



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2025 – 03:12 PM EDT

PDB ID : 9B0F  
EMDB ID : EMD-44039  
Title : In situ human Hibernating class3 80S ribosome  
Authors : Wei, Z.; Yong, X.  
Deposited on : 2024-03-12  
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

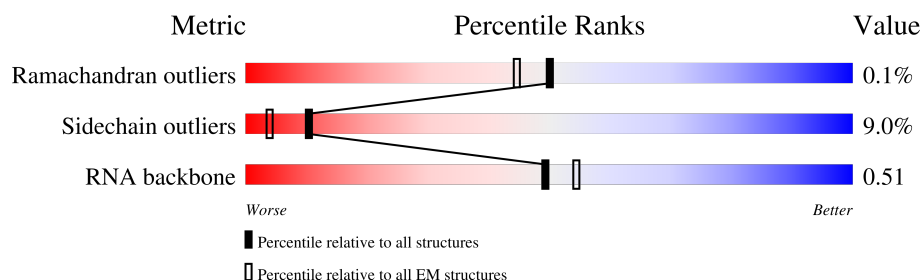
EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.78 Å.

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





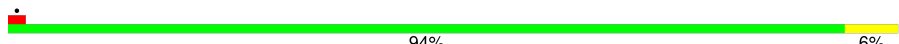
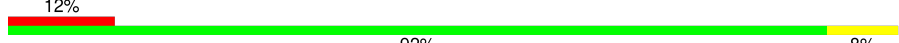

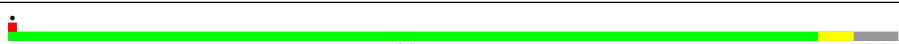


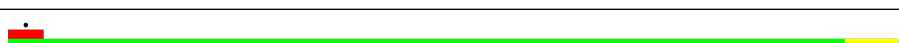
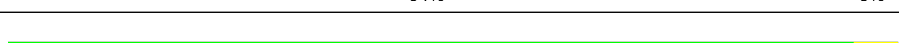
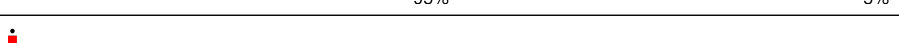
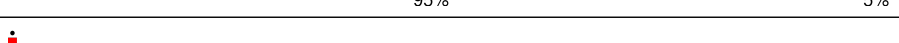
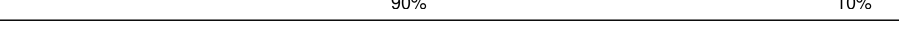
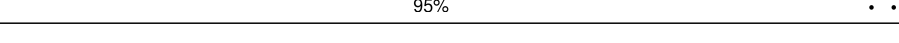
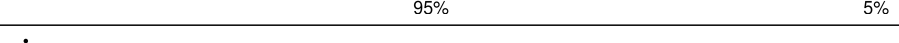
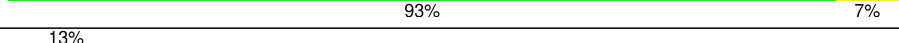

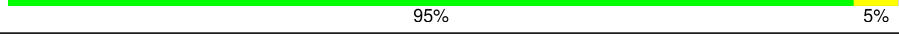
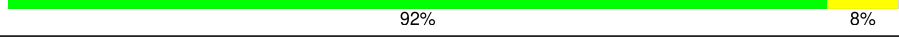
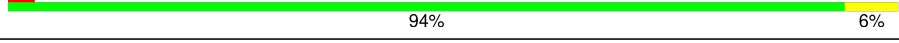
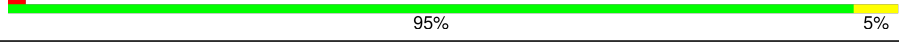
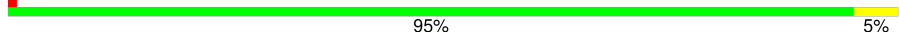


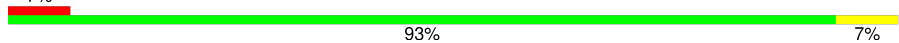
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |
| RNA backbone          | 6643                        | 2191                        |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | LR    | 187    | <div> <div>12%</div> <div>90%</div> <div>10%</div> </div>               |
| 2   | S2    | 1869   | <div> <div>9%</div> <div>68%</div> <div>25%</div> <div>7%</div> </div>  |
| 3   | L5    | 5070   | <div> <div>7%</div> <div>56%</div> <div>18%</div> <div>26%</div> </div> |
| 4   | L7    | 120    | <div> <div>88%</div> <div>12%</div> </div>                              |
| 5   | L8    | 156    | <div> <div>5%</div> <div>81%</div> <div>19%</div> </div>                |
| 6   | LA    | 248    | <div> <div>93%</div> <div>6%</div> </div>                               |
| 7   | LB    | 402    | <div> <div>94%</div> <div>6%</div> </div>                               |
| 8   | LC    | 368    | <div> <div>95%</div> <div>5%</div> </div>                               |

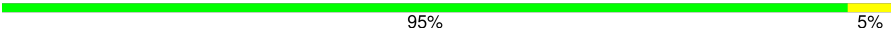
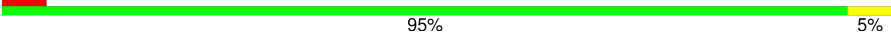
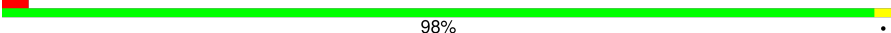
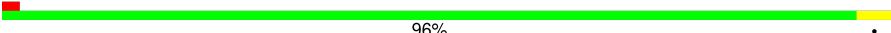
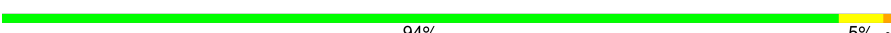







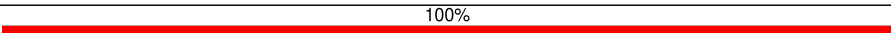





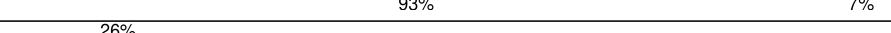

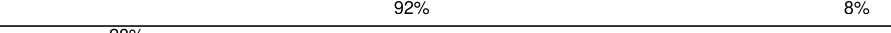




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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | LD    | 293    |    |
| 10  | LE    | 247    |    |
| 11  | LF    | 225    |    |
| 12  | LG    | 241    |    |
| 13  | LH    | 190    |    |
| 14  | LI    | 213    |    |
| 15  | LJ    | 176    |    |
| 16  | LL    | 210    |    |
| 17  | LM    | 139    |    |
| 18  | LN    | 203    |    |
| 19  | LO    | 201    |    |
| 20  | LP    | 153    |    |
| 21  | LQ    | 187    |  |
| 22  | LS    | 175    |  |
| 23  | LT    | 159    |  |
| 24  | LU    | 101    |  |
| 25  | LV    | 131    |  |
| 26  | LX    | 120    |  |
| 27  | LY    | 134    |  |
| 28  | LZ    | 135    |  |
| 29  | La    | 147    |  |
| 30  | Lb    | 121    |  |
| 31  | Lc    | 98     |  |
| 32  | Ld    | 107    |  |
| 33  | Le    | 128    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | Lf    | 109    |    |
| 35  | Lg    | 114    |    |
| 36  | Lh    | 122    |    |
| 37  | Li    | 102    |    |
| 38  | Lj    | 86     |    |
| 39  | Lk    | 69     |    |
| 40  | Ll    | 50     |    |
| 41  | Lm    | 52     |    |
| 42  | Ln    | 24     |    |
| 43  | Lo    | 105    |    |
| 44  | Lp    | 91     |    |
| 45  | Lr    | 125    |    |
| 46  | Lz    | 217    |  |
| 47  | CA    | 356    |  |
| 48  | Ls    | 196    |  |
| 49  | Lt    | 141    |  |
| 50  | SD    | 227    |  |
| 51  | SF    | 189    |  |
| 52  | SK    | 98     |  |
| 53  | SP    | 121    |  |
| 54  | SQ    | 144    |  |
| 55  | SS    | 145    |  |
| 56  | ST    | 143    |  |
| 57  | SU    | 104    |  |
| 58  | Sc    | 64     |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 59  | Sd    | 55     |                  |
| 60  | Sg    | 313    |                  |
| 61  | SM    | 122    |                  |
| 62  | SZ    | 75     |                  |
| 63  | Sf    | 67     |                  |
| 64  | CD    | 55     |                  |
| 65  | LW    | 124    |                  |
| 66  | SE    | 262    |                  |
| 67  | SI    | 206    |                  |
| 68  | SL    | 153    |                  |
| 69  | SX    | 141    |                  |
| 70  | SG    | 237    |                  |
| 71  | SJ    | 185    |                  |
| 72  | SY    | 131    |                  |
| 73  | Se    | 58     |                  |
| 74  | SA    | 221    |                  |
| 75  | SB    | 214    |                  |
| 76  | SH    | 189    |                  |
| 77  | SV    | 83     |                  |
| 78  | Sa    | 102    |                  |
| 79  | SC    | 222    |                  |
| 80  | SN    | 150    |                  |
| 81  | SO    | 140    |                  |
| 82  | SW    | 129    |                  |
| 83  | Sb    | 83     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 84  | CB    | 856    | <div><div></div><div>29%</div><div></div><div>89%</div><div></div><div>9%</div><div></div></div>               |
| 85  | Et    | 75     | <div><div></div><div>27%</div><div></div><div>73%</div><div></div><div>68%</div><div></div><div>5%</div></div> |

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 229857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | LR    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 971 | 336 | 250 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 2   | S2    | 1740     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36898 | 16459 | 6599 | 12101 | 1739 |         |       |

- Molecule 3 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | L5    | 3740     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 79860 | 35549 | 14585 | 25987 | 3739 |         |       |

- Molecule 4 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | L7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2561  | 1141 | 456 | 844 | 120 |         |       |

- Molecule 5 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5   | L8    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3314  | 1480 | 585 | 1094 | 155 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | LA    | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1898  | 1189 | 389 | 314 | 6 |         |       |

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | LB    | 402      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3238  | 2060 | 608 | 556 | 14 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | LC    | 368      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2927  | 1840 | 583 | 489 | 15 |         |       |

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | LD    | 293      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2382  | 1507 | 434 | 427 | 14 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | LE    | 236      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1904  | 1222 | 361 | 317 | 4 |         |       |

- Molecule 11 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | LF    | 225      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1870  | 1202 | 358 | 301 | 9 |         |       |

- Molecule 12 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | LG    | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1927  | 1228 | 371 | 324 | 4 |         |       |

- Molecule 13 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | LH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 956 | 284 | 272 | 6 |         |       |

- Molecule 14 is a protein called Ribosomal protein uL16-like.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | LI    | 202      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1037 | 314 | 269 | 14 |         |       |

- Molecule 15 is a protein called 60S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | LJ    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1410  | 888 | 263 | 253 | 6 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | LL    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1064 | 352 | 281 | 4 |         |       |

- Molecule 17 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | LM    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 730 | 218 | 183 | 7 |         |       |

- Molecule 18 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | LN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 19 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | LO    | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1650  | 1063 | 321 | 261 | 5 |         |       |

- Molecule 20 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | LP    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1242  | 776 | 241 | 216 | 9 |         |       |

- Molecule 21 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | LQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1513  | 944 | 314 | 250 | 5 |         |       |

- Molecule 22 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | LS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | LT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 24 is a protein called Heparin-binding protein HBp15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 529 | 144 | 150 | 2 |         |       |

- Molecule 25 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 630 | 185 | 169 | 1 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Lb    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 546 | 189 | 137 | 4 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | Lc    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Ld    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Le    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Lg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Lj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 39  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 41 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | Lm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | Ln    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Lo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L10a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | Lz    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1113 | 312 | 307 | 9 |         |       |

- Molecule 47 is a protein called Proliferation-associated protein 2G4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | CA    | 354      | Total | C    | N   | O   | S  | 4       | 0     |
|     |       |          | 2764  | 1744 | 475 | 528 | 17 |         |       |

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48  | Ls    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1496  | 952 | 259 | 276 | 9 |         |       |

- Molecule 49 is a protein called 60S ribosomal protein L12 [Homo sapiens].

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Lt    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1046  | 652 | 191 | 199 | 4 |         |       |

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | SD    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | SF    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | SK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | SP    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 623 | 185 | 170 | 7 |         |       |

- Molecule 54 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | SQ    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1142  | 726 | 216 | 197 | 3 |         |       |

- Molecule 55 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | SS    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 751 | 242 | 203 | 2 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56  | ST    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 697 | 214 | 198 | 3 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SU    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 58  | Sc    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 59  | Sd    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 60 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 60  | Sg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 61 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SM    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 940   | 590 | 164 | 177 | 9 |         |       |

- Molecule 62 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | SZ    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 63  | Sf    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 548   | 346 | 102 | 93 | 7 |         |       |

- Molecule 64 is a protein called Serbp1.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 64  | CD    | 55       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 440   | 263 | 87 | 90 |  |         |       |

- Molecule 65 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | LW    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 965   | 604 | 199 | 158 | 4 |         |       |

- Molecule 66 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 66  | SE    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 67  | SI    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | SL    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 793 | 234 | 214 | 6 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | SX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S6.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 70  | SG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | SJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | SY    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 673 | 209 | 178 | 5 |         |       |

- Molecule 73 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 73  | Se    | 58       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 459   | 284 | 100 | 74 | 1 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 74  | SA    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1106 | 305 | 322 | 8 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 75  | SB    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |

- Molecule 76 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | SH    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1497  | 956 | 274 | 266 | 1 |         |       |

- Molecule 77 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | SV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 78 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | Sa    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 512 | 171 | 133 | 5 |         |       |

- Molecule 79 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 79  | SC    | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1115 | 298 | 302 | 10 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 81 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | SO    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 642 | 204 | 197 | 6 |         |       |

- Molecule 82 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 83 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 84 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 84  | CB    | 846      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6605  | 4193 | 1136 | 1232 | 44 |         |       |

- Molecule 85 is a RNA chain called E site tRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 85  | Et    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1593  | 712 | 281 | 526 | 74 |         |       |

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 86  | S2    | 29       | Total | Mg  | 0       |
|     |       |          | 29    | 29  |         |
| 86  | L5    | 213      | Total | Mg  | 0       |
|     |       |          | 213   | 213 |         |
| 86  | L7    | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |
| 86  | L8    | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 86  | LA    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 86  | LI    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 86  | LP    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 86  | LV    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 86  | Le    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 86  | Lg    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 87  | Lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 87  | Lj    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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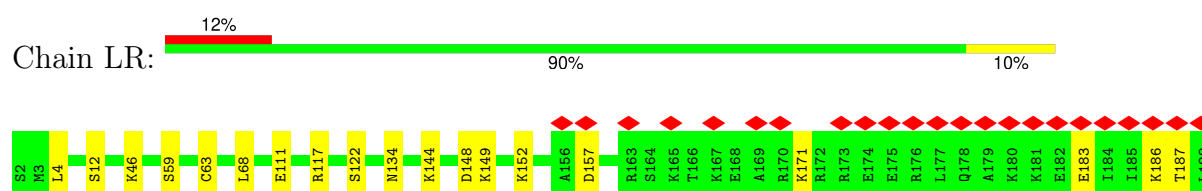
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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 87  | Lm    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 87  | Lo    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 87  | Lp    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 87  | Sa    | 1        | Total<br>1 | Zn<br>1 | 0       |

