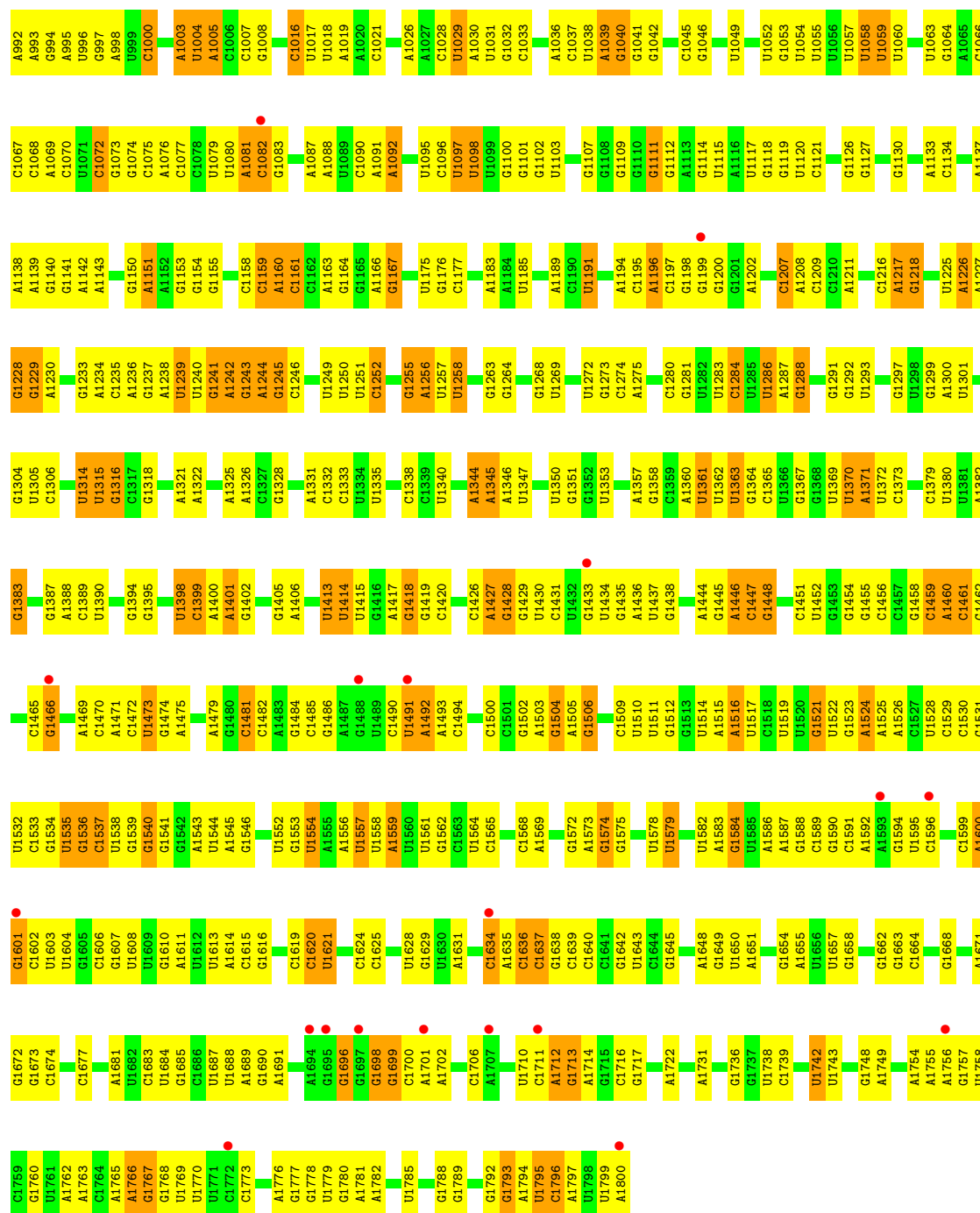




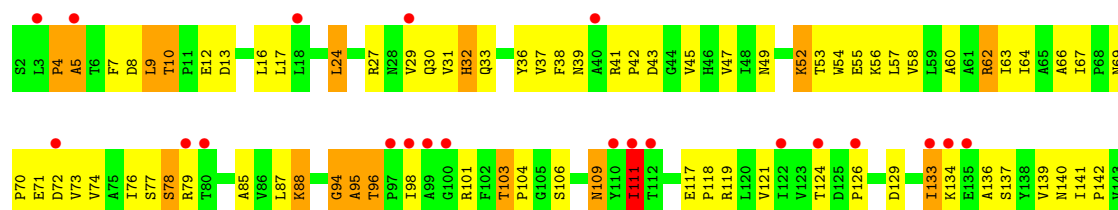


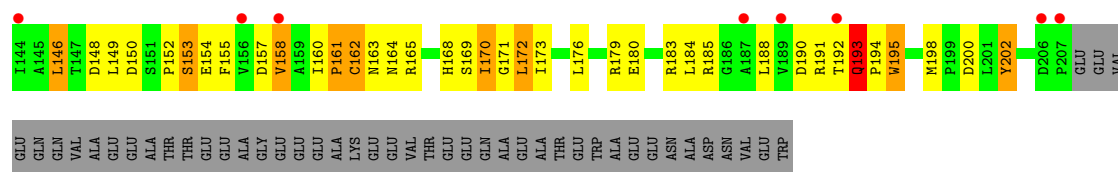
• Molecule 1: 18S ribosomal RNA



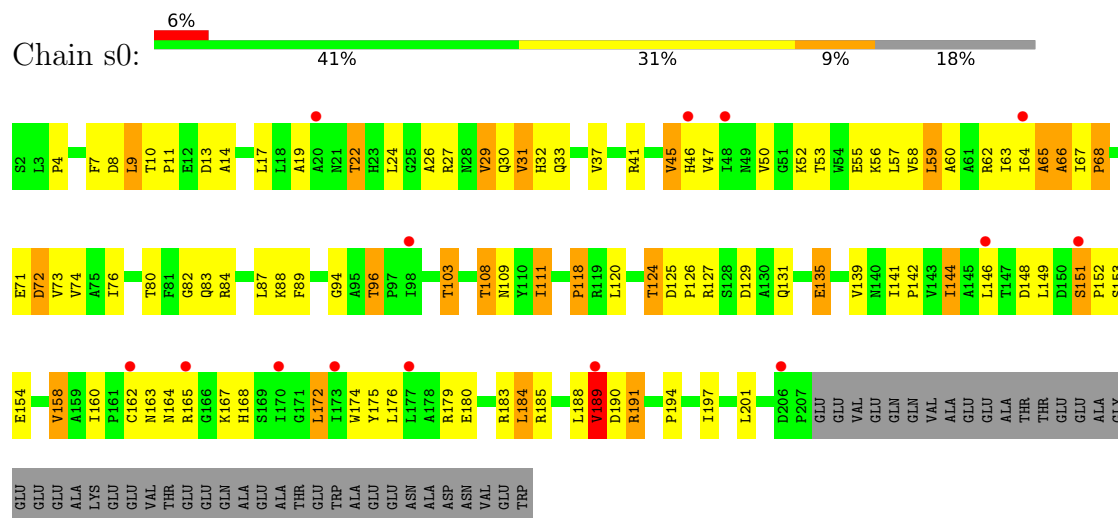


• Molecule 2: 40S ribosomal protein S0-A

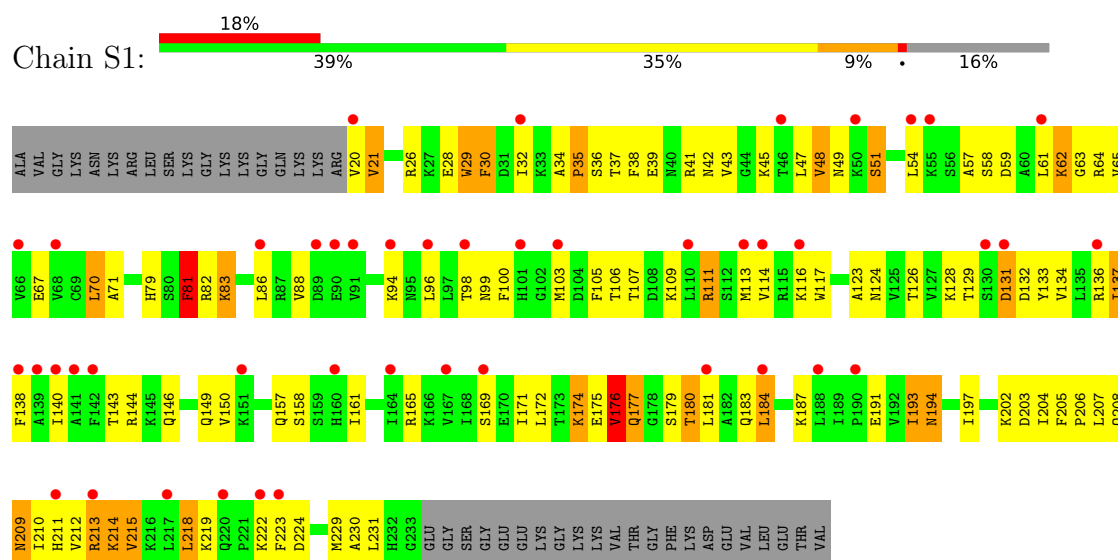




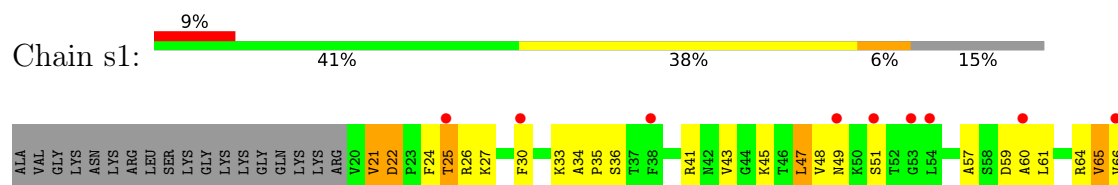
• Molecule 2: 40S ribosomal protein S0-A

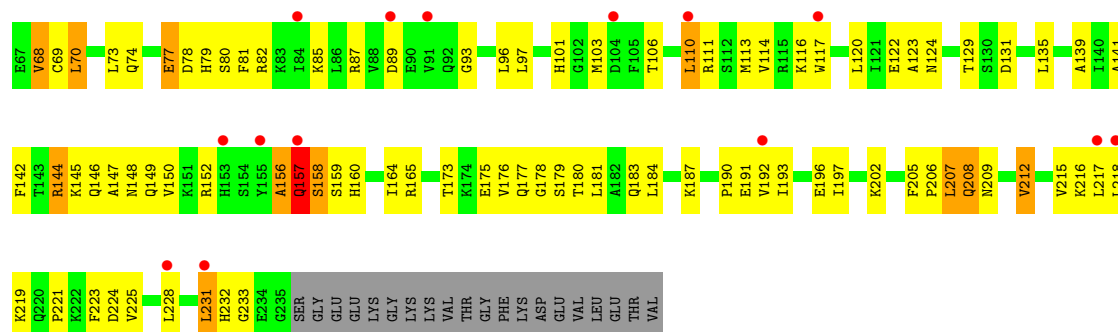


• Molecule 3: 40S ribosomal protein S1-A

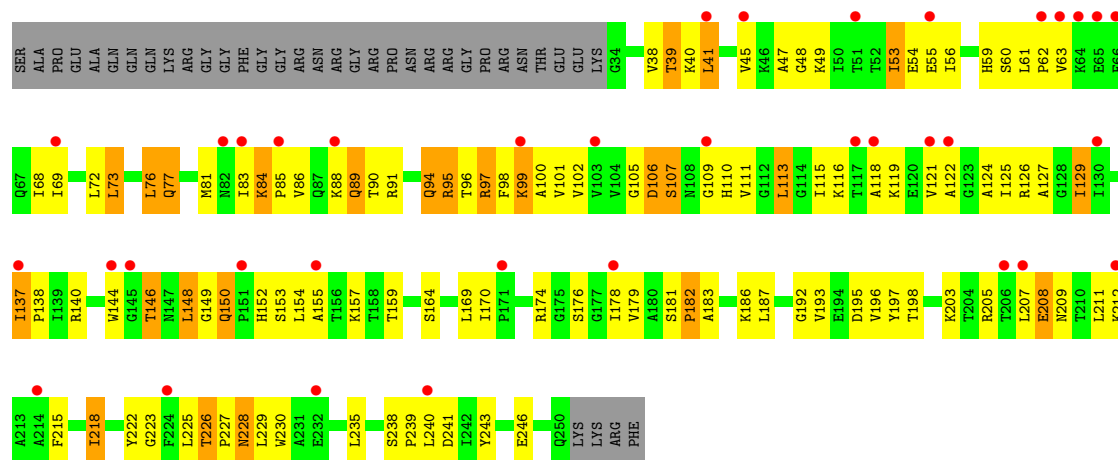


• Molecule 3: 40S ribosomal protein S1-A

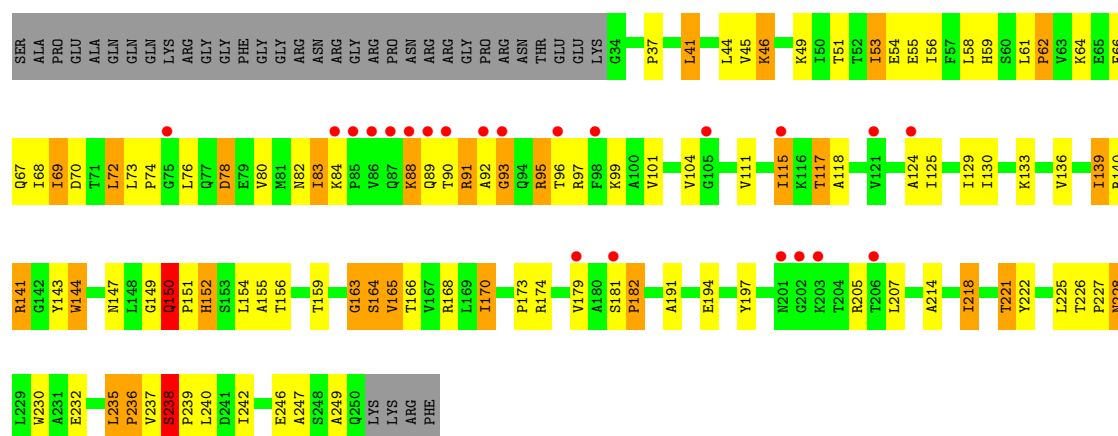




• Molecule 4: 40S ribosomal protein S2

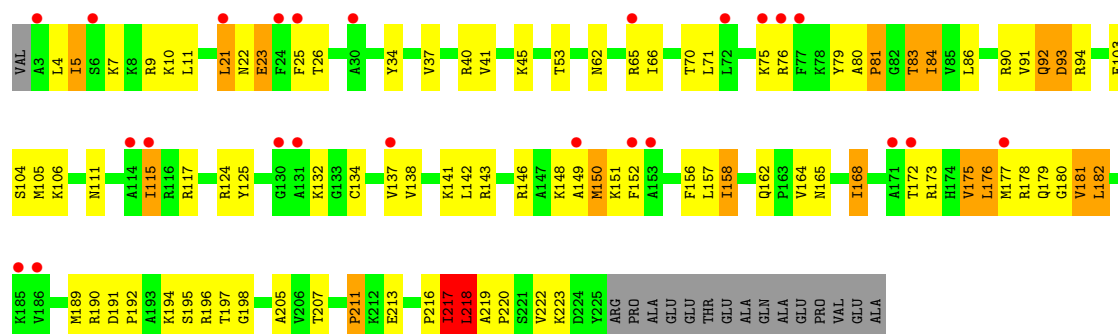


• Molecule 4: 40S ribosomal protein S2

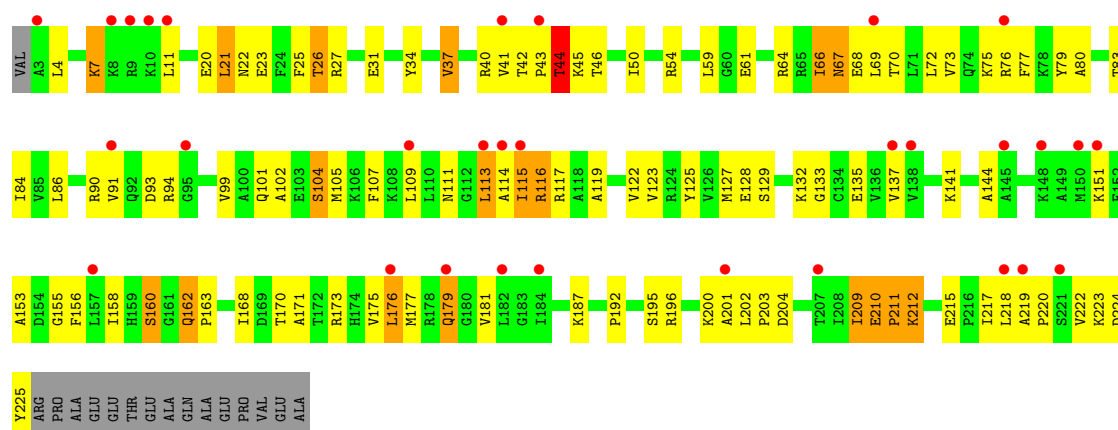


• Molecule 5: 40S ribosomal protein S3

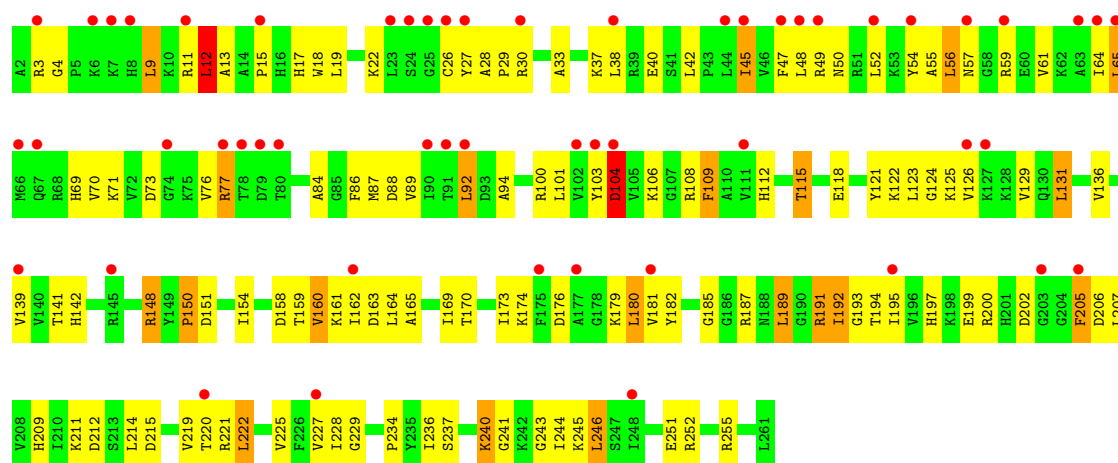




• Molecule 5: 40S ribosomal protein S3

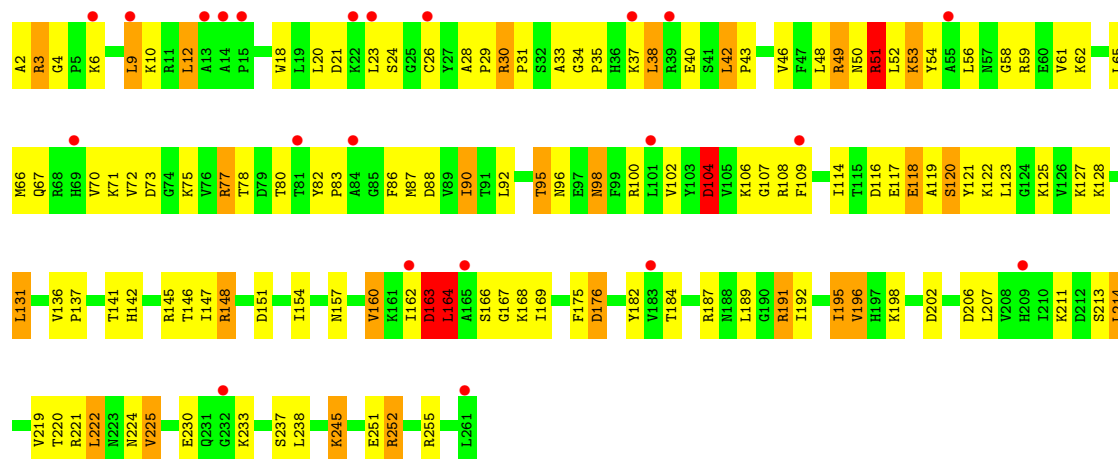


• Molecule 6: 40S ribosomal protein S4-A

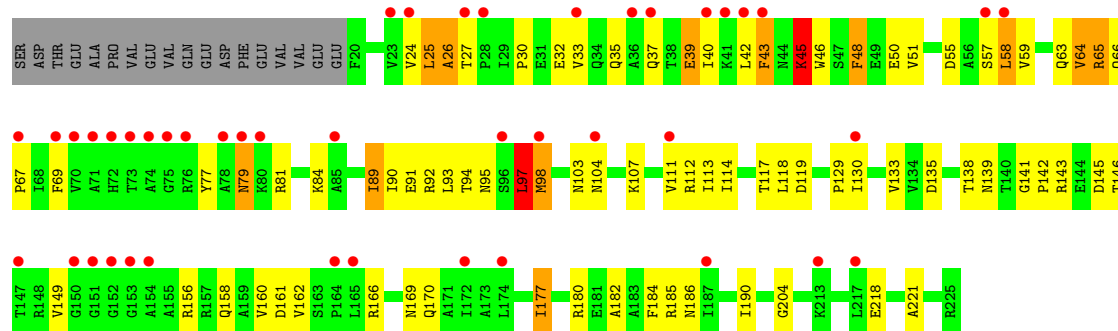


• Molecule 6: 40S ribosomal protein S4-A

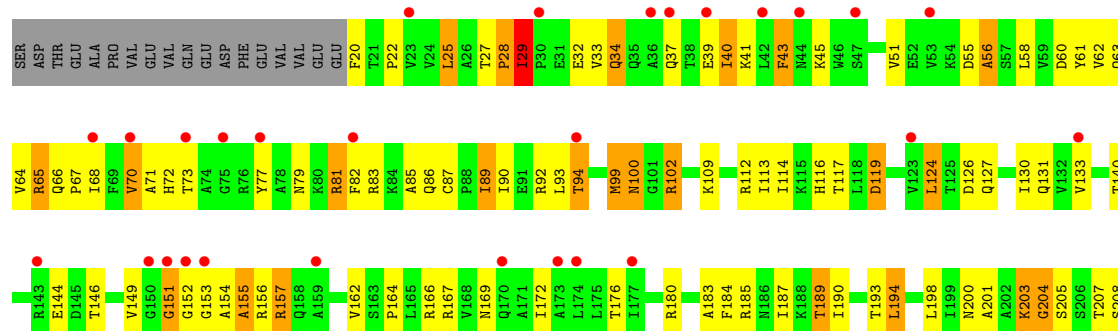




• Molecule 7: 40S ribosomal protein S5

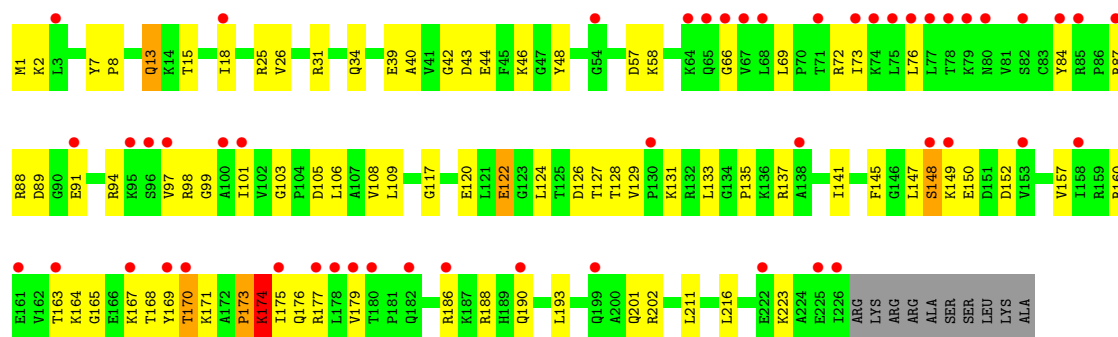


• Molecule 7: 40S ribosomal protein S5

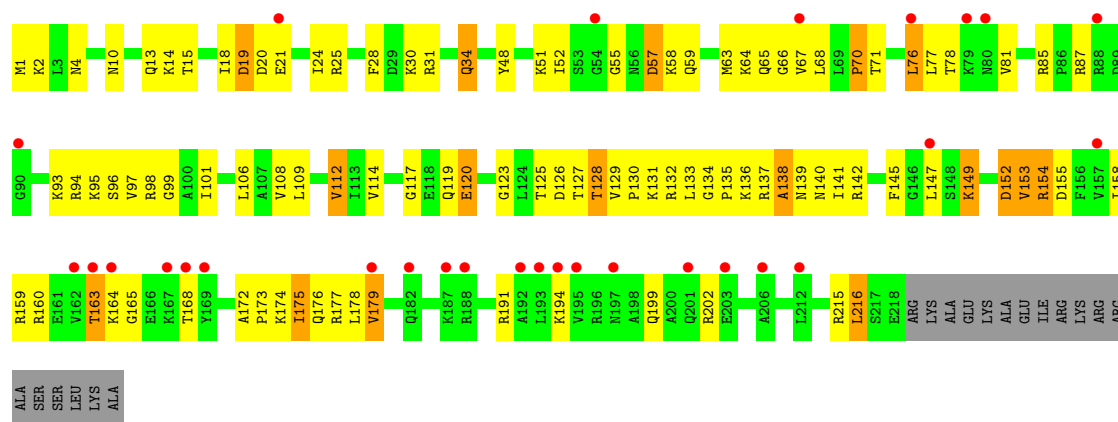


• Molecule 8: 40S ribosomal protein S6-A

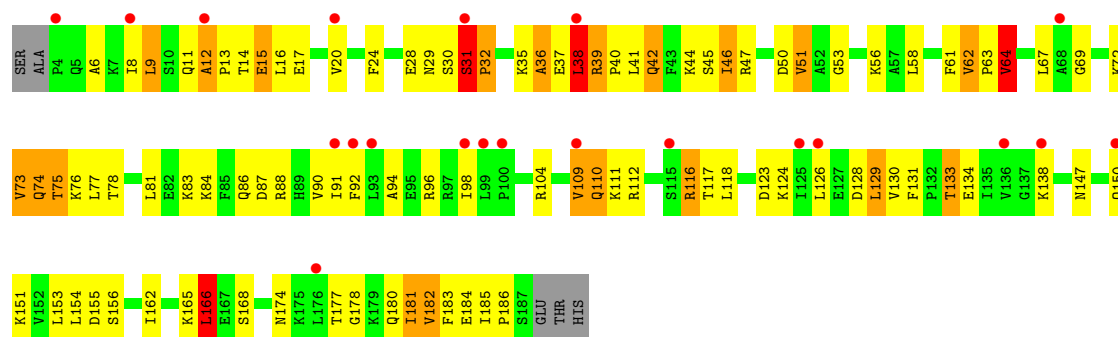




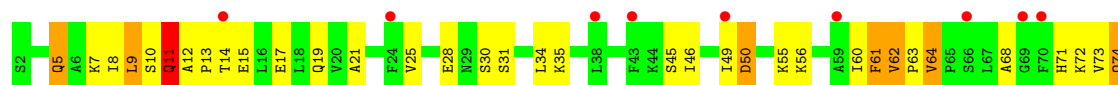
• Molecule 8: 40S ribosomal protein S6-A

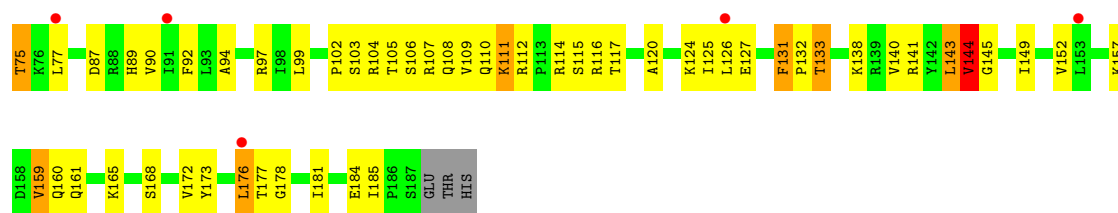


• Molecule 9: 40S ribosomal protein S7-A

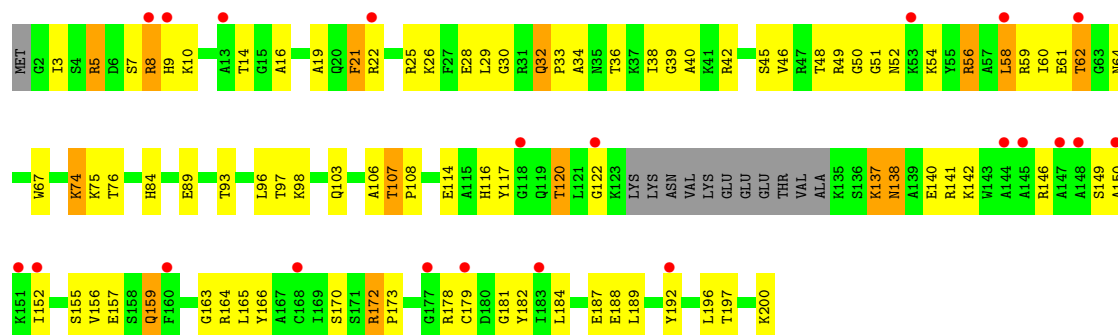


• Molecule 9: 40S ribosomal protein S7-A

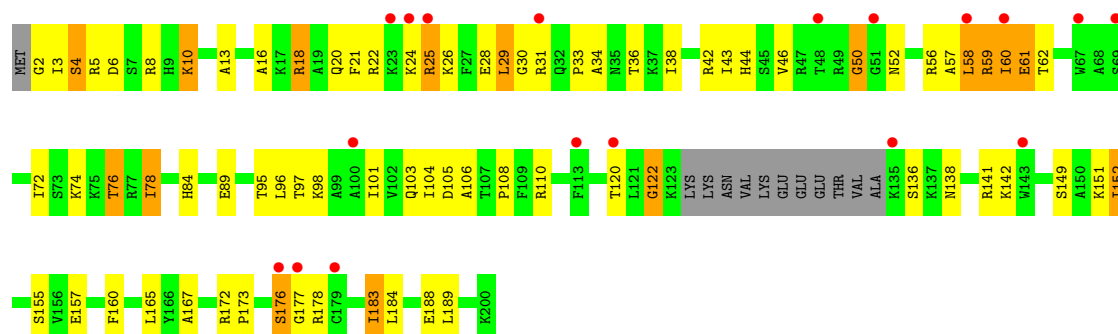




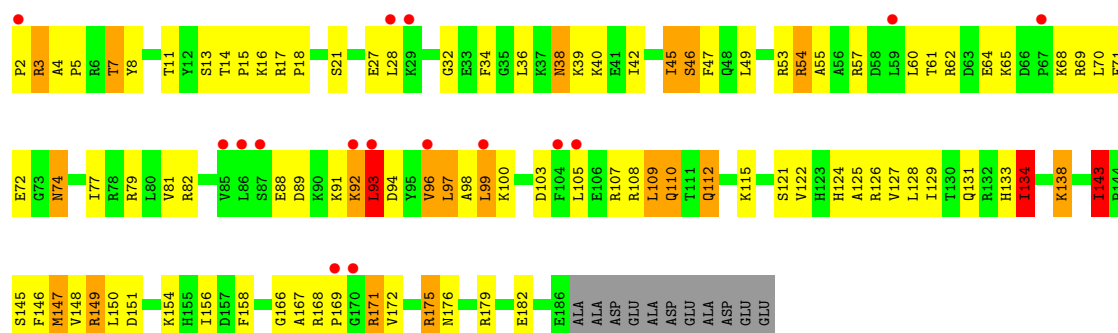
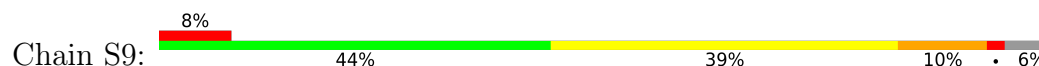
• Molecule 10: 40S ribosomal protein S8-A



• Molecule 10: 40S ribosomal protein S8-A



• Molecule 11: 40S ribosomal protein S9-A



Chain s9:

7% 40% 44% 10% 6%

P2 P5 T7 Y8 R10 T11 T14 K16 R17 S22 E27 L28 K29 L30 A31 F34 G35 L36 K40 E41 I42 Y43 R44 I45 S46 F47 Q48 L49 S50 K51 I52 R53 R54 R57 D58 L59 L60 T61 D62 D63 E64 K65 D66 P67 R69 L70 F71 F72

Chain C0:

| Amino Acid | Count |
|------------|-------|
| M1         | 1     |
| L2         | 1     |
| M3         | 1     |
| P4         | 1     |
| K5         | 1     |
| F6         | 1     |
| D7         | 1     |
| K10        | 1     |
| I11        | 1     |
| H12        | 1     |
| Q13        | 1     |
| Y14        | 1     |
| L15        | 1     |
| V20        | 1     |
| V21        | 1     |
| K24        | 1     |
| D26        | 1     |
| F27        | 1     |
| N28        | 1     |
| Q29        | 1     |
| A30        | 1     |
| K31        | 1     |
| E34        | 1     |
| I35        | 1     |
| D36        | 1     |
| T37        | 1     |
| K38        | 1     |
| N39        | 1     |
| L40        | 1     |
| Y41        | 1     |
| W42        | 1     |
| I43        | 1     |
| K44        | 1     |
| Q47        | 1     |
| S48        | 1     |
| L49        | 1     |
| T50        | 1     |
| S51        | 1     |
| K52        | 1     |
| G53        | 1     |
| Y54        | 1     |
| V55        | 1     |
| K56        | 1     |
| S60        | 1     |
| Q62        | 1     |
| Y63        | 1     |
| Y64        | 1     |
| Y65        | 1     |
| Y66        | 1     |
| T67        | 1     |
| L68        | 1     |
| T69        | 1     |

Chain c0:

| Amino Acid Type | Percentage |
|-----------------|------------|
| Red             | 21%        |
| Green           | 56%        |
| Yellow          | 30%        |
| Orange          | 14%        |

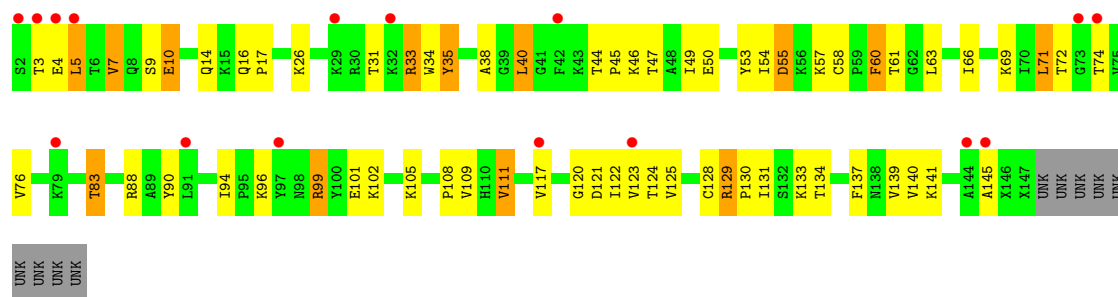
Chain C1:

7% 55% 38% 6%

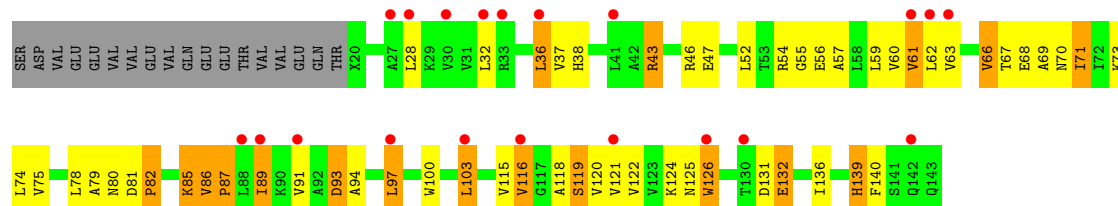
32 T3 E4 L5 T6 V7 Q8 S9 F13 Q14 K15 H18 I19 F20 N21 N22 P23 K24 V25 K26 R30 K36 N37 A38 G39 L40 T44 P45 K46 T49 Y53 I54 P55 K56 K57 C58 R67 T72 G73 T74 V75 V76 T77 T78 K79 R80 T83 T84 V85 T86

L91 N98 R99 Y100 E101 L102 V107 P108 H109 H110 V111 S112 P113 A114 F115 Q118 V119 G120 D121 I122 V123 T124 V125 C128 I131 S132 K133 T134 V135 R136 F137 M138 V139 V142 S143 A144 A145 X156

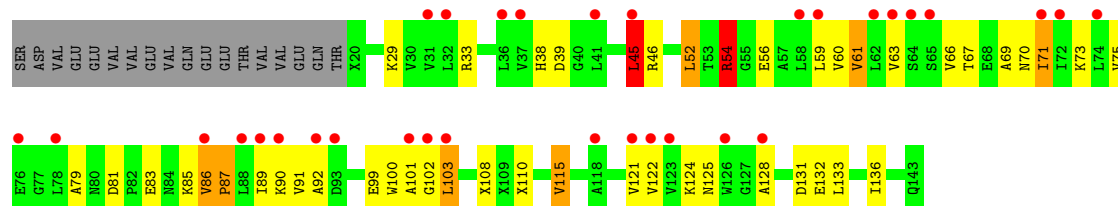
Chain c1: 



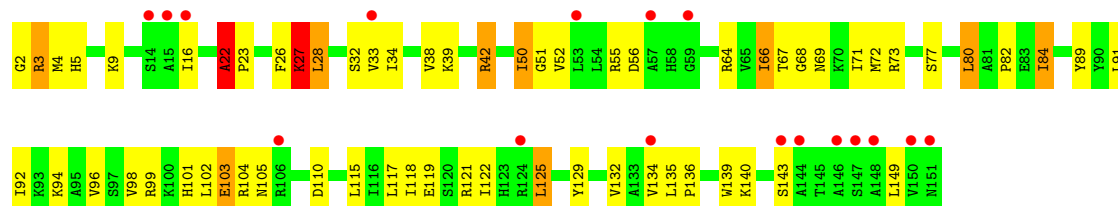
• Molecule 14: 40S ribosomal protein S12



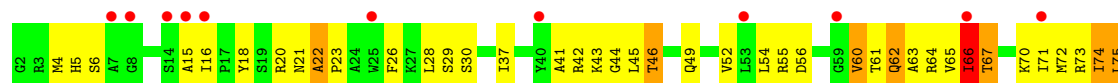
• Molecule 14: 40S ribosomal protein S12



• Molecule 15: 40S ribosomal protein S13

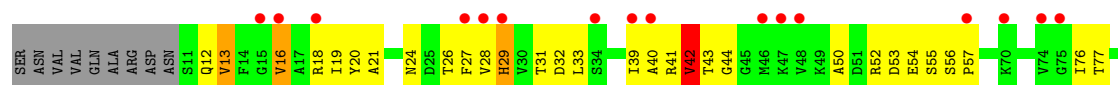


• Molecule 15: 40S ribosomal protein S13

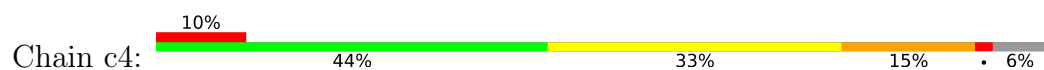




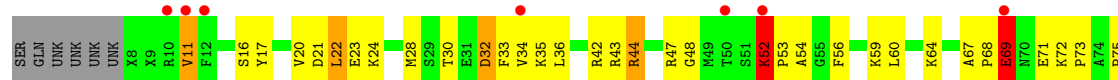
• Molecule 16: 40S ribosomal protein S14-A



• Molecule 16: 40S ribosomal protein S14-A

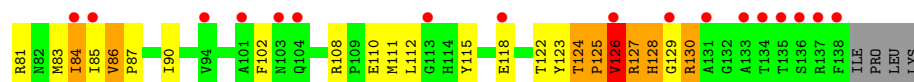


• Molecule 17: 40S ribosomal protein S15 (uS19)

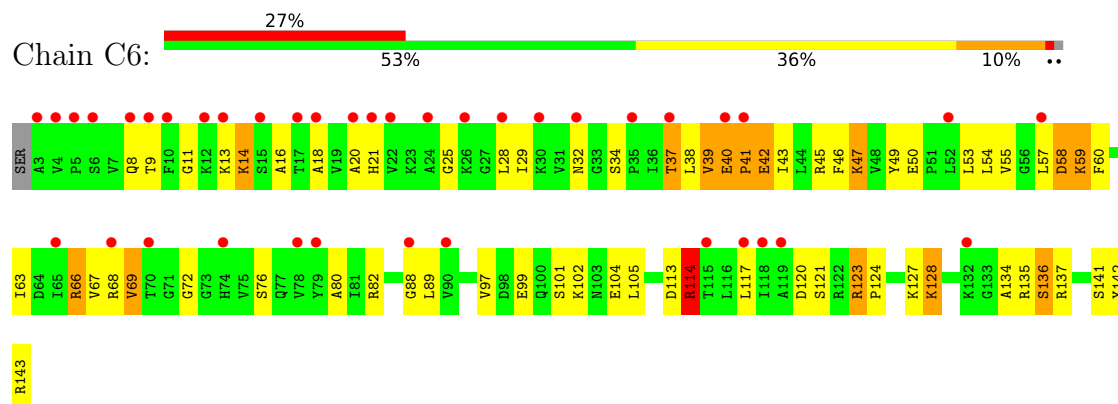


LYS

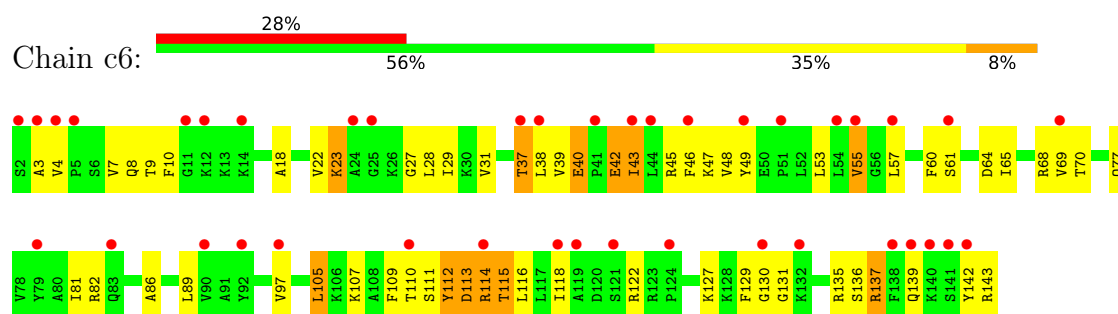
• Molecule 17: 40S ribosomal protein S15 (uS19)



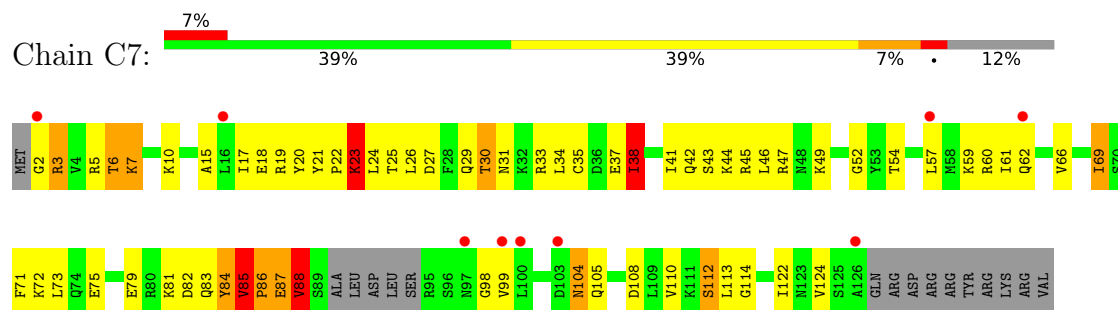
- Molecule 18: 40S ribosomal protein S16-A



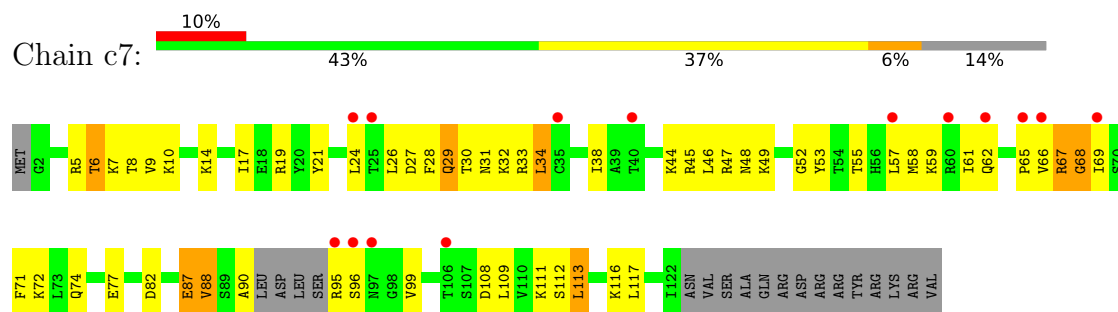
- Molecule 18: 40S ribosomal protein S16-A



- Molecule 19: 40S ribosomal protein S17-A

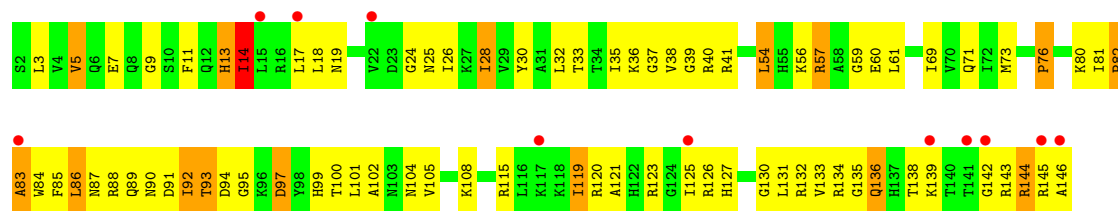


- Molecule 19: 40S ribosomal protein S17-A

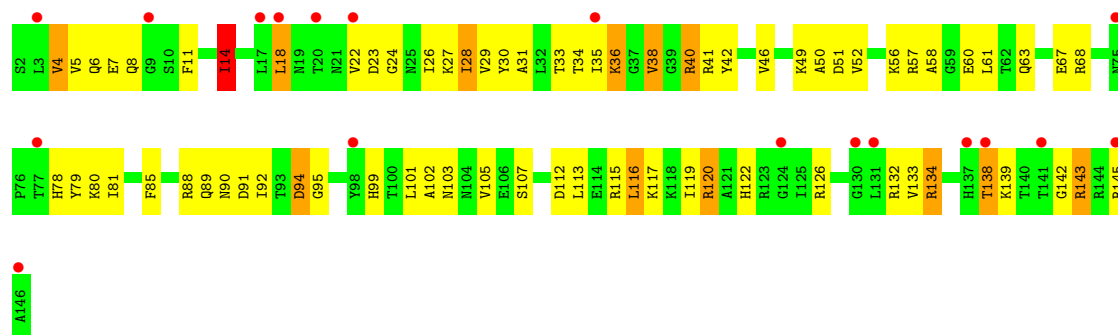


- Molecule 20: 40S ribosomal protein S18-A

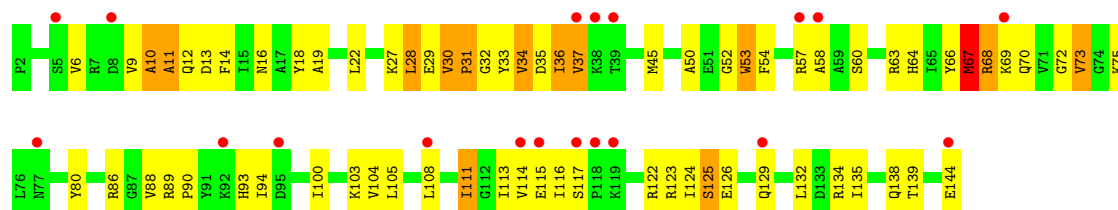




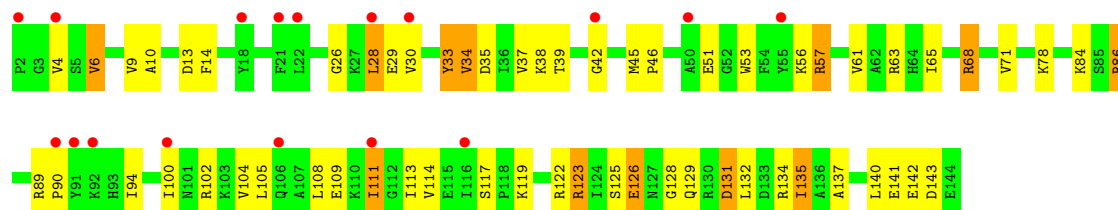
• Molecule 20: 40S ribosomal protein S18-A



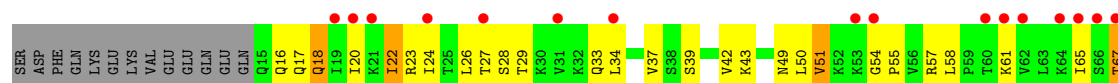
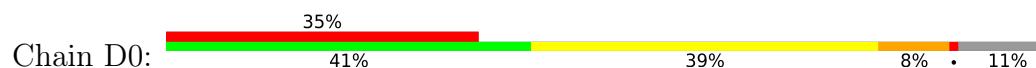
• Molecule 21: 40S ribosomal protein S19-A

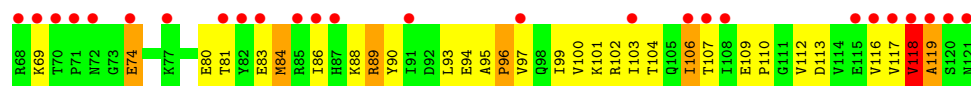


• Molecule 21: 40S ribosomal protein S19-A



• Molecule 22: 40S ribosomal protein S20

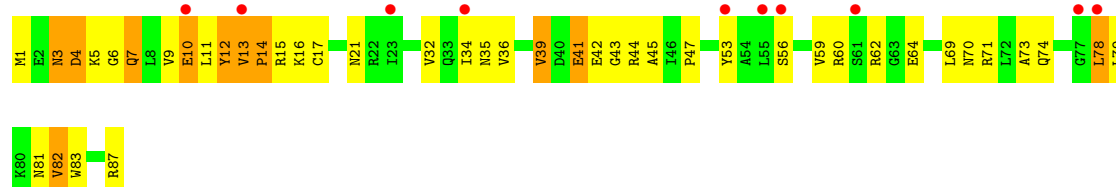




• Molecule 22: 40S ribosomal protein S20



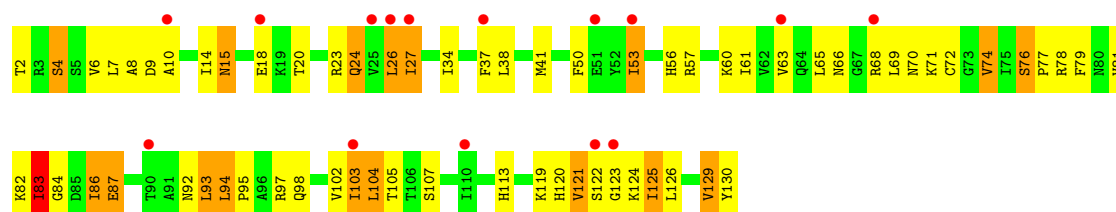
• Molecule 23: 40S ribosomal protein S21-A



• Molecule 23: 40S ribosomal protein S21-A

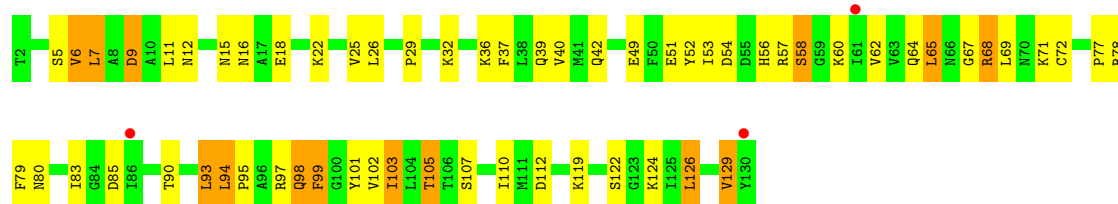


• Molecule 24: 40S ribosomal protein S22-A

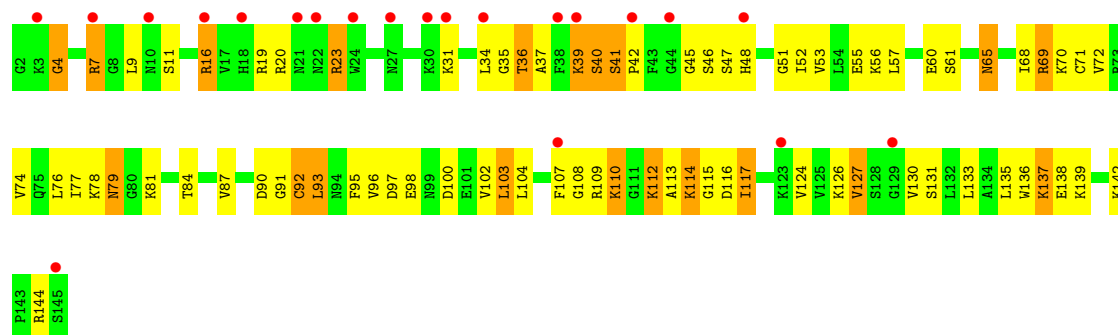


• Molecule 24: 40S ribosomal protein S22-A

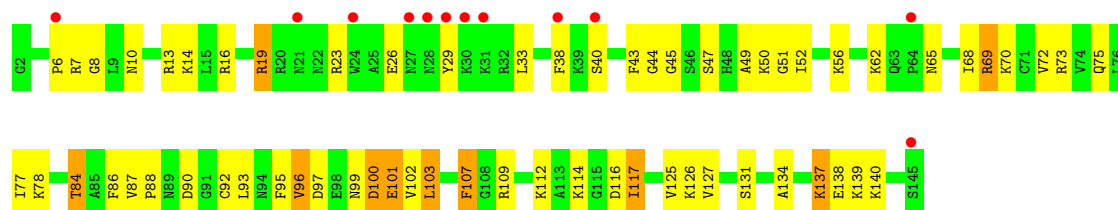




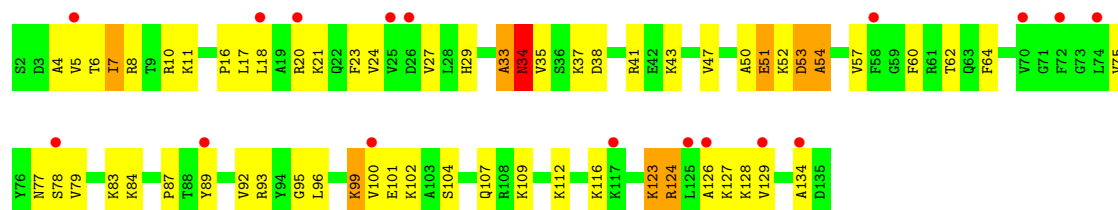
• Molecule 25: 40S ribosomal protein S23-A



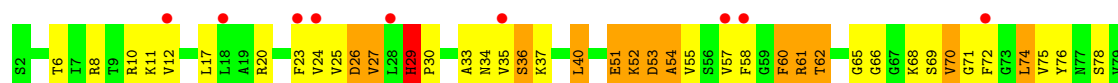
• Molecule 25: 40S ribosomal protein S23-A

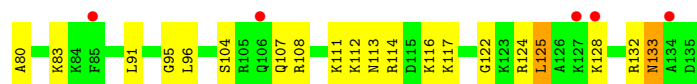


• Molecule 26: 40S ribosomal protein S24-A

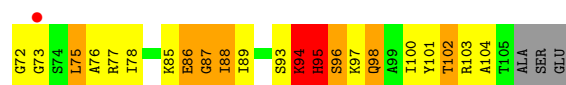
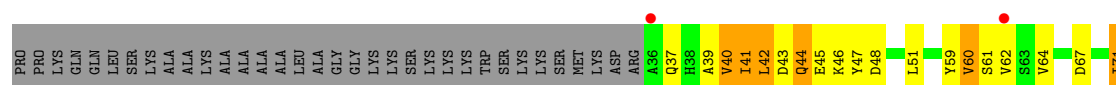
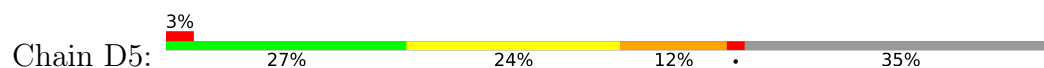


• Molecule 26: 40S ribosomal protein S24-A

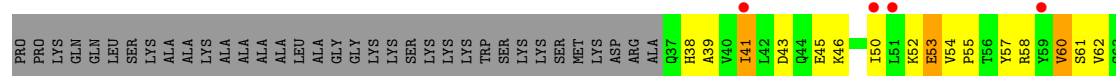
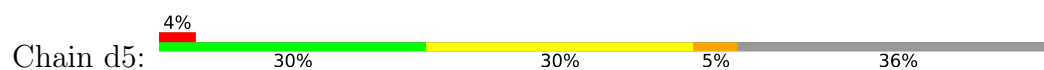




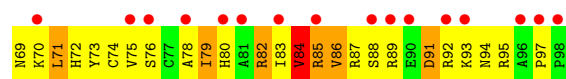
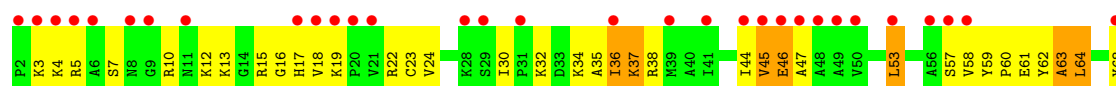
- Molecule 27: 40S ribosomal protein S25-A



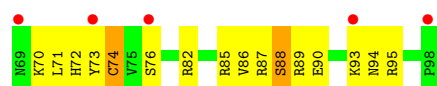
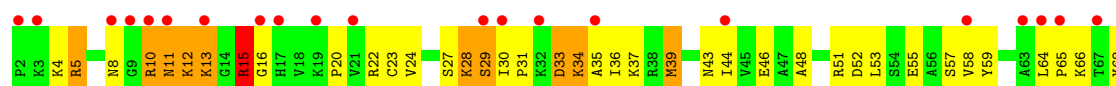
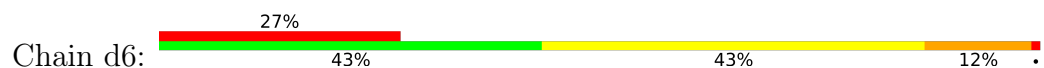
- Molecule 27: 40S ribosomal protein S25-A



- Molecule 28: 40S ribosomal protein S26-B

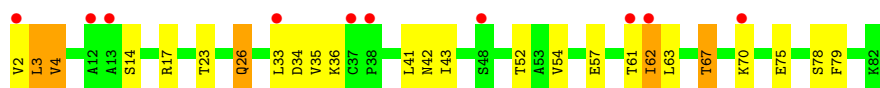


- Molecule 28: 40S ribosomal protein S26-B

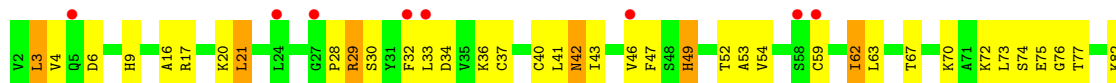


- Molecule 29: 40S ribosomal protein S27-A

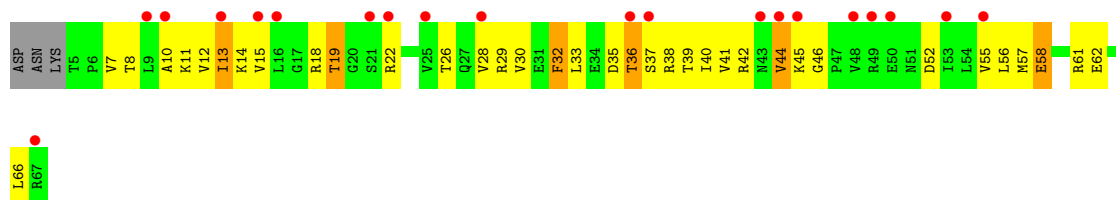




- Molecule 29: 40S ribosomal protein S27-A



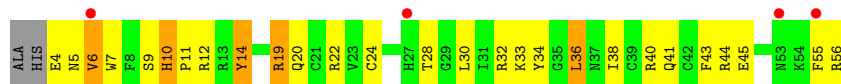
- Molecule 30: 40S ribosomal protein S28-A



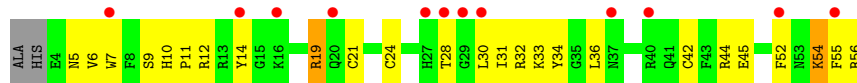
- Molecule 30: 40S ribosomal protein S28-A



- Molecule 31: 40S ribosomal protein S29-A

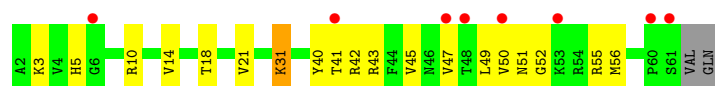


- Molecule 31: 40S ribosomal protein S29-A



- Molecule 32: 40S ribosomal protein S30-A

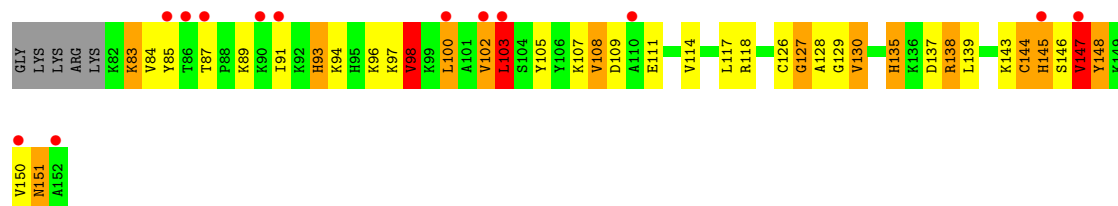




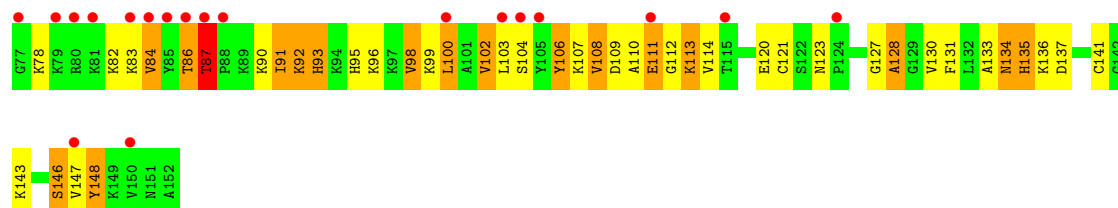
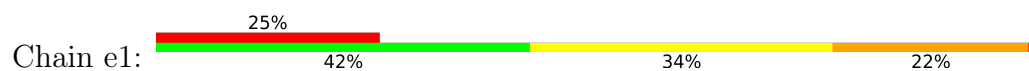
- Molecule 32: 40S ribosomal protein S30-A



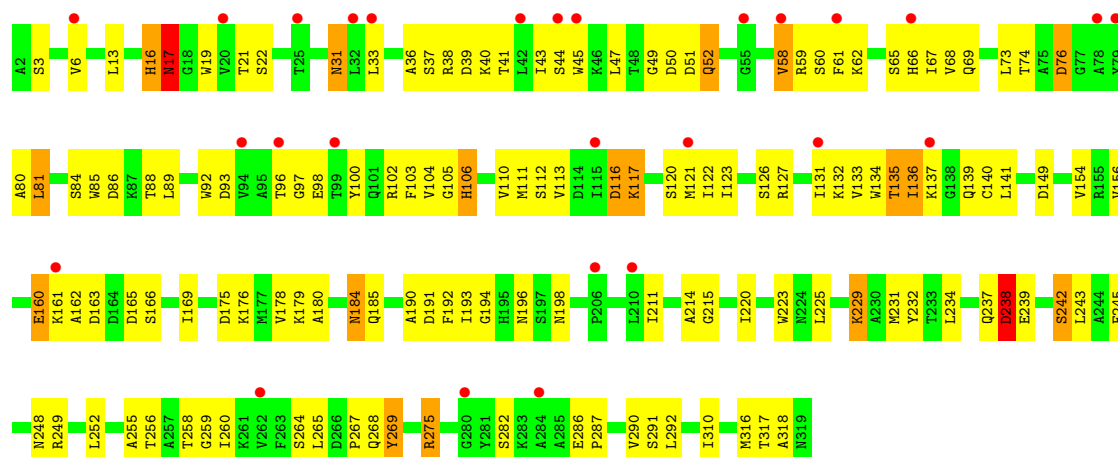
- Molecule 33: Ubiquitin-40S ribosomal protein S31



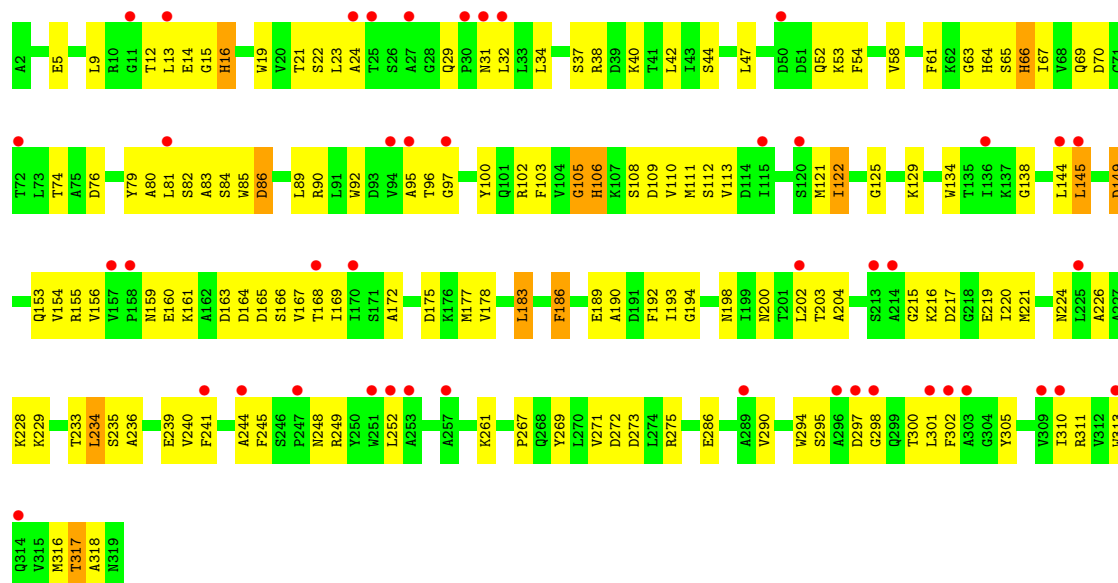
- Molecule 33: Ubiquitin-40S ribosomal protein S31