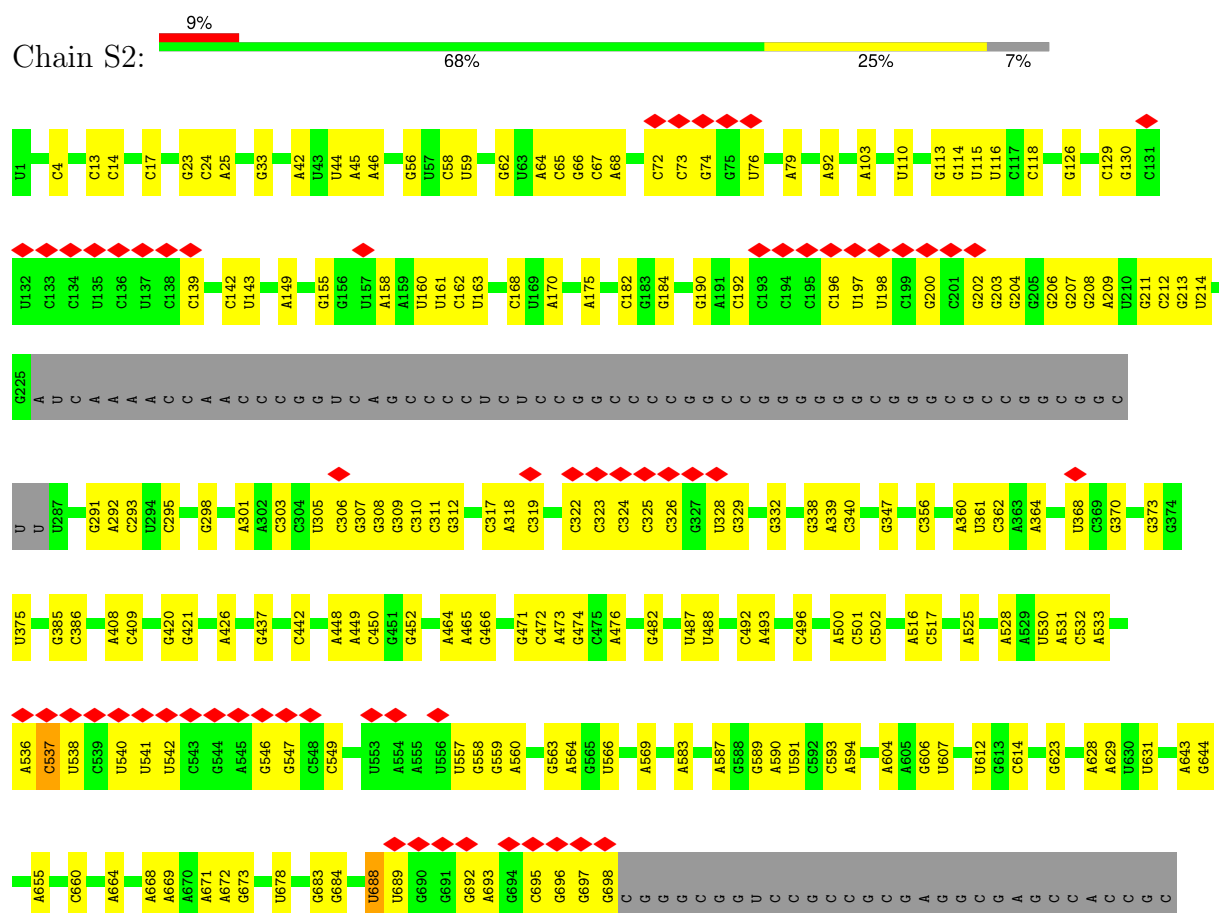
### 3 Residue-property plots

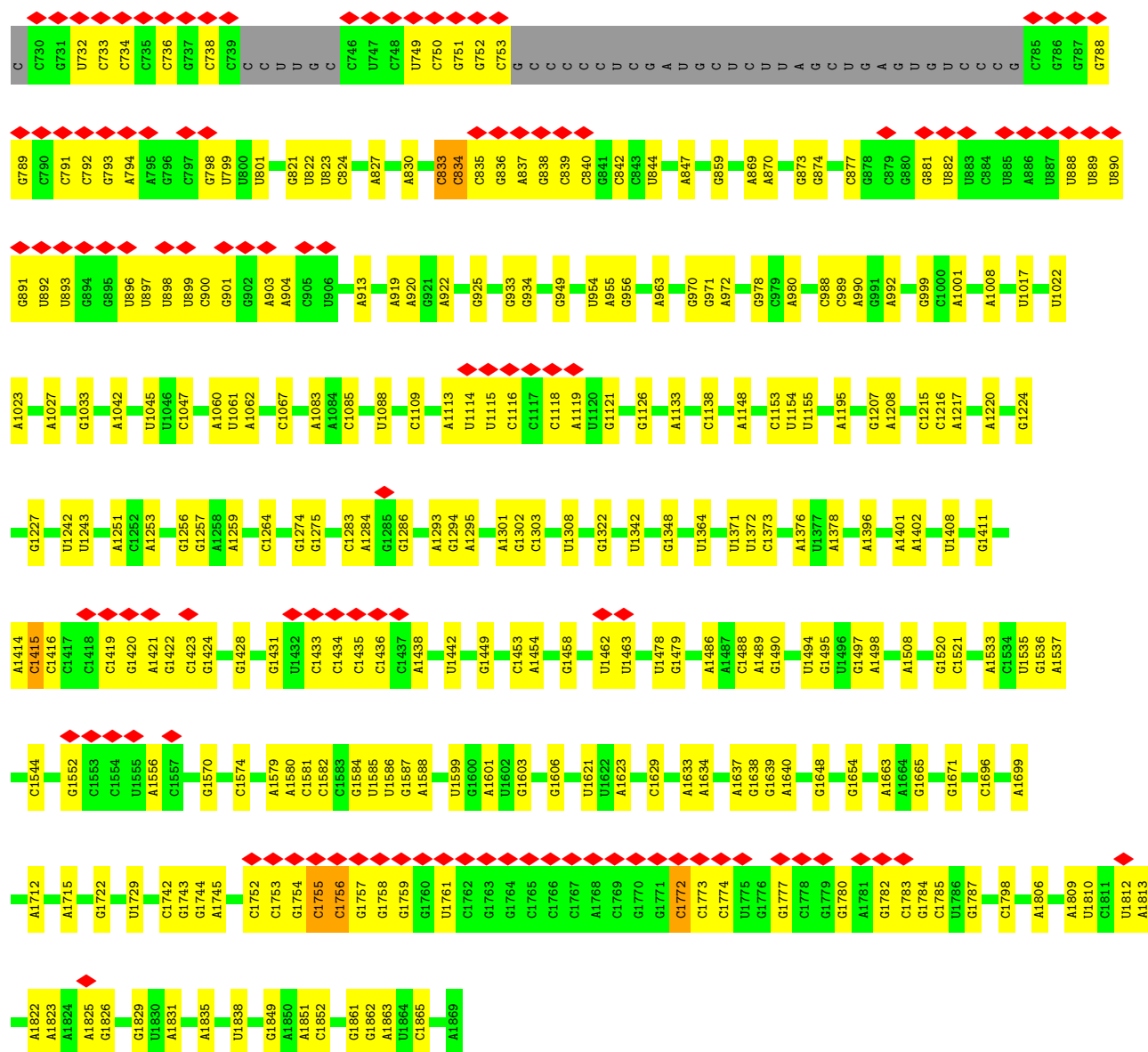
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 60S ribosomal protein L19

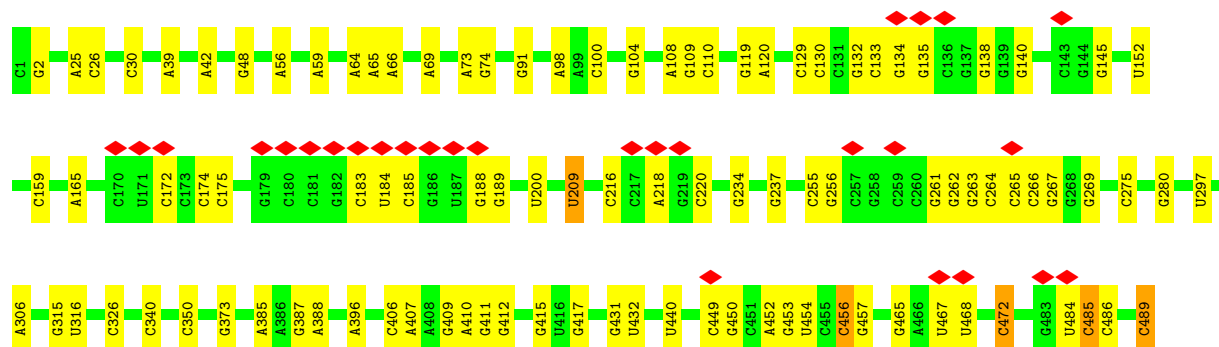


- Molecule 2: 18S rRNA





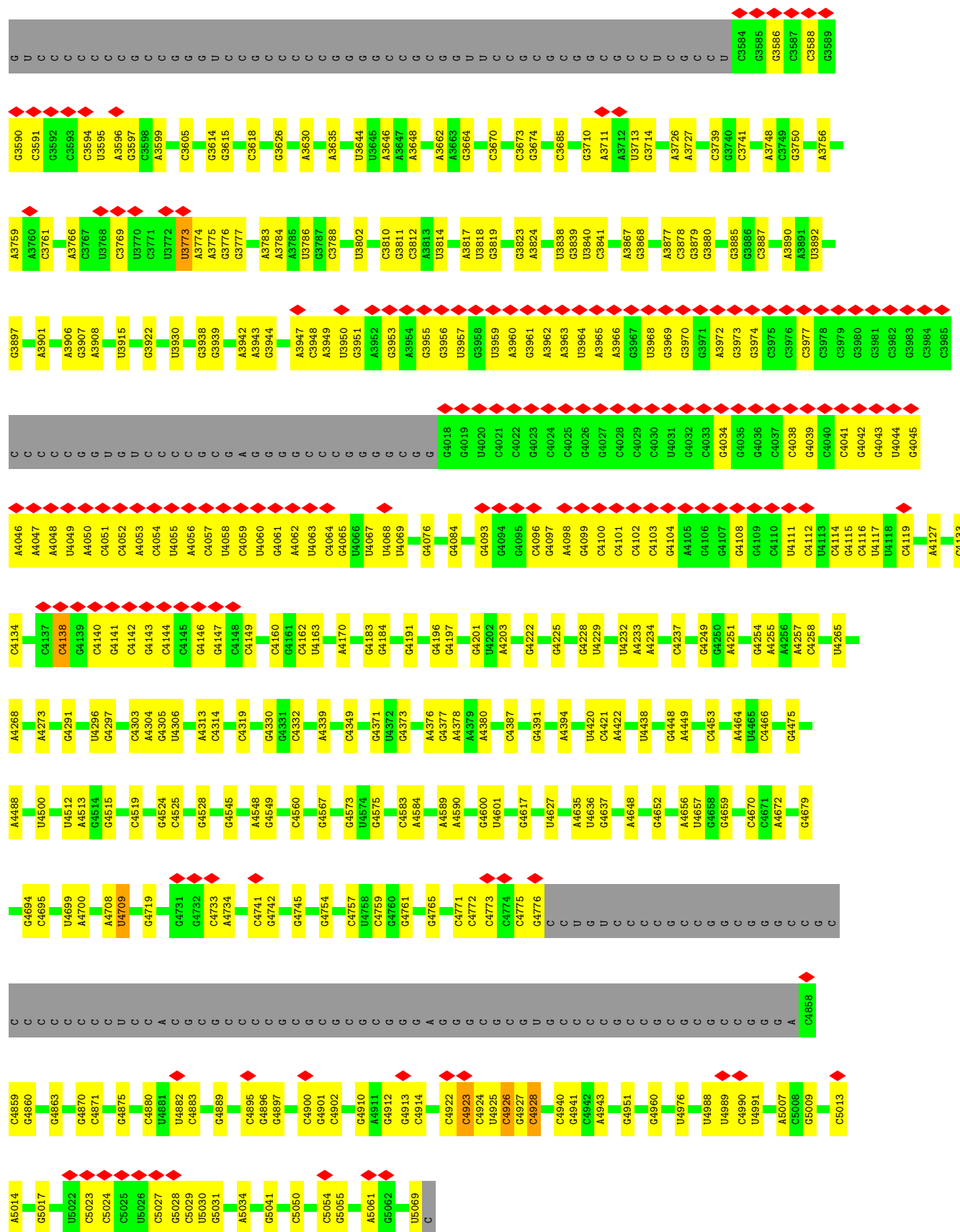
• Molecule 3: 28S rRNA



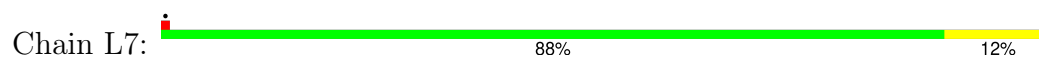




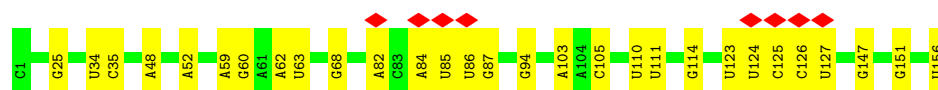
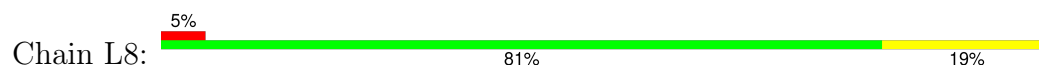




• Molecule 4: 5S rRNA



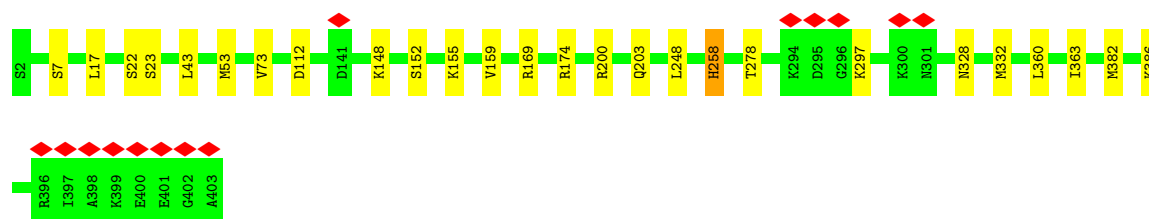
- Molecule 5: 5.8S rRNA



- Molecule 6: 60S ribosomal protein L8



- Molecule 7: Large ribosomal subunit protein uL3



- Molecule 8: 60S ribosomal protein L4

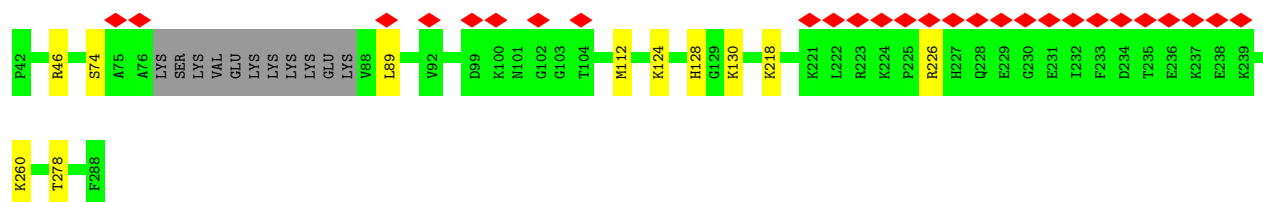


- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6

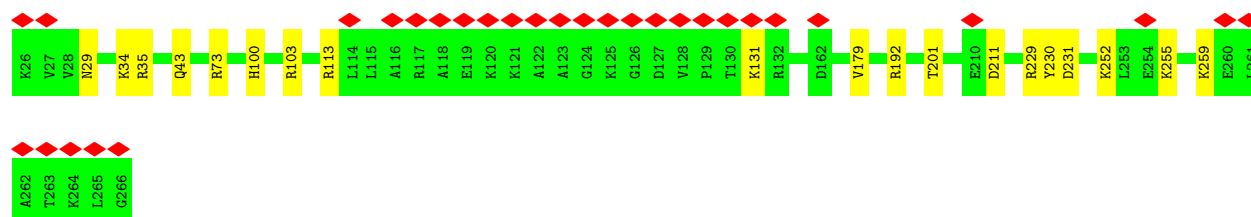




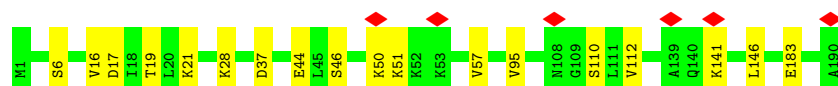
- Molecule 11: 60S ribosomal protein L7



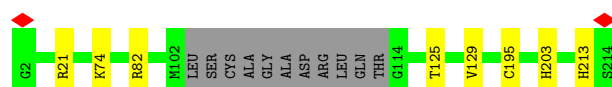
- Molecule 12: 60S ribosomal protein L7a



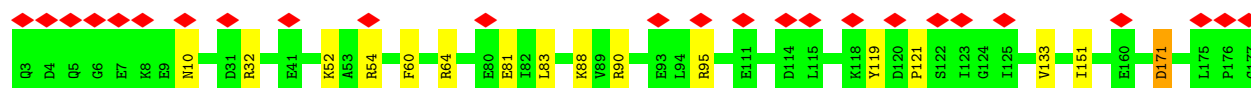
- Molecule 13: 60S ribosomal protein L9



- Molecule 14: Ribosomal protein uL16-like

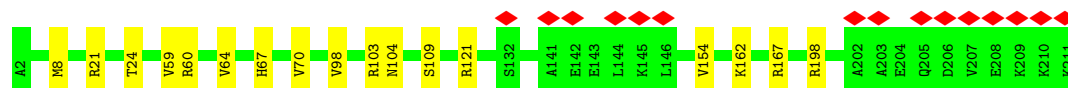
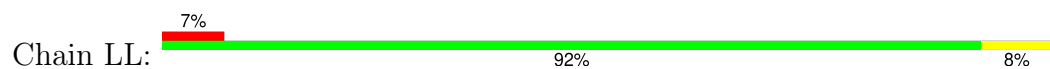


- Molecule 15: 60S ribosomal protein L11





- Molecule 16: Large ribosomal subunit protein eL13



- Molecule 17: 60S ribosomal protein L14



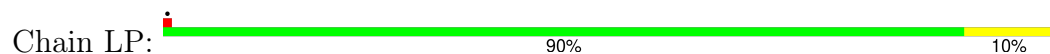
- Molecule 18: 60S ribosomal protein L15



- Molecule 19: 60S ribosomal protein L13a



- Molecule 20: 60S ribosomal protein L17

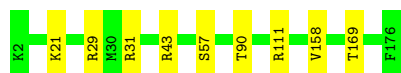


- Molecule 21: 60S ribosomal protein L18



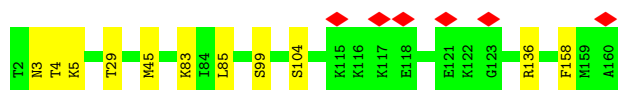
- Molecule 22: 60S ribosomal protein L18a

Chain LS:  95% 5%




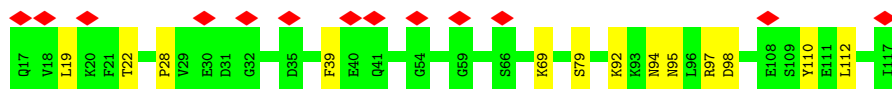
- Molecule 23: 60S ribosomal protein L21

Chain LT:  93% 7%



- Molecule 24: Heparin-binding protein HBp15

Chain LU:  13% 87% 13%



- Molecule 25: 60S ribosomal protein L23

Chain LV:  95% 5%



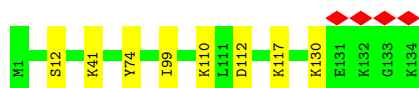
- Molecule 26: 60S ribosomal protein L23a

Chain LX:  92% 8%



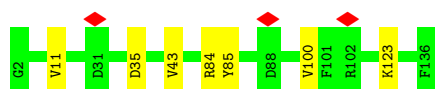
- Molecule 27: 60S ribosomal protein L26

Chain LY:  94% 6%



- Molecule 28: 60S ribosomal protein L27

Chain LZ:  95% 5%




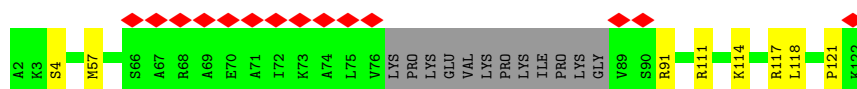
- Molecule 29: 60S ribosomal protein L27a

Chain La:  95% 5%

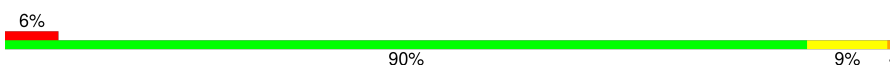


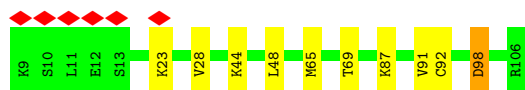
- Molecule 30: Large ribosomal subunit protein eL29

Chain Lb:  12% 83% 7% 10%



- Molecule 31: 60S ribosomal protein L30

Chain Lc:  6% 90% 9%



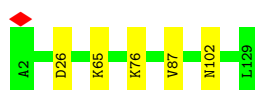
- Molecule 32: 60S ribosomal protein L31

Chain Ld:  7% 93% 7%



- Molecule 33: 60S ribosomal protein L32

Chain Le:  96%



- Molecule 34: 60S ribosomal protein L35a

Chain Lf:  95% 5%

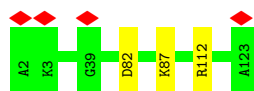


- Molecule 35: 60S ribosomal protein L34

Chain Lg:  5% 95% 5%



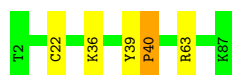
- Molecule 36: 60S ribosomal protein L35



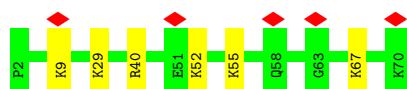
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37



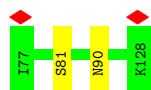
- Molecule 39: 60S ribosomal protein L38



- Molecule 40: 60S ribosomal protein L39

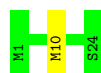


- Molecule 41: Large ribosomal subunit protein eL40



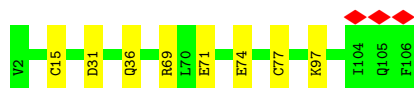
- Molecule 42: 60S ribosomal protein L41

Chain Ln:  96% .