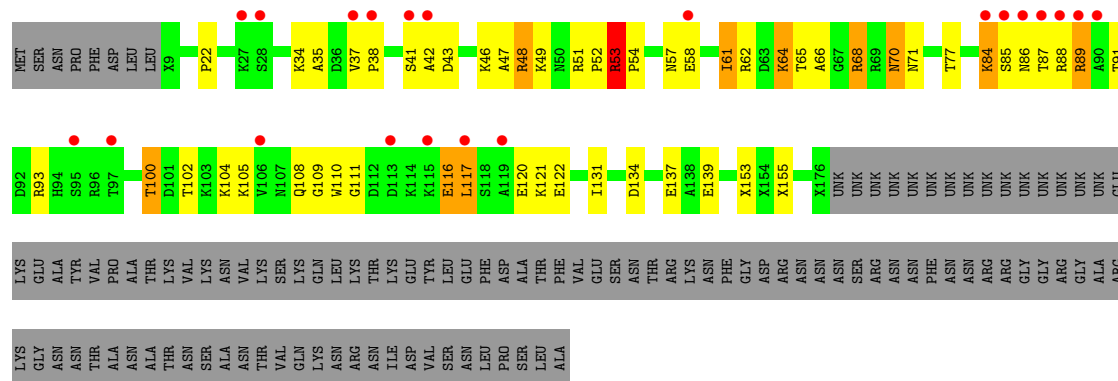
- Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein



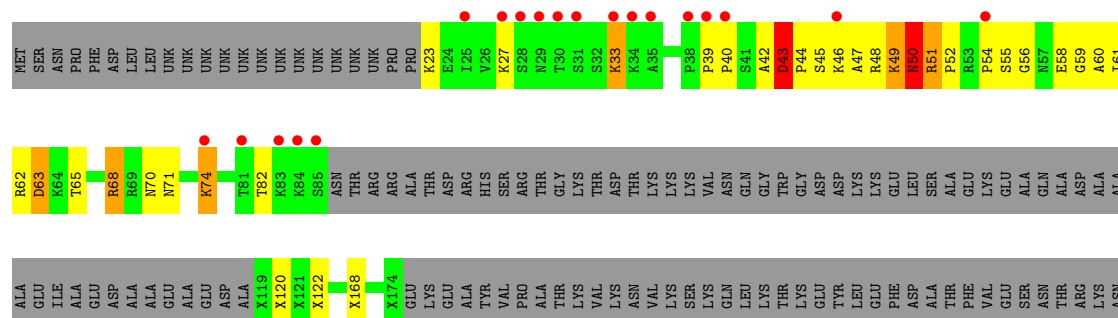
Chain sR: 



Chain SM: 



Chain sM: 



Chain 1:  %



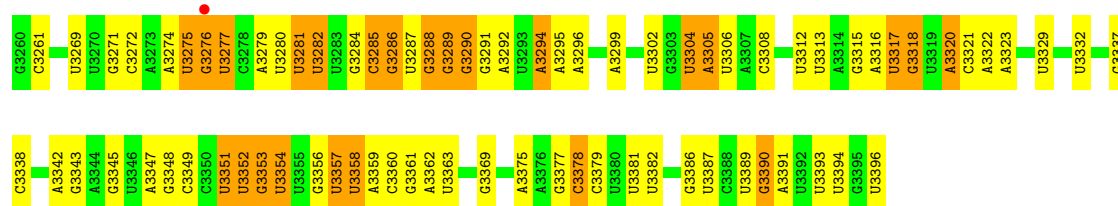


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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U2337 | G3238 | U1160 | A3163 | A3164 | A3165 | A3166 | A3167 | A3168 | A3169 | A3170 | A3171 | A3172 | A3173 | A3174 | U3175 | U3176 | U3177 | A3178 | U3179 | A3180 | A3181 | A3182 | A3183 | U3187 | C3272 | A3193 | A3194 | A3195 | U3196 | A3197 | U3198 | A3199 | C3204 | A3205 | U3206 | U3207 | G3208 | A3209 | U3287 | G3288 | G3289 | A3215 | G3216 | A3217 | A3218 | A3219 | A3220 | A3221 | A3222 | A3223 | A3224 | A3225 | A3226 | U3227 | A3228 | A3229 | A3232 | A3233 | A3234 | A3235 | A3236 | A3237 | A3238 | A3239 | A3240 | A3241 | A3242 | A3243 | A3244 | A3245 | A3246 | G3247 | G3248 | G3249 | G3250 | G3251 | A3252 | G3253 | G3254 | A3255 | A3256 | A3259 | U3260 | G3261 | A3262 | G3263 | G3264 | G3265 | G3266 | G3267 | G3268 | G3269 | G3270 | G3271 | C3272 | A3273 | A3274 | A3275 | A3276 | U3277 | C3278 | A3279 | A3280 | A3281 | A3282 | A3283 | A3284 | A3285 | A3286 | A3287 | A3288 | A3289 | A3290 | A3291 | A3292 | A3293 | A3294 | A3295 | A3296 | A3297 | A3298 | A3299 | A3300 | A3301 | A3302 | A3303 | A3304 | A3305 | A3306 | A3307 | G3308 | G3309 |
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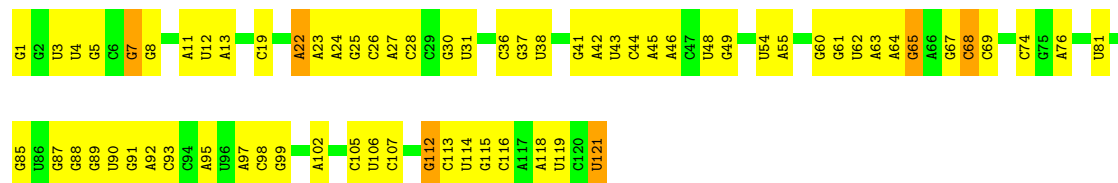




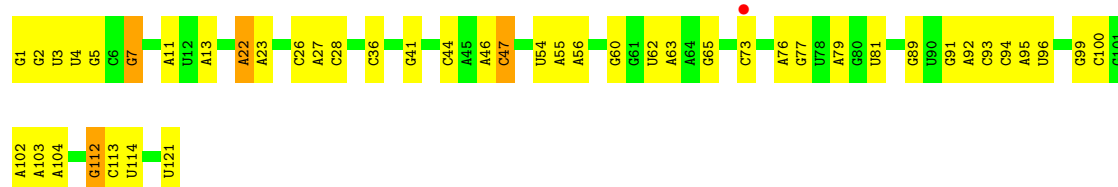
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| A3213 | A3139 | U3056 | U2966 | U2883 | U2722 | U2635 | A2637 | C2551 | G | G2414 | A2243 | G2157 |
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| A3215 | C3143 | C3060 | G2968 | U2885 | U2724 | A2643 | A2643 | C2553 | A | A2419 | G2246 | C2163 |
| C3217 | G3147 | G3061 | C2970 | U2886 | C2726 | G2644 | G2645 | C2554 | U | C2422 | G2249 | A2168 |
| A3218 | U3148 | G3062 | A2971 | U2887 | G2727 | G2645 |       | C2555 | A | U2423 | G2250 | G2169 |
| G3219 | C3063 | U3066 | C2977 | U2888 | U2728 |       |       | C2556 | C | U2424 | G2251 | U2170 |
| U3222 | A3150 | U3067 | U2980 | U2889 | C2737 | U2655 | U2655 | C2557 | A | A2425 | G2252 | G2171 |
| A3223 | G3151 | G3068 | U2981 | C2899 | A2738 | U2656 | A2657 | C2558 | C | G2426 | G2253 | A2172 |
| G3224 | U3152 | U3069 | U2982 | A2900 | G2739 | A2657 | A2657 | C2559 | U | U2427 | U2254 | U2173 |
| A3226 | C3153 | C3070 | C2983 | G2901 | U2740 | A2658 | G2660 | C2560 | G | U2428 | A2255 | G2174 |
| G3229 | U3154 | A3072 | U2984 | U2904 | U2741 | U2659 |       | C2561 | A | G2429 | A2256 |       |
| C3230 | C3073 | G3074 | U2985 | U2905 | A2742 | U2660 |       | C2562 | C | U2430 | G2257 | G2177 |
| U3231 | U3155 | G3075 | U2986 | C2906 | A2743 | C2661 |       | C2563 | U | U2431 | A2258 | A2178 |
| G3232 | G3156 | U3078 | A2987 | U2907 | A2744 | U2662 |       | C2564 | C | U2432 | U2259 | G2179 |
| C3233 | U3157 | U3079 | U2988 | U2908 | U2745 | U2663 |       | C2565 | A | U2433 | G2260 | G2180 |
| A3234 | U3160 | G3080 | G2989 | C2909 | A2746 | C2664 |       | C2566 | C | G2440 | A2261 | C2181 |
| C3235 | C3161 | U3081 | U2990 | C2910 | A2747 | U2665 |       | C2567 | U | U2441 | A2262 |       |
| A3236 | C3162 | G3082 | A2991 | C2911 | U2748 | U2666 |       | C2568 | C | A2442 | G2263 | G2187 |
| U3237 | A3163 | A3083 | U2992 | C2912 | G2749 | C2667 |       | C2569 | A | G2443 | U2266 | A2188 |
| G3238 | C3164 | A3084 | G2993 | C2913 | G2750 | A2667 |       | C2570 | C | C2444 | U2267 | U2189 |
| C3239 | A3165 | A3087 | U2996 | G2918 | G2751 |       |       | C2571 | U | A2445 | G2268 |       |
| G3240 | A3168 | U2997 | G2997 | U2923 | U2752 | C2672 |       | C2572 | C | U2446 | U2269 | C2192 |
| A3241 | U3169 | A3091 | A3006 | C2927 | G2753 | A2673 |       | C2573 | U | A2447 | U2193 | U2193 |
| G3242 | C3170 | C3092 | U3007 | C2928 | C2755 | A2674 |       | C2574 | C | G2448 | A2270 | G2194 |
| A3243 | A3171 | G3102 | A3008 | C2931 | C2756 | A2675 |       | C2575 | A | U2449 | A2271 |       |
| G3244 | C3172 |       | G3009 | U2932 | G2761 | A2676 |       | C2576 | C | G2450 | G2272 | C2197 |
| A3245 | A3173 | A3106 | U3010 | A2933 | U2762 | A2677 |       | C2577 | U | G2451 | G2273 | A2198 |
| G3246 | U3174 | U3107 | A3012 | A2934 | U2763 | A2678 |       | C2578 | C | A2452 | G2276 |       |
| C3247 | C3175 | U3013 | U3013 | U2935 | A2764 |       |       | C2579 | A | U     | G2277 | G2201 |
| G3248 | G3176 | U3014 | U3014 | A2936 | U2765 |       |       | C2580 | C | G     | A2279 | U2205 |
| U3251 | A3177 | C3110 | G3015 | G2937 | C2766 |       |       | C2581 | A | A     | G2280 | G2206 |
| G3252 | C3178 | U3111 | G3016 | U2938 | U2767 |       |       | C2582 | C | G     | A2281 | A2207 |
| U3258 | A3180 | G3112 | A3017 | C2939 | U2768 |       |       | C2583 | A | A     | G2287 | U2208 |
| C3259 | C3181 | A3114 | C3018 | A2940 | A2769 |       |       | C2584 | U | A     | G2288 | G2210 |
|       |       |       |       |       | G2770 |       |       | C2585 | C | U     | U2289 | U2211 |
|       |       |       |       |       | U2771 |       |       | C2586 | A | A     | C2290 | C2212 |
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|       |       |       |       |       |       |       |       | C2589 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2590 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2591 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2592 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2593 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2594 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2595 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2596 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2597 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2598 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2599 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2600 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2601 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2602 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2603 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2604 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2605 | C | G     |       |       |
|       |       |       |       |       |       |       |       | C2606 | A | A     |       |       |
|       |       |       |       |       |       |       |       | C2607 | C | G     |       |       |



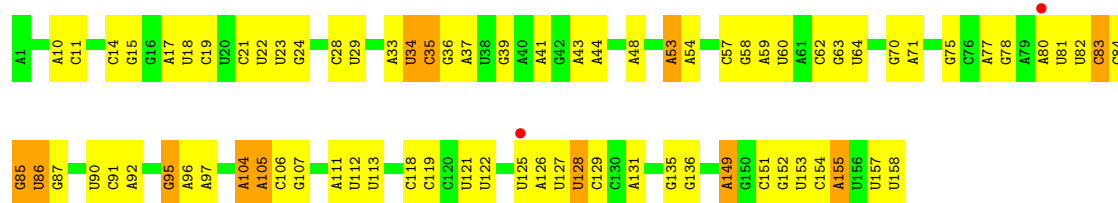
• Molecule 37: 5S ribosomal RNA



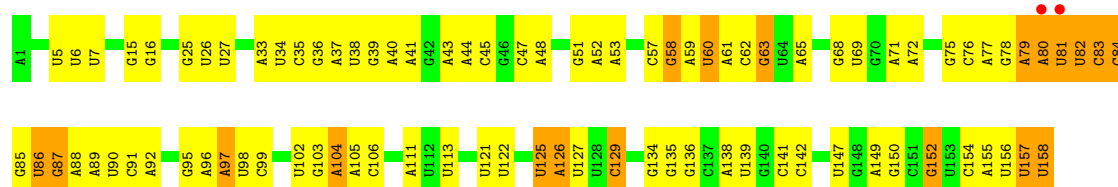
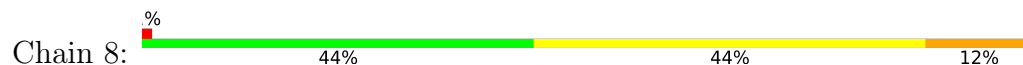
• Molecule 37: 5S ribosomal RNA



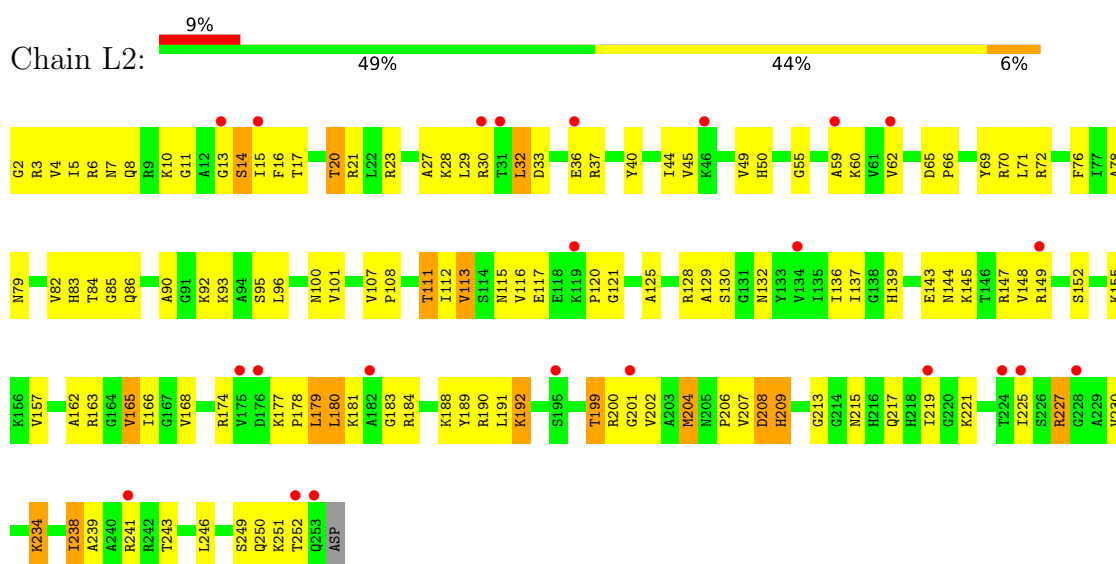
• Molecule 38: 5.8S ribosomal RNA



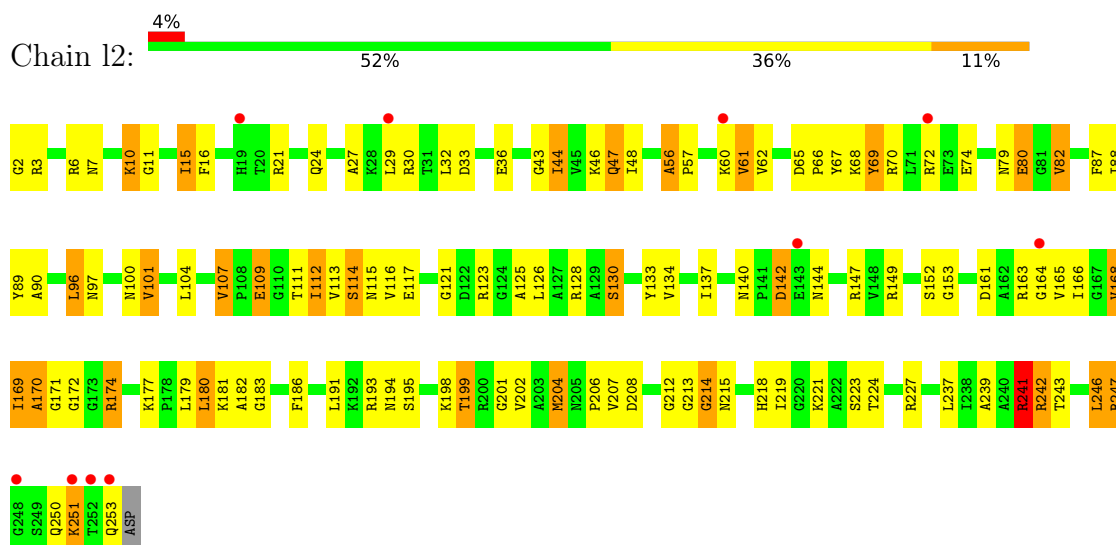
• Molecule 38: 5.8S ribosomal RNA



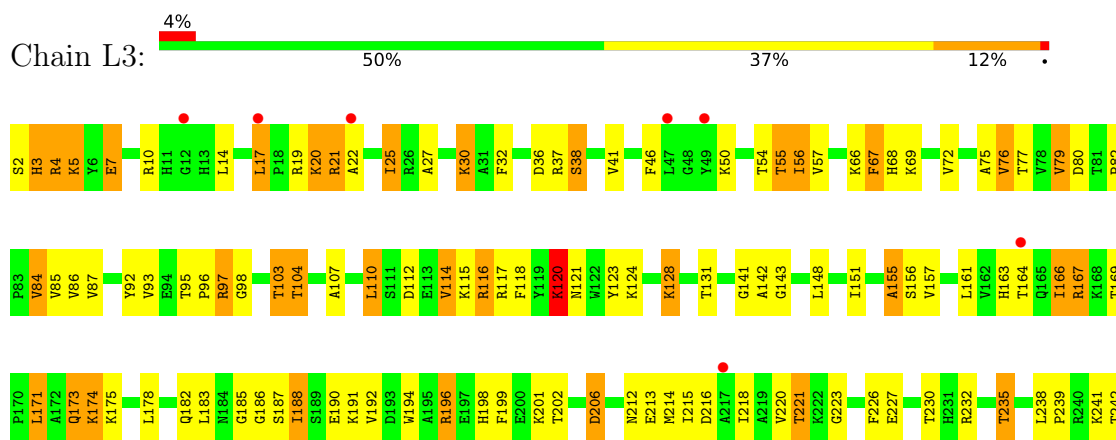
• Molecule 39: 60S ribosomal protein L2-A

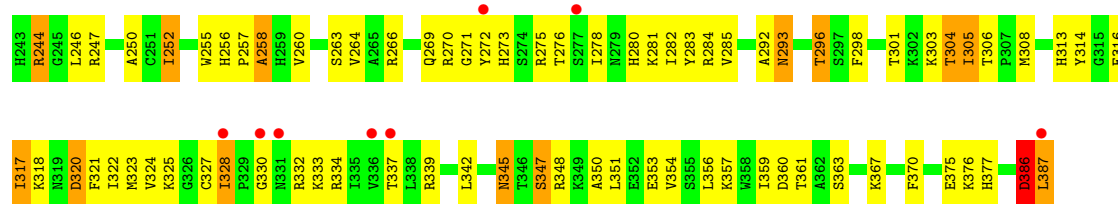


• Molecule 39: 60S ribosomal protein L2-A

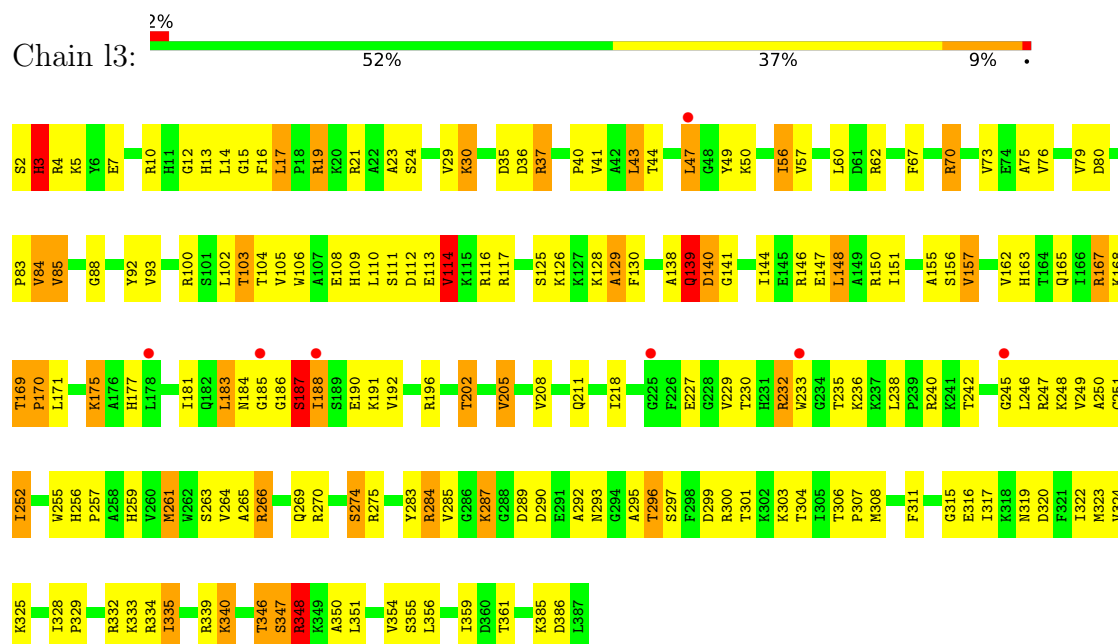


• Molecule 40: 60S ribosomal protein L3

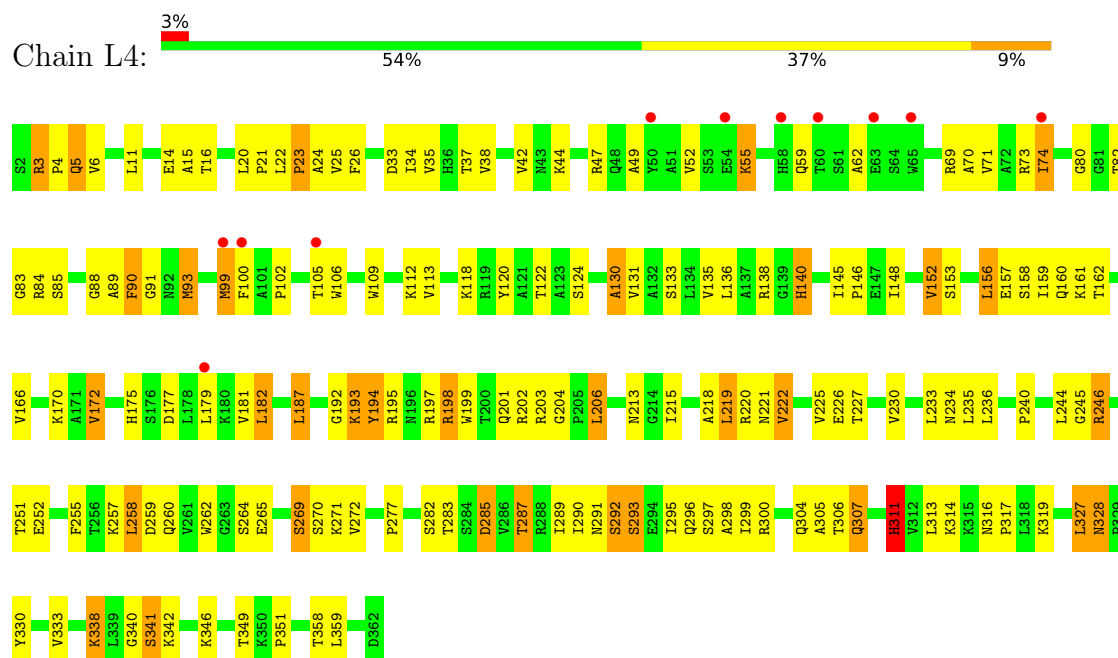




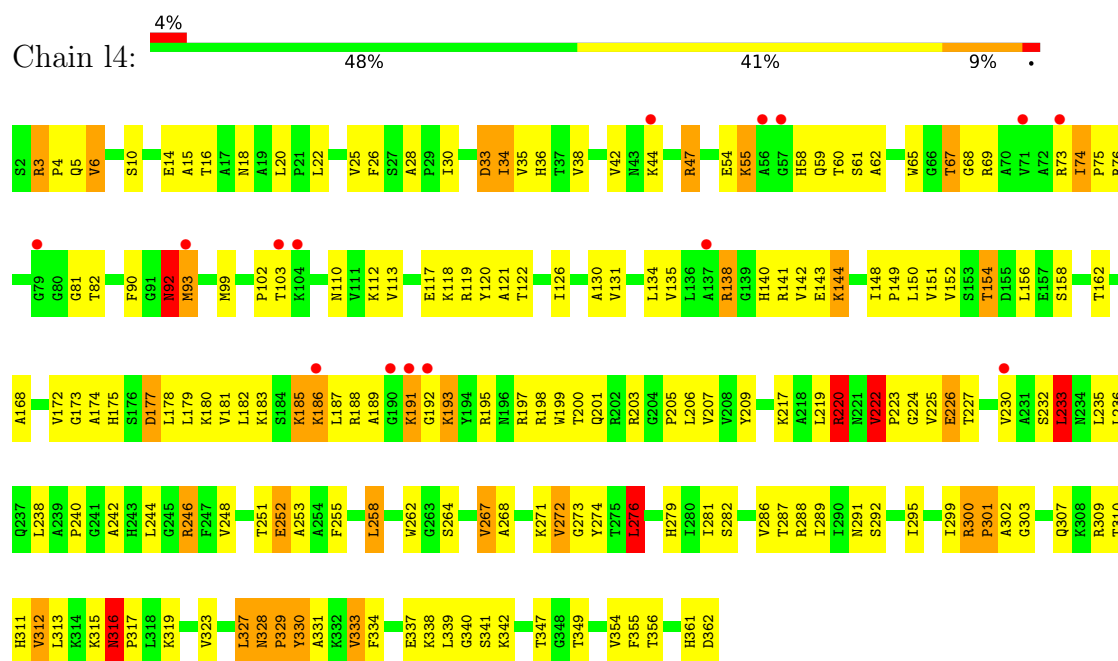
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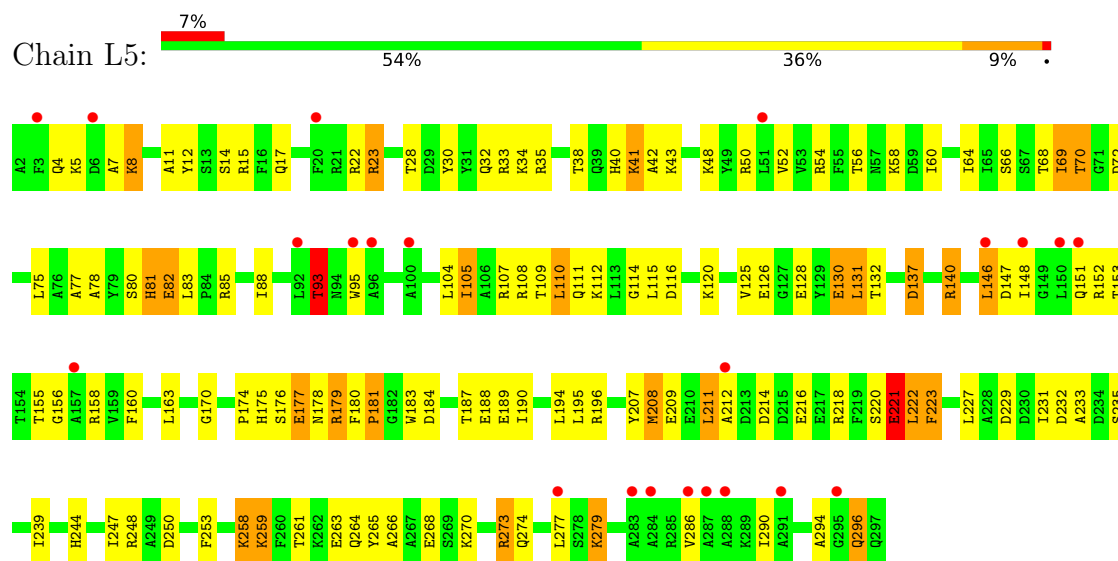
• Molecule 41: 60S ribosomal protein L4-A



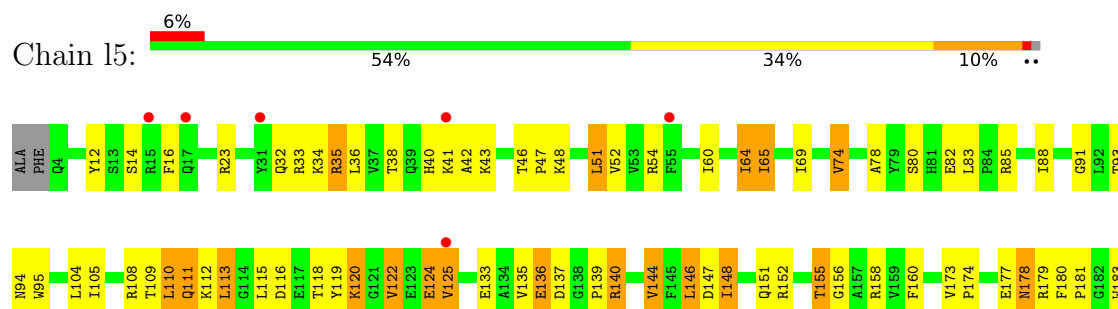
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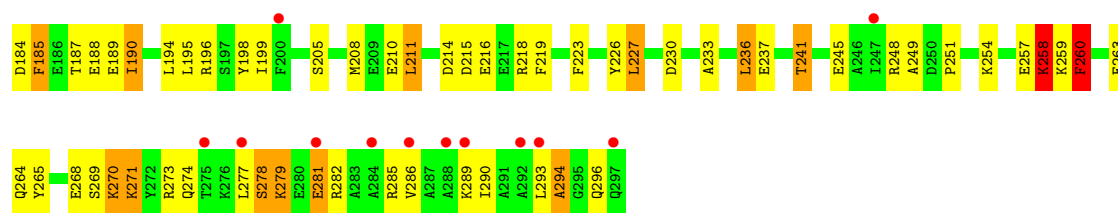