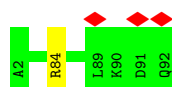
- Molecule 43: 60S ribosomal protein L36a

Chain Lo:  92% 8%




- Molecule 44: 60S ribosomal protein L37a

Chain Lp:  99% .



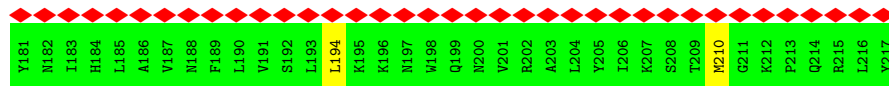
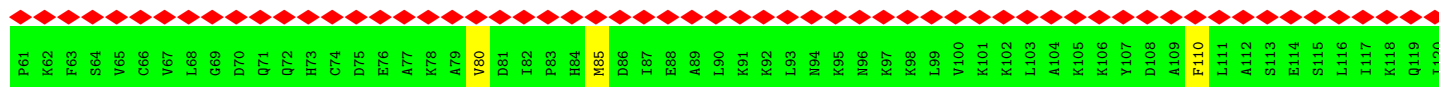
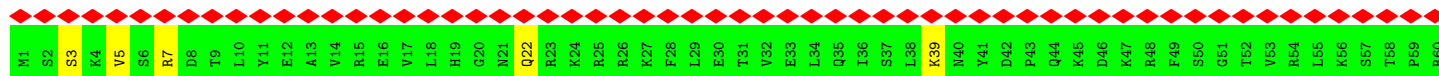
- Molecule 45: 60S ribosomal protein L28

Chain Lr:  87% 13%



- Molecule 46: 60S ribosomal protein L10a

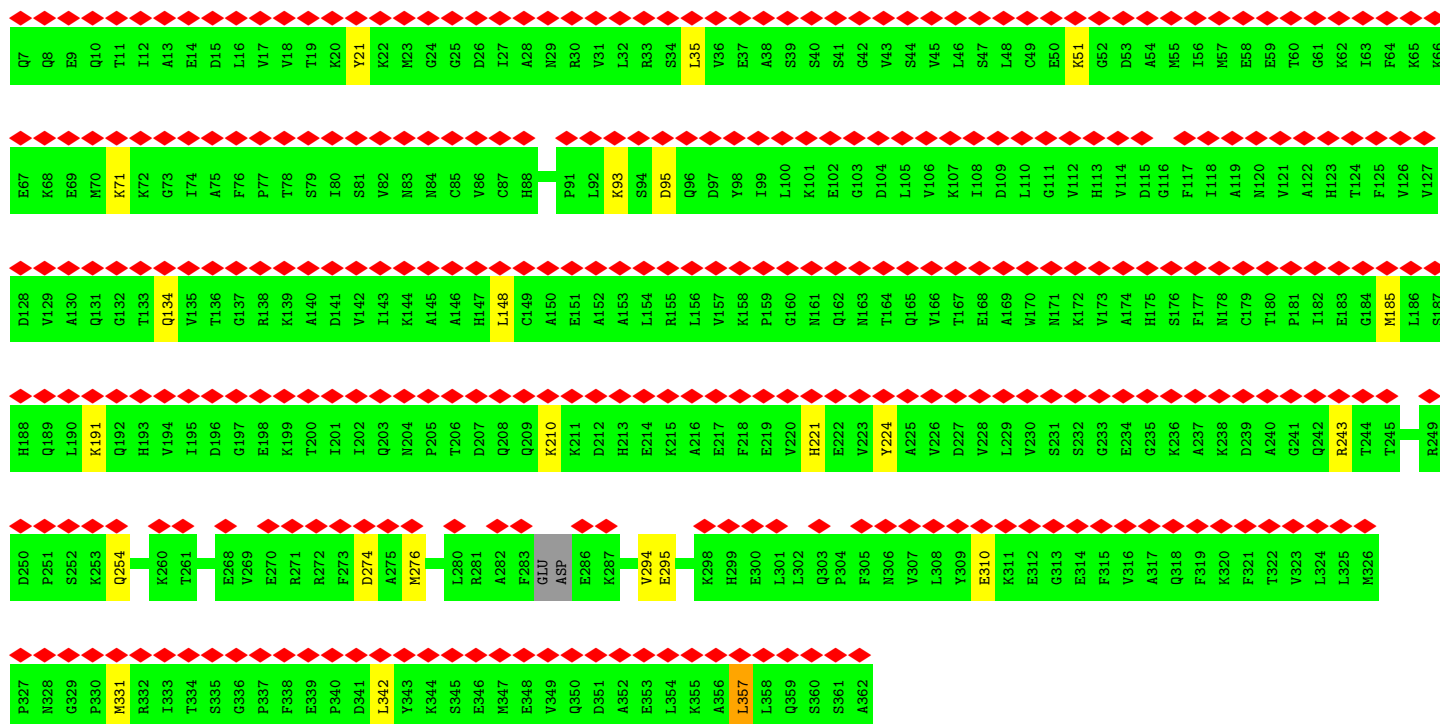
Chain Lz:  100% 93% 7%



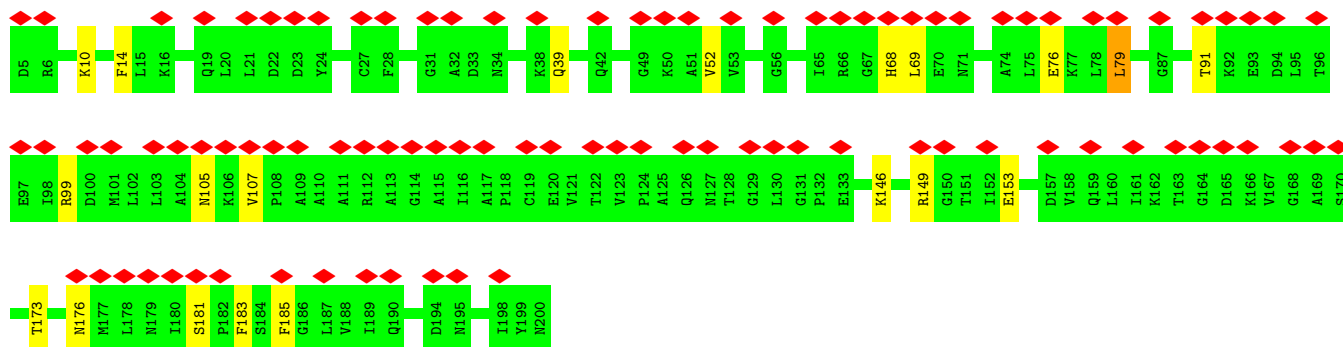
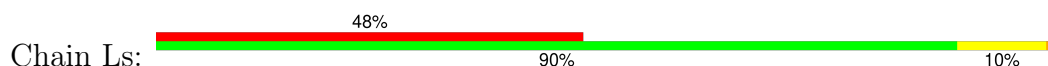
- Molecule 47: Proliferation-associated protein 2G4

Chain CA:  90% 93% 6% .

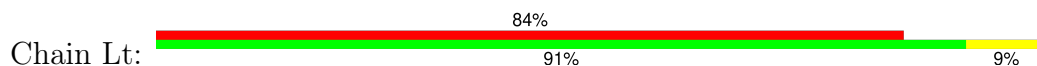




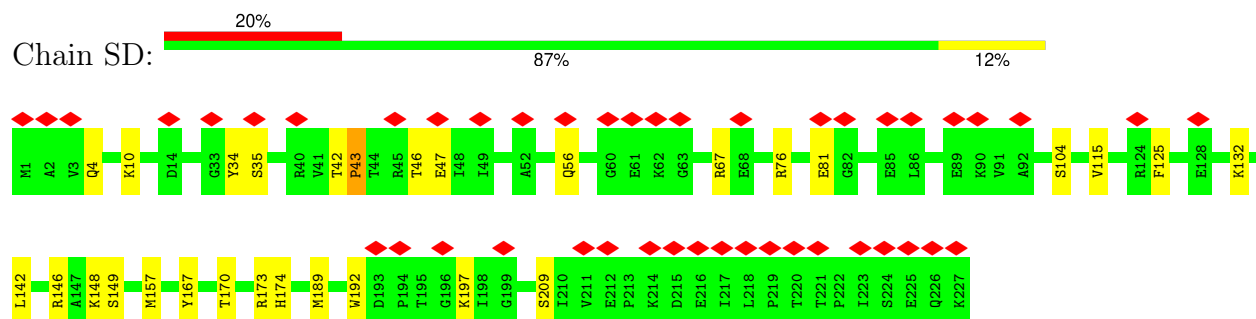
• Molecule 48: 60S acidic ribosomal protein P0



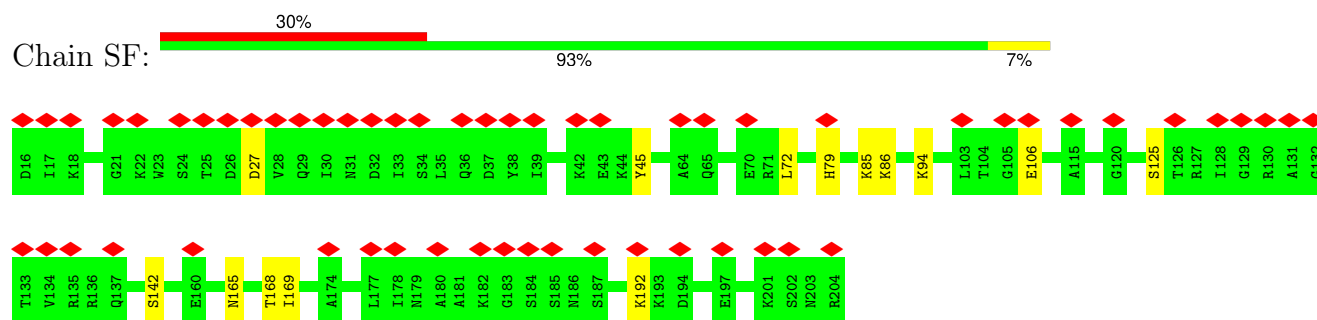
• Molecule 49: 60S ribosomal protein L12 [Homo sapiens]



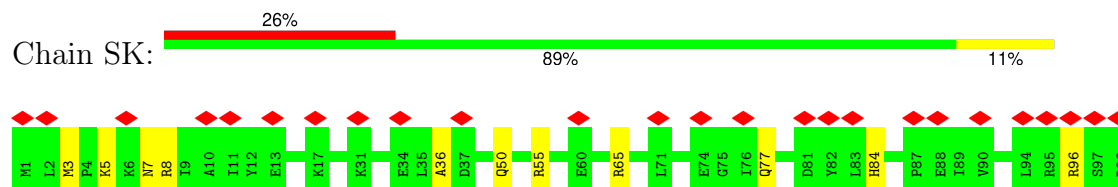
- Molecule 50: Small ribosomal subunit protein uS3



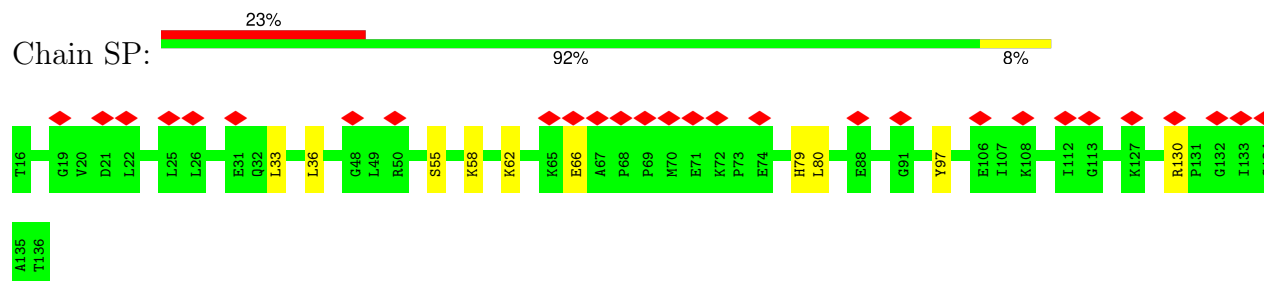
- Molecule 51: 40S ribosomal protein S5



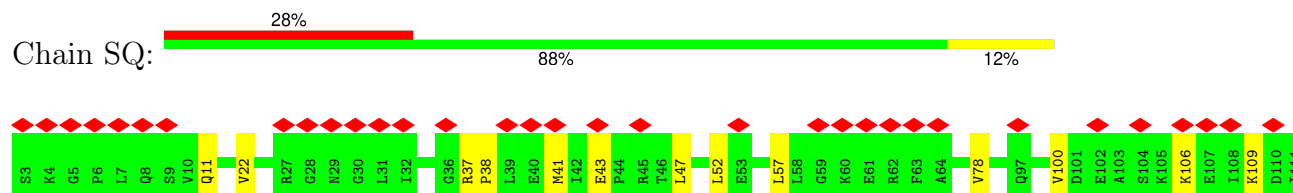
- Molecule 52: 40S ribosomal protein S10

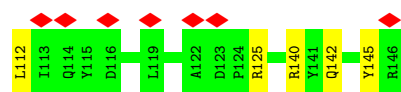


- Molecule 53: Small ribosomal subunit protein uS19

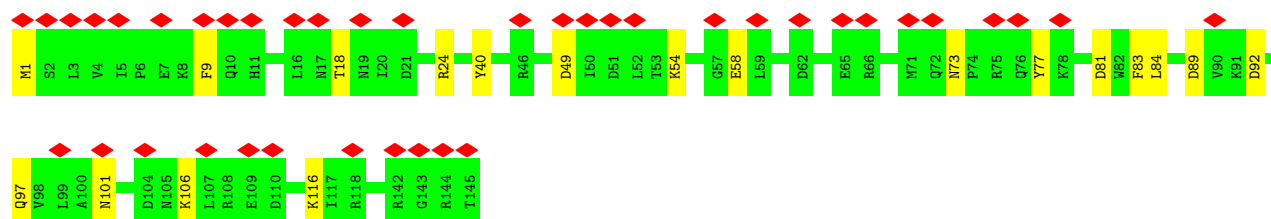
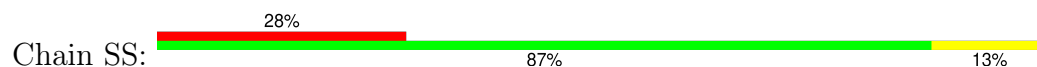


- Molecule 54: Small ribosomal subunit protein uS9

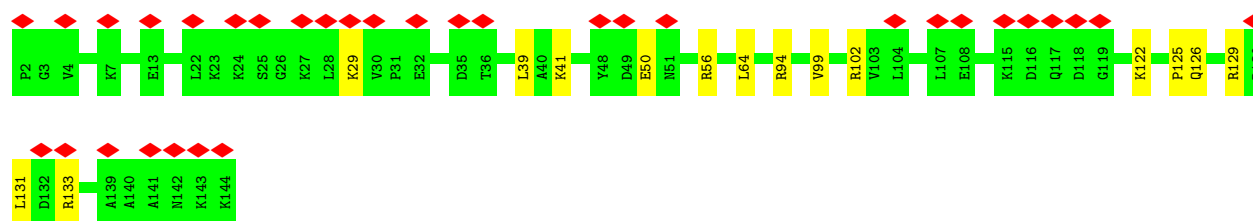
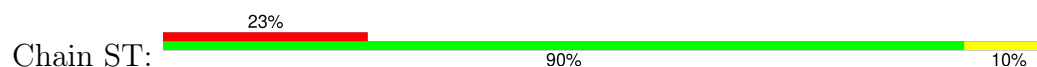




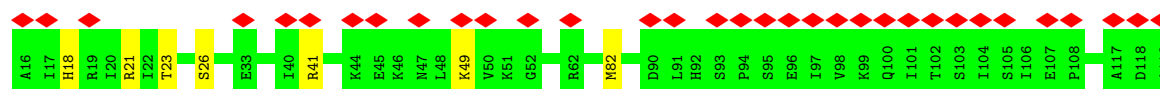
- Molecule 55: 40S ribosomal protein S18



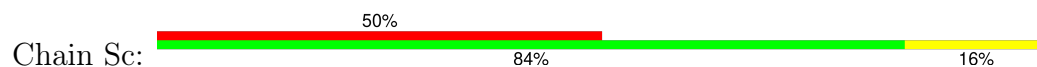
- Molecule 56: 40S ribosomal protein S19



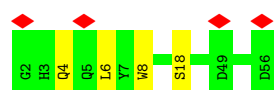
- Molecule 57: 40S ribosomal protein S20



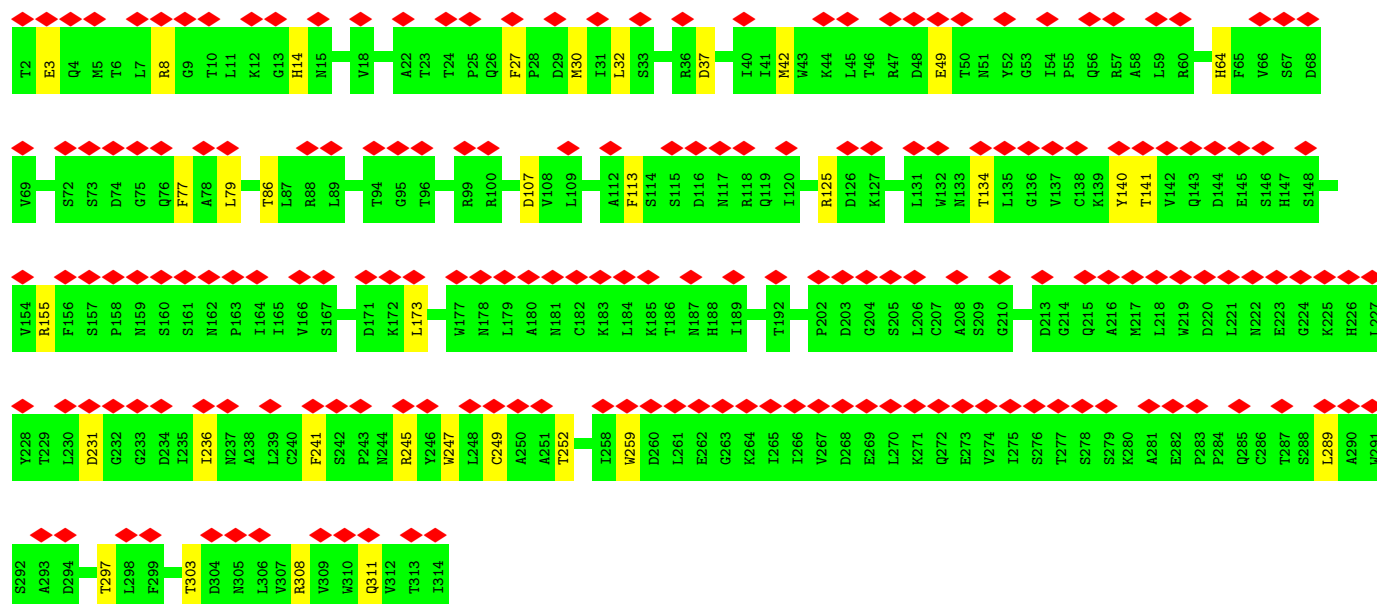
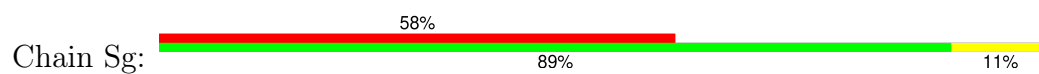
- Molecule 58: 40S ribosomal protein S28



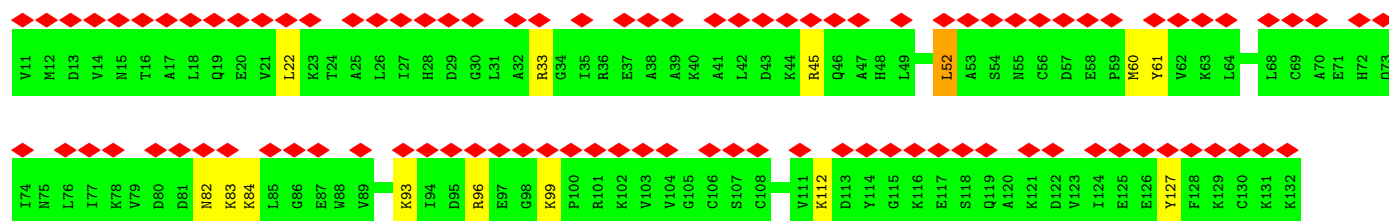
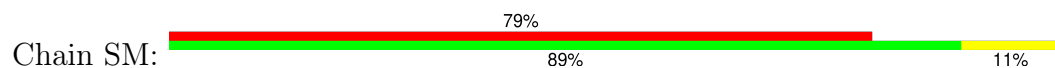
- Molecule 59: 40S ribosomal protein S29



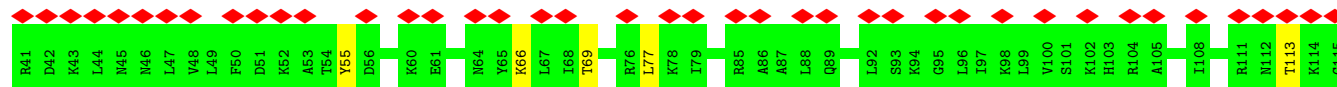
- Molecule 60: Receptor of activated protein C kinase 1



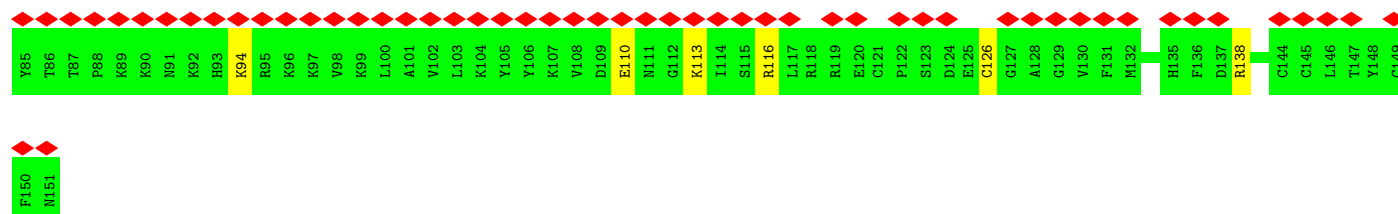
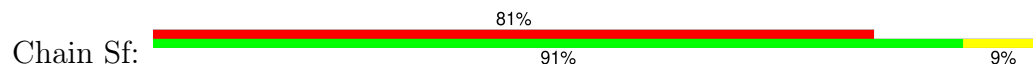
- Molecule 61: Small ribosomal subunit protein eS12



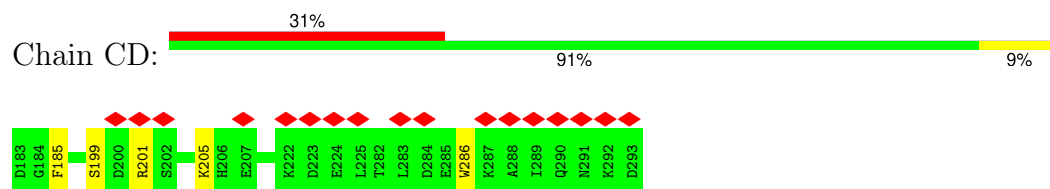
- Molecule 62: Small ribosomal subunit protein eS25



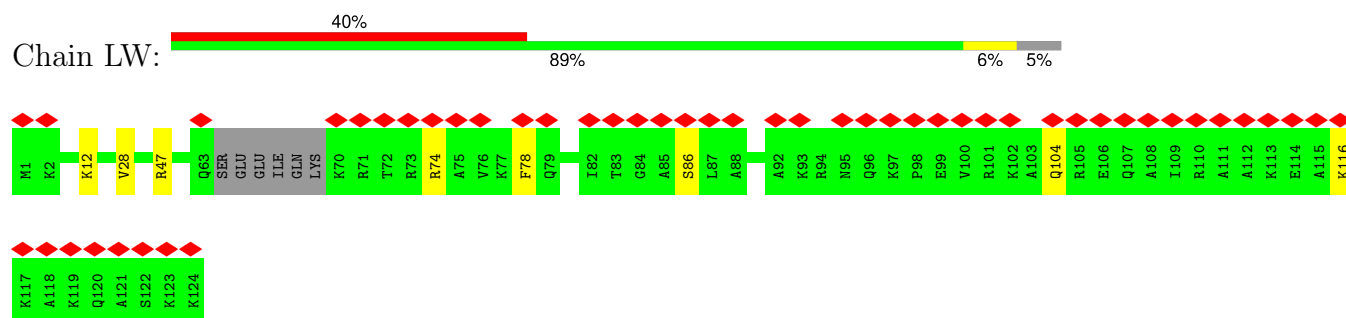
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



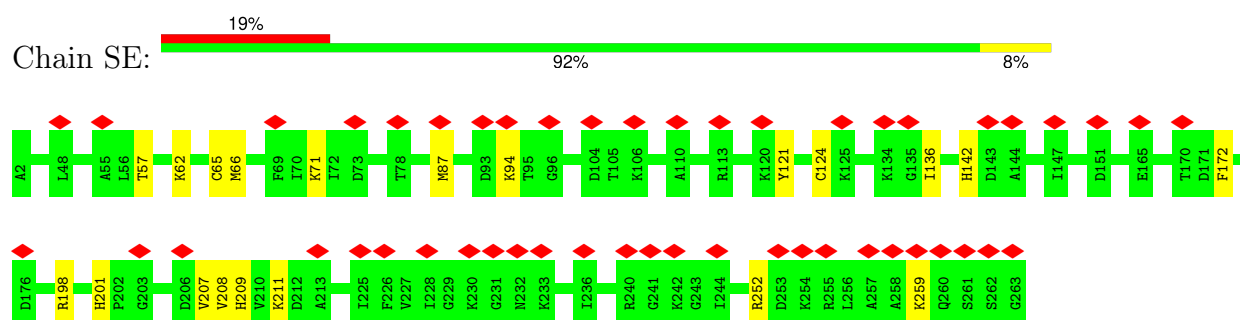
- Molecule 64: Serbp1



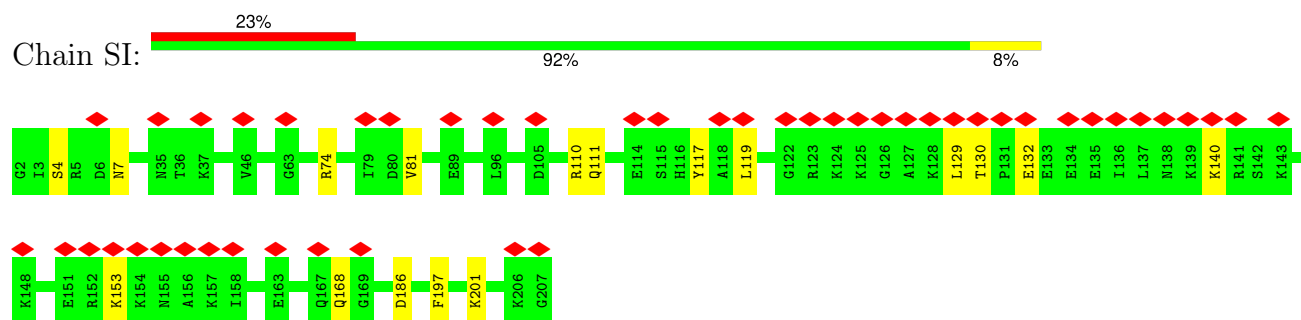
- Molecule 65: Ribosomal protein L24



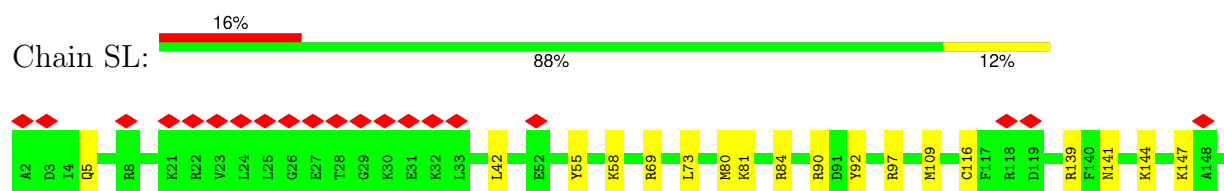
- Molecule 66: Small ribosomal subunit protein eS4, X isoform

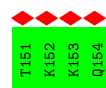


- Molecule 67: 40S ribosomal protein S8

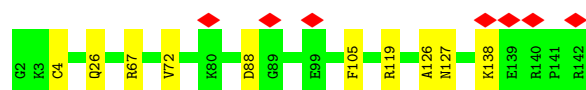


- Molecule 68: 40S ribosomal protein S11

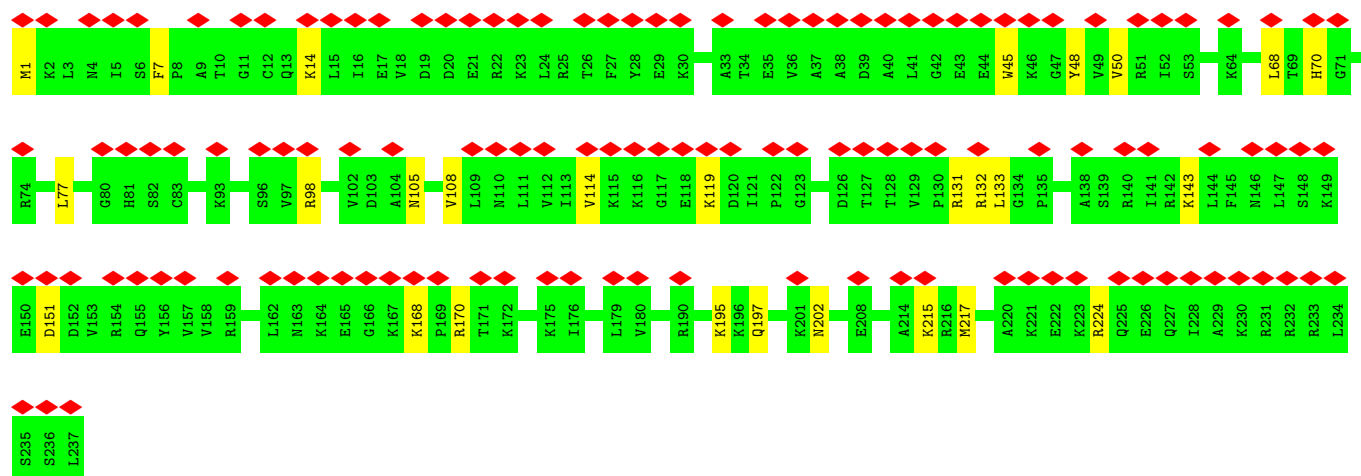
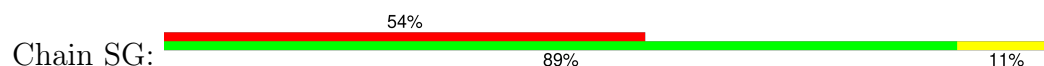




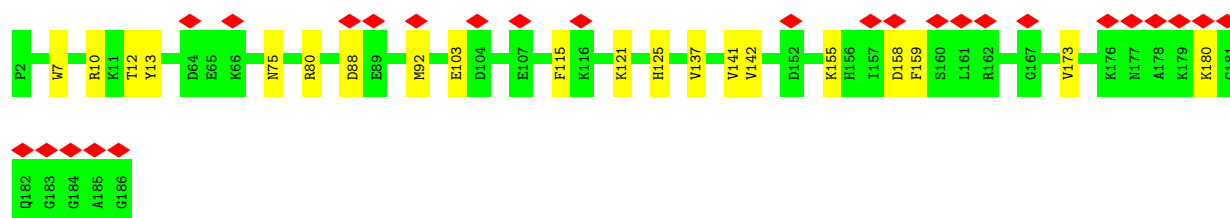
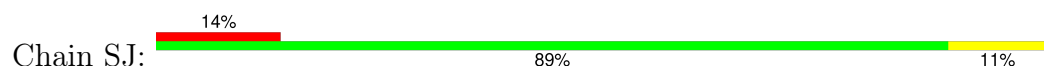
- Molecule 69: 40S ribosomal protein S23



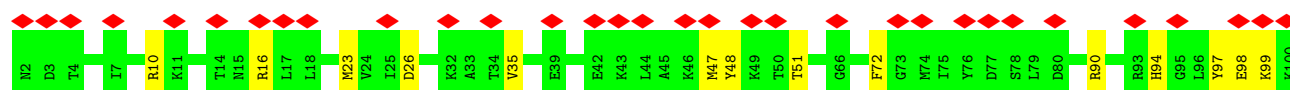
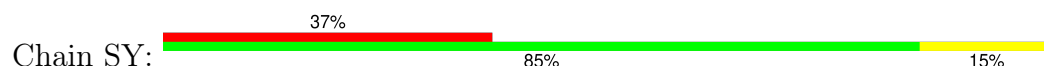
- Molecule 70: 40S ribosomal protein S6

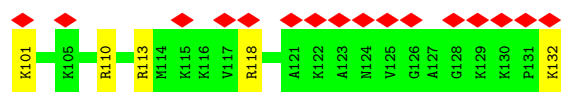


- Molecule 71: 40S ribosomal protein S9

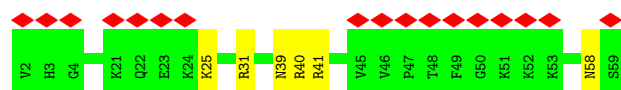
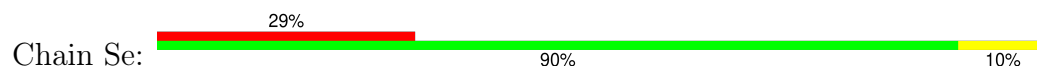


- Molecule 72: 40S ribosomal protein S24

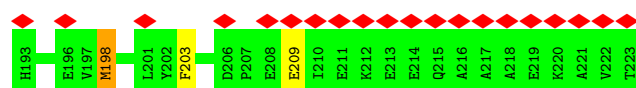
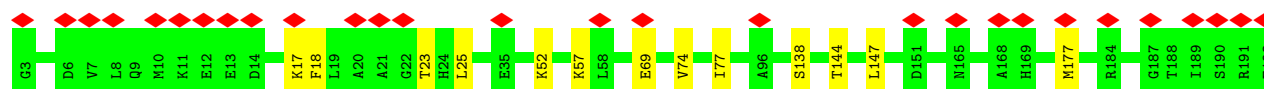