• Molecule 42: 60S ribosomal protein L5

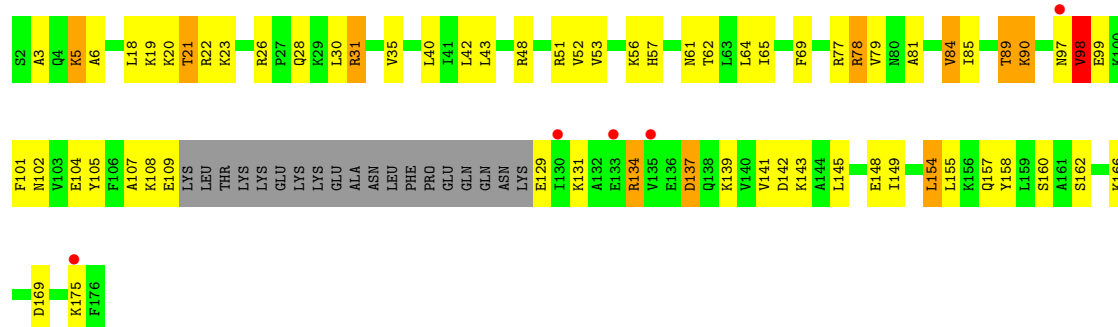


• Molecule 42: 60S ribosomal protein L5

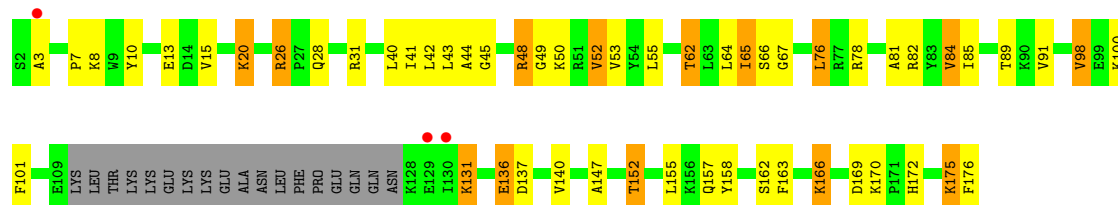




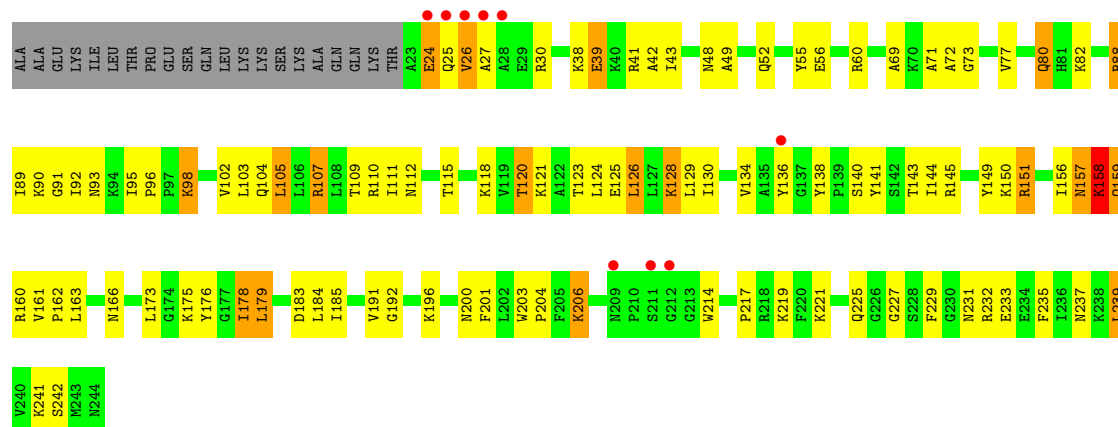
• Molecule 43: 60S ribosomal protein L6-A



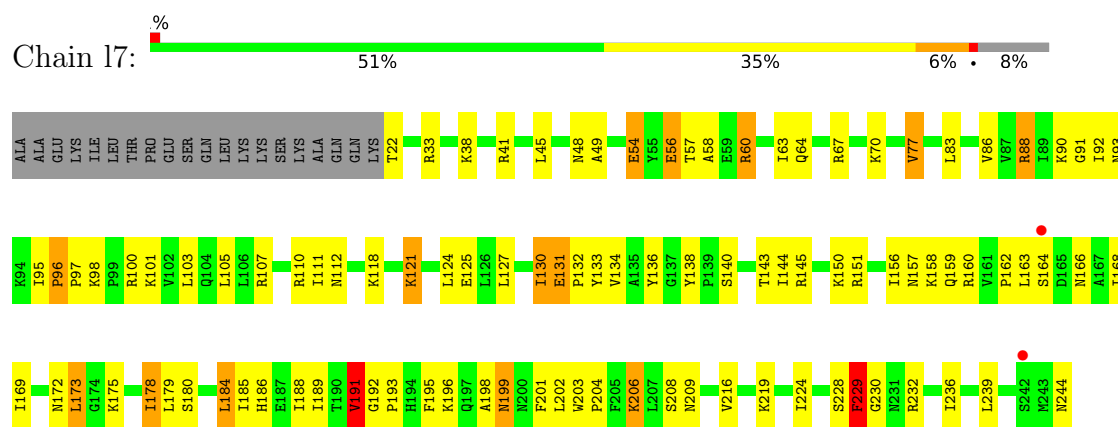
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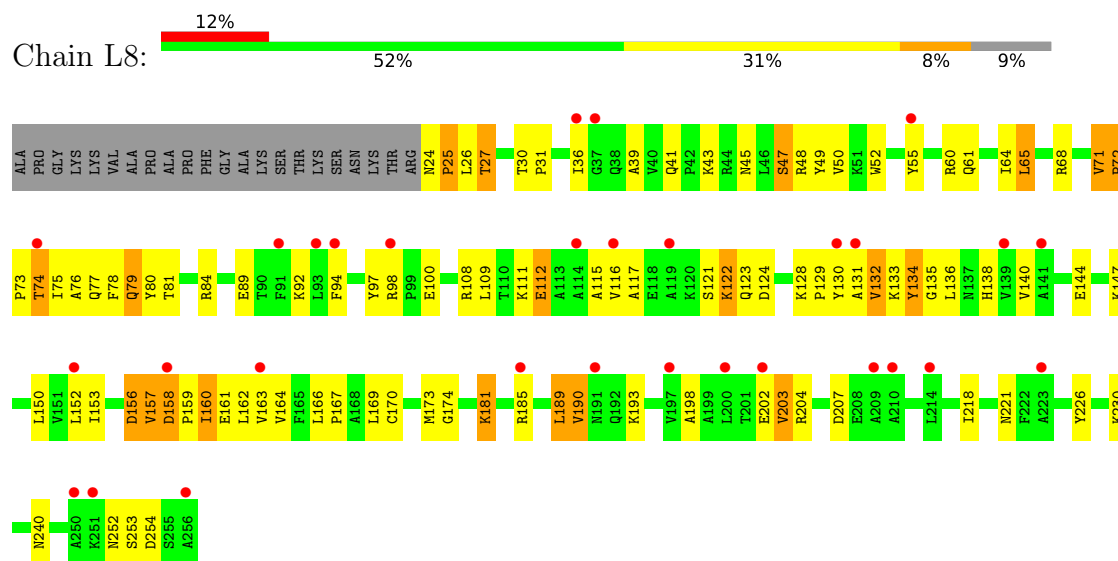
• Molecule 44: 60S ribosomal protein L7-A



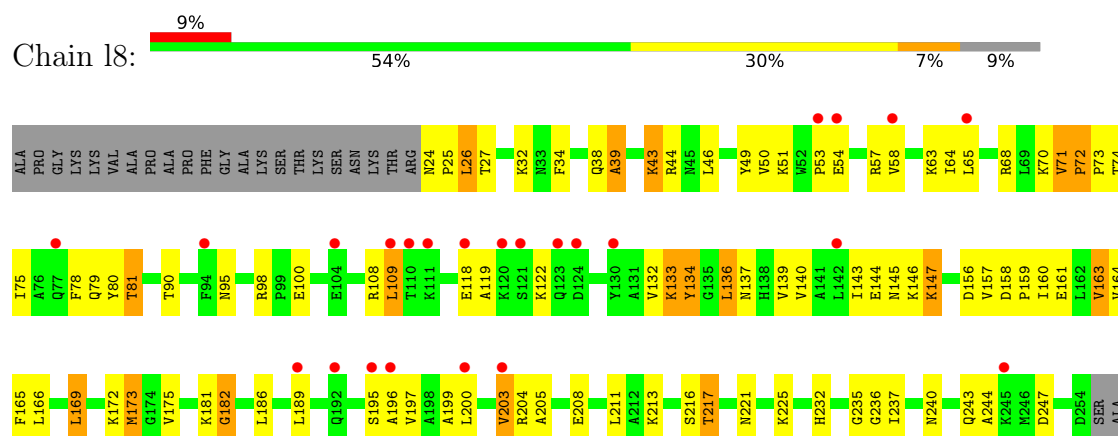
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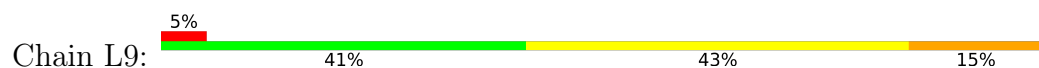
• Molecule 45: 60S ribosomal protein L8-A

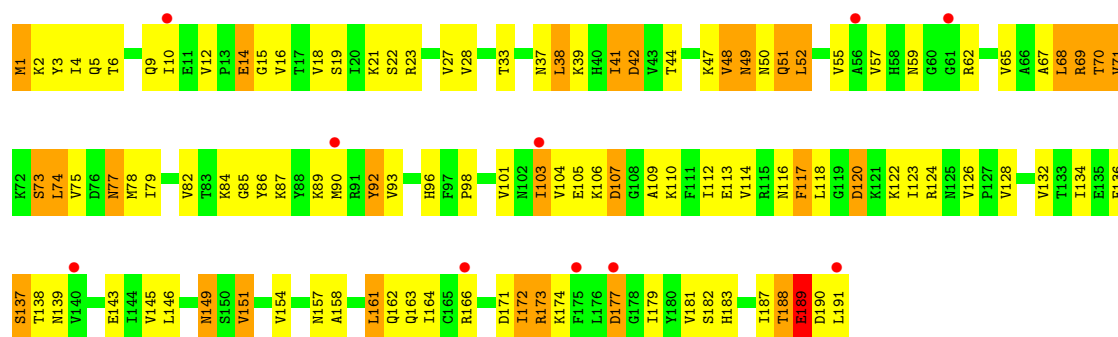


• Molecule 45: 60S ribosomal protein L8-A



• Molecule 46: 60S ribosomal protein L9-A

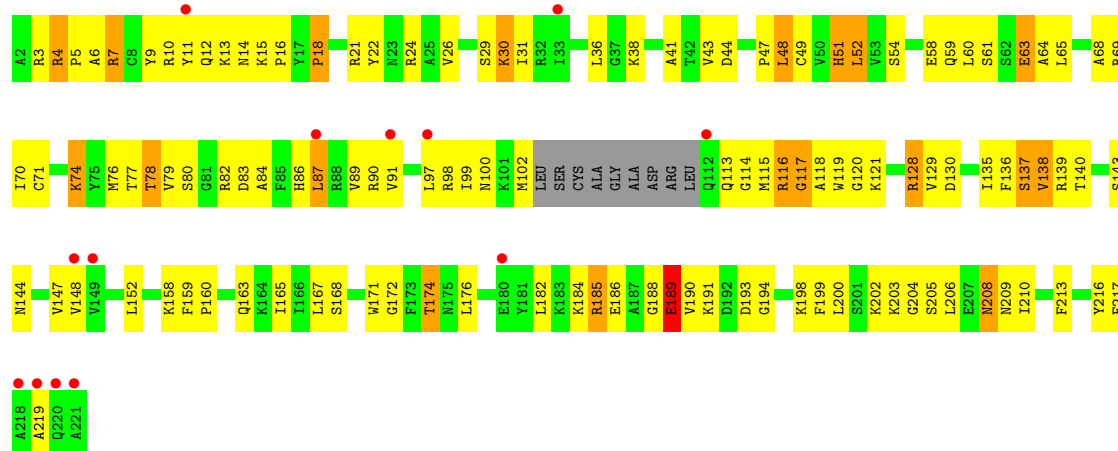
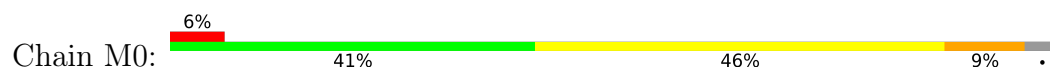




• Molecule 46: 60S ribosomal protein L9-A

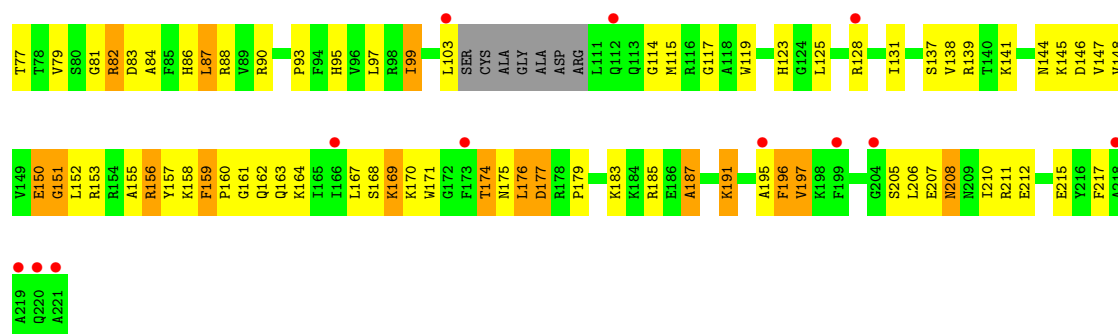


• Molecule 47: 60S ribosomal protein L10

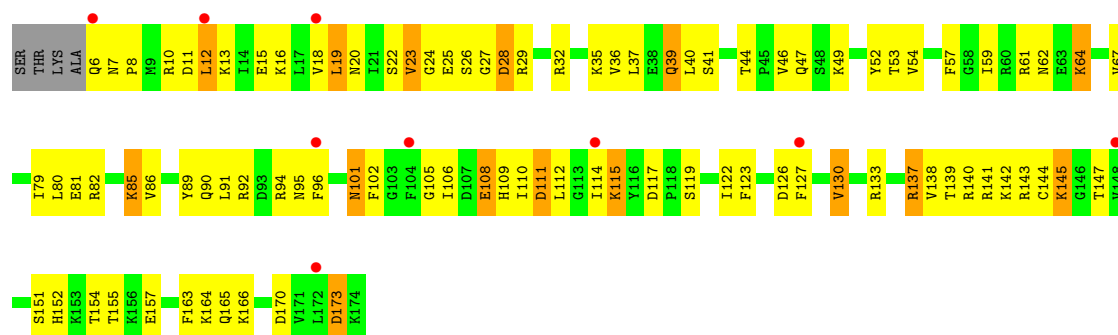


• Molecule 47: 60S ribosomal protein L10

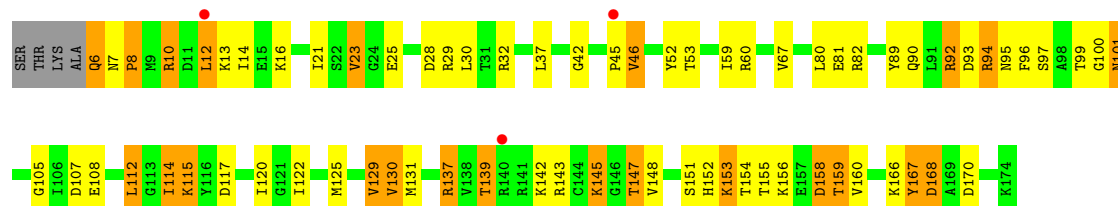




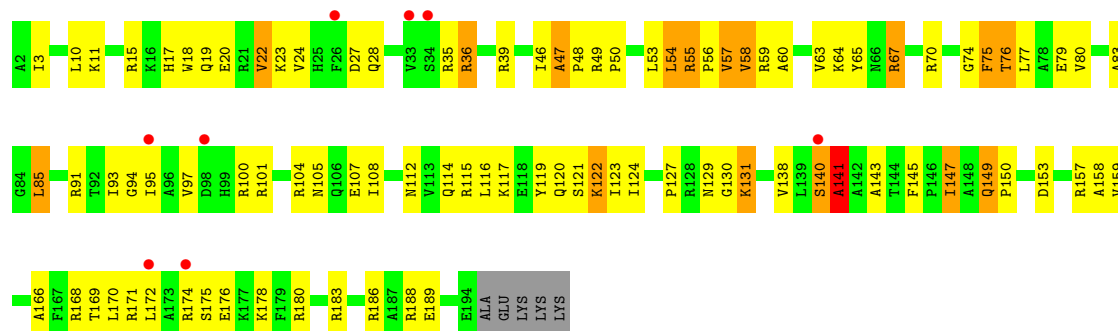
• Molecule 48: 60S ribosomal protein L11-B



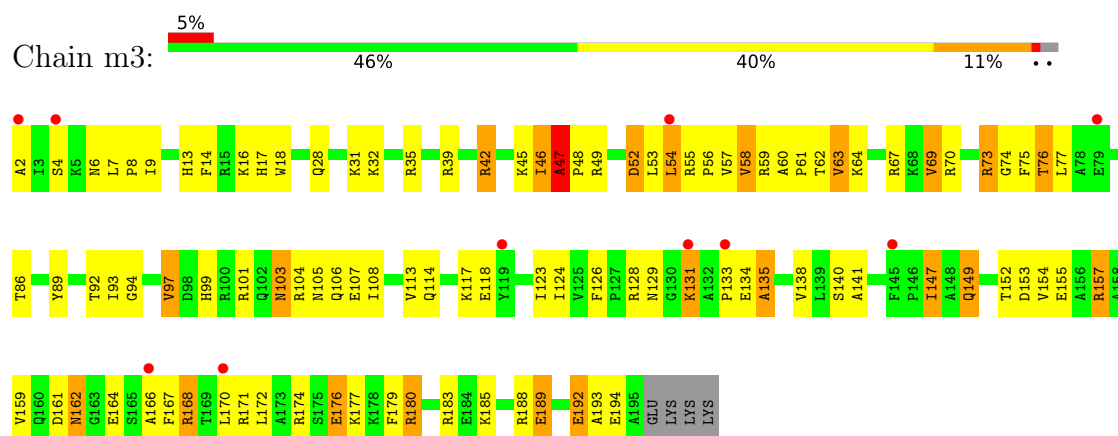
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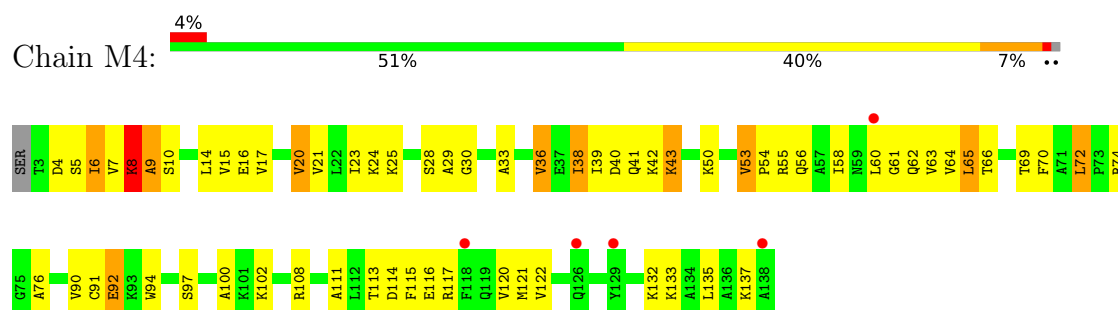
• Molecule 49: 60S ribosomal protein L13-A



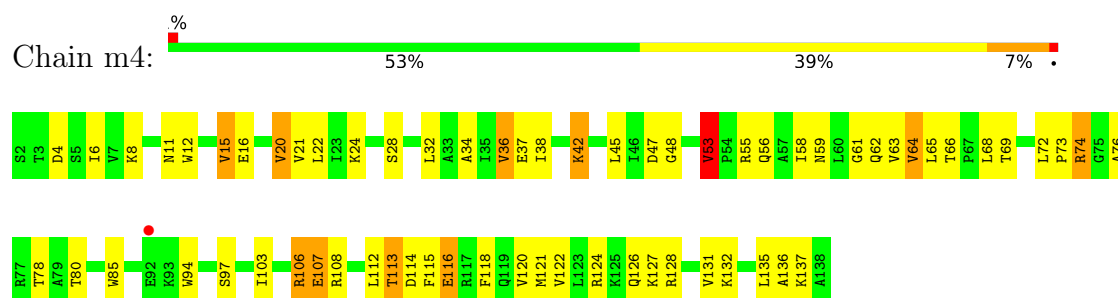
- Molecule 49: 60S ribosomal protein L13-A



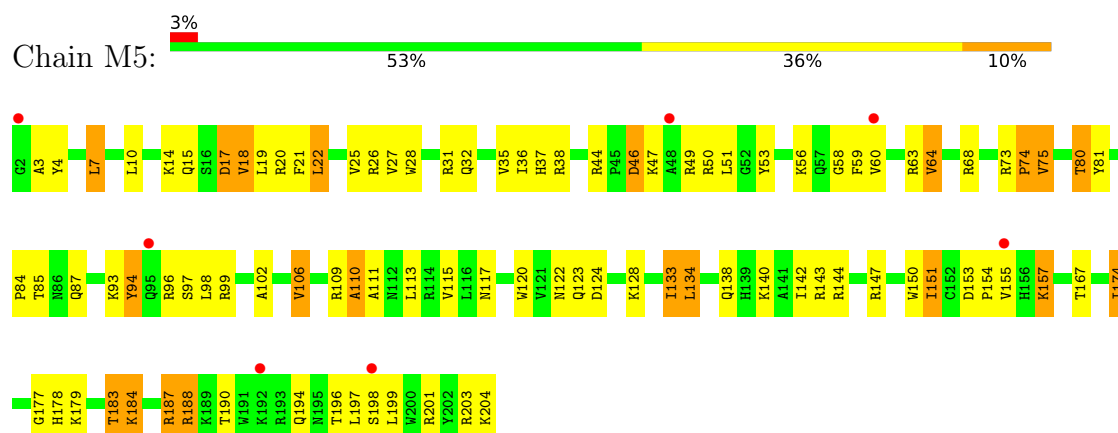
- Molecule 50: 60S ribosomal protein L14-A



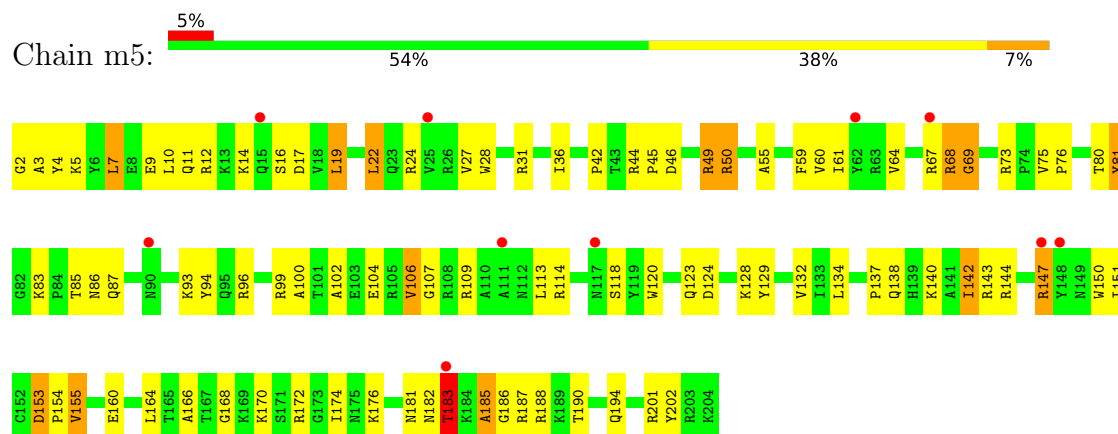
- Molecule 50: 60S ribosomal protein L14-A



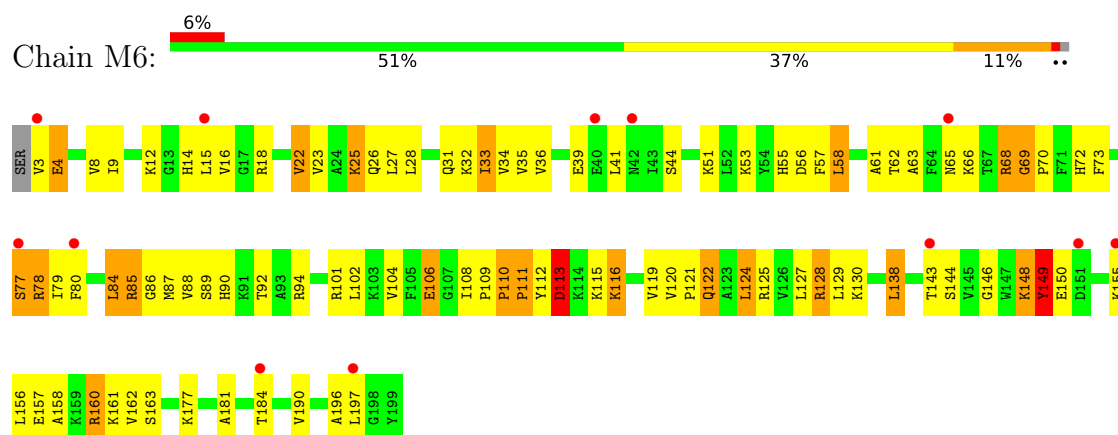
- Molecule 51: 60S ribosomal protein L15-A



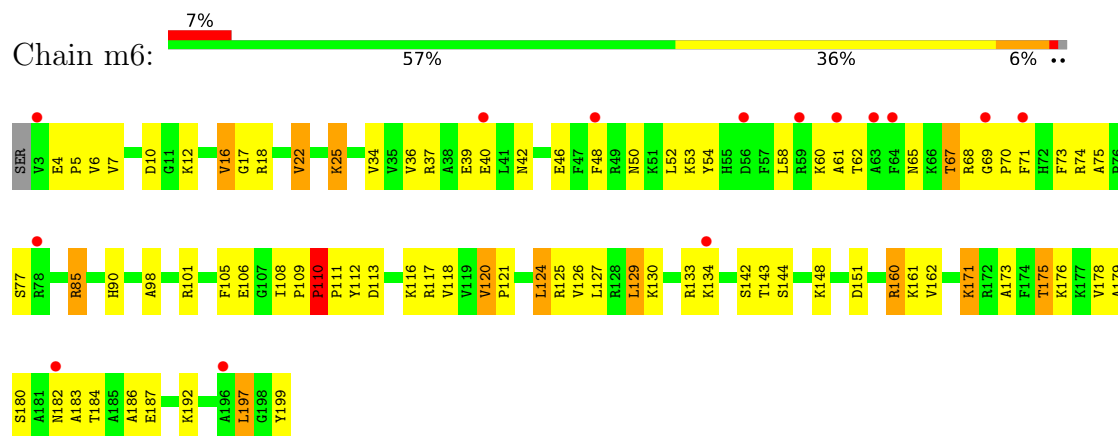
- Molecule 51: 60S ribosomal protein L15-A



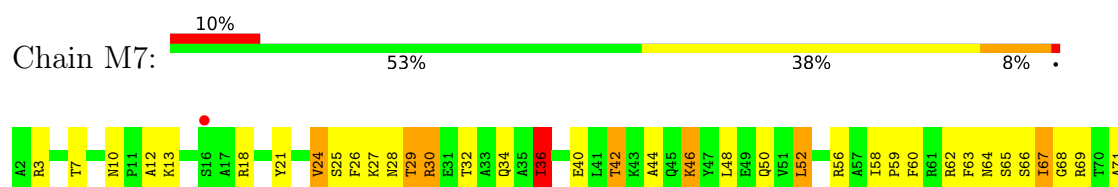
- Molecule 52: 60S ribosomal protein L16-A

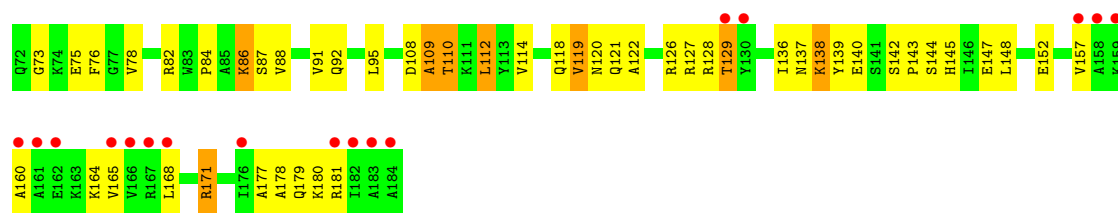


- Molecule 52: 60S ribosomal protein L16-A

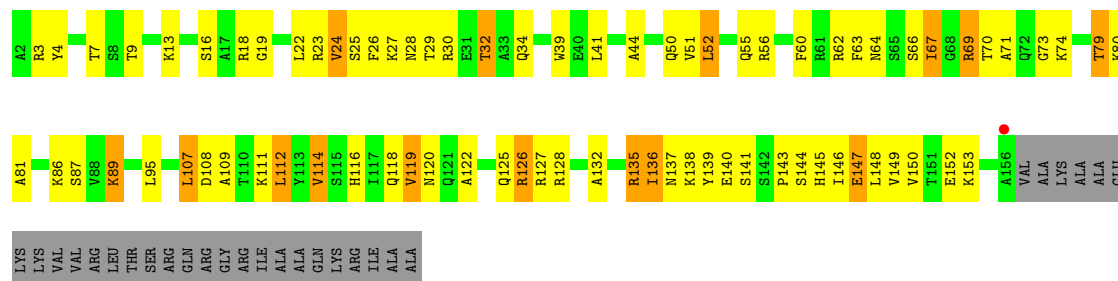
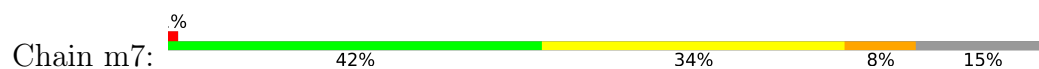


- Molecule 53: 60S ribosomal protein L17-A

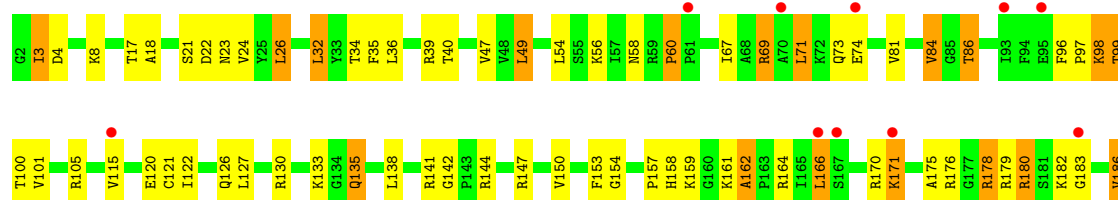




• Molecule 53: 60S ribosomal protein L17-A



• Molecule 54: 60S ribosomal protein L18-A

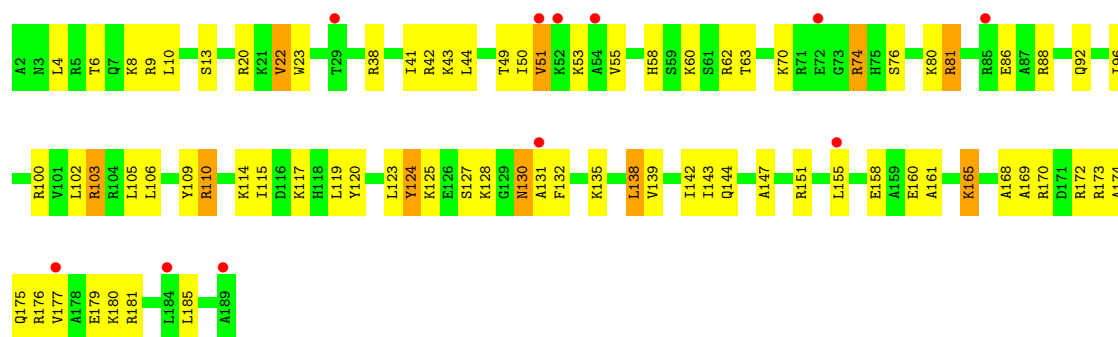


• Molecule 54: 60S ribosomal protein L18-A

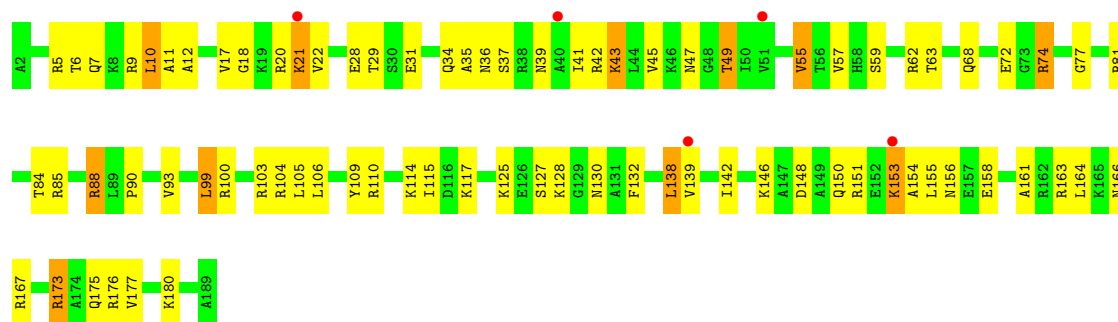


• Molecule 55: 60S ribosomal protein L19-A

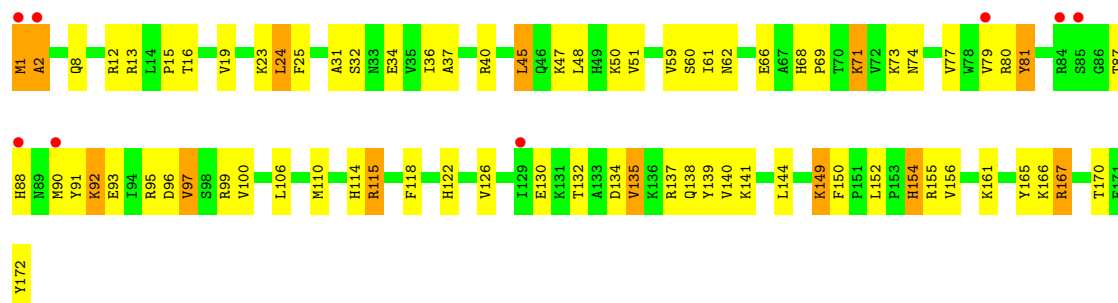




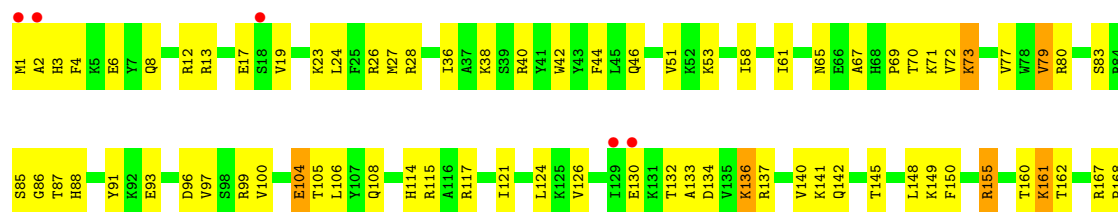
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• Molecule 56: 60S ribosomal protein L20-A

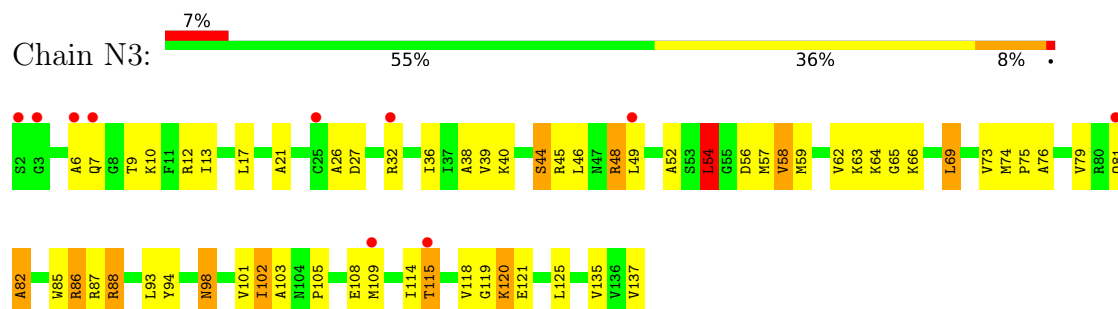


• Molecule 56: 60S ribosomal protein L20-A

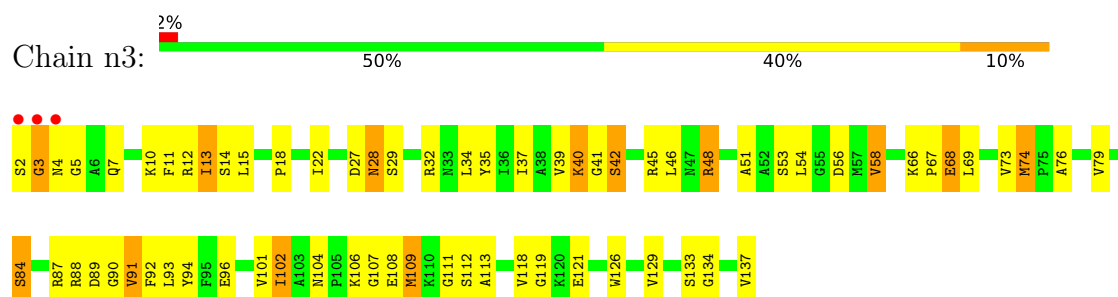




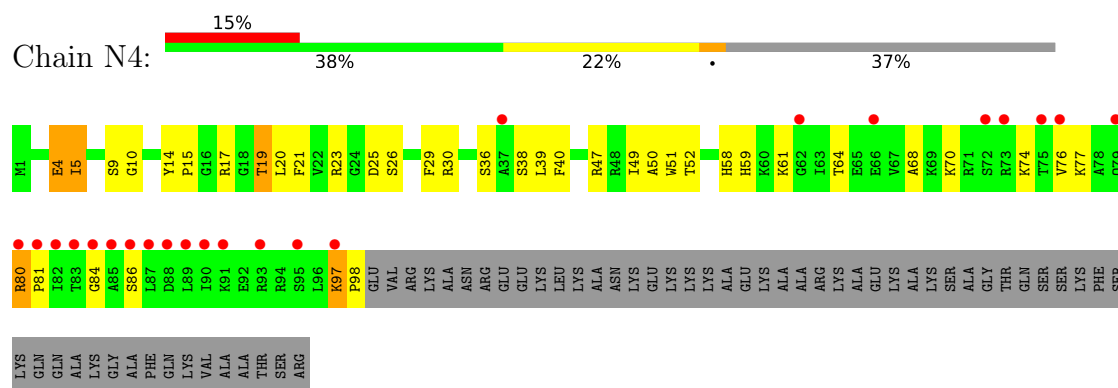
- Molecule 59: 60S ribosomal protein L23-A



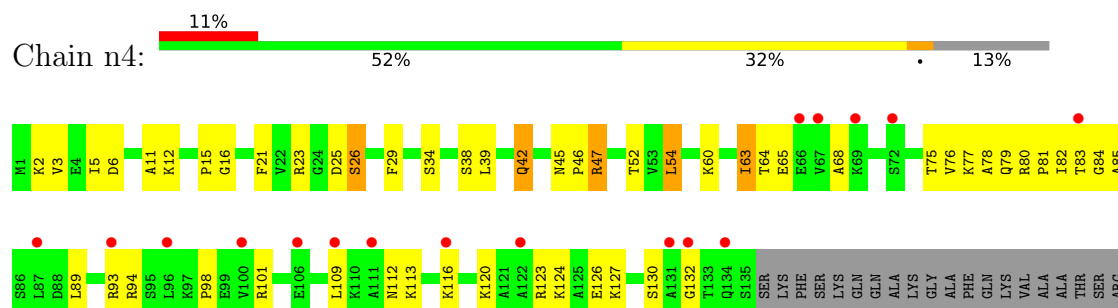
- Molecule 59: 60S ribosomal protein L23-A



- Molecule 60: 60S ribosomal protein L24-A



- Molecule 60: 60S ribosomal protein L24-A

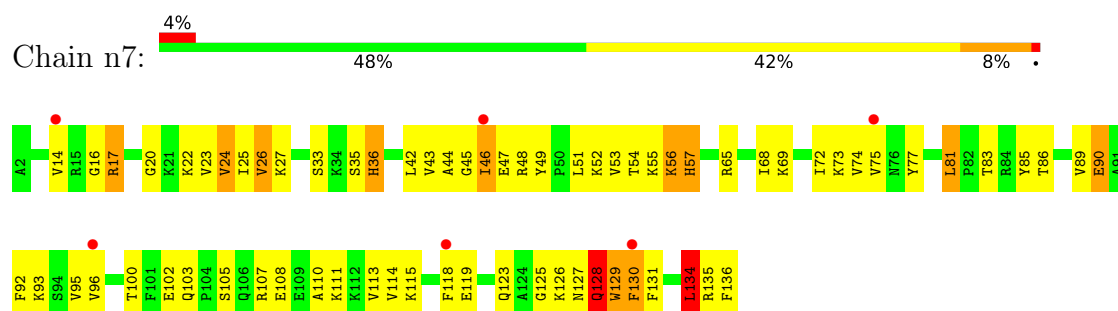


- Molecule 61: 60S ribosomal protein L25





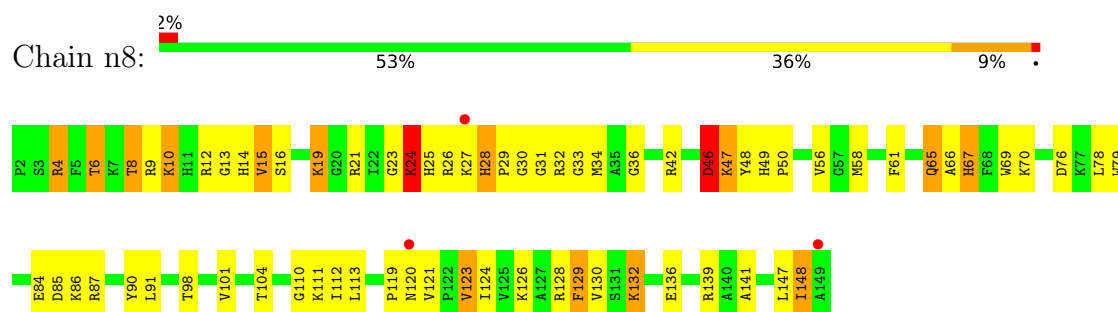
- Molecule 63: 60S ribosomal protein L27-A



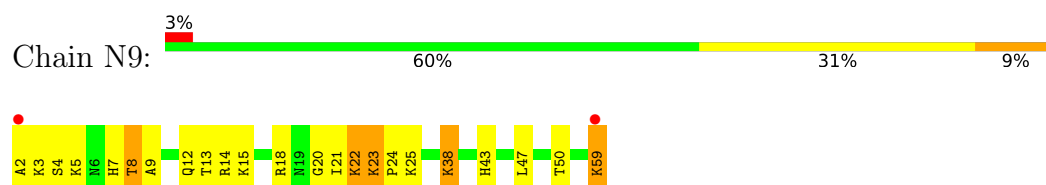
- Molecule 64: 60S ribosomal protein L28



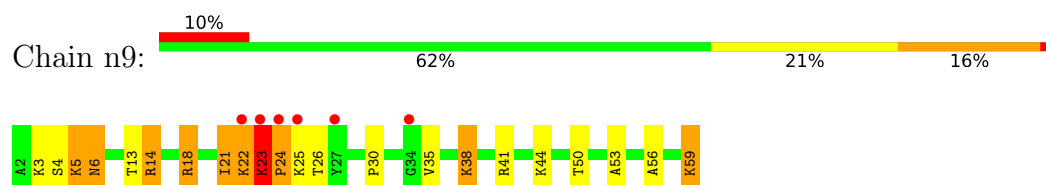
- Molecule 64: 60S ribosomal protein L28



- Molecule 65: 60S ribosomal protein L29

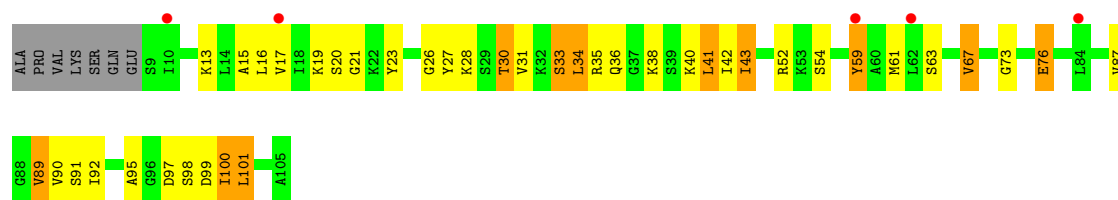


- Molecule 65: 60S ribosomal protein L29

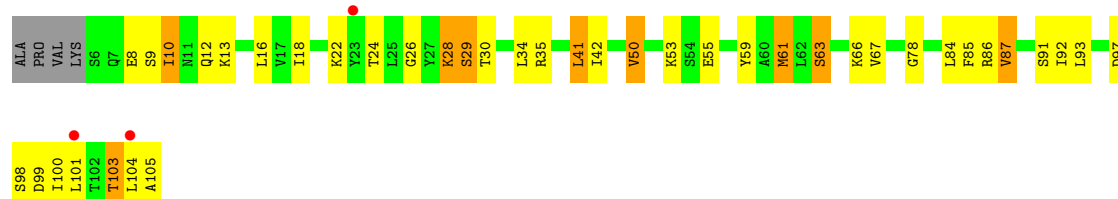


- Molecule 66: 60S ribosomal protein L30

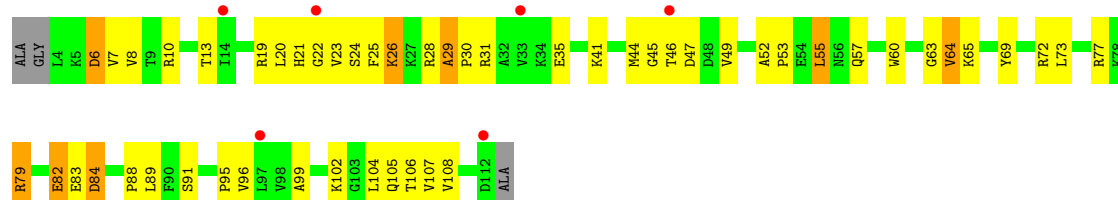




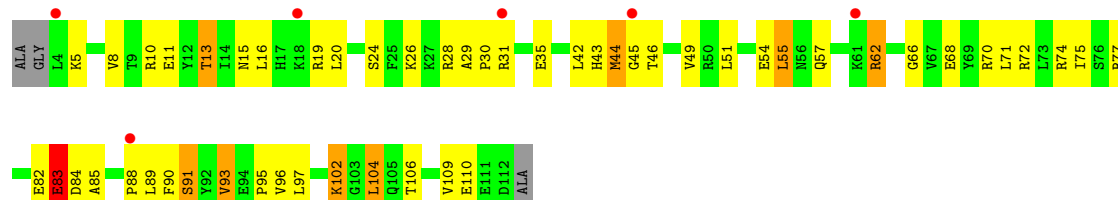
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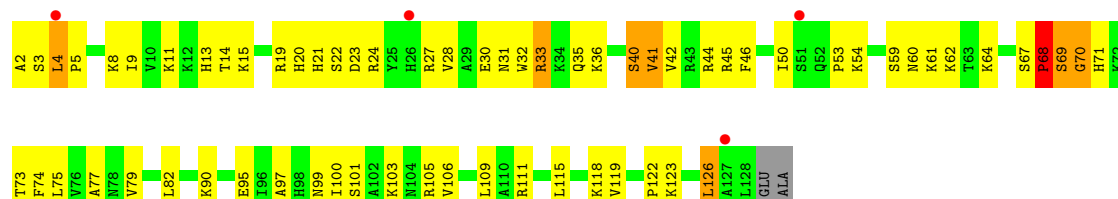
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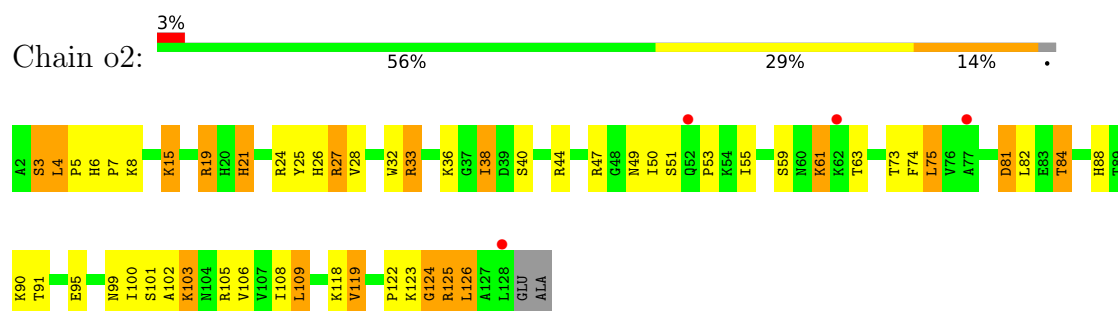
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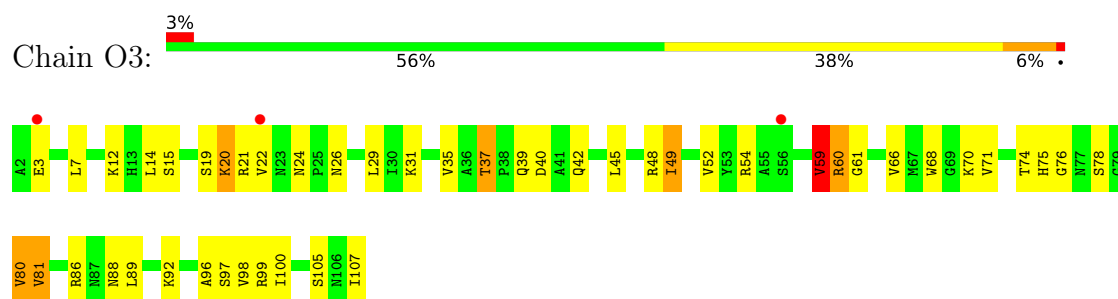
• Molecule 68: 60S ribosomal protein L32



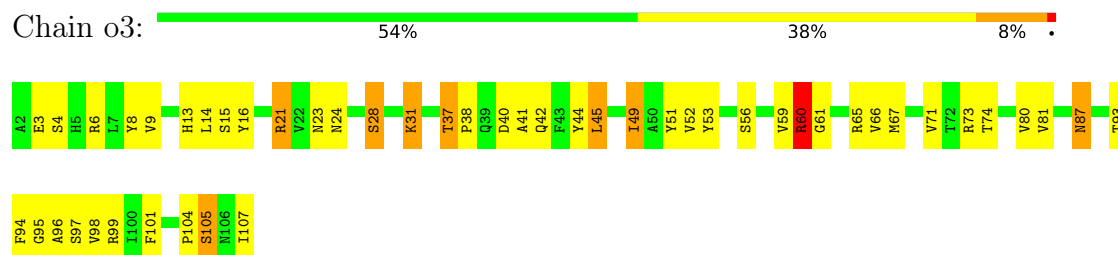
- Molecule 68: 60S ribosomal protein L32



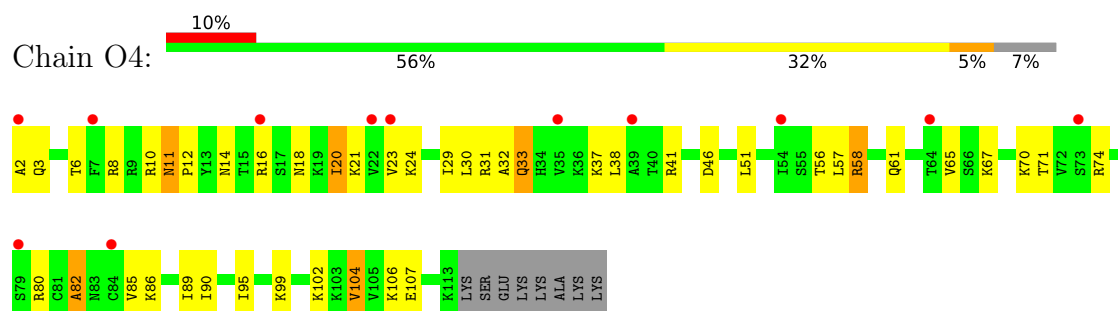
- Molecule 69: 60S ribosomal protein L33-A



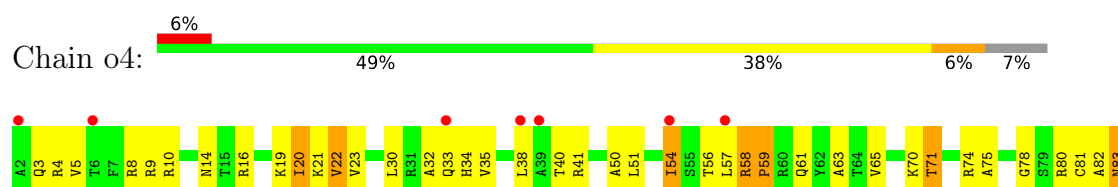
- Molecule 69: 60S ribosomal protein L33-A

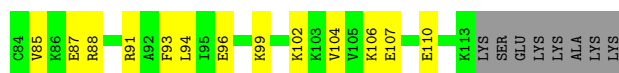


- Molecule 70: 60S ribosomal protein L34-A



- Molecule 70: 60S ribosomal protein L34-A

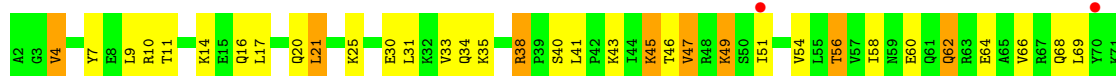




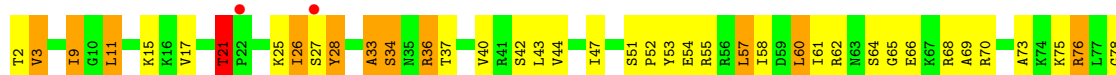
- Molecule 71: 60S ribosomal protein L35-A



- Molecule 71: 60S ribosomal protein L35-A



- Molecule 72: 60S ribosomal protein L36-A

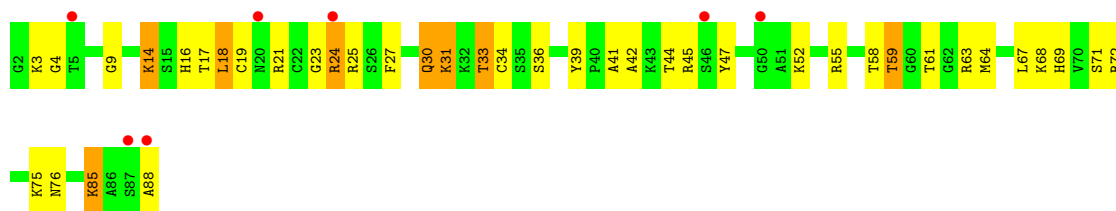


- Molecule 72: 60S ribosomal protein L36-A

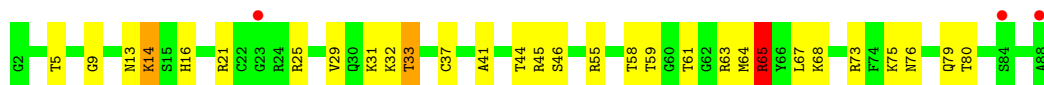


- Molecule 73: 60S ribosomal protein L37-A

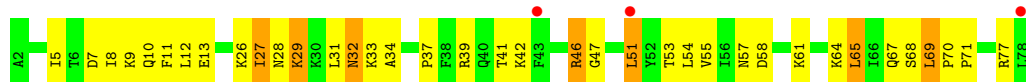




- Molecule 73: 60S ribosomal protein L37-A



- Molecule 74: 60S ribosomal protein L38



- Molecule 74: 60S ribosomal protein L38



- Molecule 75: 60S ribosomal protein L39

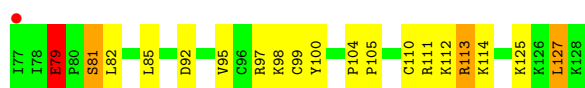


- Molecule 75: 60S ribosomal protein L39



- Molecule 76: Ubiquitin-60S ribosomal protein L40

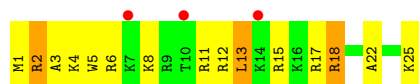




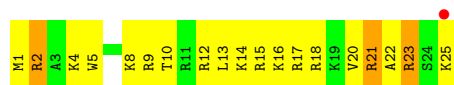
- Molecule 76: Ubiquitin-60S ribosomal protein L40



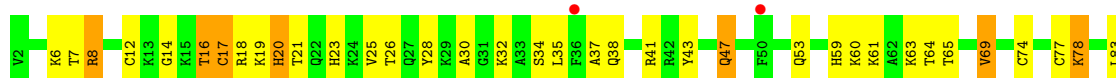
- Molecule 77: 60S ribosomal protein L41-A



- Molecule 77: 60S ribosomal protein L41-A



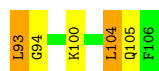
- Molecule 78: 60S ribosomal protein L42-A



- Molecule 78: 60S ribosomal protein L42-A

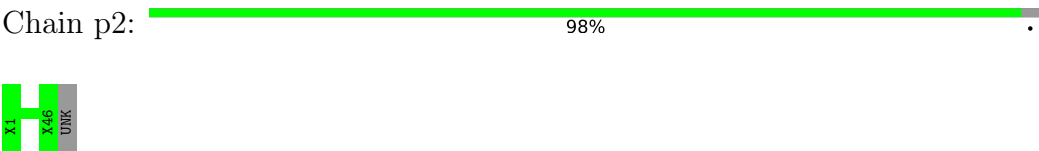


- Molecule 79: 60S ribosomal protein L43-A

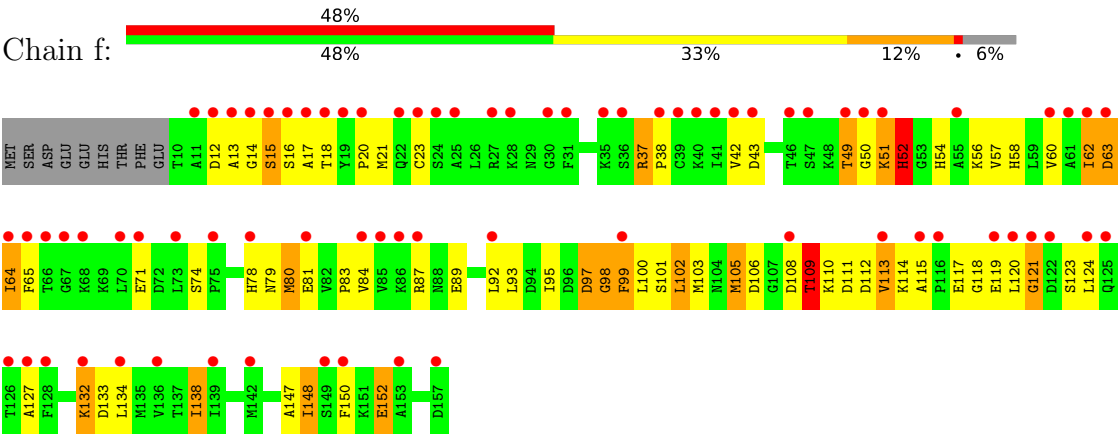




- Molecule 82: 60S ribosomal protein P1 alpha/P2 beta



- Molecule 83: Eukaryotic translation initiation factor 5A-1



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 435.58Å 287.33Å 303.82Å<br>90.00° 98.95° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 99.53 – 3.30<br>99.53 – 3.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (99.53-3.30)<br>99.9 (99.53-3.30)                     | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.59                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.34 (at 3.33Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.251 , 0.310<br>0.256 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.176                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 61.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 404292                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 79.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, MG, ZN, SPS, CH, OHX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | 2     | 0.21         | 0/42467     | 0.39        | 2/66169 (0.0%) |
| 1   | 6     | 0.24         | 0/42790     | 0.42        | 0/66673        |
| 2   | S0    | 0.39         | 0/1617      | 0.89        | 7/2215 (0.3%)  |
| 2   | s0    | 0.40         | 0/1623      | 0.90        | 2/2222 (0.1%)  |
| 3   | S1    | 0.32         | 0/1735      | 0.80        | 3/2335 (0.1%)  |
| 3   | s1    | 0.41         | 0/1748      | 0.87        | 7/2352 (0.3%)  |
| 4   | S2    | 0.42         | 0/1665      | 0.90        | 6/2263 (0.3%)  |
| 4   | s2    | 0.45         | 0/1665      | 0.94        | 6/2263 (0.3%)  |
| 5   | S3    | 0.38         | 0/1759      | 0.84        | 4/2368 (0.2%)  |
| 5   | s3    | 0.36         | 0/1759      | 0.87        | 6/2368 (0.3%)  |
| 6   | S4    | 0.37         | 0/2109      | 0.87        | 4/2839 (0.1%)  |
| 6   | s4    | 0.43         | 0/2109      | 0.86        | 4/2839 (0.1%)  |
| 7   | S5    | 0.35         | 0/1629      | 0.85        | 2/2202 (0.1%)  |
| 7   | s5    | 0.36         | 0/1629      | 0.83        | 4/2202 (0.2%)  |
| 8   | S6    | 0.35         | 0/1823      | 0.79        | 0/2439         |
| 8   | s6    | 0.40         | 0/1779      | 0.83        | 0/2379         |
| 9   | S7    | 0.36         | 0/1506      | 0.88        | 8/2028 (0.4%)  |
| 9   | s7    | 0.39         | 0/1516      | 0.89        | 5/2043 (0.2%)  |
| 10  | S8    | 0.38         | 0/1514      | 0.84        | 2/2021 (0.1%)  |
| 10  | s8    | 0.45         | 0/1514      | 0.82        | 0/2021         |
| 11  | S9    | 0.37         | 0/1519      | 0.85        | 5/2035 (0.2%)  |
| 11  | s9    | 0.39         | 0/1519      | 0.86        | 4/2035 (0.2%)  |
| 12  | C0    | 0.34         | 0/725       | 0.71        | 0/978          |
| 12  | c0    | 0.33         | 0/713       | 0.82        | 1/961 (0.1%)   |
| 13  | C1    | 0.41         | 0/1185      | 0.85        | 2/1598 (0.1%)  |
| 13  | c1    | 0.49         | 0/1185      | 0.85        | 1/1598 (0.1%)  |
| 14  | C2    | 0.35         | 0/819       | 0.77        | 0/1109         |
| 14  | c2    | 0.31         | 0/819       | 0.77        | 0/1109         |
| 15  | C3    | 0.39         | 0/1215      | 0.85        | 3/1638 (0.2%)  |
| 15  | c3    | 0.44         | 0/1215      | 0.87        | 2/1638 (0.1%)  |
| 16  | C4    | 0.39         | 0/901       | 0.89        | 2/1217 (0.2%)  |
| 16  | c4    | 0.39         | 0/960       | 0.90        | 4/1290 (0.3%)  |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 17  | C5    | 0.40         | 0/988   | 1.00        | 8/1327 (0.6%)   |
| 17  | c5    | 0.39         | 0/1030  | 0.94        | 4/1384 (0.3%)   |
| 18  | C6    | 0.37         | 0/1125  | 0.83        | 3/1510 (0.2%)   |
| 18  | c6    | 0.39         | 0/1131  | 0.84        | 0/1518          |
| 19  | C7    | 0.42         | 0/935   | 0.87        | 3/1254 (0.2%)   |
| 19  | c7    | 0.36         | 0/914   | 0.84        | 0/1224          |
| 20  | C8    | 0.37         | 0/1211  | 0.79        | 0/1628          |
| 20  | c8    | 0.36         | 0/1211  | 0.80        | 0/1628          |
| 21  | C9    | 0.38         | 0/1130  | 0.85        | 2/1517 (0.1%)   |
| 21  | c9    | 0.38         | 0/1130  | 0.81        | 0/1517          |
| 22  | D0    | 0.40         | 0/865   | 0.90        | 2/1169 (0.2%)   |
| 22  | d0    | 0.37         | 0/892   | 0.81        | 0/1205          |
| 23  | D1    | 0.38         | 0/693   | 0.86        | 2/935 (0.2%)    |
| 23  | d1    | 0.38         | 0/693   | 0.84        | 0/935           |
| 24  | D2    | 0.38         | 0/1038  | 0.93        | 4/1395 (0.3%)   |
| 24  | d2    | 0.46         | 0/1038  | 0.89        | 2/1395 (0.1%)   |
| 25  | D3    | 0.44         | 0/1139  | 0.88        | 4/1518 (0.3%)   |
| 25  | d3    | 0.48         | 0/1139  | 0.87        | 1/1518 (0.1%)   |
| 26  | D4    | 0.37         | 0/1087  | 0.82        | 0/1449          |
| 26  | d4    | 0.40         | 0/1087  | 0.90        | 6/1449 (0.4%)   |
| 27  | D5    | 0.39         | 0/571   | 0.90        | 1/768 (0.1%)    |
| 27  | d5    | 0.39         | 0/566   | 0.89        | 1/761 (0.1%)    |
| 28  | D6    | 0.42         | 0/782   | 0.89        | 3/1047 (0.3%)   |
| 28  | d6    | 0.43         | 0/782   | 0.85        | 0/1047          |
| 29  | D7    | 0.43         | 0/620   | 0.83        | 0/838           |
| 29  | d7    | 0.38         | 0/620   | 0.85        | 0/838           |
| 30  | D8    | 0.37         | 0/499   | 0.80        | 0/670           |
| 30  | d8    | 0.39         | 0/499   | 0.79        | 0/670           |
| 31  | D9    | 0.39         | 0/452   | 0.89        | 3/600 (0.5%)    |
| 31  | d9    | 0.38         | 0/452   | 0.80        | 0/600           |
| 32  | E0    | 0.39         | 0/483   | 0.86        | 0/643           |
| 32  | e0    | 0.40         | 0/499   | 1.02        | 4/665 (0.6%)    |
| 33  | E1    | 0.40         | 0/577   | 0.89        | 1/770 (0.1%)    |
| 33  | e1    | 0.43         | 0/619   | 0.94        | 4/822 (0.5%)    |
| 34  | SR    | 0.35         | 0/2490  | 0.78        | 1/3389 (0.0%)   |
| 34  | sR    | 0.32         | 0/2495  | 0.73        | 0/3395          |
| 35  | SM    | 0.45         | 0/925   | 0.95        | 4/1240 (0.3%)   |
| 35  | sM    | 0.45         | 0/480   | 0.93        | 3/642 (0.5%)    |
| 36  | 1     | 0.31         | 0/75394 | 0.49        | 2/117545 (0.0%) |
| 36  | 5     | 0.33         | 0/75865 | 0.50        | 1/118275 (0.0%) |
| 37  | 3     | 0.25         | 0/2883  | 0.41        | 0/4491          |
| 37  | 7     | 0.31         | 0/2883  | 0.47        | 0/4491          |
| 38  | 4     | 0.30         | 0/3746  | 0.47        | 0/5832          |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 38  | 8     | 0.29         | 0/3746  | 0.46        | 0/5832         |
| 39  | L2    | 0.50         | 0/1948  | 0.91        | 2/2617 (0.1%)  |
| 39  | l2    | 0.55         | 0/1946  | 0.95        | 2/2614 (0.1%)  |
| 40  | L3    | 0.49         | 0/3146  | 0.87        | 3/4228 (0.1%)  |
| 40  | l3    | 0.55         | 0/3146  | 0.91        | 6/4228 (0.1%)  |
| 41  | L4    | 0.52         | 0/2800  | 0.96        | 9/3790 (0.2%)  |
| 41  | l4    | 0.53         | 0/2800  | 1.01        | 16/3790 (0.4%) |
| 42  | L5    | 0.42         | 0/2425  | 0.83        | 2/3271 (0.1%)  |
| 42  | l5    | 0.49         | 0/2408  | 0.87        | 1/3248 (0.0%)  |
| 43  | L6    | 0.49         | 0/1260  | 0.89        | 2/1694 (0.1%)  |
| 43  | l6    | 0.50         | 0/1269  | 0.90        | 3/1705 (0.2%)  |
| 44  | L7    | 0.52         | 0/1821  | 0.93        | 4/2451 (0.2%)  |
| 44  | l7    | 0.54         | 0/1828  | 0.99        | 13/2461 (0.5%) |
| 45  | L8    | 0.41         | 0/1836  | 0.92        | 8/2481 (0.3%)  |
| 45  | l8    | 0.42         | 0/1796  | 0.90        | 6/2431 (0.2%)  |
| 46  | L9    | 0.46         | 0/1539  | 0.85        | 0/2073         |
| 46  | l9    | 0.52         | 0/1539  | 0.87        | 0/2073         |
| 47  | M0    | 0.47         | 0/1741  | 0.88        | 2/2335 (0.1%)  |
| 47  | m0    | 0.53         | 0/1758  | 0.95        | 6/2358 (0.3%)  |
| 48  | M1    | 0.41         | 0/1374  | 0.85        | 3/1842 (0.2%)  |
| 48  | m1    | 0.46         | 0/1374  | 0.90        | 2/1842 (0.1%)  |
| 49  | M3    | 0.51         | 0/1568  | 0.90        | 4/2106 (0.2%)  |
| 49  | m3    | 0.47         | 0/1573  | 0.97        | 9/2113 (0.4%)  |
| 50  | M4    | 0.50         | 0/1068  | 0.96        | 3/1438 (0.2%)  |
| 50  | m4    | 0.54         | 0/1074  | 0.94        | 2/1446 (0.1%)  |
| 51  | M5    | 0.49         | 0/1757  | 0.88        | 4/2354 (0.2%)  |
| 51  | m5    | 0.46         | 0/1757  | 0.89        | 5/2354 (0.2%)  |
| 52  | M6    | 0.55         | 0/1585  | 0.97        | 8/2128 (0.4%)  |
| 52  | m6    | 0.61         | 0/1585  | 1.00        | 8/2128 (0.4%)  |
| 53  | M7    | 0.54         | 0/1443  | 0.94        | 3/1944 (0.2%)  |
| 53  | m7    | 0.58         | 0/1250  | 0.91        | 1/1683 (0.1%)  |
| 54  | M8    | 0.51         | 0/1465  | 1.02        | 4/1965 (0.2%)  |
| 54  | m8    | 0.53         | 0/1465  | 0.99        | 3/1965 (0.2%)  |
| 55  | M9    | 0.41         | 0/1538  | 0.86        | 1/2050 (0.0%)  |
| 55  | m9    | 0.46         | 0/1538  | 0.87        | 1/2050 (0.0%)  |
| 56  | N0    | 0.49         | 0/1481  | 0.91        | 5/1990 (0.3%)  |
| 56  | n0    | 0.54         | 0/1481  | 0.95        | 8/1990 (0.4%)  |
| 57  | N1    | 0.49         | 0/1300  | 0.83        | 1/1743 (0.1%)  |
| 57  | n1    | 0.51         | 0/1300  | 0.92        | 4/1743 (0.2%)  |
| 58  | N2    | 0.37         | 0/812   | 0.76        | 0/1099         |
| 58  | n2    | 0.36         | 0/794   | 0.87        | 0/1076         |
| 59  | N3    | 0.51         | 0/1018  | 0.92        | 1/1369 (0.1%)  |
| 59  | n3    | 0.58         | 0/1018  | 1.02        | 3/1369 (0.2%)  |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 60  | N4    | 0.42         | 0/712         | 1.13        | 3/958 (0.3%)  |
| 60  | n4    | 0.45         | 0/1052        | 0.87        | 1/1398 (0.1%) |
| 61  | N5    | 0.41         | 0/979         | 0.81        | 0/1321        |
| 61  | n5    | 0.44         | 0/974         | 0.85        | 2/1314 (0.2%) |
| 62  | N6    | 0.47         | 0/1004        | 0.93        | 1/1341 (0.1%) |
| 62  | n6    | 0.46         | 0/1004        | 0.88        | 1/1341 (0.1%) |
| 63  | N7    | 0.36         | 0/1118        | 0.87        | 4/1497 (0.3%) |
| 63  | n7    | 0.39         | 0/1118        | 0.79        | 0/1497        |
| 64  | N8    | 0.51         | 0/1204        | 0.92        | 1/1612 (0.1%) |
| 64  | n8    | 0.51         | 0/1204        | 0.94        | 4/1612 (0.2%) |
| 65  | N9    | 0.50         | 0/473         | 0.93        | 2/629 (0.3%)  |
| 65  | n9    | 0.54         | 0/473         | 1.07        | 1/629 (0.2%)  |
| 66  | O0    | 0.38         | 0/751         | 0.75        | 0/1008        |
| 66  | o0    | 0.39         | 0/775         | 0.83        | 0/1040        |
| 67  | O1    | 0.41         | 0/890         | 0.84        | 2/1196 (0.2%) |
| 67  | o1    | 0.50         | 0/897         | 0.87        | 1/1205 (0.1%) |
| 68  | O2    | 0.54         | 0/1041        | 1.04        | 4/1394 (0.3%) |
| 68  | o2    | 0.55         | 0/1041        | 0.96        | 2/1394 (0.1%) |
| 69  | O3    | 0.57         | 0/868         | 0.89        | 0/1168        |
| 69  | o3    | 0.59         | 0/868         | 0.88        | 0/1168        |
| 70  | O4    | 0.45         | 0/890         | 0.90        | 2/1189 (0.2%) |
| 70  | o4    | 0.46         | 0/890         | 0.95        | 1/1189 (0.1%) |
| 71  | O5    | 0.46         | 0/978         | 0.92        | 0/1301        |
| 71  | o5    | 0.40         | 0/974         | 0.86        | 0/1297        |
| 72  | O6    | 0.50         | 0/778         | 0.93        | 2/1034 (0.2%) |
| 72  | o6    | 0.42         | 0/777         | 0.82        | 0/1033        |
| 73  | O7    | 0.54         | 0/696         | 0.91        | 1/923 (0.1%)  |
| 73  | o7    | 0.52         | 0/696         | 0.88        | 2/923 (0.2%)  |
| 74  | O8    | 0.39         | 0/618         | 0.85        | 2/826 (0.2%)  |
| 74  | o8    | 0.37         | 0/614         | 0.84        | 0/822         |
| 75  | O9    | 0.50         | 0/443         | 0.85        | 0/588         |
| 75  | o9    | 0.50         | 0/443         | 0.76        | 0/588         |
| 76  | Q0    | 0.51         | 0/423         | 0.93        | 2/562 (0.4%)  |
| 76  | q0    | 0.53         | 0/423         | 0.78        | 0/562         |
| 77  | Q1    | 0.45         | 0/234         | 0.92        | 1/300 (0.3%)  |
| 77  | q1    | 0.55         | 0/234         | 0.96        | 0/300         |
| 78  | Q2    | 0.55         | 0/860         | 0.91        | 0/1136        |
| 78  | q2    | 0.54         | 0/860         | 0.93        | 1/1136 (0.1%) |
| 79  | Q3    | 0.44         | 0/701         | 0.92        | 1/934 (0.1%)  |
| 79  | q3    | 0.52         | 0/701         | 0.88        | 0/934         |
| 81  | p0    | 0.32         | 0/977         | 0.81        | 0/1313        |
| 83  | f     | 0.52         | 1/1131 (0.1%) | 0.91        | 2/1522 (0.1%) |
| 84  | B     | 0.31         | 0/15          | 0.46        | 0/20          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 84  | C     | 0.40         | 0/15            | 0.70        | 0/20              |
| All | All   | 0.37         | 1/431576 (0.0%) | 0.66        | 379/633602 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 18  | c6    | 0                   | 1                   |
| 19  | C7    | 0                   | 1                   |
| 27  | D5    | 0                   | 1                   |
| 39  | l2    | 0                   | 1                   |
| 44  | L7    | 0                   | 1                   |
| 52  | M6    | 0                   | 1                   |
| 64  | n8    | 0                   | 1                   |
| 65  | N9    | 0                   | 1                   |
| 65  | n9    | 0                   | 1                   |
| 83  | f     | 0                   | 1                   |
| All | All   | 0                   | 10                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 83  | f     | 12  | ASP  | CA-C  | 5.52 | 1.55        | 1.52     |