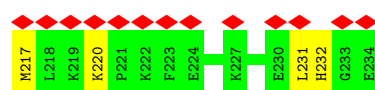
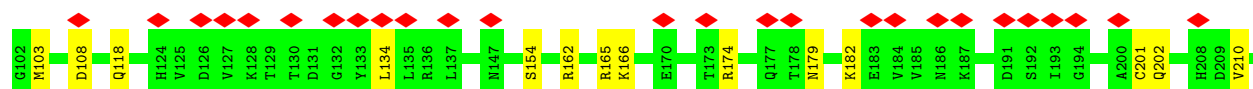
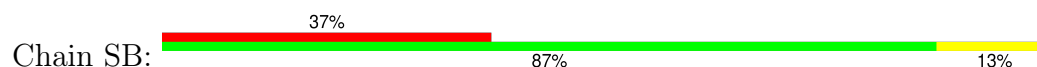
- Molecule 73: Small ribosomal subunit protein eS30



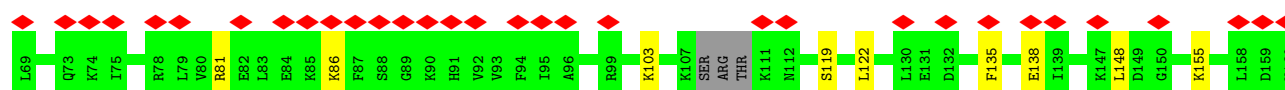
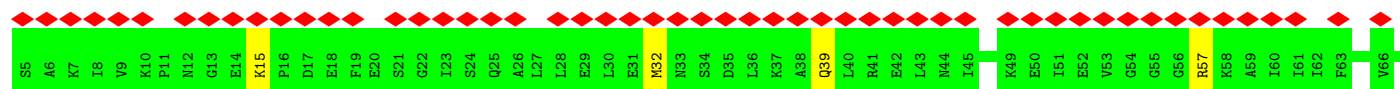
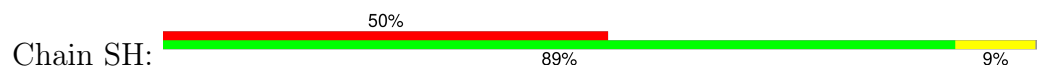
- Molecule 74: 40S ribosomal protein SA

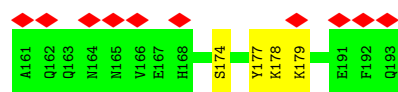


- Molecule 75: 40S ribosomal protein S3a

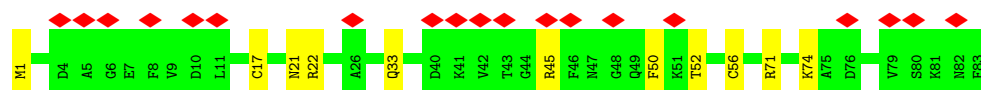
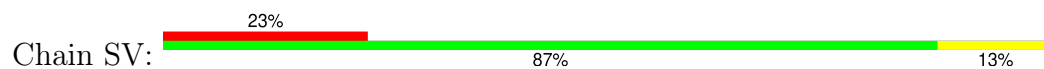


- Molecule 76: Small ribosomal subunit protein eS7

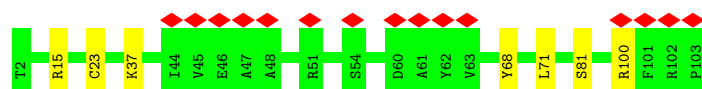




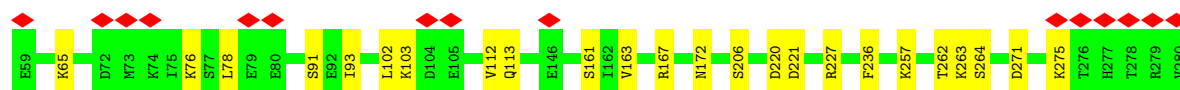
- Molecule 77: 40S ribosomal protein S21



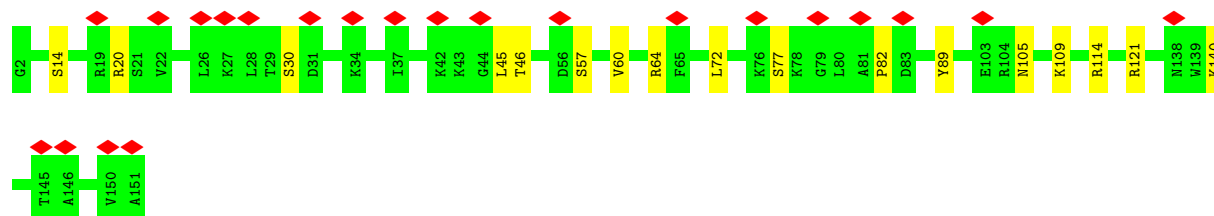
- Molecule 78: 40S ribosomal protein S26



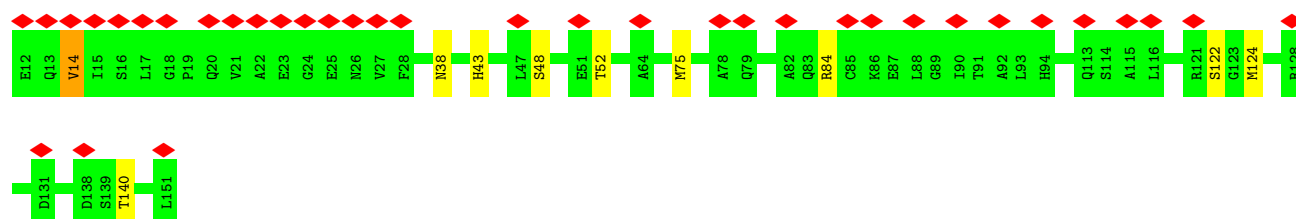
- Molecule 79: 40S ribosomal protein S2



- Molecule 80: 40S ribosomal protein S13



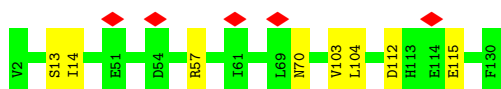
- Molecule 81: Small ribosomal subunit protein uS11




- Molecule 82: 40S ribosomal protein S15a

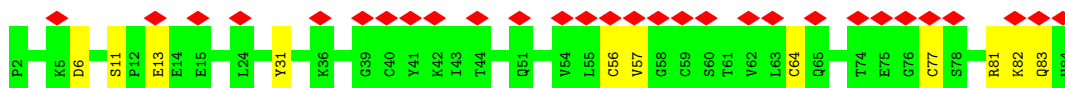


Chain SW:  94% 6%



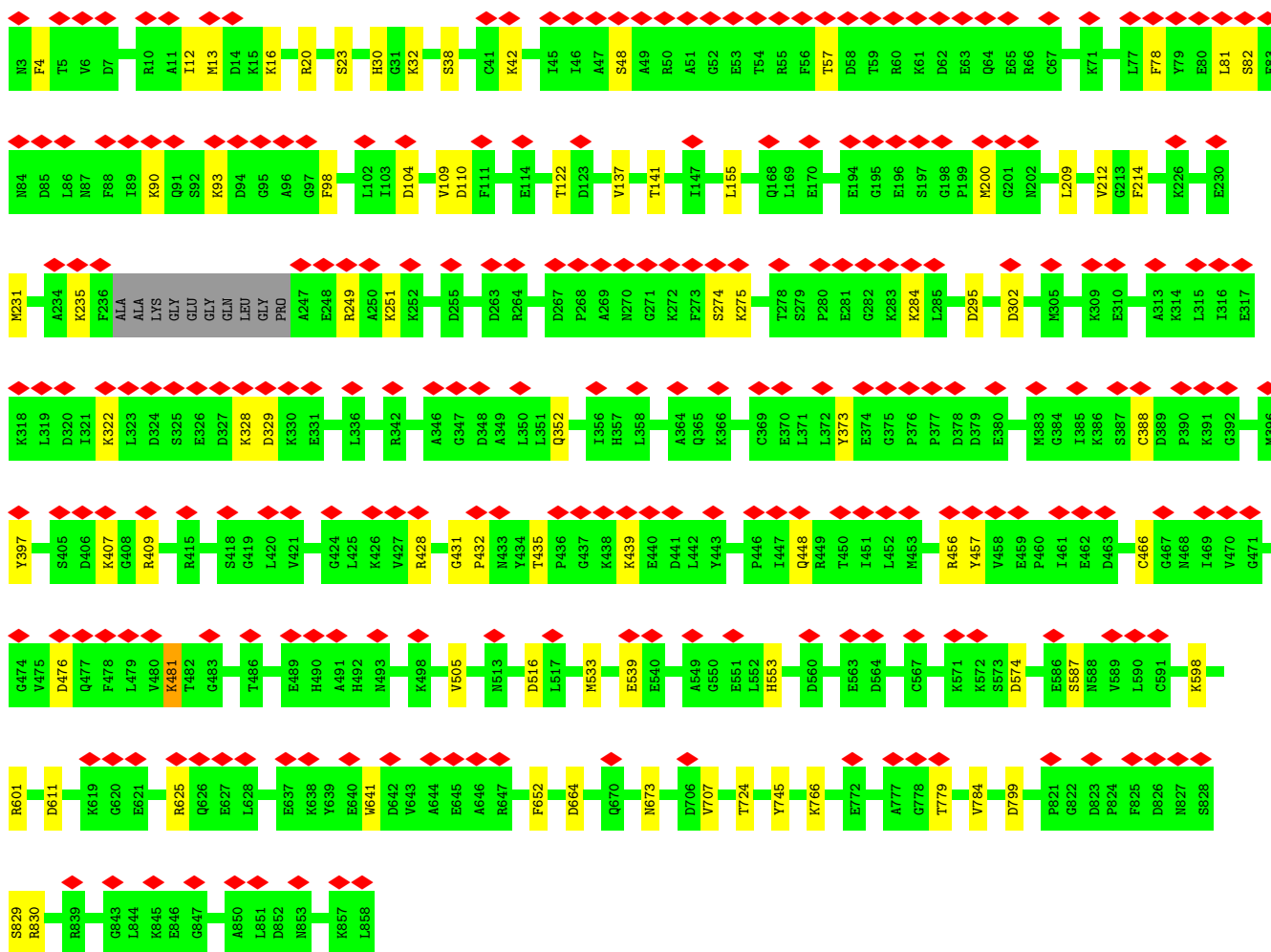
- Molecule 83: Small ribosomal subunit protein eS27

Chain Sb:  35% 87% 13%




- Molecule 84: Elongation factor 2

Chain CB:  29% 89% 9%



- Molecule 85: E site tRNA [Homo sapiens]

Chain Et:  27% 73% 68% 5%



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 54480                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | 1200                      | Depositor |
| Maximum defocus (nm)                 | 2500                      | Depositor |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K3 (6k x 4k)        | Depositor |
| Maximum map value                    | 0.495                     | Depositor |
| Minimum map value                    | -0.198                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.014                     | Depositor |
| Recommended contour level            | 0.05                      | Depositor |
| Map size ( $\text{\AA}$ )            | 546.816, 546.816, 546.816 | wwPDB     |
| Map dimensions                       | 512, 512, 512             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.068, 1.068, 1.068       | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | LR    | 0.31         | 0/1582      | 0.58        | 0/2091           |
| 2   | S2    | 0.41         | 0/41244     | 0.81        | 31/64263 (0.0%)  |
| 3   | L5    | 0.64         | 0/89313     | 0.86        | 97/139291 (0.1%) |
| 4   | L7    | 0.62         | 0/2861      | 0.78        | 0/4459           |
| 5   | L8    | 0.64         | 0/3701      | 0.78        | 0/5766           |
| 6   | LA    | 0.40         | 0/1936      | 0.62        | 0/2596           |
| 7   | LB    | 0.39         | 0/3306      | 0.59        | 0/4424           |
| 8   | LC    | 0.36         | 0/2981      | 0.59        | 1/4002 (0.0%)    |
| 9   | LD    | 0.36         | 0/2428      | 0.55        | 0/3252           |
| 10  | LE    | 0.34         | 0/1942      | 0.58        | 0/2606           |
| 11  | LF    | 0.38         | 0/1905      | 0.55        | 0/2539           |
| 12  | LG    | 0.34         | 0/1960      | 0.57        | 0/2637           |
| 13  | LH    | 0.36         | 0/1537      | 0.58        | 0/2066           |
| 14  | LI    | 0.36         | 0/1673      | 0.56        | 0/2233           |
| 15  | LJ    | 0.35         | 0/1433      | 0.68        | 2/1915 (0.1%)    |
| 16  | LL    | 0.36         | 0/1732      | 0.59        | 0/2315           |
| 17  | LM    | 0.36         | 0/1161      | 0.58        | 1/1554 (0.1%)    |
| 18  | LN    | 0.39         | 0/1746      | 0.59        | 0/2338           |
| 19  | LO    | 0.37         | 0/1682      | 0.56        | 0/2250           |
| 20  | LP    | 0.37         | 0/1268      | 0.53        | 0/1701           |
| 21  | LQ    | 0.37         | 0/1537      | 0.63        | 1/2052 (0.0%)    |
| 22  | LS    | 0.39         | 0/1493      | 0.58        | 0/2003           |
| 23  | LT    | 0.37         | 0/1326      | 0.56        | 0/1770           |
| 24  | LU    | 0.38         | 0/839       | 0.66        | 2/1126 (0.2%)    |
| 25  | LV    | 0.38         | 0/993       | 0.55        | 0/1332           |
| 26  | LX    | 0.35         | 0/1002      | 0.58        | 0/1345           |
| 27  | LY    | 0.37         | 0/1132      | 0.59        | 0/1504           |
| 28  | LZ    | 0.36         | 0/1130      | 0.58        | 0/1507           |
| 29  | La    | 0.38         | 0/1191      | 0.56        | 0/1591           |
| 30  | Lb    | 0.34         | 0/889       | 0.65        | 2/1175 (0.2%)    |
| 31  | Lc    | 0.35         | 0/774       | 0.58        | 1/1038 (0.1%)    |
| 32  | Ld    | 0.35         | 0/903       | 0.61        | 0/1216           |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 33  | Le    | 0.39         | 0/1071        | 0.56        | 0/1429        |
| 34  | Lf    | 0.41         | 0/895         | 0.63        | 0/1198        |
| 35  | Lg    | 0.36         | 0/916         | 0.61        | 0/1220        |
| 36  | Lh    | 0.32         | 0/1023        | 0.58        | 0/1351        |
| 37  | Li    | 0.32         | 0/843         | 0.58        | 0/1115        |
| 38  | Lj    | 1.03         | 3/720 (0.4%)  | 1.40        | 5/952 (0.5%)  |
| 39  | Lk    | 0.31         | 0/575         | 0.60        | 0/761         |
| 40  | Ll    | 0.33         | 0/454         | 0.59        | 0/599         |
| 41  | Lm    | 0.34         | 0/435         | 0.56        | 0/575         |
| 42  | Ln    | 0.28         | 0/231         | 0.74        | 0/294         |
| 43  | Lo    | 0.38         | 0/876         | 0.61        | 0/1156        |
| 44  | Lp    | 0.38         | 0/718         | 0.53        | 0/953         |
| 45  | Lr    | 0.36         | 0/1017        | 0.59        | 0/1364        |
| 46  | Lz    | 0.25         | 0/1769        | 0.57        | 1/2371 (0.0%) |
| 47  | CA    | 0.28         | 0/2810        | 0.53        | 1/3780 (0.0%) |
| 48  | Ls    | 0.29         | 0/1519        | 0.58        | 1/2052 (0.0%) |
| 49  | Lt    | 0.26         | 0/1058        | 0.64        | 1/1430 (0.1%) |
| 50  | SD    | 0.50         | 1/1793 (0.1%) | 0.83        | 3/2414 (0.1%) |
| 51  | SF    | 0.29         | 0/1516        | 0.60        | 0/2037        |
| 52  | SK    | 0.33         | 0/851         | 0.63        | 0/1147        |
| 53  | SP    | 0.29         | 0/1003        | 0.67        | 2/1342 (0.1%) |
| 54  | SQ    | 0.30         | 0/1160        | 0.65        | 1/1553 (0.1%) |
| 55  | SS    | 0.28         | 0/1216        | 0.64        | 0/1628        |
| 56  | ST    | 0.30         | 0/1131        | 0.62        | 1/1515 (0.1%) |
| 57  | SU    | 0.27         | 0/831         | 0.62        | 0/1115        |
| 58  | Sc    | 0.28         | 0/508         | 0.66        | 0/680         |
| 59  | Sd    | 0.31         | 0/470         | 0.58        | 0/623         |
| 60  | Sg    | 0.28         | 0/2493        | 0.61        | 0/3394        |
| 61  | SM    | 0.30         | 0/950         | 0.70        | 2/1275 (0.2%) |
| 62  | SZ    | 0.27         | 0/604         | 0.57        | 0/810         |
| 63  | Sf    | 0.29         | 0/560         | 0.61        | 0/745         |
| 64  | CD    | 0.28         | 0/447         | 0.57        | 0/592         |
| 65  | LW    | 0.33         | 0/979         | 0.57        | 0/1295        |
| 66  | SE    | 0.30         | 0/2118        | 0.59        | 0/2849        |
| 67  | SI    | 0.29         | 0/1715        | 0.62        | 0/2287        |
| 68  | SL    | 0.30         | 0/1268        | 0.60        | 0/1696        |
| 69  | SX    | 0.32         | 0/1116        | 0.56        | 0/1490        |
| 70  | SG    | 0.28         | 0/1946        | 0.66        | 0/2590        |
| 71  | SJ    | 0.30         | 0/1550        | 0.59        | 0/2069        |
| 72  | SY    | 0.28         | 0/1083        | 0.61        | 0/1438        |
| 73  | Se    | 0.29         | 0/465         | 0.57        | 0/612         |
| 74  | SA    | 0.28         | 0/1778        | 0.63        | 2/2416 (0.1%) |
| 75  | SB    | 0.29         | 0/1765        | 0.61        | 0/2362        |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 76  | SH    | 0.27         | 0/1519          | 0.59        | 1/2033 (0.0%)     |
| 77  | SV    | 0.30         | 0/643           | 0.61        | 0/860             |
| 78  | Sa    | 0.33         | 0/836           | 0.64        | 0/1121            |
| 79  | SC    | 0.31         | 0/1762          | 0.54        | 0/2381            |
| 80  | SN    | 0.50         | 2/1232 (0.2%)   | 0.92        | 4/1656 (0.2%)     |
| 81  | SO    | 0.28         | 0/1062          | 0.64        | 1/1425 (0.1%)     |
| 82  | SW    | 0.31         | 0/1051          | 0.60        | 0/1406            |
| 83  | Sb    | 0.28         | 0/665           | 0.55        | 0/891             |
| 84  | CB    | 0.46         | 3/6734 (0.0%)   | 0.65        | 7/9094 (0.1%)     |
| 85  | Et    | 0.37         | 0/1778          | 1.07        | 4/2767 (0.1%)     |
| All | All   | 0.49         | 9/246128 (0.0%) | 0.76        | 175/360165 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | LA    | 0                   | 2                   |
| 7   | LB    | 0                   | 2                   |
| 16  | LL    | 0                   | 1                   |
| 17  | LM    | 0                   | 1                   |
| 19  | LO    | 0                   | 1                   |
| 23  | LT    | 0                   | 1                   |
| 34  | Lf    | 0                   | 1                   |
| 38  | Lj    | 0                   | 2                   |
| 54  | SQ    | 0                   | 1                   |
| 69  | SX    | 0                   | 1                   |
| 76  | SH    | 0                   | 1                   |
| All | All   | 0                   | 14                  |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 84  | CB    | 432 | PRO  | CB-CG | 19.48  | 2.47        | 1.50     |
| 38  | Lj    | 40  | PRO  | CB-CG | 19.12  | 2.45        | 1.50     |
| 84  | CB    | 432 | PRO  | CG-CD | -17.08 | 0.94        | 1.50     |
| 50  | SD    | 43  | PRO  | CG-CD | -15.46 | 0.99        | 1.50     |
| 38  | Lj    | 40  | PRO  | CG-CD | -15.07 | 1.00        | 1.50     |
| 80  | SN    | 82  | PRO  | CB-CG | -9.98  | 1.00        | 1.50     |
| 80  | SN    | 82  | PRO  | CG-CD | -9.74  | 1.18        | 1.50     |
| 84  | CB    | 432 | PRO  | N-CD  | 9.60   | 1.61        | 1.47     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 38  | Lj    | 40  | PRO  | N-CD  | 5.64 | 1.55        | 1.47     |