The worst 5 of 379 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 60  | N4    | 80  | ARG  | CA-C-N | 15.66 | 139.41      | 119.84   |
| 60  | N4    | 80  | ARG  | C-N-CA | 15.66 | 139.41      | 119.84   |
| 65  | n9    | 14  | ARG  | N-CA-C | -9.89 | 100.48      | 111.07   |
| 54  | m8    | 18  | ALA  | CA-C-N | -9.52 | 110.05      | 120.14   |
| 54  | m8    | 18  | ALA  | C-N-CA | -9.52 | 110.05      | 120.14   |

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 19  | C7    | 85  | VAL  | Peptide |
| 27  | D5    | 94  | LYS  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 44  | L7    | 157 | ASN  | Peptide |
| 52  | M6    | 110 | PRO  | Peptide |
| 65  | N9    | 20  | GLY  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 37970 | 0        | 19106    | 815     | 0            |
| 1   | 6     | 38260 | 0        | 19252    | 802     | 0            |
| 2   | S0    | 1577  | 0        | 1567     | 82      | 0            |
| 2   | s0    | 1583  | 0        | 1578     | 77      | 0            |
| 3   | S1    | 1709  | 0        | 1784     | 66      | 0            |
| 3   | s1    | 1722  | 0        | 1793     | 69      | 0            |
| 4   | S2    | 1635  | 0        | 1723     | 78      | 0            |
| 4   | s2    | 1635  | 0        | 1723     | 66      | 0            |
| 5   | S3    | 1734  | 0        | 1817     | 59      | 0            |
| 5   | s3    | 1734  | 0        | 1817     | 68      | 0            |
| 6   | S4    | 2068  | 0        | 2154     | 94      | 0            |
| 6   | s4    | 2068  | 0        | 2154     | 95      | 0            |
| 7   | S5    | 1609  | 0        | 1675     | 63      | 0            |
| 7   | s5    | 1609  | 0        | 1675     | 65      | 0            |
| 8   | S6    | 1799  | 0        | 1879     | 49      | 0            |
| 8   | s6    | 1755  | 0        | 1846     | 72      | 0            |
| 9   | S7    | 1481  | 0        | 1572     | 65      | 0            |
| 9   | s7    | 1491  | 0        | 1578     | 56      | 0            |
| 10  | S8    | 1489  | 0        | 1525     | 64      | 0            |
| 10  | s8    | 1489  | 0        | 1525     | 57      | 0            |
| 11  | S9    | 1494  | 0        | 1573     | 69      | 0            |
| 11  | s9    | 1494  | 0        | 1573     | 88      | 0            |
| 12  | C0    | 773   | 0        | 714      | 34      | 0            |
| 12  | c0    | 762   | 0        | 689      | 25      | 0            |
| 13  | C1    | 1214  | 0        | 1237     | 43      | 0            |
| 13  | c1    | 1168  | 0        | 1226     | 45      | 0            |
| 14  | C2    | 892   | 0        | 872      | 36      | 0            |
| 14  | c2    | 892   | 0        | 869      | 29      | 0            |
| 15  | C3    | 1192  | 0        | 1255     | 43      | 0            |
| 15  | c3    | 1192  | 0        | 1255     | 55      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | C4    | 891   | 0        | 883      | 43      | 0            |
| 16  | c4    | 949   | 0        | 985      | 52      | 0            |
| 17  | C5    | 977   | 0        | 1004     | 48      | 0            |
| 17  | c5    | 1039  | 0        | 1041     | 40      | 0            |
| 18  | C6    | 1105  | 0        | 1166     | 48      | 0            |
| 18  | c6    | 1111  | 0        | 1171     | 43      | 0            |
| 19  | C7    | 926   | 0        | 930      | 50      | 0            |
| 19  | c7    | 906   | 0        | 909      | 43      | 0            |
| 20  | C8    | 1192  | 0        | 1222     | 59      | 0            |
| 20  | c8    | 1192  | 0        | 1222     | 50      | 0            |
| 21  | C9    | 1112  | 0        | 1124     | 51      | 0            |
| 21  | c9    | 1112  | 0        | 1124     | 44      | 0            |
| 22  | D0    | 855   | 0        | 917      | 42      | 0            |
| 22  | d0    | 882   | 0        | 939      | 33      | 0            |
| 23  | D1    | 684   | 0        | 672      | 40      | 0            |
| 23  | d1    | 684   | 0        | 672      | 37      | 0            |
| 24  | D2    | 1021  | 0        | 1060     | 47      | 0            |
| 24  | d2    | 1021  | 0        | 1060     | 56      | 0            |
| 25  | D3    | 1121  | 0        | 1196     | 58      | 0            |
| 25  | d3    | 1121  | 0        | 1196     | 42      | 0            |
| 26  | D4    | 1073  | 0        | 1132     | 48      | 0            |
| 26  | d4    | 1073  | 0        | 1132     | 45      | 0            |
| 27  | D5    | 563   | 0        | 603      | 25      | 0            |
| 27  | d5    | 558   | 0        | 598      | 29      | 0            |
| 28  | D6    | 769   | 0        | 814      | 45      | 0            |
| 28  | d6    | 769   | 0        | 814      | 40      | 0            |
| 29  | D7    | 610   | 0        | 630      | 14      | 0            |
| 29  | d7    | 610   | 0        | 631      | 27      | 0            |
| 30  | D8    | 497   | 0        | 535      | 28      | 0            |
| 30  | d8    | 497   | 0        | 535      | 16      | 0            |
| 31  | D9    | 442   | 0        | 428      | 20      | 0            |
| 31  | d9    | 442   | 0        | 428      | 13      | 0            |
| 32  | E0    | 475   | 0        | 525      | 12      | 0            |
| 32  | e0    | 491   | 0        | 542      | 19      | 0            |
| 33  | E1    | 566   | 0        | 602      | 26      | 0            |
| 33  | e1    | 608   | 0        | 657      | 24      | 0            |
| 34  | SR    | 2437  | 0        | 2386     | 87      | 0            |
| 34  | sR    | 2442  | 0        | 2392     | 85      | 1            |
| 35  | SM    | 1105  | 0        | 959      | 44      | 0            |
| 35  | sM    | 680   | 0        | 542      | 25      | 0            |
| 36  | 1     | 67355 | 0        | 33848    | 1255    | 1            |
| 36  | 5     | 67780 | 0        | 34065    | 1218    | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37  | 3     | 2579  | 0        | 1304     | 64      | 0            |
| 37  | 7     | 2579  | 0        | 1304     | 46      | 0            |
| 38  | 4     | 3353  | 0        | 1695     | 59      | 0            |
| 38  | 8     | 3353  | 0        | 1695     | 71      | 0            |
| 39  | L2    | 1914  | 0        | 1981     | 85      | 0            |
| 39  | l2    | 1912  | 0        | 1976     | 97      | 0            |
| 40  | L3    | 3075  | 0        | 3142     | 140     | 0            |
| 40  | l3    | 3075  | 0        | 3142     | 125     | 0            |
| 41  | L4    | 2748  | 0        | 2859     | 104     | 0            |
| 41  | l4    | 2748  | 0        | 2859     | 133     | 0            |
| 42  | L5    | 2375  | 0        | 2325     | 104     | 0            |
| 42  | l5    | 2359  | 0        | 2311     | 102     | 0            |
| 43  | L6    | 1239  | 0        | 1326     | 49      | 0            |
| 43  | l6    | 1248  | 0        | 1339     | 38      | 0            |
| 44  | L7    | 1784  | 0        | 1862     | 73      | 0            |
| 44  | l7    | 1791  | 0        | 1869     | 73      | 0            |
| 45  | L8    | 1804  | 0        | 1875     | 70      | 0            |
| 45  | l8    | 1764  | 0        | 1821     | 50      | 0            |
| 46  | L9    | 1518  | 0        | 1587     | 78      | 0            |
| 46  | l9    | 1518  | 0        | 1587     | 52      | 0            |
| 47  | M0    | 1705  | 0        | 1736     | 85      | 0            |
| 47  | m0    | 1722  | 0        | 1755     | 77      | 0            |
| 48  | M1    | 1353  | 0        | 1383     | 45      | 0            |
| 48  | m1    | 1353  | 0        | 1383     | 42      | 0            |
| 49  | M3    | 1543  | 0        | 1608     | 76      | 0            |
| 49  | m3    | 1548  | 0        | 1613     | 73      | 0            |
| 50  | M4    | 1053  | 0        | 1149     | 45      | 0            |
| 50  | m4    | 1059  | 0        | 1154     | 46      | 0            |
| 51  | M5    | 1720  | 0        | 1779     | 73      | 0            |
| 51  | m5    | 1720  | 0        | 1779     | 75      | 0            |
| 52  | M6    | 1555  | 0        | 1659     | 64      | 0            |
| 52  | m6    | 1555  | 0        | 1659     | 48      | 0            |
| 53  | M7    | 1420  | 0        | 1437     | 56      | 0            |
| 53  | m7    | 1227  | 0        | 1236     | 57      | 0            |
| 54  | M8    | 1441  | 0        | 1543     | 51      | 0            |
| 54  | m8    | 1441  | 0        | 1543     | 66      | 0            |
| 55  | M9    | 1521  | 0        | 1617     | 62      | 0            |
| 55  | m9    | 1521  | 0        | 1617     | 52      | 0            |
| 56  | N0    | 1445  | 0        | 1487     | 50      | 0            |
| 56  | n0    | 1445  | 0        | 1487     | 55      | 0            |
| 57  | N1    | 1276  | 0        | 1323     | 46      | 0            |
| 57  | n1    | 1276  | 0        | 1323     | 57      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58  | N2    | 796   | 0        | 812      | 26      | 0            |
| 58  | n2    | 778   | 0        | 791      | 17      | 0            |
| 59  | N3    | 1003  | 0        | 1048     | 41      | 0            |
| 59  | n3    | 1003  | 0        | 1048     | 39      | 0            |
| 60  | N4    | 699   | 0        | 640      | 24      | 0            |
| 60  | n4    | 1038  | 0        | 1071     | 36      | 0            |
| 61  | N5    | 964   | 0        | 1025     | 44      | 0            |
| 61  | n5    | 959   | 0        | 1023     | 36      | 0            |
| 62  | N6    | 993   | 0        | 1081     | 40      | 0            |
| 62  | n6    | 993   | 0        | 1081     | 42      | 0            |
| 63  | N7    | 1092  | 0        | 1155     | 58      | 0            |
| 63  | n7    | 1092  | 0        | 1155     | 46      | 0            |
| 64  | N8    | 1173  | 0        | 1215     | 66      | 0            |
| 64  | n8    | 1173  | 0        | 1215     | 53      | 0            |
| 65  | N9    | 462   | 0        | 491      | 19      | 0            |
| 65  | n9    | 462   | 0        | 491      | 18      | 0            |
| 66  | O0    | 743   | 0        | 797      | 26      | 0            |
| 66  | o0    | 767   | 0        | 816      | 28      | 0            |
| 67  | O1    | 876   | 0        | 912      | 35      | 0            |
| 67  | o1    | 883   | 0        | 918      | 28      | 0            |
| 68  | O2    | 1020  | 0        | 1090     | 43      | 0            |
| 68  | o2    | 1020  | 0        | 1090     | 40      | 0            |
| 69  | O3    | 850   | 0        | 880      | 36      | 0            |
| 69  | o3    | 850   | 0        | 880      | 33      | 0            |
| 70  | O4    | 880   | 0        | 945      | 32      | 0            |
| 70  | o4    | 880   | 0        | 945      | 36      | 0            |
| 71  | O5    | 969   | 0        | 1078     | 37      | 0            |
| 71  | o5    | 965   | 0        | 1067     | 59      | 0            |
| 72  | O6    | 771   | 0        | 849      | 39      | 0            |
| 72  | o6    | 770   | 0        | 846      | 35      | 0            |
| 73  | O7    | 681   | 0        | 683      | 35      | 0            |
| 73  | o7    | 681   | 0        | 683      | 19      | 0            |
| 74  | O8    | 612   | 0        | 682      | 20      | 0            |
| 74  | o8    | 608   | 0        | 671      | 22      | 0            |
| 75  | O9    | 436   | 0        | 475      | 18      | 0            |
| 75  | o9    | 436   | 0        | 475      | 22      | 0            |
| 76  | Q0    | 417   | 0        | 455      | 10      | 0            |
| 76  | q0    | 417   | 0        | 455      | 14      | 0            |
| 77  | Q1    | 233   | 0        | 284      | 14      | 0            |
| 77  | q1    | 233   | 0        | 284      | 11      | 0            |
| 78  | Q2    | 847   | 0        | 914      | 26      | 0            |
| 78  | q2    | 847   | 0        | 914      | 25      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 79  | Q3    | 694    | 0        | 734      | 29      | 0            |
| 79  | q3    | 694    | 0        | 734      | 28      | 0            |
| 80  | m2    | 750    | 0        | 185      | 10      | 0            |
| 81  | p0    | 1077   | 0        | 1012     | 29      | 0            |
| 82  | p1    | 235    | 0        | 53       | 2       | 0            |
| 82  | p2    | 230    | 0        | 52       | 0       | 0            |
| 83  | f     | 1116   | 0        | 1108     | 49      | 0            |
| 84  | B     | 76     | 0        | 49       | 3       | 0            |
| 84  | C     | 73     | 0        | 49       | 4       | 0            |
| 85  | D6    | 1      | 0        | 0        | 0       | 0            |
| 85  | D7    | 1      | 0        | 0        | 0       | 0            |
| 85  | D9    | 1      | 0        | 0        | 0       | 0            |
| 85  | E1    | 1      | 0        | 0        | 0       | 0            |
| 85  | O7    | 1      | 0        | 0        | 0       | 0            |
| 85  | Q0    | 1      | 0        | 0        | 0       | 0            |
| 85  | Q2    | 1      | 0        | 0        | 0       | 0            |
| 85  | Q3    | 1      | 0        | 0        | 0       | 0            |
| 85  | d6    | 1      | 0        | 0        | 0       | 0            |
| 85  | d7    | 1      | 0        | 0        | 0       | 0            |
| 85  | d9    | 1      | 0        | 0        | 0       | 0            |
| 85  | e1    | 1      | 0        | 0        | 0       | 0            |
| 85  | o7    | 1      | 0        | 0        | 0       | 0            |
| 85  | q0    | 1      | 0        | 0        | 0       | 0            |
| 85  | q2    | 1      | 0        | 0        | 0       | 0            |
| 85  | q3    | 1      | 0        | 0        | 0       | 0            |
| 86  | 1     | 23     | 0        | 18       | 3       | 0            |
| 86  | B     | 23     | 0        | 18       | 2       | 0            |
| 87  | 1     | 3      | 0        | 0        | 0       | 0            |
| 87  | 5     | 5      | 0        | 0        | 0       | 0            |
| 87  | B     | 1      | 0        | 0        | 0       | 0            |
| 87  | C     | 1      | 0        | 0        | 0       | 0            |
| 87  | f     | 2      | 0        | 0        | 0       | 0            |
| 88  | 1     | 14     | 0        | 0        | 0       | 0            |
| 88  | 5     | 7      | 0        | 0        | 0       | 0            |
| 89  | 5     | 2      | 0        | 0        | 0       | 0            |
| 89  | f     | 10     | 0        | 0        | 0       | 0            |
| All | All   | 404292 | 0        | 298868   | 9865    | 1            |

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 14.

The worst 5 of 9865 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) |
|-----------------|------------------|--------------------------|-------------------|
| 83:f:110:LYS:NZ | 83:f:112:ASP:OD1 | 1.85                     | 1.09              |
| 83:f:99:PHE:HA  | 83:f:100:LEU:HB2 | 1.45                     | 0.98              |
| 1:6:514:G:HO2'  | 1:6:515:A:H8     | 1.13                     | 0.97              |
| 1:6:104:A:H61   | 1:6:308:C:H5'    | 1.29                     | 0.96              |
| 1:2:1456:C:H5'' | 1:2:1457:C:H5''  | 1.49                     | 0.94              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 36:1:3153:U:O4 | 34:sR:79:TYR:OH[2_656] | 2.12                     | 0.08              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2   | S0    | 204/251 (81%) | 151 (74%) | 30 (15%) | 23 (11%) | 0           | 2  |
| 2   | s0    | 204/251 (81%) | 164 (80%) | 25 (12%) | 15 (7%)  | 1           | 6  |
| 3   | S1    | 212/254 (84%) | 152 (72%) | 38 (18%) | 22 (10%) | 0           | 2  |
| 3   | s1    | 214/254 (84%) | 168 (78%) | 33 (15%) | 13 (6%)  | 1           | 9  |
| 4   | S2    | 215/253 (85%) | 168 (78%) | 33 (15%) | 14 (6%)  | 1           | 8  |
| 4   | s2    | 215/253 (85%) | 168 (78%) | 33 (15%) | 14 (6%)  | 1           | 8  |
| 5   | S3    | 221/239 (92%) | 187 (85%) | 26 (12%) | 8 (4%)   | 2           | 17 |
| 5   | s3    | 221/239 (92%) | 176 (80%) | 35 (16%) | 10 (4%)  | 2           | 13 |
| 6   | S4    | 258/260 (99%) | 202 (78%) | 46 (18%) | 10 (4%)  | 2           | 16 |
| 6   | s4    | 258/260 (99%) | 189 (73%) | 53 (20%) | 16 (6%)  | 1           | 9  |
| 7   | S5    | 204/224 (91%) | 155 (76%) | 37 (18%) | 12 (6%)  | 1           | 9  |
| 7   | s5    | 204/224 (91%) | 160 (78%) | 29 (14%) | 15 (7%)  | 1           | 6  |
| 8   | S6    | 224/236 (95%) | 193 (86%) | 22 (10%) | 9 (4%)   | 2           | 15 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 8   | s6    | 216/236 (92%) | 182 (84%) | 22 (10%) | 12 (6%)  | 1           | 9  |
| 9   | S7    | 182/189 (96%) | 134 (74%) | 27 (15%) | 21 (12%) | 0           | 2  |
| 9   | s7    | 184/189 (97%) | 152 (83%) | 20 (11%) | 12 (6%)  | 1           | 8  |
| 10  | S8    | 184/200 (92%) | 151 (82%) | 24 (13%) | 9 (5%)   | 1           | 12 |
| 10  | s8    | 184/200 (92%) | 157 (85%) | 20 (11%) | 7 (4%)   | 2           | 16 |
| 11  | S9    | 183/196 (93%) | 149 (81%) | 23 (13%) | 11 (6%)  | 1           | 9  |
| 11  | s9    | 183/196 (93%) | 147 (80%) | 27 (15%) | 9 (5%)   | 1           | 12 |
| 12  | C0    | 82/96 (85%)   | 71 (87%)  | 8 (10%)  | 3 (4%)   | 2           | 17 |
| 12  | c0    | 82/96 (85%)   | 56 (68%)  | 16 (20%) | 10 (12%) | 0           | 1  |
| 13  | C1    | 143/155 (92%) | 116 (81%) | 18 (13%) | 9 (6%)   | 1           | 8  |
| 13  | c1    | 143/155 (92%) | 115 (80%) | 21 (15%) | 7 (5%)   | 1           | 12 |
| 14  | C2    | 107/142 (75%) | 70 (65%)  | 27 (25%) | 10 (9%)  | 0           | 3  |
| 14  | c2    | 107/142 (75%) | 75 (70%)  | 22 (21%) | 10 (9%)  | 0           | 3  |
| 15  | C3    | 148/150 (99%) | 124 (84%) | 20 (14%) | 4 (3%)   | 4           | 22 |
| 15  | c3    | 148/150 (99%) | 116 (78%) | 23 (16%) | 9 (6%)   | 1           | 9  |
| 16  | C4    | 125/136 (92%) | 81 (65%)  | 33 (26%) | 11 (9%)  | 0           | 4  |
| 16  | c4    | 126/136 (93%) | 96 (76%)  | 15 (12%) | 15 (12%) | 0           | 1  |
| 17  | C5    | 121/141 (86%) | 95 (78%)  | 12 (10%) | 14 (12%) | 0           | 2  |
| 17  | c5    | 128/141 (91%) | 98 (77%)  | 19 (15%) | 11 (9%)  | 0           | 4  |
| 18  | C6    | 139/142 (98%) | 116 (84%) | 14 (10%) | 9 (6%)   | 1           | 8  |
| 18  | c6    | 140/142 (99%) | 118 (84%) | 13 (9%)  | 9 (6%)   | 1           | 8  |
| 19  | C7    | 116/136 (85%) | 82 (71%)  | 23 (20%) | 11 (10%) | 0           | 3  |
| 19  | c7    | 113/136 (83%) | 93 (82%)  | 13 (12%) | 7 (6%)   | 1           | 9  |
| 20  | C8    | 143/145 (99%) | 116 (81%) | 17 (12%) | 10 (7%)  | 1           | 7  |
| 20  | c8    | 143/145 (99%) | 120 (84%) | 16 (11%) | 7 (5%)   | 1           | 12 |
| 21  | C9    | 141/143 (99%) | 115 (82%) | 18 (13%) | 8 (6%)   | 1           | 9  |
| 21  | c9    | 141/143 (99%) | 120 (85%) | 15 (11%) | 6 (4%)   | 2           | 14 |
| 22  | D0    | 105/120 (88%) | 89 (85%)  | 9 (9%)   | 7 (7%)   | 1           | 7  |
| 22  | d0    | 108/120 (90%) | 89 (82%)  | 14 (13%) | 5 (5%)   | 2           | 13 |
| 23  | D1    | 85/87 (98%)   | 66 (78%)  | 11 (13%) | 8 (9%)   | 0           | 3  |
| 23  | d1    | 85/87 (98%)   | 63 (74%)  | 17 (20%) | 5 (6%)   | 1           | 9  |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|----------|-------------|----|
| 24  | D2    | 127/129 (98%)  | 116 (91%) | 8 (6%)   | 3 (2%)   | 4           | 24 |
| 24  | d2    | 127/129 (98%)  | 107 (84%) | 17 (13%) | 3 (2%)   | 4           | 24 |
| 25  | D3    | 142/144 (99%)  | 109 (77%) | 21 (15%) | 12 (8%)  | 0           | 4  |
| 25  | d3    | 142/144 (99%)  | 117 (82%) | 20 (14%) | 5 (4%)   | 3           | 18 |
| 26  | D4    | 132/134 (98%)  | 109 (83%) | 13 (10%) | 10 (8%)  | 1           | 6  |
| 26  | d4    | 132/134 (98%)  | 110 (83%) | 15 (11%) | 7 (5%)   | 1           | 10 |
| 27  | D5    | 68/107 (64%)   | 48 (71%)  | 13 (19%) | 7 (10%)  | 0           | 2  |
| 27  | d5    | 67/107 (63%)   | 51 (76%)  | 15 (22%) | 1 (2%)   | 8           | 32 |
| 28  | D6    | 95/97 (98%)    | 56 (59%)  | 21 (22%) | 18 (19%) | 0           | 0  |
| 28  | d6    | 95/97 (98%)    | 66 (70%)  | 20 (21%) | 9 (10%)  | 0           | 3  |
| 29  | D7    | 79/81 (98%)    | 61 (77%)  | 15 (19%) | 3 (4%)   | 2           | 16 |
| 29  | d7    | 79/81 (98%)    | 61 (77%)  | 14 (18%) | 4 (5%)   | 1           | 11 |
| 30  | D8    | 61/66 (92%)    | 50 (82%)  | 9 (15%)  | 2 (3%)   | 3           | 19 |
| 30  | d8    | 61/66 (92%)    | 47 (77%)  | 11 (18%) | 3 (5%)   | 1           | 12 |
| 31  | D9    | 51/55 (93%)    | 39 (76%)  | 9 (18%)  | 3 (6%)   | 1           | 9  |
| 31  | d9    | 51/55 (93%)    | 41 (80%)  | 8 (16%)  | 2 (4%)   | 2           | 16 |
| 32  | E0    | 58/62 (94%)    | 46 (79%)  | 10 (17%) | 2 (3%)   | 3           | 18 |
| 32  | e0    | 60/62 (97%)    | 40 (67%)  | 12 (20%) | 8 (13%)  | 0           | 1  |
| 33  | E1    | 69/76 (91%)    | 35 (51%)  | 17 (25%) | 17 (25%) | 0           | 0  |
| 33  | e1    | 74/76 (97%)    | 36 (49%)  | 21 (28%) | 17 (23%) | 0           | 0  |
| 34  | SR    | 316/318 (99%)  | 263 (83%) | 36 (11%) | 17 (5%)  | 1           | 10 |
| 34  | sR    | 316/318 (99%)  | 252 (80%) | 53 (17%) | 11 (4%)  | 3           | 18 |
| 35  | SM    | 120/273 (44%)  | 91 (76%)  | 18 (15%) | 11 (9%)  | 0           | 3  |
| 35  | sM    | 61/273 (22%)   | 42 (69%)  | 11 (18%) | 8 (13%)  | 0           | 1  |
| 39  | L2    | 250/253 (99%)  | 213 (85%) | 27 (11%) | 10 (4%)  | 2           | 15 |
| 39  | l2    | 250/253 (99%)  | 205 (82%) | 30 (12%) | 15 (6%)  | 1           | 9  |
| 40  | L3    | 384/386 (100%) | 316 (82%) | 49 (13%) | 19 (5%)  | 1           | 12 |
| 40  | l3    | 384/386 (100%) | 330 (86%) | 39 (10%) | 15 (4%)  | 2           | 16 |
| 41  | L4    | 359/361 (99%)  | 291 (81%) | 46 (13%) | 22 (6%)  | 1           | 9  |
| 41  | l4    | 359/361 (99%)  | 296 (82%) | 43 (12%) | 20 (6%)  | 1           | 9  |
| 42  | L5    | 294/296 (99%)  | 232 (79%) | 44 (15%) | 18 (6%)  | 1           | 9  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 42  | l5    | 292/296 (99%) | 248 (85%) | 38 (13%) | 6 (2%)   | 5           | 26 |
| 43  | L6    | 152/175 (87%) | 122 (80%) | 27 (18%) | 3 (2%)   | 6           | 27 |
| 43  | l6    | 153/175 (87%) | 125 (82%) | 24 (16%) | 4 (3%)   | 4           | 23 |
| 44  | L7    | 220/243 (90%) | 185 (84%) | 24 (11%) | 11 (5%)  | 1           | 11 |
| 44  | l7    | 221/243 (91%) | 192 (87%) | 21 (10%) | 8 (4%)   | 2           | 17 |
| 45  | L8    | 231/255 (91%) | 190 (82%) | 30 (13%) | 11 (5%)  | 2           | 12 |
| 45  | l8    | 229/255 (90%) | 174 (76%) | 40 (18%) | 15 (7%)  | 1           | 7  |
| 46  | L9    | 189/191 (99%) | 145 (77%) | 29 (15%) | 15 (8%)  | 1           | 5  |
| 46  | l9    | 189/191 (99%) | 158 (84%) | 24 (13%) | 7 (4%)   | 2           | 17 |
| 47  | M0    | 207/220 (94%) | 161 (78%) | 37 (18%) | 9 (4%)   | 2           | 14 |
| 47  | m0    | 209/220 (95%) | 169 (81%) | 29 (14%) | 11 (5%)  | 1           | 10 |
| 48  | M1    | 167/173 (96%) | 128 (77%) | 27 (16%) | 12 (7%)  | 1           | 6  |
| 48  | m1    | 167/173 (96%) | 145 (87%) | 9 (5%)   | 13 (8%)  | 1           | 5  |
| 49  | M3    | 191/198 (96%) | 153 (80%) | 30 (16%) | 8 (4%)   | 2           | 14 |
| 49  | m3    | 192/198 (97%) | 152 (79%) | 27 (14%) | 13 (7%)  | 1           | 7  |
| 50  | M4    | 134/137 (98%) | 116 (87%) | 12 (9%)  | 6 (4%)   | 2           | 13 |
| 50  | m4    | 135/137 (98%) | 117 (87%) | 15 (11%) | 3 (2%)   | 5           | 26 |
| 51  | M5    | 201/203 (99%) | 175 (87%) | 20 (10%) | 6 (3%)   | 3           | 20 |
| 51  | m5    | 201/203 (99%) | 178 (89%) | 18 (9%)  | 5 (2%)   | 4           | 23 |
| 52  | M6    | 195/198 (98%) | 174 (89%) | 12 (6%)  | 9 (5%)   | 2           | 13 |
| 52  | m6    | 195/198 (98%) | 172 (88%) | 20 (10%) | 3 (2%)   | 8           | 32 |
| 53  | M7    | 181/183 (99%) | 151 (83%) | 25 (14%) | 5 (3%)   | 4           | 21 |
| 53  | m7    | 153/183 (84%) | 137 (90%) | 14 (9%)  | 2 (1%)   | 9           | 35 |
| 54  | M8    | 183/185 (99%) | 156 (85%) | 20 (11%) | 7 (4%)   | 2           | 16 |
| 54  | m8    | 183/185 (99%) | 154 (84%) | 21 (12%) | 8 (4%)   | 2           | 13 |
| 55  | M9    | 186/188 (99%) | 164 (88%) | 17 (9%)  | 5 (3%)   | 4           | 22 |
| 55  | m9    | 186/188 (99%) | 164 (88%) | 20 (11%) | 2 (1%)   | 11          | 39 |
| 56  | N0    | 170/172 (99%) | 151 (89%) | 15 (9%)  | 4 (2%)   | 4           | 24 |
| 56  | n0    | 170/172 (99%) | 159 (94%) | 9 (5%)   | 2 (1%)   | 10          | 37 |
| 57  | N1    | 157/159 (99%) | 131 (83%) | 20 (13%) | 6 (4%)   | 2           | 16 |
| 57  | n1    | 157/159 (99%) | 138 (88%) | 16 (10%) | 3 (2%)   | 6           | 28 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 58  | N2    | 98/120 (82%)  | 73 (74%)  | 20 (20%) | 5 (5%)   | 1           | 11 |
| 58  | n2    | 96/120 (80%)  | 80 (83%)  | 13 (14%) | 3 (3%)   | 3           | 20 |
| 59  | N3    | 134/136 (98%) | 117 (87%) | 12 (9%)  | 5 (4%)   | 2           | 17 |
| 59  | n3    | 134/136 (98%) | 122 (91%) | 4 (3%)   | 8 (6%)   | 1           | 9  |
| 60  | N4    | 96/155 (62%)  | 66 (69%)  | 21 (22%) | 9 (9%)   | 0           | 3  |
| 60  | n4    | 133/155 (86%) | 102 (77%) | 23 (17%) | 8 (6%)   | 1           | 9  |
| 61  | N5    | 119/141 (84%) | 103 (87%) | 12 (10%) | 4 (3%)   | 3           | 18 |
| 61  | n5    | 118/141 (84%) | 91 (77%)  | 17 (14%) | 10 (8%)  | 0           | 4  |
| 62  | N6    | 124/126 (98%) | 104 (84%) | 19 (15%) | 1 (1%)   | 16          | 45 |
| 62  | n6    | 124/126 (98%) | 102 (82%) | 17 (14%) | 5 (4%)   | 2           | 15 |
| 63  | N7    | 133/135 (98%) | 112 (84%) | 12 (9%)  | 9 (7%)   | 1           | 7  |
| 63  | n7    | 133/135 (98%) | 100 (75%) | 26 (20%) | 7 (5%)   | 1           | 10 |
| 64  | N8    | 146/148 (99%) | 113 (77%) | 26 (18%) | 7 (5%)   | 2           | 12 |
| 64  | n8    | 146/148 (99%) | 110 (75%) | 25 (17%) | 11 (8%)  | 1           | 6  |
| 65  | N9    | 56/58 (97%)   | 46 (82%)  | 8 (14%)  | 2 (4%)   | 2           | 17 |
| 65  | n9    | 56/58 (97%)   | 41 (73%)  | 9 (16%)  | 6 (11%)  | 0           | 2  |
| 66  | O0    | 95/104 (91%)  | 83 (87%)  | 11 (12%) | 1 (1%)   | 11          | 39 |
| 66  | o0    | 98/104 (94%)  | 86 (88%)  | 10 (10%) | 2 (2%)   | 6           | 27 |
| 67  | O1    | 107/112 (96%) | 96 (90%)  | 6 (6%)   | 5 (5%)   | 2           | 12 |
| 67  | o1    | 107/112 (96%) | 85 (79%)  | 15 (14%) | 7 (6%)   | 1           | 8  |
| 68  | O2    | 125/129 (97%) | 110 (88%) | 11 (9%)  | 4 (3%)   | 3           | 19 |
| 68  | o2    | 125/129 (97%) | 105 (84%) | 16 (13%) | 4 (3%)   | 3           | 19 |
| 69  | O3    | 104/106 (98%) | 96 (92%)  | 6 (6%)   | 2 (2%)   | 6           | 28 |
| 69  | o3    | 104/106 (98%) | 93 (89%)  | 9 (9%)   | 2 (2%)   | 6           | 28 |
| 70  | O4    | 110/120 (92%) | 96 (87%)  | 11 (10%) | 3 (3%)   | 4           | 22 |
| 70  | o4    | 110/120 (92%) | 88 (80%)  | 18 (16%) | 4 (4%)   | 2           | 17 |
| 71  | O5    | 117/119 (98%) | 95 (81%)  | 12 (10%) | 10 (8%)  | 0           | 4  |
| 71  | o5    | 117/119 (98%) | 94 (80%)  | 21 (18%) | 2 (2%)   | 7           | 30 |
| 72  | O6    | 97/99 (98%)   | 76 (78%)  | 12 (12%) | 9 (9%)   | 0           | 3  |
| 72  | o6    | 97/99 (98%)   | 76 (78%)  | 11 (11%) | 10 (10%) | 0           | 2  |
| 73  | O7    | 85/87 (98%)   | 69 (81%)  | 14 (16%) | 2 (2%)   | 4           | 24 |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers  | Percentiles |     |
|-----|-------|-------------------|-------------|------------|-----------|-------------|-----|
| 73  | o7    | 85/87 (98%)       | 70 (82%)    | 14 (16%)   | 1 (1%)    | 10          | 37  |
| 74  | O8    | 75/77 (97%)       | 66 (88%)    | 7 (9%)     | 2 (3%)    | 4           | 22  |
| 74  | o8    | 75/77 (97%)       | 61 (81%)    | 9 (12%)    | 5 (7%)    | 1           | 7   |
| 75  | O9    | 48/50 (96%)       | 35 (73%)    | 10 (21%)   | 3 (6%)    | 1           | 8   |
| 75  | o9    | 48/50 (96%)       | 39 (81%)    | 9 (19%)    | 0         | 100         | 100 |
| 76  | Q0    | 50/52 (96%)       | 43 (86%)    | 6 (12%)    | 1 (2%)    | 6           | 27  |
| 76  | q0    | 50/52 (96%)       | 48 (96%)    | 1 (2%)     | 1 (2%)    | 6           | 27  |
| 77  | Q1    | 23/25 (92%)       | 21 (91%)    | 2 (9%)     | 0         | 100         | 100 |
| 77  | q1    | 23/25 (92%)       | 20 (87%)    | 2 (9%)     | 1 (4%)    | 2           | 14  |
| 78  | Q2    | 103/105 (98%)     | 85 (82%)    | 13 (13%)   | 5 (5%)    | 1           | 12  |
| 78  | q2    | 103/105 (98%)     | 88 (85%)    | 9 (9%)     | 6 (6%)    | 1           | 9   |
| 79  | Q3    | 89/91 (98%)       | 70 (79%)    | 13 (15%)   | 6 (7%)    | 1           | 7   |
| 79  | q3    | 89/91 (98%)       | 79 (89%)    | 9 (10%)    | 1 (1%)    | 11          | 39  |
| 81  | p0    | 117/311 (38%)     | 97 (83%)    | 14 (12%)   | 6 (5%)    | 1           | 11  |
| 83  | f     | 146/157 (93%)     | 91 (62%)    | 35 (24%)   | 20 (14%)  | 0           | 1   |
| All | All   | 22316/24284 (92%) | 18108 (81%) | 2992 (13%) | 1216 (5%) | 1           | 10  |

5 of 1216 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S0    | 95  | ALA  |
| 2   | S0    | 158 | VAL  |
| 2   | S0    | 190 | ASP  |
| 2   | S0    | 192 | THR  |
| 3   | S1    | 35  | PRO  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | S0    | 164/209 (78%) | 143 (87%) | 21 (13%) | 4           | 18 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | s0    | 165/209 (79%)  | 141 (86%) | 24 (14%) | 3           | 14 |
| 3   | S1    | 191/223 (86%)  | 165 (86%) | 26 (14%) | 3           | 16 |
| 3   | s1    | 192/223 (86%)  | 165 (86%) | 27 (14%) | 3           | 14 |
| 4   | S2    | 176/204 (86%)  | 149 (85%) | 27 (15%) | 3           | 13 |
| 4   | s2    | 176/204 (86%)  | 134 (76%) | 42 (24%) | 1           | 4  |
| 5   | S3    | 182/194 (94%)  | 152 (84%) | 30 (16%) | 2           | 11 |
| 5   | s3    | 182/194 (94%)  | 157 (86%) | 25 (14%) | 3           | 16 |
| 6   | S4    | 221/221 (100%) | 193 (87%) | 28 (13%) | 4           | 18 |
| 6   | s4    | 221/221 (100%) | 183 (83%) | 38 (17%) | 2           | 10 |
| 7   | S5    | 173/190 (91%)  | 157 (91%) | 16 (9%)  | 8           | 30 |
| 7   | s5    | 173/190 (91%)  | 143 (83%) | 30 (17%) | 2           | 9  |
| 8   | S6    | 188/201 (94%)  | 163 (87%) | 25 (13%) | 4           | 17 |
| 8   | s6    | 187/201 (93%)  | 160 (86%) | 27 (14%) | 3           | 14 |
| 9   | S7    | 165/169 (98%)  | 145 (88%) | 20 (12%) | 5           | 20 |
| 9   | s7    | 165/169 (98%)  | 150 (91%) | 15 (9%)  | 9           | 31 |
| 10  | S8    | 150/161 (93%)  | 133 (89%) | 17 (11%) | 5           | 21 |
| 10  | s8    | 150/161 (93%)  | 129 (86%) | 21 (14%) | 3           | 15 |
| 11  | S9    | 158/165 (96%)  | 129 (82%) | 29 (18%) | 1           | 7  |
| 11  | s9    | 158/165 (96%)  | 132 (84%) | 26 (16%) | 2           | 11 |
| 12  | C0    | 77/77 (100%)   | 70 (91%)  | 7 (9%)   | 9           | 31 |
| 12  | c0    | 73/77 (95%)    | 63 (86%)  | 10 (14%) | 3           | 16 |
| 13  | C1    | 129/129 (100%) | 117 (91%) | 12 (9%)  | 8           | 30 |
| 13  | c1    | 129/129 (100%) | 109 (84%) | 20 (16%) | 2           | 12 |
| 14  | C2    | 88/106 (83%)   | 71 (81%)  | 17 (19%) | 1           | 6  |
| 14  | c2    | 88/106 (83%)   | 77 (88%)  | 11 (12%) | 4           | 19 |
| 15  | C3    | 127/127 (100%) | 108 (85%) | 19 (15%) | 3           | 13 |
| 15  | c3    | 127/127 (100%) | 107 (84%) | 20 (16%) | 2           | 12 |
| 16  | C4    | 81/104 (78%)   | 63 (78%)  | 18 (22%) | 1           | 5  |
| 16  | c4    | 97/104 (93%)   | 79 (81%)  | 18 (19%) | 1           | 7  |
| 17  | C5    | 101/113 (89%)  | 84 (83%)  | 17 (17%) | 2           | 11 |
| 17  | c5    | 103/113 (91%)  | 85 (82%)  | 18 (18%) | 2           | 9  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 18  | C6    | 117/118 (99%)  | 101 (86%) | 16 (14%) | 3           | 16 |
| 18  | c6    | 118/118 (100%) | 104 (88%) | 14 (12%) | 5           | 20 |
| 19  | C7    | 94/124 (76%)   | 77 (82%)  | 17 (18%) | 2           | 8  |
| 19  | c7    | 92/124 (74%)   | 82 (89%)  | 10 (11%) | 6           | 23 |
| 20  | C8    | 128/128 (100%) | 105 (82%) | 23 (18%) | 2           | 8  |
| 20  | c8    | 128/128 (100%) | 109 (85%) | 19 (15%) | 3           | 13 |
| 21  | C9    | 115/115 (100%) | 96 (84%)  | 19 (16%) | 2           | 11 |
| 21  | c9    | 115/115 (100%) | 99 (86%)  | 16 (14%) | 3           | 15 |
| 22  | D0    | 100/113 (88%)  | 87 (87%)  | 13 (13%) | 4           | 17 |
| 22  | d0    | 103/113 (91%)  | 88 (85%)  | 15 (15%) | 3           | 14 |
| 23  | D1    | 74/74 (100%)   | 66 (89%)  | 8 (11%)  | 6           | 23 |
| 23  | d1    | 74/74 (100%)   | 69 (93%)  | 5 (7%)   | 14          | 42 |
| 24  | D2    | 110/110 (100%) | 89 (81%)  | 21 (19%) | 1           | 7  |
| 24  | d2    | 110/110 (100%) | 96 (87%)  | 14 (13%) | 4           | 18 |
| 25  | D3    | 119/119 (100%) | 104 (87%) | 15 (13%) | 4           | 18 |
| 25  | d3    | 119/119 (100%) | 105 (88%) | 14 (12%) | 5           | 20 |
| 26  | D4    | 112/112 (100%) | 101 (90%) | 11 (10%) | 7           | 28 |
| 26  | d4    | 112/112 (100%) | 98 (88%)  | 14 (12%) | 4           | 19 |
| 27  | D5    | 61/88 (69%)    | 48 (79%)  | 13 (21%) | 1           | 5  |
| 27  | d5    | 61/88 (69%)    | 49 (80%)  | 12 (20%) | 1           | 6  |
| 28  | D6    | 83/83 (100%)   | 71 (86%)  | 12 (14%) | 3           | 14 |
| 28  | d6    | 83/83 (100%)   | 70 (84%)  | 13 (16%) | 2           | 12 |
| 29  | D7    | 70/70 (100%)   | 62 (89%)  | 8 (11%)  | 5           | 21 |
| 29  | d7    | 70/70 (100%)   | 58 (83%)  | 12 (17%) | 2           | 10 |
| 30  | D8    | 56/59 (95%)    | 48 (86%)  | 8 (14%)  | 3           | 14 |
| 30  | d8    | 56/59 (95%)    | 46 (82%)  | 10 (18%) | 2           | 8  |
| 31  | D9    | 47/48 (98%)    | 40 (85%)  | 7 (15%)  | 3           | 13 |
| 31  | d9    | 47/48 (98%)    | 38 (81%)  | 9 (19%)  | 1           | 7  |
| 32  | E0    | 51/53 (96%)    | 46 (90%)  | 5 (10%)  | 7           | 28 |
| 32  | e0    | 53/53 (100%)   | 38 (72%)  | 15 (28%) | 0           | 2  |
| 33  | E1    | 62/66 (94%)    | 48 (77%)  | 14 (23%) | 1           | 5  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 33  | e1    | 66/66 (100%)   | 52 (79%)  | 14 (21%) | 1           | 5  |
| 34  | SR    | 259/261 (99%)  | 228 (88%) | 31 (12%) | 5           | 20 |
| 34  | sR    | 260/261 (100%) | 239 (92%) | 21 (8%)  | 11          | 36 |
| 35  | SM    | 97/183 (53%)   | 82 (84%)  | 15 (16%) | 2           | 12 |
| 35  | sM    | 54/183 (30%)   | 46 (85%)  | 8 (15%)  | 3           | 13 |
| 39  | L2    | 193/195 (99%)  | 162 (84%) | 31 (16%) | 2           | 12 |
| 39  | l2    | 192/195 (98%)  | 158 (82%) | 34 (18%) | 2           | 8  |
| 40  | L3    | 319/322 (99%)  | 263 (82%) | 56 (18%) | 2           | 9  |
| 40  | l3    | 319/322 (99%)  | 253 (79%) | 66 (21%) | 1           | 6  |
| 41  | L4    | 288/288 (100%) | 244 (85%) | 44 (15%) | 3           | 13 |
| 41  | l4    | 288/288 (100%) | 236 (82%) | 52 (18%) | 2           | 8  |
| 42  | L5    | 244/244 (100%) | 209 (86%) | 35 (14%) | 3           | 14 |
| 42  | l5    | 243/244 (100%) | 194 (80%) | 49 (20%) | 1           | 6  |
| 43  | L6    | 134/152 (88%)  | 115 (86%) | 19 (14%) | 3           | 14 |
| 43  | l6    | 135/152 (89%)  | 111 (82%) | 24 (18%) | 2           | 8  |
| 44  | L7    | 186/204 (91%)  | 163 (88%) | 23 (12%) | 4           | 19 |
| 44  | l7    | 187/204 (92%)  | 162 (87%) | 25 (13%) | 4           | 16 |
| 45  | L8    | 187/207 (90%)  | 163 (87%) | 24 (13%) | 4           | 18 |
| 45  | l8    | 177/207 (86%)  | 151 (85%) | 26 (15%) | 3           | 14 |
| 46  | L9    | 171/171 (100%) | 134 (78%) | 37 (22%) | 1           | 5  |
| 46  | l9    | 171/171 (100%) | 141 (82%) | 30 (18%) | 2           | 9  |
| 47  | M0    | 177/186 (95%)  | 146 (82%) | 31 (18%) | 2           | 9  |
| 47  | m0    | 179/186 (96%)  | 146 (82%) | 33 (18%) | 1           | 7  |
| 48  | M1    | 147/150 (98%)  | 119 (81%) | 28 (19%) | 1           | 7  |
| 48  | m1    | 147/150 (98%)  | 123 (84%) | 24 (16%) | 2           | 11 |
| 49  | M3    | 154/158 (98%)  | 132 (86%) | 22 (14%) | 3           | 14 |
| 49  | m3    | 154/158 (98%)  | 128 (83%) | 26 (17%) | 2           | 10 |
| 50  | M4    | 107/108 (99%)  | 89 (83%)  | 18 (17%) | 2           | 11 |
| 50  | m4    | 108/108 (100%) | 89 (82%)  | 19 (18%) | 2           | 9  |
| 51  | M5    | 175/175 (100%) | 148 (85%) | 27 (15%) | 2           | 12 |
| 51  | m5    | 175/175 (100%) | 152 (87%) | 23 (13%) | 4           | 17 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 52  | M6    | 160/161 (99%)  | 132 (82%) | 28 (18%) | 2           | 9  |
| 52  | m6    | 160/161 (99%)  | 132 (82%) | 28 (18%) | 2           | 9  |
| 53  | M7    | 140/145 (97%)  | 112 (80%) | 28 (20%) | 1           | 6  |
| 53  | m7    | 125/145 (86%)  | 103 (82%) | 22 (18%) | 2           | 9  |
| 54  | M8    | 150/150 (100%) | 130 (87%) | 20 (13%) | 4           | 17 |
| 54  | m8    | 150/150 (100%) | 120 (80%) | 30 (20%) | 1           | 6  |
| 55  | M9    | 153/153 (100%) | 134 (88%) | 19 (12%) | 4           | 19 |
| 55  | m9    | 153/153 (100%) | 130 (85%) | 23 (15%) | 3           | 13 |
| 56  | N0    | 156/156 (100%) | 132 (85%) | 24 (15%) | 2           | 12 |
| 56  | n0    | 156/156 (100%) | 134 (86%) | 22 (14%) | 3           | 14 |
| 57  | N1    | 136/136 (100%) | 105 (77%) | 31 (23%) | 1           | 4  |
| 57  | n1    | 136/136 (100%) | 109 (80%) | 27 (20%) | 1           | 6  |
| 58  | N2    | 87/106 (82%)   | 78 (90%)  | 9 (10%)  | 7           | 25 |
| 58  | n2    | 85/106 (80%)   | 74 (87%)  | 11 (13%) | 4           | 17 |
| 59  | N3    | 104/104 (100%) | 88 (85%)  | 16 (15%) | 2           | 12 |
| 59  | n3    | 104/104 (100%) | 86 (83%)  | 18 (17%) | 2           | 9  |
| 60  | N4    | 57/129 (44%)   | 53 (93%)  | 4 (7%)   | 14          | 41 |
| 60  | n4    | 100/129 (78%)  | 94 (94%)  | 6 (6%)   | 17          | 46 |
| 61  | N5    | 104/117 (89%)  | 81 (78%)  | 23 (22%) | 1           | 5  |
| 61  | n5    | 104/117 (89%)  | 87 (84%)  | 17 (16%) | 2           | 11 |
| 62  | N6    | 109/109 (100%) | 86 (79%)  | 23 (21%) | 1           | 5  |
| 62  | n6    | 109/109 (100%) | 89 (82%)  | 20 (18%) | 2           | 7  |
| 63  | N7    | 115/115 (100%) | 98 (85%)  | 17 (15%) | 3           | 13 |
| 63  | n7    | 115/115 (100%) | 97 (84%)  | 18 (16%) | 2           | 12 |
| 64  | N8    | 118/118 (100%) | 103 (87%) | 15 (13%) | 4           | 18 |
| 64  | n8    | 118/118 (100%) | 98 (83%)  | 20 (17%) | 2           | 10 |
| 65  | N9    | 46/46 (100%)   | 40 (87%)  | 6 (13%)  | 4           | 17 |
| 65  | n9    | 46/46 (100%)   | 39 (85%)  | 7 (15%)  | 3           | 13 |
| 66  | O0    | 81/87 (93%)    | 66 (82%)  | 15 (18%) | 1           | 7  |
| 66  | o0    | 84/87 (97%)    | 72 (86%)  | 12 (14%) | 3           | 14 |
| 67  | O1    | 92/96 (96%)    | 79 (86%)  | 13 (14%) | 3           | 14 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers   | Percentiles |    |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 67  | o1    | 94/96 (98%)       | 76 (81%)    | 18 (19%)   | 1           | 7  |
| 68  | O2    | 109/110 (99%)     | 94 (86%)    | 15 (14%)   | 3           | 15 |
| 68  | o2    | 109/110 (99%)     | 83 (76%)    | 26 (24%)   | 1           | 4  |
| 69  | O3    | 90/90 (100%)      | 72 (80%)    | 18 (20%)   | 1           | 6  |
| 69  | o3    | 90/90 (100%)      | 74 (82%)    | 16 (18%)   | 2           | 8  |
| 70  | O4    | 95/102 (93%)      | 82 (86%)    | 13 (14%)   | 3           | 16 |
| 70  | o4    | 95/102 (93%)      | 81 (85%)    | 14 (15%)   | 3           | 14 |
| 71  | O5    | 104/104 (100%)    | 94 (90%)    | 10 (10%)   | 8           | 29 |
| 71  | o5    | 103/104 (99%)     | 86 (84%)    | 17 (16%)   | 2           | 11 |
| 72  | O6    | 81/81 (100%)      | 64 (79%)    | 17 (21%)   | 1           | 5  |
| 72  | o6    | 80/81 (99%)       | 58 (72%)    | 22 (28%)   | 0           | 2  |
| 73  | O7    | 70/70 (100%)      | 59 (84%)    | 11 (16%)   | 2           | 12 |
| 73  | o7    | 70/70 (100%)      | 61 (87%)    | 9 (13%)    | 4           | 17 |
| 74  | O8    | 68/68 (100%)      | 53 (78%)    | 15 (22%)   | 1           | 5  |
| 74  | o8    | 67/68 (98%)       | 57 (85%)    | 10 (15%)   | 3           | 13 |
| 75  | O9    | 45/45 (100%)      | 39 (87%)    | 6 (13%)    | 4           | 17 |
| 75  | o9    | 45/45 (100%)      | 41 (91%)    | 4 (9%)     | 9           | 32 |
| 76  | Q0    | 47/47 (100%)      | 37 (79%)    | 10 (21%)   | 1           | 5  |
| 76  | q0    | 47/47 (100%)      | 39 (83%)    | 8 (17%)    | 2           | 10 |
| 77  | Q1    | 23/23 (100%)      | 20 (87%)    | 3 (13%)    | 4           | 17 |
| 77  | q1    | 23/23 (100%)      | 16 (70%)    | 7 (30%)    | 0           | 1  |
| 78  | Q2    | 90/90 (100%)      | 71 (79%)    | 19 (21%)   | 1           | 5  |
| 78  | q2    | 90/90 (100%)      | 71 (79%)    | 19 (21%)   | 1           | 5  |
| 79  | Q3    | 71/71 (100%)      | 56 (79%)    | 15 (21%)   | 1           | 5  |
| 79  | q3    | 71/71 (100%)      | 60 (84%)    | 11 (16%)   | 2           | 12 |
| 81  | p0    | 105/232 (45%)     | 94 (90%)    | 11 (10%)   | 6           | 25 |
| 83  | f     | 124/133 (93%)     | 102 (82%)   | 22 (18%)   | 2           | 8  |
| All | All   | 18849/20177 (93%) | 15893 (84%) | 2956 (16%) | 2           | 12 |

5 of 2956 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | c9    | 135 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | l8    | 134 | TYR  |
| 26  | d4    | 40  | LEU  |
| 21  | c9    | 131 | ASP  |
| 40  | l3    | 84  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | c8    | 25  | ASN  |
| 46  | l9    | 58  | HIS  |
| 25  | d3    | 22  | ASN  |
| 40  | l3    | 211 | GLN  |
| 50  | m4    | 59  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed          | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1   | 2     | 1777/1800 (98%)   | 456 (25%)         | 40 (2%)         |
| 1   | 6     | 1791/1800 (99%)   | 447 (24%)         | 29 (1%)         |
| 36  | 1     | 3145/3396 (92%)   | 677 (21%)         | 53 (1%)         |
| 36  | 5     | 3163/3396 (93%)   | 651 (20%)         | 52 (1%)         |
| 37  | 3     | 120/121 (99%)     | 11 (9%)           | 0               |
| 37  | 7     | 120/121 (99%)     | 13 (10%)          | 0               |
| 38  | 4     | 157/158 (99%)     | 32 (20%)          | 3 (1%)          |
| 38  | 8     | 157/158 (99%)     | 34 (21%)          | 0               |
| All | All   | 10430/10950 (95%) | 2321 (22%)        | 177 (1%)        |

5 of 2321 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 2   | A    |
| 1   | 2     | 4   | C    |
| 1   | 2     | 6   | G    |
| 1   | 2     | 17  | C    |
| 1   | 2     | 23  | G    |

5 of 177 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 6     | 1097 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 36  | 5     | 1331 | U    |
| 1   | 6     | 1481 | C    |
| 36  | 5     | 916  | G    |
| 36  | 5     | 1816 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 28 are monoatomic - leaving 5 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 86  | SPS  | B     | 3401 | 87   | 20,23,23     | 3.62 | 13 (65%) | 23,30,30    | 2.48 | 11 (47%) |
| 86  | SPS  | 1     | 3401 | -    | 20,23,23     | 3.62 | 15 (75%) | 23,30,30    | 2.82 | 10 (43%) |
| 88  | OHX  | 5     | 3406 | -    | 0,6,6        | -    | -        | -           |      |          |
| 88  | OHX  | 1     | 3406 | -    | 0,6,6        | -    | -        | -           |      |          |
| 88  | OHX  | 1     | 3405 | -    | 0,6,6        | -    | -        | -           |      |          |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 86  | SPS  | B     | 3401 | 87   | -       | 3/15/18/18 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 86  | SPS  | 1     | 3401 | -    | -       | 2/15/18/18 | 0/1/1/1 |

The worst 5 of 28 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 86  | 1     | 3401 | SPS  | C9-C10  | -8.18 | 1.31        | 1.48     |
| 86  | B     | 3401 | SPS  | C9-C10  | -7.90 | 1.31        | 1.48     |
| 86  | B     | 3401 | SPS  | C9-C8   | 6.78  | 1.53        | 1.33     |
| 86  | 1     | 3401 | SPS  | C9-C8   | 6.51  | 1.52        | 1.33     |
| 86  | B     | 3401 | SPS  | O13-C13 | -5.48 | 1.19        | 1.42     |

The worst 5 of 21 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 86  | 1     | 3401 | SPS  | C7-C5-N4    | 6.32  | 120.77      | 113.42   |
| 86  | 1     | 3401 | SPS  | C7-C5-C6    | -6.31 | 118.29      | 126.47   |
| 86  | B     | 3401 | SPS  | C7-C5-C6    | -4.80 | 120.25      | 126.47   |
| 86  | 1     | 3401 | SPS  | C5-N4-C3    | -4.61 | 120.13      | 123.70   |
| 86  | B     | 3401 | SPS  | C18-S17-C16 | 4.12  | 111.12      | 100.14   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 86  | 1     | 3401 | SPS  | C14-C12-C13-O13 |
| 86  | B     | 3401 | SPS  | N11-C12-C13-O13 |
| 86  | B     | 3401 | SPS  | C14-C12-C13-O13 |
| 86  | 1     | 3401 | SPS  | N11-C12-C13-O13 |
| 86  | B     | 3401 | SPS  | C5-C6-C8-C9     |