All (175) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 38  | Lj    | 40   | PRO  | CB-CG-CD   | -26.47 | 3.27        | 106.50   |
| 84  | CB    | 432  | PRO  | CB-CG-CD   | -23.04 | 16.63       | 106.50   |
| 50  | SD    | 43   | PRO  | N-CD-CG    | -19.95 | 73.28       | 103.20   |
| 38  | Lj    | 40   | PRO  | CA-N-CD    | -19.71 | 83.90       | 111.50   |
| 80  | SN    | 82   | PRO  | CA-CB-CG   | -18.40 | 69.04       | 104.00   |
| 80  | SN    | 82   | PRO  | N-CD-CG    | -18.35 | 75.67       | 103.20   |
| 50  | SD    | 43   | PRO  | CA-CB-CG   | -15.81 | 73.97       | 104.00   |
| 38  | Lj    | 40   | PRO  | N-CA-CB    | -14.65 | 85.72       | 103.30   |
| 84  | CB    | 432  | PRO  | N-CA-CB    | -13.92 | 86.60       | 103.30   |
| 3   | L5    | 655  | C    | N3-C2-O2   | -12.75 | 112.97      | 121.90   |
| 3   | L5    | 4923 | C    | N3-C2-O2   | -11.45 | 113.88      | 121.90   |
| 38  | Lj    | 40   | PRO  | CA-CB-CG   | -11.19 | 82.74       | 104.00   |
| 84  | CB    | 432  | PRO  | N-CD-CG    | -11.09 | 86.57       | 103.20   |
| 3   | L5    | 129  | C    | N3-C2-O2   | -10.56 | 114.50      | 121.90   |
| 3   | L5    | 499  | G    | O4'-C1'-N9 | 10.42  | 116.54      | 108.20   |
| 80  | SN    | 82   | PRO  | CB-CG-CD   | 10.38  | 146.97      | 106.50   |
| 50  | SD    | 43   | PRO  | N-CA-CB    | -9.97  | 91.34       | 103.30   |
| 3   | L5    | 485  | C    | C2-N1-C1'  | 9.75   | 129.52      | 118.80   |
| 3   | L5    | 655  | C    | N1-C2-O2   | 9.67   | 124.70      | 118.90   |
| 3   | L5    | 174  | C    | N3-C2-O2   | -9.38  | 115.33      | 121.90   |
| 2   | S2    | 1772 | C    | N3-C2-O2   | -9.17  | 115.48      | 121.90   |
| 3   | L5    | 2710 | C    | N1-C2-O2   | 9.09   | 124.35      | 118.90   |
| 2   | S2    | 1772 | C    | N1-C2-O2   | 9.06   | 124.33      | 118.90   |
| 3   | L5    | 2710 | C    | C2-N1-C1'  | 8.79   | 128.47      | 118.80   |
| 2   | S2    | 1453 | C    | C2-N1-C1'  | 8.76   | 128.43      | 118.80   |
| 3   | L5    | 4923 | C    | N1-C2-O2   | 8.53   | 124.02      | 118.90   |
| 3   | L5    | 1447 | C    | N3-C2-O2   | -8.53  | 115.93      | 121.90   |
| 84  | CB    | 432  | PRO  | CA-N-CD    | -8.40  | 99.74       | 111.50   |
| 2   | S2    | 356  | C    | N1-C2-O2   | 8.35   | 123.91      | 118.90   |
| 3   | L5    | 654  | C    | N1-C2-O2   | 8.26   | 123.86      | 118.90   |
| 3   | L5    | 4924 | C    | N3-C2-O2   | -8.25  | 116.13      | 121.90   |
| 2   | S2    | 1453 | C    | N1-C2-O2   | 8.13   | 123.78      | 118.90   |
| 3   | L5    | 417  | G    | O4'-C1'-N9 | 8.04   | 114.63      | 108.20   |
| 3   | L5    | 971  | U    | C2-N1-C1'  | 7.83   | 127.10      | 117.70   |
| 2   | S2    | 356  | C    | C2-N1-C1'  | 7.73   | 127.31      | 118.80   |
| 3   | L5    | 1414 | C    | N3-C2-O2   | -7.71  | 116.51      | 121.90   |
| 3   | L5    | 456  | C    | N3-C2-O2   | -7.60  | 116.58      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | L5    | 130  | C    | N3-C2-O2   | -7.56 | 116.61      | 121.90   |
| 3   | L5    | 485  | C    | C6-N1-C1'  | -7.54 | 111.75      | 120.80   |
| 3   | L5    | 3773 | U    | N3-C2-O2   | -7.51 | 116.95      | 122.20   |
| 3   | L5    | 490  | C    | N3-C2-O2   | -7.44 | 116.69      | 121.90   |
| 3   | L5    | 1252 | C    | N3-C2-O2   | -7.38 | 116.74      | 121.90   |
| 80  | SN    | 82   | PRO  | CA-N-CD    | -7.33 | 101.24      | 111.50   |
| 3   | L5    | 1082 | C    | O4'-C1'-N1 | 7.27  | 114.02      | 108.20   |
| 3   | L5    | 655  | C    | C6-N1-C2   | -7.26 | 117.40      | 120.30   |
| 3   | L5    | 1191 | C    | N3-C2-O2   | -7.24 | 116.83      | 121.90   |
| 3   | L5    | 925  | C    | N3-C2-O2   | -7.24 | 116.83      | 121.90   |
| 84  | CB    | 431  | GLY  | C-N-CD     | 7.23  | 143.59      | 128.40   |
| 3   | L5    | 925  | C    | N1-C2-O2   | 7.21  | 123.22      | 118.90   |
| 3   | L5    | 4138 | C    | N3-C2-O2   | -7.16 | 116.89      | 121.90   |
| 3   | L5    | 2710 | C    | N3-C2-O2   | -7.12 | 116.91      | 121.90   |
| 3   | L5    | 175  | C    | N3-C2-O2   | -7.10 | 116.93      | 121.90   |
| 3   | L5    | 4897 | G    | N1-C6-O6   | -7.02 | 115.69      | 119.90   |
| 30  | Lb    | 118  | LEU  | CA-CB-CG   | 6.98  | 131.36      | 115.30   |
| 38  | Lj    | 40   | PRO  | N-CD-CG    | -6.98 | 92.74       | 103.20   |
| 3   | L5    | 971  | U    | N1-C2-O2   | 6.92  | 127.64      | 122.80   |
| 2   | S2    | 1416 | C    | N3-C2-O2   | -6.86 | 117.10      | 121.90   |
| 74  | SA    | 147  | LEU  | CA-CB-CG   | 6.83  | 131.02      | 115.30   |
| 56  | ST    | 125  | PRO  | CA-N-CD    | -6.83 | 101.94      | 111.50   |
| 3   | L5    | 456  | C    | O4'-C1'-N1 | 6.83  | 113.66      | 108.20   |
| 3   | L5    | 4897 | G    | C5-C6-O6   | 6.80  | 132.68      | 128.60   |
| 31  | Lc    | 98   | ASP  | CB-CG-OD1  | 6.80  | 124.42      | 118.30   |
| 3   | L5    | 4147 | G    | C5-C6-O6   | 6.78  | 132.67      | 128.60   |
| 53  | SP    | 80   | LEU  | CA-CB-CG   | 6.78  | 130.89      | 115.30   |
| 3   | L5    | 1077 | C    | N3-C2-O2   | -6.77 | 117.16      | 121.90   |
| 3   | L5    | 4709 | U    | C2-N1-C1'  | 6.76  | 125.81      | 117.70   |
| 3   | L5    | 1414 | C    | N1-C2-O2   | 6.71  | 122.92      | 118.90   |
| 15  | LJ    | 121  | PRO  | CA-N-CD    | -6.69 | 102.14      | 111.50   |
| 2   | S2    | 1022 | U    | C2-N1-C1'  | 6.68  | 125.72      | 117.70   |
| 61  | SM    | 52   | LEU  | CB-CG-CD2  | 6.65  | 122.31      | 111.00   |
| 2   | S2    | 356  | C    | N3-C2-O2   | -6.65 | 117.25      | 121.90   |
| 84  | CB    | 432  | PRO  | CA-CB-CG   | -6.62 | 91.42       | 104.00   |
| 3   | L5    | 1082 | C    | N3-C2-O2   | -6.61 | 117.27      | 121.90   |
| 3   | L5    | 4897 | G    | N1-C2-N2   | -6.59 | 110.27      | 116.20   |
| 3   | L5    | 129  | C    | C6-N1-C2   | -6.59 | 117.67      | 120.30   |
| 3   | L5    | 129  | C    | N1-C2-O2   | 6.55  | 122.83      | 118.90   |
| 3   | L5    | 485  | C    | N1-C2-O2   | 6.51  | 122.81      | 118.90   |
| 81  | SO    | 14   | VAL  | C-N-CA     | 6.47  | 137.87      | 121.70   |
| 48  | Ls    | 79   | LEU  | CA-CB-CG   | 6.37  | 129.96      | 115.30   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | S2    | 1453 | C    | C6-N1-C1' | -6.31 | 113.22      | 120.80   |
| 3   | L5    | 971  | U    | N3-C2-O2  | -6.27 | 117.81      | 122.20   |
| 61  | SM    | 52   | LEU  | CA-CB-CG  | 6.25  | 129.68      | 115.30   |
| 3   | L5    | 3741 | C    | N3-C2-O2  | -6.24 | 117.53      | 121.90   |
| 76  | SH    | 148  | LEU  | CA-CB-CG  | 6.19  | 129.55      | 115.30   |
| 3   | L5    | 4147 | G    | N1-C6-O6  | -6.17 | 116.20      | 119.90   |
| 3   | L5    | 2410 | C    | C2-N1-C1' | 6.15  | 125.56      | 118.80   |
| 46  | Lz    | 194  | LEU  | CA-CB-CG  | 6.14  | 129.42      | 115.30   |
| 3   | L5    | 2710 | C    | C6-N1-C1' | -6.13 | 113.44      | 120.80   |
| 3   | L5    | 4928 | C    | C2-N1-C1' | 6.12  | 125.53      | 118.80   |
| 85  | Et    | 4    | C    | C2-N1-C1' | 6.07  | 125.48      | 118.80   |
| 15  | LJ    | 171  | ASP  | CB-CG-OD2 | 6.05  | 123.74      | 118.30   |
| 3   | L5    | 2560 | C    | C2-N1-C1' | 6.02  | 125.43      | 118.80   |
| 2   | S2    | 1415 | C    | N1-C2-O2  | 5.99  | 122.49      | 118.90   |
| 2   | S2    | 1453 | C    | N3-C2-O2  | -5.99 | 117.71      | 121.90   |
| 3   | L5    | 100  | C    | C2-N1-C1' | 5.91  | 125.30      | 118.80   |
| 3   | L5    | 654  | C    | C2-N1-C1' | 5.86  | 125.25      | 118.80   |
| 3   | L5    | 174  | C    | N1-C2-O2  | 5.84  | 122.41      | 118.90   |
| 3   | L5    | 499  | G    | N3-C2-N2  | 5.79  | 123.96      | 119.90   |
| 3   | L5    | 262  | G    | N1-C6-O6  | -5.78 | 116.43      | 119.90   |
| 8   | LC    | 2    | ALA  | C-N-CA    | 5.77  | 136.13      | 121.70   |
| 3   | L5    | 3761 | C    | C2-N1-C1' | 5.76  | 125.14      | 118.80   |
| 85  | Et    | 49   | C    | C2-N1-C1' | 5.72  | 125.09      | 118.80   |
| 3   | L5    | 489  | C    | N1-C2-O2  | 5.70  | 122.32      | 118.90   |
| 2   | S2    | 834  | C    | N3-C2-O2  | -5.68 | 117.93      | 121.90   |
| 30  | Lb    | 121  | PRO  | CA-N-CD   | -5.66 | 103.57      | 111.50   |
| 3   | L5    | 4709 | U    | C5-C4-O4  | -5.65 | 122.51      | 125.90   |
| 2   | S2    | 322  | C    | N1-C2-O2  | 5.64  | 122.29      | 118.90   |
| 24  | LU    | 28   | PRO  | N-CD-CG   | -5.61 | 94.78       | 103.20   |
| 21  | LQ    | 4    | ASP  | CB-CG-OD1 | 5.60  | 123.34      | 118.30   |
| 3   | L5    | 1447 | C    | C6-N1-C2  | -5.60 | 118.06      | 120.30   |
| 47  | CA    | 357  | LEU  | CA-CB-CG  | 5.59  | 128.15      | 115.30   |
| 2   | S2    | 1755 | C    | C2-N1-C1' | 5.57  | 124.93      | 118.80   |
| 2   | S2    | 1520 | G    | C4-N9-C1' | 5.56  | 133.73      | 126.50   |
| 3   | L5    | 1367 | C    | C2-N1-C1' | 5.55  | 124.91      | 118.80   |
| 3   | L5    | 2710 | C    | C6-N1-C2  | -5.54 | 118.08      | 120.30   |
| 3   | L5    | 209  | U    | C2-N1-C1' | 5.52  | 124.33      | 117.70   |
| 3   | L5    | 262  | G    | C5-C6-O6  | 5.52  | 131.91      | 128.60   |
| 2   | S2    | 118  | C    | C2-N1-C1' | 5.52  | 124.87      | 118.80   |
| 3   | L5    | 1077 | C    | C6-N1-C2  | -5.51 | 118.09      | 120.30   |
| 3   | L5    | 1417 | C    | C2-N1-C1' | 5.49  | 124.84      | 118.80   |
| 3   | L5    | 1082 | C    | C2-N1-C1' | -5.48 | 112.77      | 118.80   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | S2    | 1755 | C    | N1-C2-O2  | 5.48  | 122.19      | 118.90   |
| 3   | L5    | 1755 | C    | C2-N1-C1' | 5.48  | 124.83      | 118.80   |
| 3   | L5    | 1082 | C    | C6-N1-C1' | 5.47  | 127.37      | 120.80   |
| 49  | Lt    | 121  | LEU  | CA-CB-CG  | 5.45  | 127.84      | 115.30   |
| 3   | L5    | 472  | C    | C2-N1-C1' | 5.45  | 124.79      | 118.80   |
| 3   | L5    | 1216 | C    | C2-N1-C1' | 5.43  | 124.78      | 118.80   |
| 85  | Et    | 71   | G    | N3-C4-N9  | 5.42  | 129.25      | 126.00   |
| 2   | S2    | 356  | C    | C6-N1-C1' | -5.42 | 114.29      | 120.80   |
| 3   | L5    | 3761 | C    | N1-C2-O2  | 5.42  | 122.15      | 118.90   |
| 2   | S2    | 833  | C    | N1-C2-O2  | 5.41  | 122.15      | 118.90   |
| 2   | S2    | 1756 | C    | C6-N1-C1' | 5.41  | 127.29      | 120.80   |
| 3   | L5    | 138  | G    | N3-C4-N9  | 5.40  | 129.24      | 126.00   |
| 3   | L5    | 1241 | C    | C2-N1-C1' | 5.40  | 124.74      | 118.80   |
| 2   | S2    | 293  | C    | N1-C2-O2  | 5.38  | 122.13      | 118.90   |
| 3   | L5    | 654  | C    | N3-C2-O2  | -5.37 | 118.14      | 121.90   |
| 2   | S2    | 501  | C    | N1-C2-O2  | 5.35  | 122.11      | 118.90   |
| 3   | L5    | 1173 | G    | N3-C4-N9  | -5.33 | 122.81      | 126.00   |
| 3   | L5    | 4926 | C    | N1-C2-O2  | 5.33  | 122.09      | 118.90   |
| 3   | L5    | 3773 | U    | C2-N1-C1' | 5.32  | 124.09      | 117.70   |
| 24  | LU    | 28   | PRO  | CA-N-CD   | -5.32 | 104.05      | 111.50   |
| 3   | L5    | 3773 | U    | N1-C2-O2  | 5.31  | 126.52      | 122.80   |
| 53  | SP    | 33   | LEU  | CA-CB-CG  | 5.31  | 127.52      | 115.30   |
| 3   | L5    | 500  | G    | N1-C2-N2  | -5.30 | 111.43      | 116.20   |
| 2   | S2    | 501  | C    | C2-N1-C1' | 5.29  | 124.62      | 118.80   |
| 3   | L5    | 456  | C    | C6-N1-C2  | -5.29 | 118.18      | 120.30   |
| 2   | S2    | 688  | U    | P-O3'-C3' | 5.29  | 126.04      | 119.70   |
| 3   | L5    | 4709 | U    | C6-N1-C1' | -5.28 | 113.81      | 121.20   |
| 2   | S2    | 1520 | G    | N3-C4-N9  | 5.26  | 129.15      | 126.00   |
| 2   | S2    | 834  | C    | C6-N1-C2  | -5.23 | 118.21      | 120.30   |
| 54  | SQ    | 38   | PRO  | CA-N-CD   | -5.23 | 104.17      | 111.50   |
| 74  | SA    | 198  | MET  | CA-CB-CG  | 5.22  | 122.17      | 113.30   |
| 3   | L5    | 2257 | C    | N1-C2-O2  | 5.22  | 122.03      | 118.90   |
| 3   | L5    | 971  | U    | C6-N1-C1' | -5.20 | 113.92      | 121.20   |
| 3   | L5    | 1182 | C    | N1-C2-O2  | 5.19  | 122.02      | 118.90   |
| 2   | S2    | 1520 | G    | C8-N9-C1' | -5.18 | 120.26      | 127.00   |
| 3   | L5    | 1447 | C    | N1-C2-O2  | 5.18  | 122.01      | 118.90   |
| 3   | L5    | 3741 | C    | N1-C2-O2  | 5.17  | 122.00      | 118.90   |
| 3   | L5    | 1191 | C    | N1-C2-O2  | 5.16  | 122.00      | 118.90   |
| 3   | L5    | 4924 | C    | C6-N1-C2  | -5.16 | 118.24      | 120.30   |
| 3   | L5    | 1241 | C    | N1-C2-O2  | 5.13  | 121.98      | 118.90   |
| 2   | S2    | 537  | C    | C2-N1-C1' | 5.11  | 124.42      | 118.80   |
| 2   | S2    | 834  | C    | N1-C2-O2  | 5.09  | 121.96      | 118.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 17  | LM    | 136  | LEU  | CA-CB-CG   | 5.09  | 127.02      | 115.30   |
| 3   | L5    | 2257 | C    | C2-N1-C1'  | 5.09  | 124.40      | 118.80   |
| 3   | L5    | 4303 | C    | C2-N1-C1'  | 5.07  | 124.38      | 118.80   |
| 3   | L5    | 3775 | A    | O4'-C1'-N9 | 5.07  | 112.25      | 108.20   |
| 85  | Et    | 72   | C    | N3-C2-O2   | -5.05 | 118.37      | 121.90   |
| 3   | L5    | 140  | G    | C5-C6-O6   | 5.04  | 131.63      | 128.60   |
| 3   | L5    | 1597 | G    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 3   | L5    | 4924 | C    | C5-C4-N4   | 5.02  | 123.72      | 120.20   |
| 2   | S2    | 1453 | C    | C5-C6-N1   | 5.02  | 123.51      | 121.00   |
| 3   | L5    | 1446 | C    | N1-C2-O2   | 5.02  | 121.91      | 118.90   |
| 84  | CB    | 664  | ASP  | CB-CG-OD2  | 5.02  | 122.81      | 118.30   |
| 3   | L5    | 963  | G    | C4-N9-C1'  | 5.01  | 133.02      | 126.50   |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 6   | LA    | 13  | GLY  | Peptide |
| 6   | LA    | 54  | ARG  | Peptide |
| 7   | LB    | 17  | LEU  | Peptide |
| 7   | LB    | 258 | HIS  | Peptide |
| 16  | LL    | 154 | VAL  | Peptide |
| 17  | LM    | 87  | ALA  | Peptide |
| 19  | LO    | 110 | PRO  | Peptide |
| 23  | LT    | 136 | ARG  | Peptide |
| 34  | Lf    | 106 | TYR  | Peptide |
| 38  | Lj    | 39  | TYR  | Peptide |
| 38  | Lj    | 40  | PRO  | Peptide |
| 76  | SH    | 15  | LYS  | Peptide |
| 54  | SQ    | 43  | GLU  | Peptide |
| 69  | SX    | 126 | ALA  | Peptide |

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | LR    | 185/187 (99%)  | 180 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 6   | LA    | 246/248 (99%)  | 222 (90%) | 23 (9%)  | 1 (0%)   | 30          | 58  |
| 7   | LB    | 400/402 (100%) | 373 (93%) | 27 (7%)  | 0        | 100         | 100 |
| 8   | LC    | 366/368 (100%) | 342 (93%) | 24 (7%)  | 0        | 100         | 100 |
| 9   | LD    | 291/293 (99%)  | 277 (95%) | 14 (5%)  | 0        | 100         | 100 |
| 10  | LE    | 232/247 (94%)  | 207 (89%) | 25 (11%) | 0        | 100         | 100 |
| 11  | LF    | 223/225 (99%)  | 213 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 12  | LG    | 239/241 (99%)  | 225 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 13  | LH    | 188/190 (99%)  | 173 (92%) | 15 (8%)  | 0        | 100         | 100 |
| 14  | LI    | 198/213 (93%)  | 184 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 15  | LJ    | 174/176 (99%)  | 158 (91%) | 16 (9%)  | 0        | 100         | 100 |
| 16  | LL    | 208/210 (99%)  | 192 (92%) | 16 (8%)  | 0        | 100         | 100 |
| 17  | LM    | 137/139 (99%)  | 130 (95%) | 6 (4%)   | 1 (1%)   | 19          | 45  |
| 18  | LN    | 201/203 (99%)  | 192 (96%) | 8 (4%)   | 1 (0%)   | 25          | 52  |
| 19  | LO    | 199/201 (99%)  | 189 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 20  | LP    | 151/153 (99%)  | 139 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 21  | LQ    | 185/187 (99%)  | 180 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 22  | LS    | 173/175 (99%)  | 163 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 23  | LT    | 157/159 (99%)  | 146 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 24  | LU    | 99/101 (98%)   | 81 (82%)  | 18 (18%) | 0        | 100         | 100 |
| 25  | LV    | 129/131 (98%)  | 125 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 26  | LX    | 118/120 (98%)  | 116 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 27  | LY    | 132/134 (98%)  | 128 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 28  | LZ    | 133/135 (98%)  | 121 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 29  | La    | 145/147 (99%)  | 138 (95%) | 7 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 30  | Lb    | 105/121 (87%) | 97 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 31  | Lc    | 96/98 (98%)   | 89 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 32  | Ld    | 105/107 (98%) | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 33  | Le    | 126/128 (98%) | 118 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 34  | Lf    | 107/109 (98%) | 96 (90%)  | 10 (9%)  | 1 (1%)   | 14          | 38  |
| 35  | Lg    | 112/114 (98%) | 110 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 36  | Lh    | 120/122 (98%) | 118 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 37  | Li    | 100/102 (98%) | 97 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 38  | Lj    | 84/86 (98%)   | 80 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 39  | Lk    | 67/69 (97%)   | 65 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 40  | Ll    | 48/50 (96%)   | 44 (92%)  | 4 (8%)   | 0        | 100         | 100 |
| 41  | Lm    | 50/52 (96%)   | 50 (100%) | 0        | 0        | 100         | 100 |
| 42  | Ln    | 22/24 (92%)   | 22 (100%) | 0        | 0        | 100         | 100 |
| 43  | Lo    | 103/105 (98%) | 99 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 44  | Lp    | 89/91 (98%)   | 86 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 45  | Lr    | 123/125 (98%) | 115 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 46  | Lz    | 215/217 (99%) | 172 (80%) | 43 (20%) | 0        | 100         | 100 |
| 47  | CA    | 350/356 (98%) | 333 (95%) | 17 (5%)  | 0        | 100         | 100 |
| 48  | Ls    | 194/196 (99%) | 185 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 49  | Lt    | 137/141 (97%) | 106 (77%) | 29 (21%) | 2 (2%)   | 8           | 25  |
| 50  | SD    | 225/227 (99%) | 200 (89%) | 25 (11%) | 0        | 100         | 100 |
| 51  | SF    | 187/189 (99%) | 169 (90%) | 18 (10%) | 0        | 100         | 100 |
| 52  | SK    | 96/98 (98%)   | 80 (83%)  | 14 (15%) | 2 (2%)   | 5           | 18  |
| 53  | SP    | 119/121 (98%) | 112 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 54  | SQ    | 142/144 (99%) | 124 (87%) | 18 (13%) | 0        | 100         | 100 |
| 55  | SS    | 143/145 (99%) | 134 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 56  | ST    | 141/143 (99%) | 128 (91%) | 11 (8%)  | 2 (1%)   | 9           | 27  |
| 57  | SU    | 102/104 (98%) | 92 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 58  | Sc    | 62/64 (97%)   | 51 (82%)  | 11 (18%) | 0        | 100         | 100 |
| 59  | Sd    | 53/55 (96%)   | 50 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 60  | Sg    | 311/313 (99%) | 274 (88%) | 37 (12%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 61  | SM    | 120/122 (98%)     | 108 (90%)   | 11 (9%)  | 1 (1%)   | 16          | 41  |
| 62  | SZ    | 73/75 (97%)       | 62 (85%)    | 11 (15%) | 0        | 100         | 100 |
| 63  | Sf    | 65/67 (97%)       | 56 (86%)    | 9 (14%)  | 0        | 100         | 100 |
| 64  | CD    | 51/55 (93%)       | 46 (90%)    | 5 (10%)  | 0        | 100         | 100 |
| 65  | LW    | 114/124 (92%)     | 109 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 66  | SE    | 260/262 (99%)     | 243 (94%)   | 17 (6%)  | 0        | 100         | 100 |
| 67  | SI    | 204/206 (99%)     | 200 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 68  | SL    | 151/153 (99%)     | 144 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 69  | SX    | 139/141 (99%)     | 122 (88%)   | 16 (12%) | 1 (1%)   | 19          | 45  |
| 70  | SG    | 235/237 (99%)     | 219 (93%)   | 16 (7%)  | 0        | 100         | 100 |
| 71  | SJ    | 183/185 (99%)     | 168 (92%)   | 15 (8%)  | 0        | 100         | 100 |
| 72  | SY    | 129/131 (98%)     | 120 (93%)   | 9 (7%)   | 0        | 100         | 100 |
| 73  | Se    | 56/58 (97%)       | 51 (91%)    | 5 (9%)   | 0        | 100         | 100 |
| 74  | SA    | 219/221 (99%)     | 196 (90%)   | 23 (10%) | 0        | 100         | 100 |
| 75  | SB    | 212/214 (99%)     | 206 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 76  | SH    | 182/189 (96%)     | 159 (87%)   | 23 (13%) | 0        | 100         | 100 |
| 77  | SV    | 81/83 (98%)       | 70 (86%)    | 11 (14%) | 0        | 100         | 100 |
| 78  | Sa    | 100/102 (98%)     | 90 (90%)    | 10 (10%) | 0        | 100         | 100 |
| 79  | SC    | 220/222 (99%)     | 206 (94%)   | 13 (6%)  | 1 (0%)   | 25          | 52  |
| 80  | SN    | 148/150 (99%)     | 143 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 81  | SO    | 138/140 (99%)     | 123 (89%)   | 15 (11%) | 0        | 100         | 100 |
| 82  | SW    | 127/129 (98%)     | 124 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 83  | Sb    | 81/83 (98%)       | 70 (86%)    | 11 (14%) | 0        | 100         | 100 |
| 84  | CB    | 842/856 (98%)     | 795 (94%)   | 43 (5%)  | 4 (0%)   | 25          | 52  |
| All | All   | 12973/13206 (98%) | 12018 (93%) | 938 (7%) | 17 (0%)  | 50          | 76  |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | Lt    | 144 | ASP  |
| 52  | SK    | 96  | ARG  |
| 56  | ST    | 39  | LEU  |
| 84  | CB    | 407 | LYS  |
| 84  | CB    | 779 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | LN    | 124 | ASP  |
| 52  | SK    | 36  | ALA  |
| 69  | SX    | 127 | ASN  |
| 17  | LM    | 88  | ALA  |
| 49  | Lt    | 13  | VAL  |
| 61  | SM    | 96  | ARG  |
| 84  | CB    | 481 | LYS  |
| 84  | CB    | 611 | ASP  |
| 56  | ST    | 41  | LYS  |
| 79  | SC    | 78  | LEU  |
| 6   | LA    | 55  | GLY  |
| 34  | Lf    | 107 | PRO  |

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

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | LR    | 166/166 (100%) | 147 (89%) | 19 (11%) | 4           | 14 |
| 6   | LA    | 190/190 (100%) | 175 (92%) | 15 (8%)  | 10          | 28 |
| 7   | LB    | 348/348 (100%) | 323 (93%) | 25 (7%)  | 12          | 31 |
| 8   | LC    | 306/306 (100%) | 288 (94%) | 18 (6%)  | 16          | 41 |
| 9   | LD    | 246/247 (100%) | 229 (93%) | 17 (7%)  | 13          | 34 |
| 10  | LE    | 209/220 (95%)  | 198 (95%) | 11 (5%)  | 19          | 46 |
| 11  | LF    | 194/194 (100%) | 180 (93%) | 14 (7%)  | 12          | 31 |
| 12  | LG    | 203/205 (99%)  | 184 (91%) | 19 (9%)  | 7           | 20 |
| 13  | LH    | 169/169 (100%) | 151 (89%) | 18 (11%) | 5           | 15 |
| 14  | LI    | 172/180 (96%)  | 164 (95%) | 8 (5%)   | 22          | 51 |
| 15  | LJ    | 148/148 (100%) | 133 (90%) | 15 (10%) | 6           | 17 |
| 16  | LL    | 176/176 (100%) | 160 (91%) | 16 (9%)  | 7           | 22 |
| 17  | LM    | 118/118 (100%) | 112 (95%) | 6 (5%)   | 20          | 47 |
| 18  | LN    | 171/171 (100%) | 162 (95%) | 9 (5%)   | 19          | 46 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 19  | LO    | 173/173 (100%) | 163 (94%) | 10 (6%)  | 17          | 42 |
| 20  | LP    | 134/134 (100%) | 118 (88%) | 16 (12%) | 4           | 12 |
| 21  | LQ    | 164/164 (100%) | 155 (94%) | 9 (6%)   | 18          | 44 |
| 22  | LS    | 156/156 (100%) | 147 (94%) | 9 (6%)   | 17          | 42 |
| 23  | LT    | 139/139 (100%) | 129 (93%) | 10 (7%)  | 12          | 31 |
| 24  | LU    | 91/91 (100%)   | 79 (87%)  | 12 (13%) | 3           | 9  |
| 25  | LV    | 101/101 (100%) | 95 (94%)  | 6 (6%)   | 16          | 41 |
| 26  | LX    | 108/108 (100%) | 98 (91%)  | 10 (9%)  | 7           | 21 |
| 27  | LY    | 124/124 (100%) | 116 (94%) | 8 (6%)   | 14          | 37 |
| 28  | LZ    | 117/117 (100%) | 110 (94%) | 7 (6%)   | 16          | 40 |
| 29  | La    | 120/120 (100%) | 113 (94%) | 7 (6%)   | 17          | 42 |
| 30  | Lb    | 88/101 (87%)   | 82 (93%)  | 6 (7%)   | 13          | 34 |
| 31  | Lc    | 83/83 (100%)   | 73 (88%)  | 10 (12%) | 4           | 12 |
| 32  | Ld    | 98/98 (100%)   | 91 (93%)  | 7 (7%)   | 12          | 32 |
| 33  | Le    | 114/114 (100%) | 109 (96%) | 5 (4%)   | 24          | 53 |
| 34  | Lf    | 88/88 (100%)   | 85 (97%)  | 3 (3%)   | 32          | 63 |
| 35  | Lg    | 98/98 (100%)   | 92 (94%)  | 6 (6%)   | 15          | 40 |
| 36  | Lh    | 109/109 (100%) | 106 (97%) | 3 (3%)   | 38          | 69 |
| 37  | Li    | 86/86 (100%)   | 82 (95%)  | 4 (5%)   | 22          | 51 |
| 38  | Lj    | 73/73 (100%)   | 70 (96%)  | 3 (4%)   | 26          | 56 |
| 39  | Lk    | 64/64 (100%)   | 58 (91%)  | 6 (9%)   | 7           | 20 |
| 40  | Ll    | 47/47 (100%)   | 44 (94%)  | 3 (6%)   | 14          | 37 |
| 41  | Lm    | 48/48 (100%)   | 46 (96%)  | 2 (4%)   | 25          | 55 |
| 42  | Ln    | 23/23 (100%)   | 22 (96%)  | 1 (4%)   | 25          | 54 |
| 43  | Lo    | 93/93 (100%)   | 85 (91%)  | 8 (9%)   | 8           | 24 |
| 44  | Lp    | 74/74 (100%)   | 73 (99%)  | 1 (1%)   | 62          | 85 |
| 45  | Lr    | 109/109 (100%) | 93 (85%)  | 16 (15%) | 2           | 7  |
| 46  | Lz    | 195/196 (100%) | 181 (93%) | 14 (7%)  | 12          | 31 |
| 47  | CA    | 303/305 (99%)  | 280 (92%) | 23 (8%)  | 11          | 29 |
| 48  | Ls    | 162/164 (99%)  | 142 (88%) | 20 (12%) | 4           | 11 |
| 49  | Lt    | 112/115 (97%)  | 103 (92%) | 9 (8%)   | 10          | 27 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 50  | SD    | 190/190 (100%) | 161 (85%) | 29 (15%) | 2           | 6  |
| 51  | SF    | 159/159 (100%) | 145 (91%) | 14 (9%)  | 8           | 23 |
| 52  | SK    | 89/89 (100%)   | 80 (90%)  | 9 (10%)  | 6           | 17 |
| 53  | SP    | 107/107 (100%) | 99 (92%)  | 8 (8%)   | 11          | 30 |
| 54  | SQ    | 119/119 (100%) | 103 (87%) | 16 (13%) | 3           | 9  |
| 55  | SS    | 126/126 (100%) | 107 (85%) | 19 (15%) | 2           | 6  |
| 56  | ST    | 113/113 (100%) | 101 (89%) | 12 (11%) | 5           | 16 |
| 57  | SU    | 94/94 (100%)   | 87 (93%)  | 7 (7%)   | 11          | 30 |
| 58  | Sc    | 57/57 (100%)   | 47 (82%)  | 10 (18%) | 1           | 4  |
| 59  | Sd    | 48/48 (100%)   | 44 (92%)  | 4 (8%)   | 9           | 26 |
| 60  | Sg    | 272/272 (100%) | 238 (88%) | 34 (12%) | 3           | 11 |
| 61  | SM    | 102/104 (98%)  | 89 (87%)  | 13 (13%) | 3           | 11 |
| 62  | SZ    | 66/66 (100%)   | 61 (92%)  | 5 (8%)   | 11          | 29 |
| 63  | Sf    | 60/60 (100%)   | 54 (90%)  | 6 (10%)  | 6           | 18 |
| 64  | CD    | 46/46 (100%)   | 41 (89%)  | 5 (11%)  | 5           | 15 |
| 65  | LW    | 97/103 (94%)   | 89 (92%)  | 8 (8%)   | 9           | 26 |
| 66  | SE    | 224/224 (100%) | 204 (91%) | 20 (9%)  | 8           | 23 |
| 67  | SI    | 178/178 (100%) | 161 (90%) | 17 (10%) | 7           | 19 |
| 68  | SL    | 137/137 (100%) | 119 (87%) | 18 (13%) | 3           | 9  |
| 69  | SX    | 113/113 (100%) | 105 (93%) | 8 (7%)   | 12          | 32 |
| 70  | SG    | 207/207 (100%) | 180 (87%) | 27 (13%) | 3           | 10 |
| 71  | SJ    | 161/161 (100%) | 141 (88%) | 20 (12%) | 4           | 11 |
| 72  | SY    | 113/113 (100%) | 94 (83%)  | 19 (17%) | 1           | 5  |
| 73  | Se    | 47/47 (100%)   | 41 (87%)  | 6 (13%)  | 3           | 10 |
| 74  | SA    | 183/183 (100%) | 168 (92%) | 15 (8%)  | 9           | 26 |
| 75  | SB    | 195/195 (100%) | 167 (86%) | 28 (14%) | 2           | 7  |
| 76  | SH    | 166/169 (98%)  | 151 (91%) | 15 (9%)  | 8           | 22 |
| 77  | SV    | 67/67 (100%)   | 56 (84%)  | 11 (16%) | 2           | 5  |
| 78  | Sa    | 89/89 (100%)   | 82 (92%)  | 7 (8%)   | 10          | 28 |
| 79  | SC    | 188/188 (100%) | 165 (88%) | 23 (12%) | 4           | 11 |
| 80  | SN    | 130/130 (100%) | 114 (88%) | 16 (12%) | 4           | 11 |