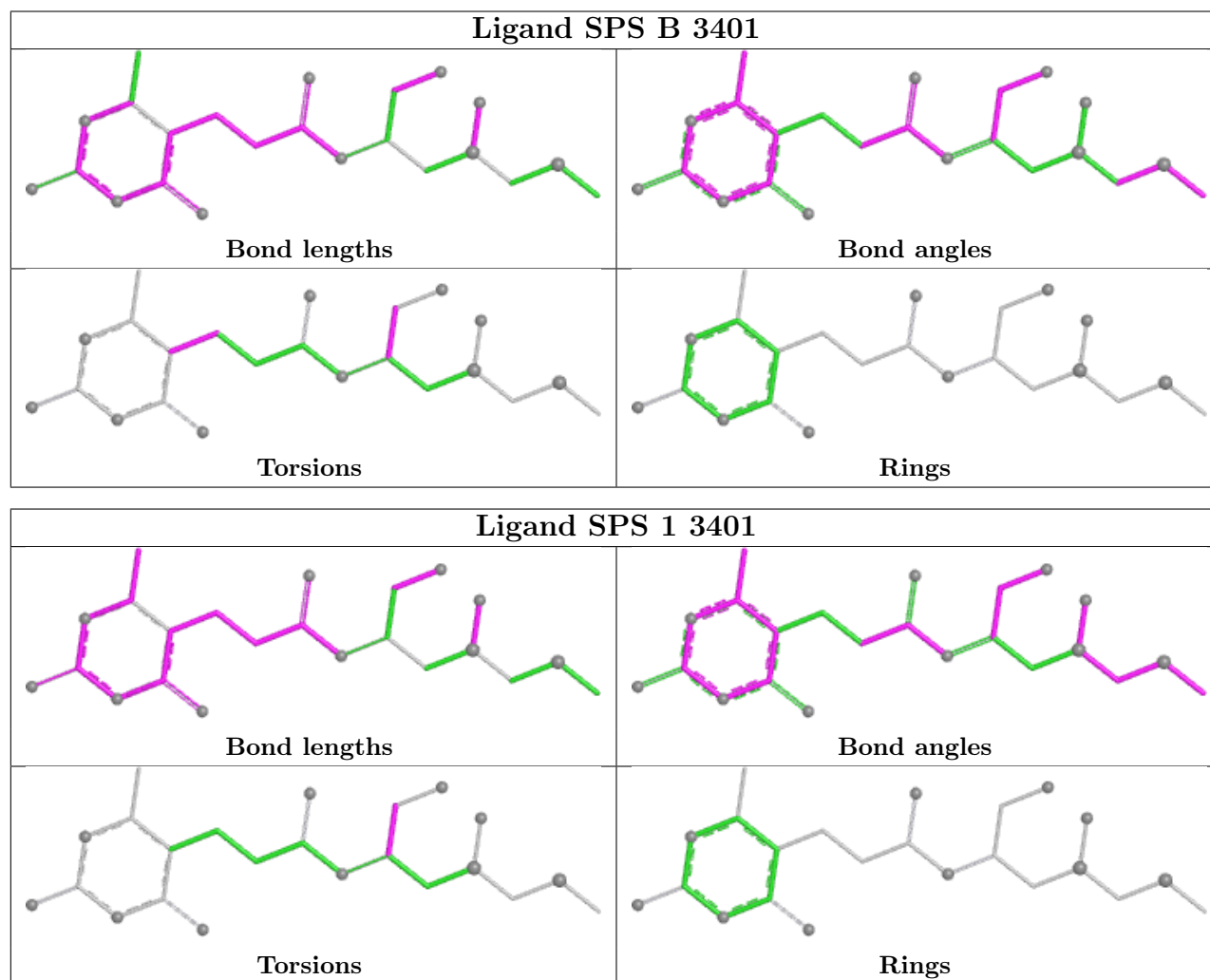
There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 86  | B     | 3401 | SPS  | 2       | 0            |
| 86  | 1     | 3401 | SPS  | 3       | 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](#)

10 such 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 |
| 84  | CH   | B     | 75  | 84,87 | 16,21,22     | 0.74 | 0        | 19,30,33    | 1.96 | 2 (10%)  |
| 84  | 8AN  | B     | 76  | 84,87 | 21,24,25     | 1.56 | 4 (19%)  | 26,35,38    | 2.26 | 9 (34%)  |
| 84  | 8AN  | C     | 76  | 84,87 | 21,24,25     | 1.56 | 4 (19%)  | 26,35,38    | 2.25 | 9 (34%)  |
| 84  | CH   | B     | 74  | 84    | 16,21,22     | 1.03 | 1 (6%)   | 19,30,33    | 1.86 | 2 (10%)  |
| 84  | CH   | C     | 75  | 84,87 | 16,21,22     | 0.97 | 2 (12%)  | 19,30,33    | 1.96 | 2 (10%)  |
| 84  | CH   | C     | 74  | 84    | 16,18,22     | 0.94 | 1 (6%)   | 20,26,33    | 1.76 | 2 (10%)  |

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   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 84  | CH   | B     | 75  | 84,87 | -       | 0/5/25/26 | 0/2/2/2 |
| 84  | 8AN  | B     | 76  | 84,87 | -       | 3/7/25/26 | 0/3/3/3 |
| 84  | 8AN  | C     | 76  | 84,87 | -       | 3/7/25/26 | 0/3/3/3 |
| 84  | CH   | B     | 74  | 84    | -       | 0/5/25/26 | 0/2/2/2 |
| 84  | CH   | C     | 75  | 84,87 | -       | 1/5/25/26 | 0/2/2/2 |
| 84  | CH   | C     | 74  | 84    | -       | 2/4/22/26 | 0/2/2/2 |

The worst 5 of 12 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 84  | B     | 76  | 8AN  | C5-C4 | 4.90  | 1.47        | 1.39     |
| 84  | C     | 76  | 8AN  | C5-C4 | 4.50  | 1.47        | 1.39     |
| 84  | B     | 74  | CH   | C4-N3 | -3.06 | 1.33        | 1.37     |
| 84  | C     | 74  | CH   | C4-N3 | -2.86 | 1.33        | 1.37     |
| 84  | B     | 76  | 8AN  | C5-C6 | 2.65  | 1.48        | 1.41     |

The worst 5 of 26 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 84  | B     | 74  | CH   | C5-C4-N3 | 7.27  | 122.18      | 118.04   |
| 84  | C     | 75  | CH   | C5-C4-N3 | 7.25  | 122.17      | 118.04   |
| 84  | B     | 75  | CH   | C5-C4-N3 | 6.07  | 121.50      | 118.04   |
| 84  | C     | 76  | 8AN  | C5-C4-N3 | -5.97 | 118.50      | 126.72   |
| 84  | C     | 74  | CH   | C5-C4-N3 | 5.87  | 121.38      | 118.04   |

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 84  | C     | 74  | CH   | C3'-C4'-C5'-O5' |
| 84  | C     | 74  | CH   | O4'-C4'-C5'-O5' |
| 84  | C     | 76  | 8AN  | C3'-C4'-C5'-O5' |
| 84  | B     | 76  | 8AN  | C3'-C4'-C5'-O5' |
| 84  | C     | 76  | 8AN  | O4'-C4'-C5'-O5' |

There are no ring outliers.

5 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 84  | B     | 75  | CH   | 1       | 0            |
| 84  | B     | 76  | 8AN  | 1       | 0            |
| 84  | B     | 74  | CH   | 1       | 0            |
| 84  | C     | 75  | CH   | 1       | 0            |
| 84  | C     | 74  | CH   | 3       | 0            |

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | 2     | 2                |
| 80  | m2    | 2                |
| 35  | sM    | 1                |
| 35  | SM    | 1                |
| 12  | c0    | 1                |
| 36  | 5     | 1                |

The worst 5 of 8 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | sM    | 139:UNK   | C      | 155:UNK   | N      | 38.68        |
| 1     | SM    | 141:ALA   | C      | 151:UNK   | N      | 26.53        |
| 1     | c0    | 84:UNK    | C      | 87:UNK    | N      | 8.84         |
| 1     | 2     | 1716:C    | O3'    | 1717:G    | P      | 5.83         |
| 1     | 5     | 2437:G    | O3'    | 2438:A    | P      | 4.00         |

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|----------------|-----------------------|--------|
| 1   | 2     | 1781/1800 (98%) | 0.42   | 49 (2%) 55 36  | 41, 98, 170, 210      | 1 (0%) |
| 1   | 6     | 1795/1800 (99%) | 0.25   | 35 (1%) 66 48  | 34, 86, 157, 204      | 1 (0%) |
| 2   | S0    | 206/251 (82%)   | 1.09   | 29 (14%) 6 5   | 100, 112, 123, 128    | 0      |
| 2   | s0    | 206/251 (82%)   | 0.78   | 14 (6%) 23 16  | 80, 97, 111, 117      | 0      |
| 3   | S1    | 214/254 (84%)   | 1.24   | 45 (21%) 2 2   | 110, 145, 169, 175    | 0      |
| 3   | s1    | 216/254 (85%)   | 0.94   | 23 (10%) 11 9  | 80, 96, 114, 123      | 0      |
| 4   | S2    | 217/253 (85%)   | 1.24   | 36 (16%) 4 4   | 83, 96, 109, 113      | 0      |
| 4   | s2    | 217/253 (85%)   | 0.88   | 22 (10%) 12 10 | 68, 79, 93, 108       | 0      |
| 5   | S3    | 223/239 (93%)   | 1.07   | 24 (10%) 11 9  | 91, 100, 123, 128     | 0      |
| 5   | s3    | 223/239 (93%)   | 1.11   | 31 (13%) 6 5   | 86, 112, 131, 137     | 0      |
| 6   | S4    | 260/260 (100%)  | 1.35   | 53 (20%) 3 2   | 77, 99, 107, 124      | 0      |
| 6   | s4    | 260/260 (100%)  | 0.95   | 22 (8%) 16 13  | 60, 82, 92, 119       | 0      |
| 7   | S5    | 206/224 (91%)   | 1.43   | 44 (21%) 2 2   | 104, 124, 131, 134    | 0      |
| 7   | s5    | 206/224 (91%)   | 1.13   | 28 (13%) 7 6   | 87, 108, 123, 130     | 0      |
| 8   | S6    | 226/236 (95%)   | 1.40   | 50 (22%) 2 2   | 77, 105, 126, 132     | 0      |
| 8   | s6    | 218/236 (92%)   | 1.05   | 29 (13%) 7 6   | 60, 89, 106, 114      | 0      |
| 9   | S7    | 184/189 (97%)   | 1.07   | 21 (11%) 10 8  | 102, 121, 136, 142    | 0      |
| 9   | s7    | 186/189 (98%)   | 0.81   | 14 (7%) 20 15  | 77, 104, 130, 134     | 0      |
| 10  | S8    | 188/200 (94%)   | 0.94   | 22 (11%) 9 8   | 70, 86, 119, 129      | 0      |
| 10  | s8    | 188/200 (94%)   | 0.83   | 18 (9%) 13 11  | 56, 73, 113, 130      | 0      |
| 11  | S9    | 185/196 (94%)   | 1.03   | 16 (8%) 16 12  | 89, 106, 130, 141     | 0      |
| 11  | s9    | 185/196 (94%)   | 0.79   | 13 (7%) 22 15  | 71, 88, 115, 126      | 0      |
| 12  | C0    | 83/96 (86%)     | 0.81   | 6 (7%) 21 15   | 94, 112, 122, 126     | 0      |
| 12  | c0    | 83/96 (86%)     | 1.50   | 20 (24%) 2 1   | 103, 131, 145, 149    | 0      |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 13  | C1    | 144/155 (92%)  | 1.01   | 11 (7%) 20 14  | 73, 83, 101, 113      | 0     |
| 13  | c1    | 144/155 (92%)  | 0.93   | 16 (11%) 10 9  | 59, 70, 91, 113       | 0     |
| 14  | C2    | 108/142 (76%)  | 1.21   | 20 (18%) 3 3   | 137, 145, 150, 152    | 0     |
| 14  | c2    | 108/142 (76%)  | 1.48   | 32 (29%) 1 1   | 167, 183, 196, 199    | 0     |
| 15  | C3    | 150/150 (100%) | 1.12   | 17 (11%) 10 8  | 82, 95, 111, 115      | 0     |
| 15  | c3    | 150/150 (100%) | 0.78   | 14 (9%) 14 11  | 66, 79, 95, 100       | 0     |
| 16  | C4    | 127/136 (93%)  | 1.36   | 27 (21%) 2 2   | 84, 142, 156, 161     | 0     |
| 16  | c4    | 128/136 (94%)  | 0.94   | 13 (10%) 12 10 | 67, 101, 113, 116     | 0     |
| 17  | C5    | 122/141 (86%)  | 1.12   | 12 (9%) 13 10  | 88, 99, 111, 117      | 0     |
| 17  | c5    | 129/141 (91%)  | 1.14   | 21 (16%) 4 4   | 86, 103, 113, 119     | 0     |
| 18  | C6    | 141/142 (99%)  | 1.53   | 39 (27%) 1 1   | 91, 112, 117, 120     | 0     |
| 18  | c6    | 142/142 (100%) | 1.50   | 40 (28%) 1 1   | 83, 102, 115, 126     | 0     |
| 19  | C7    | 120/136 (88%)  | 0.95   | 9 (7%) 20 15   | 97, 109, 125, 129     | 0     |
| 19  | c7    | 117/136 (86%)  | 0.83   | 14 (11%) 9 7   | 88, 101, 115, 119     | 0     |
| 20  | C8    | 145/145 (100%) | 0.86   | 11 (7%) 20 14  | 85, 110, 131, 138     | 0     |
| 20  | c8    | 145/145 (100%) | 1.00   | 18 (12%) 8 6   | 86, 101, 116, 126     | 0     |
| 21  | C9    | 143/143 (100%) | 1.13   | 19 (13%) 7 6   | 96, 112, 122, 126     | 0     |
| 21  | c9    | 143/143 (100%) | 0.83   | 17 (11%) 9 7   | 85, 97, 112, 118      | 0     |
| 22  | D0    | 107/120 (89%)  | 2.03   | 42 (39%) 1 1   | 86, 112, 123, 125     | 0     |
| 22  | d0    | 110/120 (91%)  | 1.24   | 12 (10%) 10 9  | 84, 114, 138, 147     | 0     |
| 23  | D1    | 87/87 (100%)   | 0.90   | 10 (11%) 9 8   | 96, 104, 119, 127     | 0     |
| 23  | d1    | 87/87 (100%)   | 0.42   | 1 (1%) 78 60   | 76, 88, 104, 112      | 0     |
| 24  | D2    | 129/129 (100%) | 1.23   | 15 (11%) 9 8   | 83, 95, 101, 109      | 0     |
| 24  | d2    | 129/129 (100%) | 0.54   | 3 (2%) 61 42   | 64, 74, 81, 87        | 0     |
| 25  | D3    | 144/144 (100%) | 1.05   | 21 (14%) 6 5   | 69, 77, 86, 96        | 0     |
| 25  | d3    | 144/144 (100%) | 0.80   | 12 (8%) 17 13  | 56, 61, 71, 79        | 0     |
| 26  | D4    | 134/134 (100%) | 1.10   | 17 (12%) 8 6   | 86, 107, 118, 129     | 0     |
| 26  | d4    | 134/134 (100%) | 0.92   | 14 (10%) 11 9  | 68, 90, 105, 110      | 0     |
| 27  | D5    | 70/107 (65%)   | 0.89   | 3 (4%) 40 25   | 119, 130, 139, 140    | 0     |
| 27  | d5    | 69/107 (64%)   | 0.80   | 4 (5%) 29 19   | 99, 113, 123, 125     | 0     |
| 28  | D6    | 97/97 (100%)   | 2.17   | 47 (48%) 0 0   | 88, 106, 154, 159     | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | d6    | 97/97 (100%)    | 1.46   | 26 (26%) 1 1  | 70, 87, 116, 123      | 0     |
| 29  | D7    | 81/81 (100%)    | 1.21   | 10 (12%) 8 7  | 98, 110, 135, 141     | 0     |
| 29  | d7    | 81/81 (100%)    | 1.03   | 8 (9%) 13 10  | 80, 93, 121, 128      | 0     |
| 30  | D8    | 63/66 (95%)     | 1.65   | 20 (31%) 1 1  | 111, 127, 139, 143    | 0     |
| 30  | d8    | 63/66 (95%)     | 1.23   | 9 (14%) 6 5   | 104, 116, 127, 129    | 0     |
| 31  | D9    | 53/55 (96%)     | 0.89   | 4 (7%) 20 15  | 84, 91, 107, 112      | 0     |
| 31  | d9    | 53/55 (96%)     | 1.23   | 12 (22%) 2 2  | 82, 92, 128, 139      | 0     |
| 32  | E0    | 60/62 (96%)     | 1.03   | 8 (13%) 7 6   | 78, 107, 129, 134     | 0     |
| 32  | e0    | 62/62 (100%)    | 0.81   | 9 (14%) 6 5   | 63, 88, 109, 122      | 0     |
| 33  | E1    | 71/76 (93%)     | 1.29   | 13 (18%) 3 3  | 107, 133, 145, 148    | 0     |
| 33  | e1    | 76/76 (100%)    | 1.57   | 19 (25%) 2 1  | 112, 158, 170, 175    | 0     |
| 34  | SR    | 318/318 (100%)  | 0.90   | 27 (8%) 16 13 | 109, 120, 132, 146    | 0     |
| 34  | sR    | 318/318 (100%)  | 1.14   | 45 (14%) 6 5  | 110, 126, 140, 150    | 0     |
| 35  | SM    | 121/273 (44%)   | 1.13   | 21 (17%) 4 4  | 59, 94, 111, 116      | 0     |
| 35  | sM    | 63/273 (23%)    | 1.70   | 19 (30%) 1 1  | 55, 105, 111, 112     | 0     |
| 36  | 1     | 3149/3396 (92%) | -0.02  | 29 (0%) 81 65 | 35, 59, 123, 212      | 0     |
| 36  | 5     | 3169/3396 (93%) | -0.08  | 45 (1%) 73 55 | 35, 54, 124, 188      | 0     |
| 37  | 3     | 121/121 (100%)  | -0.14  | 0 100 100     | 43, 76, 90, 96        | 0     |
| 37  | 7     | 121/121 (100%)  | -0.28  | 1 (0%) 82 68  | 39, 59, 70, 75        | 0     |
| 38  | 4     | 158/158 (100%)  | -0.04  | 2 (1%) 75 56  | 43, 61, 91, 130       | 0     |
| 38  | 8     | 158/158 (100%)  | -0.01  | 2 (1%) 75 56  | 43, 63, 96, 120       | 0     |
| 39  | L2    | 252/253 (99%)   | 0.80   | 23 (9%) 15 11 | 42, 61, 77, 82        | 0     |
| 39  | l2    | 252/253 (99%)   | 0.44   | 10 (3%) 42 28 | 43, 59, 74, 83        | 0     |
| 40  | L3    | 386/386 (100%)  | 0.42   | 15 (3%) 43 29 | 42, 63, 77, 85        | 0     |
| 40  | l3    | 386/386 (100%)  | 0.15   | 7 (1%) 67 49  | 34, 49, 62, 77        | 0     |
| 41  | L4    | 361/361 (100%)  | 0.35   | 11 (3%) 52 35 | 40, 54, 70, 71        | 0     |
| 41  | l4    | 361/361 (100%)  | 0.45   | 15 (4%) 40 26 | 40, 57, 73, 88        | 0     |
| 42  | L5    | 296/296 (100%)  | 0.73   | 22 (7%) 20 15 | 58, 81, 97, 111       | 0     |
| 42  | l5    | 294/296 (99%)   | 0.45   | 18 (6%) 27 18 | 49, 60, 84, 93        | 0     |
| 43  | L6    | 156/175 (89%)   | 0.34   | 5 (3%) 50 34  | 49, 57, 72, 79        | 0     |
| 43  | l6    | 157/175 (89%)   | 0.35   | 3 (1%) 66 48  | 49, 57, 75, 85        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 44  | L7    | 222/243 (91%)  | 0.21   | 9 (4%) 41 27  | 40, 49, 73, 106       | 0     |
| 44  | l7    | 223/243 (91%)  | 0.21   | 2 (0%) 81 65  | 39, 49, 80, 107       | 0     |
| 45  | L8    | 233/255 (91%)  | 0.94   | 30 (12%) 7 6  | 67, 81, 104, 112      | 0     |
| 45  | l8    | 231/255 (90%)  | 0.86   | 24 (10%) 11 9 | 73, 84, 106, 114      | 0     |
| 46  | L9    | 191/191 (100%) | 0.72   | 10 (5%) 33 22 | 60, 70, 82, 93        | 0     |
| 46  | l9    | 191/191 (100%) | 0.21   | 2 (1%) 79 63  | 44, 55, 71, 81        | 0     |
| 47  | M0    | 211/220 (95%)  | 0.57   | 13 (6%) 26 18 | 45, 63, 92, 106       | 0     |
| 47  | m0    | 213/220 (96%)  | 0.52   | 12 (5%) 30 20 | 40, 55, 80, 90        | 0     |
| 48  | M1    | 169/173 (97%)  | 0.62   | 9 (5%) 32 22  | 68, 84, 94, 98        | 0     |
| 48  | m1    | 169/173 (97%)  | 0.37   | 3 (1%) 67 49  | 52, 67, 77, 82        | 0     |
| 49  | M3    | 193/198 (97%)  | 0.41   | 8 (4%) 41 27  | 39, 64, 92, 113       | 0     |
| 49  | m3    | 194/198 (97%)  | 0.62   | 10 (5%) 33 22 | 41, 69, 100, 111      | 0     |
| 50  | M4    | 136/137 (99%)  | 0.34   | 5 (3%) 45 31  | 54, 61, 73, 83        | 0     |
| 50  | m4    | 137/137 (100%) | 0.25   | 1 (0%) 84 70  | 48, 54, 69, 82        | 0     |
| 51  | M5    | 203/203 (100%) | 0.49   | 7 (3%) 48 32  | 41, 56, 66, 69        | 0     |
| 51  | m5    | 203/203 (100%) | 0.58   | 10 (4%) 35 23 | 44, 60, 71, 76        | 0     |
| 52  | M6    | 197/198 (99%)  | 0.53   | 12 (6%) 27 18 | 42, 49, 65, 68        | 0     |
| 52  | m6    | 197/198 (99%)  | 0.40   | 14 (7%) 22 15 | 34, 42, 64, 66        | 0     |
| 53  | M7    | 183/183 (100%) | 0.63   | 18 (9%) 13 10 | 47, 55, 98, 116       | 0     |
| 53  | m7    | 155/183 (84%)  | 0.10   | 1 (0%) 85 73  | 39, 46, 59, 77        | 0     |
| 54  | M8    | 185/185 (100%) | 0.47   | 10 (5%) 31 21 | 43, 55, 69, 88        | 0     |
| 54  | m8    | 185/185 (100%) | 0.43   | 5 (2%) 56 37  | 42, 57, 66, 70        | 0     |
| 55  | M9    | 188/188 (100%) | 0.78   | 11 (5%) 28 19 | 65, 77, 135, 140      | 0     |
| 55  | m9    | 188/188 (100%) | 0.51   | 5 (2%) 56 37  | 51, 65, 121, 134      | 0     |
| 56  | N0    | 172/172 (100%) | 0.42   | 8 (4%) 36 24  | 49, 57, 69, 74        | 0     |
| 56  | n0    | 172/172 (100%) | 0.18   | 5 (2%) 53 35  | 43, 49, 59, 66        | 0     |
| 57  | N1    | 159/159 (100%) | 0.41   | 4 (2%) 58 39  | 42, 56, 93, 101       | 0     |
| 57  | n1    | 159/159 (100%) | 0.47   | 5 (3%) 51 35  | 40, 49, 83, 87        | 0     |
| 58  | N2    | 100/120 (83%)  | 0.90   | 11 (11%) 10 9 | 93, 104, 120, 122     | 0     |
| 58  | n2    | 98/120 (81%)   | 0.79   | 9 (9%) 14 11  | 75, 88, 94, 97        | 0     |
| 59  | N3    | 136/136 (100%) | 0.54   | 10 (7%) 20 15 | 51, 60, 70, 74        | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 59  | n3    | 136/136 (100%) | 0.21   | 3 (2%) 62 43  | 36, 45, 55, 58        | 0     |
| 60  | N4    | 98/155 (63%)   | 1.35   | 23 (23%) 2 2  | 62, 72, 134, 147      | 0     |
| 60  | n4    | 135/155 (87%)  | 0.89   | 17 (12%) 8 6  | 46, 91, 115, 116      | 0     |
| 61  | N5    | 121/141 (85%)  | 0.66   | 10 (8%) 17 13 | 58, 69, 84, 95        | 0     |
| 61  | n5    | 120/141 (85%)  | 0.75   | 7 (5%) 29 19  | 56, 68, 85, 93        | 0     |
| 62  | N6    | 126/126 (100%) | 0.35   | 3 (2%) 59 40  | 50, 62, 74, 79        | 0     |
| 62  | n6    | 126/126 (100%) | 0.44   | 3 (2%) 59 40  | 51, 64, 77, 83        | 0     |
| 63  | N7    | 135/135 (100%) | 0.58   | 5 (3%) 45 31  | 82, 94, 103, 109      | 0     |
| 63  | n7    | 135/135 (100%) | 0.51   | 6 (4%) 39 25  | 76, 91, 102, 105      | 0     |
| 64  | N8    | 148/148 (100%) | 0.35   | 1 (0%) 84 70  | 35, 56, 74, 82        | 0     |
| 64  | n8    | 148/148 (100%) | 0.39   | 3 (2%) 65 46  | 34, 59, 74, 77        | 0     |
| 65  | N9    | 58/58 (100%)   | 0.46   | 2 (3%) 48 32  | 38, 61, 95, 106       | 0     |
| 65  | n9    | 58/58 (100%)   | 0.65   | 6 (10%) 12 10 | 38, 58, 78, 85        | 0     |
| 66  | O0    | 97/104 (93%)   | 0.69   | 5 (5%) 33 22  | 81, 89, 101, 102      | 0     |
| 66  | o0    | 100/104 (96%)  | 0.63   | 3 (3%) 52 35  | 75, 82, 102, 108      | 0     |
| 67  | O1    | 109/112 (97%)  | 0.77   | 6 (5%) 30 21  | 61, 72, 91, 103       | 0     |
| 67  | o1    | 109/112 (97%)  | 0.46   | 6 (5%) 30 21  | 47, 58, 81, 90        | 0     |
| 68  | O2    | 127/129 (98%)  | 0.26   | 4 (3%) 51 35  | 36, 49, 62, 68        | 0     |
| 68  | o2    | 127/129 (98%)  | 0.34   | 4 (3%) 51 35  | 35, 52, 63, 71        | 0     |
| 69  | O3    | 106/106 (100%) | 0.35   | 3 (2%) 55 36  | 42, 47, 71, 78        | 0     |
| 69  | o3    | 106/106 (100%) | 0.31   | 0 100 100     | 40, 46, 69, 75        | 0     |
| 70  | O4    | 112/120 (93%)  | 0.97   | 12 (10%) 11 9 | 57, 75, 101, 107      | 0     |
| 70  | o4    | 112/120 (93%)  | 0.80   | 7 (6%) 26 17  | 50, 68, 99, 103       | 0     |
| 71  | O5    | 119/119 (100%) | 0.71   | 7 (5%) 28 19  | 55, 70, 78, 82        | 0     |
| 71  | o5    | 119/119 (100%) | 0.71   | 9 (7%) 20 14  | 59, 71, 87, 96        | 0     |
| 72  | O6    | 99/99 (100%)   | 0.39   | 2 (2%) 65 46  | 60, 68, 91, 102       | 0     |
| 72  | o6    | 99/99 (100%)   | 0.43   | 2 (2%) 65 46  | 64, 72, 88, 103       | 0     |
| 73  | O7    | 87/87 (100%)   | 0.78   | 7 (8%) 18 14  | 43, 50, 65, 71        | 0     |
| 73  | o7    | 87/87 (100%)   | 0.58   | 3 (3%) 48 32  | 41, 50, 73, 84        | 0     |
| 74  | O8    | 77/77 (100%)   | 0.57   | 3 (3%) 43 29  | 83, 93, 108, 113      | 0     |
| 74  | o8    | 77/77 (100%)   | 0.65   | 3 (3%) 43 29  | 77, 86, 94, 98        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-------------------|--------|-----------------|-----------------------|----------|
| 75  | O9    | 50/50 (100%)      | 0.73   | 6 (12%) 9 7     | 52, 57, 59, 60        | 0        |
| 75  | o9    | 50/50 (100%)      | 0.55   | 4 (8%) 18 14    | 50, 55, 63, 63        | 0        |
| 76  | Q0    | 52/52 (100%)      | 0.25   | 1 (1%) 66 48    | 53, 59, 74, 79        | 0        |
| 76  | q0    | 52/52 (100%)      | -0.08  | 0 100 100       | 41, 45, 55, 58        | 0        |
| 77  | Q1    | 25/25 (100%)      | 0.89   | 3 (12%) 9 7     | 62, 66, 73, 74        | 0        |
| 77  | q1    | 25/25 (100%)      | 0.66   | 1 (4%) 42 28    | 50, 56, 58, 58        | 0        |
| 78  | Q2    | 105/105 (100%)    | 0.33   | 3 (2%) 53 35    | 41, 56, 76, 91        | 0        |
| 78  | q2    | 105/105 (100%)    | 0.29   | 3 (2%) 53 35    | 44, 56, 70, 93        | 0        |
| 79  | Q3    | 91/91 (100%)      | 0.86   | 7 (7%) 19 14    | 54, 65, 80, 85        | 0        |
| 79  | q3    | 91/91 (100%)      | 0.52   | 3 (3%) 49 33    | 46, 59, 72, 84        | 0        |
| 80  | m2    | 0/165             | -      | -               | -                     | -        |
| 81  | p0    | 120/311 (38%)     | 1.33   | 30 (25%) 2 1    | 101, 124, 144, 152    | 0        |
| 82  | p1    | 0/47              | -      | -               | -                     | -        |
| 82  | p2    | 0/47              | -      | -               | -                     | -        |
| 83  | f     | 148/157 (94%)     | 2.12   | 75 (50%) 0 0    | 44, 82, 144, 147      | 75 (50%) |
| All | All   | 33080/35493 (93%) | 0.55   | 2267 (6%) 23 16 | 34, 74, 132, 212      | 77 (0%)  |

The worst 5 of 2267 RSRZ outliers are listed below:

| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 22  | d0    | 64      | LYS  | 9.9  |
| 7   | S5    | 152     | GLY  | 9.6  |
| 60  | N4    | 86      | SER  | 8.6  |
| 47  | m0    | 221     | ALA  | 8.5  |
| 1   | 2     | 1756[A] | A    | 8.2  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 85  | ZN   | D7    | 101  | 1/1   | 0.84 | 0.11 | 141,141,141,141             | 0     |
| 85  | ZN   | d7    | 101  | 1/1   | 0.84 | 0.10 | 131,131,131,131             | 0     |
| 87  | MG   | 5     | 3402 | 1/1   | 0.84 | 0.12 | 45,45,45,45                 | 0     |
| 87  | MG   | 5     | 3404 | 1/1   | 0.84 | 0.26 | 36,36,36,36                 | 0     |
| 87  | MG   | C     | 101  | 1/1   | 0.85 | 0.26 | 49,49,49,49                 | 0     |
| 87  | MG   | 5     | 3405 | 1/1   | 0.86 | 0.32 | 42,42,42,42                 | 0     |
| 87  | MG   | 1     | 3402 | 1/1   | 0.88 | 0.45 | 21,21,21,21                 | 0     |
| 87  | MG   | B     | 3402 | 1/1   | 0.90 | 0.25 | 40,40,40,40                 | 0     |
| 87  | MG   | 1     | 3404 | 1/1   | 0.91 | 0.26 | 29,29,29,29                 | 0     |
| 85  | ZN   | E1    | 501  | 1/1   | 0.93 | 0.06 | 136,136,136,136             | 0     |
| 87  | MG   | 5     | 3401 | 1/1   | 0.94 | 0.17 | 41,41,41,41                 | 0     |
| 85  | ZN   | e1    | 501  | 1/1   | 0.94 | 0.09 | 164,164,164,164             | 0     |
| 87  | MG   | 1     | 3403 | 1/1   | 0.95 | 0.18 | 45,45,45,45                 | 0     |
| 86  | SPS  | 1     | 3401 | 23/23 | 0.95 | 0.10 | 40,43,57,59                 | 0     |
| 86  | SPS  | B     | 3401 | 23/23 | 0.96 | 0.11 | 37,40,54,56                 | 0     |
| 85  | ZN   | d6    | 500  | 1/1   | 0.97 | 0.07 | 87,87,87,87                 | 0     |
| 85  | ZN   | D6    | 500  | 1/1   | 0.97 | 0.10 | 105,105,105,105             | 0     |
| 88  | OHX  | 1     | 3405 | 7/7   | 0.97 | 0.14 | 91,91,91,91                 | 0     |
| 85  | ZN   | Q2    | 501  | 1/1   | 0.98 | 0.11 | 76,76,76,76                 | 0     |
| 85  | ZN   | q2    | 501  | 1/1   | 0.98 | 0.10 | 77,77,77,77                 | 0     |
| 88  | OHX  | 5     | 3406 | 7/7   | 0.98 | 0.14 | 95,95,95,95                 | 0     |
| 85  | ZN   | D9    | 101  | 1/1   | 0.99 | 0.06 | 88,88,88,88                 | 0     |
| 87  | MG   | f     | 1002 | 1/1   | 0.99 | 0.04 | 66,66,66,66                 | 0     |
| 85  | ZN   | d9    | 101  | 1/1   | 0.99 | 0.03 | 94,94,94,94                 | 0     |
| 85  | ZN   | Q3    | 501  | 1/1   | 0.99 | 0.03 | 77,77,77,77                 | 0     |
| 87  | MG   | 5     | 3403 | 1/1   | 0.99 | 0.36 | 23,23,23,23                 | 0     |
| 88  | OHX  | 1     | 3406 | 7/7   | 0.99 | 0.06 | 73,73,73,73                 | 0     |
| 85  | ZN   | Q0    | 500  | 1/1   | 0.99 | 0.03 | 57,57,57,57                 | 0     |
| 85  | ZN   | q3    | 501  | 1/1   | 1.00 | 0.04 | 69,69,69,69                 | 0     |
| 85  | ZN   | o7    | 501  | 1/1   | 1.00 | 0.02 | 51,51,51,51                 | 0     |
| 85  | ZN   | q0    | 500  | 1/1   | 1.00 | 0.02 | 42,42,42,42                 | 0     |
| 87  | MG   | f     | 1001 | 1/1   | 1.00 | 0.21 | 52,52,52,52                 | 0     |
| 85  | ZN   | O7    | 100  | 1/1   | 1.00 | 0.03 | 52,52,52,52                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.