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| Mol | Chain | Analysed           | Rotameric   | Outliers  | Percentiles |    |
|-----|-------|--------------------|-------------|-----------|-------------|----|
| 81  | SO    | 110/110 (100%)     | 100 (91%)   | 10 (9%)   | 7           | 22 |
| 82  | SW    | 112/112 (100%)     | 104 (93%)   | 8 (7%)    | 12          | 32 |
| 83  | Sb    | 75/75 (100%)       | 64 (85%)    | 11 (15%)  | 2           | 7  |
| 84  | CB    | 722/728 (99%)      | 646 (90%)   | 76 (10%)  | 5           | 16 |
| All | All   | 11272/11332 (100%) | 10254 (91%) | 1018 (9%) | 10          | 22 |

All (1018) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | LR    | 4   | LEU  |
| 1   | LR    | 12  | SER  |
| 1   | LR    | 46  | LYS  |
| 1   | LR    | 59  | SER  |
| 1   | LR    | 63  | CYS  |
| 1   | LR    | 68  | LEU  |
| 1   | LR    | 111 | GLU  |
| 1   | LR    | 117 | ARG  |
| 1   | LR    | 122 | SER  |
| 1   | LR    | 134 | ASN  |
| 1   | LR    | 144 | LYS  |
| 1   | LR    | 148 | ASP  |
| 1   | LR    | 149 | LYS  |
| 1   | LR    | 152 | LYS  |
| 1   | LR    | 157 | ASP  |
| 1   | LR    | 171 | LYS  |
| 1   | LR    | 183 | GLU  |
| 1   | LR    | 186 | LYS  |
| 1   | LR    | 187 | THR  |
| 6   | LA    | 3   | ARG  |
| 6   | LA    | 28  | ARG  |
| 6   | LA    | 32  | VAL  |
| 6   | LA    | 45  | VAL  |
| 6   | LA    | 54  | ARG  |
| 6   | LA    | 80  | GLU  |
| 6   | LA    | 93  | LYS  |
| 6   | LA    | 102 | LEU  |
| 6   | LA    | 111 | THR  |
| 6   | LA    | 114 | CYS  |
| 6   | LA    | 123 | ARG  |
| 6   | LA    | 140 | ASN  |
| 6   | LA    | 160 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | LA    | 169 | VAL  |
| 6   | LA    | 207 | VAL  |
| 7   | LB    | 7   | SER  |
| 7   | LB    | 22  | SER  |
| 7   | LB    | 23  | SER  |
| 7   | LB    | 43  | LEU  |
| 7   | LB    | 53  | MET  |
| 7   | LB    | 73  | VAL  |
| 7   | LB    | 112 | ASP  |
| 7   | LB    | 148 | LYS  |
| 7   | LB    | 152 | SER  |
| 7   | LB    | 155 | LYS  |
| 7   | LB    | 159 | VAL  |
| 7   | LB    | 169 | ARG  |
| 7   | LB    | 174 | ARG  |
| 7   | LB    | 200 | ARG  |
| 7   | LB    | 203 | GLN  |
| 7   | LB    | 248 | LEU  |
| 7   | LB    | 258 | HIS  |
| 7   | LB    | 278 | THR  |
| 7   | LB    | 297 | LYS  |
| 7   | LB    | 328 | ASN  |
| 7   | LB    | 332 | MET  |
| 7   | LB    | 360 | LEU  |
| 7   | LB    | 363 | ILE  |
| 7   | LB    | 382 | MET  |
| 7   | LB    | 386 | LYS  |
| 8   | LC    | 1   | MET  |
| 8   | LC    | 16  | GLU  |
| 8   | LC    | 17  | SER  |
| 8   | LC    | 56  | GLU  |
| 8   | LC    | 114 | ARG  |
| 8   | LC    | 122 | TYR  |
| 8   | LC    | 154 | VAL  |
| 8   | LC    | 158 | VAL  |
| 8   | LC    | 175 | LYS  |
| 8   | LC    | 188 | ARG  |
| 8   | LC    | 234 | LYS  |
| 8   | LC    | 254 | GLU  |
| 8   | LC    | 261 | ASP  |
| 8   | LC    | 268 | ARG  |
| 8   | LC    | 273 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | LC    | 276 | ASN  |
| 8   | LC    | 283 | LYS  |
| 8   | LC    | 313 | VAL  |
| 9   | LD    | 72  | ASP  |
| 9   | LD    | 76  | CYS  |
| 9   | LD    | 86  | TYR  |
| 9   | LD    | 89  | LYS  |
| 9   | LD    | 112 | ARG  |
| 9   | LD    | 118 | ILE  |
| 9   | LD    | 124 | GLU  |
| 9   | LD    | 136 | ASP  |
| 9   | LD    | 210 | TYR  |
| 9   | LD    | 221 | LYS  |
| 9   | LD    | 224 | SER  |
| 9   | LD    | 225 | GLN  |
| 9   | LD    | 235 | MET  |
| 9   | LD    | 239 | MET  |
| 9   | LD    | 256 | LYS  |
| 9   | LD    | 259 | LYS  |
| 9   | LD    | 263 | LYS  |
| 10  | LE    | 46  | ARG  |
| 10  | LE    | 74  | SER  |
| 10  | LE    | 89  | LEU  |
| 10  | LE    | 112 | MET  |
| 10  | LE    | 124 | LYS  |
| 10  | LE    | 128 | HIS  |
| 10  | LE    | 130 | LYS  |
| 10  | LE    | 218 | LYS  |
| 10  | LE    | 226 | ARG  |
| 10  | LE    | 260 | LYS  |
| 10  | LE    | 278 | THR  |
| 11  | LF    | 34  | ARG  |
| 11  | LF    | 73  | ARG  |
| 11  | LF    | 77  | LYS  |
| 11  | LF    | 88  | LYS  |
| 11  | LF    | 99  | ASN  |
| 11  | LF    | 149 | SER  |
| 11  | LF    | 181 | LYS  |
| 11  | LF    | 196 | THR  |
| 11  | LF    | 200 | ARG  |
| 11  | LF    | 221 | LYS  |
| 11  | LF    | 222 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | LF    | 236 | ARG  |
| 11  | LF    | 237 | GLU  |
| 11  | LF    | 248 | ASN  |
| 12  | LG    | 29  | ASN  |
| 12  | LG    | 34  | LYS  |
| 12  | LG    | 35  | ARG  |
| 12  | LG    | 43  | GLN  |
| 12  | LG    | 73  | ARG  |
| 12  | LG    | 100 | HIS  |
| 12  | LG    | 103 | ARG  |
| 12  | LG    | 113 | ARG  |
| 12  | LG    | 131 | LYS  |
| 12  | LG    | 179 | VAL  |
| 12  | LG    | 192 | ARG  |
| 12  | LG    | 201 | THR  |
| 12  | LG    | 211 | ASP  |
| 12  | LG    | 229 | ARG  |
| 12  | LG    | 230 | TYR  |
| 12  | LG    | 231 | ASP  |
| 12  | LG    | 252 | LYS  |
| 12  | LG    | 255 | LYS  |
| 12  | LG    | 259 | LYS  |
| 13  | LH    | 6   | SER  |
| 13  | LH    | 16  | VAL  |
| 13  | LH    | 17  | ASP  |
| 13  | LH    | 19  | THR  |
| 13  | LH    | 21  | LYS  |
| 13  | LH    | 28  | LYS  |
| 13  | LH    | 37  | ASP  |
| 13  | LH    | 44  | GLU  |
| 13  | LH    | 46  | SER  |
| 13  | LH    | 50  | LYS  |
| 13  | LH    | 51  | LYS  |
| 13  | LH    | 57  | VAL  |
| 13  | LH    | 95  | VAL  |
| 13  | LH    | 110 | SER  |
| 13  | LH    | 112 | VAL  |
| 13  | LH    | 141 | LYS  |
| 13  | LH    | 146 | LEU  |
| 13  | LH    | 183 | GLU  |
| 14  | LI    | 21  | ARG  |
| 14  | LI    | 74  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | LI    | 82  | ARG  |
| 14  | LI    | 125 | THR  |
| 14  | LI    | 129 | VAL  |
| 14  | LI    | 195 | CYS  |
| 14  | LI    | 203 | HIS  |
| 14  | LI    | 213 | HIS  |
| 15  | LJ    | 10  | ASN  |
| 15  | LJ    | 32  | ARG  |
| 15  | LJ    | 52  | LYS  |
| 15  | LJ    | 54  | ARG  |
| 15  | LJ    | 60  | PHE  |
| 15  | LJ    | 64  | ARG  |
| 15  | LJ    | 81  | GLU  |
| 15  | LJ    | 83  | LEU  |
| 15  | LJ    | 88  | LYS  |
| 15  | LJ    | 90  | ARG  |
| 15  | LJ    | 95  | ARG  |
| 15  | LJ    | 119 | TYR  |
| 15  | LJ    | 133 | VAL  |
| 15  | LJ    | 151 | ILE  |
| 15  | LJ    | 171 | ASP  |
| 16  | LL    | 8   | MET  |
| 16  | LL    | 21  | ARG  |
| 16  | LL    | 24  | THR  |
| 16  | LL    | 59  | VAL  |
| 16  | LL    | 60  | ARG  |
| 16  | LL    | 64  | VAL  |
| 16  | LL    | 67  | HIS  |
| 16  | LL    | 70  | VAL  |
| 16  | LL    | 98  | VAL  |
| 16  | LL    | 103 | ARG  |
| 16  | LL    | 104 | ASN  |
| 16  | LL    | 109 | SER  |
| 16  | LL    | 121 | ARG  |
| 16  | LL    | 162 | LYS  |
| 16  | LL    | 167 | ARG  |
| 16  | LL    | 198 | ARG  |
| 17  | LM    | 16  | SER  |
| 17  | LM    | 25  | VAL  |
| 17  | LM    | 30  | VAL  |
| 17  | LM    | 35  | ARG  |
| 17  | LM    | 63  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | LM    | 125 | ASN  |
| 18  | LN    | 5   | LYS  |
| 18  | LN    | 32  | GLN  |
| 18  | LN    | 38  | ARG  |
| 18  | LN    | 41  | ARG  |
| 18  | LN    | 53  | TYR  |
| 18  | LN    | 60  | VAL  |
| 18  | LN    | 80  | THR  |
| 18  | LN    | 125 | SER  |
| 18  | LN    | 148 | THR  |
| 19  | LO    | 5   | GLN  |
| 19  | LO    | 27  | VAL  |
| 19  | LO    | 61  | ARG  |
| 19  | LO    | 132 | THR  |
| 19  | LO    | 145 | VAL  |
| 19  | LO    | 158 | GLU  |
| 19  | LO    | 165 | LYS  |
| 19  | LO    | 169 | ARG  |
| 19  | LO    | 191 | LYS  |
| 19  | LO    | 201 | LEU  |
| 20  | LP    | 13  | LYS  |
| 20  | LP    | 14  | SER  |
| 20  | LP    | 18  | ARG  |
| 20  | LP    | 23  | ARG  |
| 20  | LP    | 24  | VAL  |
| 20  | LP    | 30  | ARG  |
| 20  | LP    | 42  | ARG  |
| 20  | LP    | 46  | LYS  |
| 20  | LP    | 57  | CYS  |
| 20  | LP    | 58  | VAL  |
| 20  | LP    | 69  | ARG  |
| 20  | LP    | 75  | GLN  |
| 20  | LP    | 76  | TRP  |
| 20  | LP    | 93  | HIS  |
| 20  | LP    | 118 | GLN  |
| 20  | LP    | 139 | TYR  |
| 21  | LQ    | 4   | ASP  |
| 21  | LQ    | 28  | LEU  |
| 21  | LQ    | 33  | ARG  |
| 21  | LQ    | 68  | ARG  |
| 21  | LQ    | 93  | GLN  |
| 21  | LQ    | 101 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | LQ    | 115 | ARG  |
| 21  | LQ    | 128 | LEU  |
| 21  | LQ    | 183 | SER  |
| 22  | LS    | 21  | LYS  |
| 22  | LS    | 29  | ARG  |
| 22  | LS    | 31  | ARG  |
| 22  | LS    | 43  | ARG  |
| 22  | LS    | 57  | SER  |
| 22  | LS    | 90  | THR  |
| 22  | LS    | 111 | ARG  |
| 22  | LS    | 158 | VAL  |
| 22  | LS    | 169 | THR  |
| 23  | LT    | 3   | ASN  |
| 23  | LT    | 4   | THR  |
| 23  | LT    | 5   | LYS  |
| 23  | LT    | 29  | THR  |
| 23  | LT    | 45  | MET  |
| 23  | LT    | 83  | LYS  |
| 23  | LT    | 85  | LEU  |
| 23  | LT    | 99  | SER  |
| 23  | LT    | 104 | SER  |
| 23  | LT    | 158 | PHE  |
| 24  | LU    | 19  | LEU  |
| 24  | LU    | 22  | THR  |
| 24  | LU    | 39  | PHE  |
| 24  | LU    | 69  | LYS  |
| 24  | LU    | 79  | SER  |
| 24  | LU    | 92  | LYS  |
| 24  | LU    | 94  | ASN  |
| 24  | LU    | 95  | ASN  |
| 24  | LU    | 97  | ARG  |
| 24  | LU    | 98  | ASP  |
| 24  | LU    | 110 | TYR  |
| 24  | LU    | 112 | LEU  |
| 25  | LV    | 17  | SER  |
| 25  | LV    | 35  | LYS  |
| 25  | LV    | 48  | ARG  |
| 25  | LV    | 59  | ASP  |
| 25  | LV    | 67  | LYS  |
| 25  | LV    | 131 | ARG  |
| 26  | LX    | 52  | LEU  |
| 26  | LX    | 57  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | LX    | 68  | ARG  |
| 26  | LX    | 73  | HIS  |
| 26  | LX    | 80  | PRO  |
| 26  | LX    | 95  | THR  |
| 26  | LX    | 121 | VAL  |
| 26  | LX    | 126 | THR  |
| 26  | LX    | 148 | ASP  |
| 26  | LX    | 152 | LYS  |
| 27  | LY    | 12  | SER  |
| 27  | LY    | 41  | LYS  |
| 27  | LY    | 74  | TYR  |
| 27  | LY    | 99  | ILE  |
| 27  | LY    | 110 | LYS  |
| 27  | LY    | 112 | ASP  |
| 27  | LY    | 117 | LYS  |
| 27  | LY    | 130 | LYS  |
| 28  | LZ    | 11  | VAL  |
| 28  | LZ    | 35  | ASP  |
| 28  | LZ    | 43  | VAL  |
| 28  | LZ    | 84  | ARG  |
| 28  | LZ    | 85  | TYR  |
| 28  | LZ    | 100 | VAL  |
| 28  | LZ    | 123 | LYS  |
| 29  | La    | 10  | LYS  |
| 29  | La    | 15  | VAL  |
| 29  | La    | 58  | MET  |
| 29  | La    | 66  | ASN  |
| 29  | La    | 68  | SER  |
| 29  | La    | 106 | SER  |
| 29  | La    | 139 | SER  |
| 30  | Lb    | 4   | SER  |
| 30  | Lb    | 57  | MET  |
| 30  | Lb    | 91  | ARG  |
| 30  | Lb    | 111 | ARG  |
| 30  | Lb    | 114 | LYS  |
| 30  | Lb    | 117 | ARG  |
| 31  | Lc    | 23  | LYS  |
| 31  | Lc    | 28  | VAL  |
| 31  | Lc    | 44  | LYS  |
| 31  | Lc    | 48  | LEU  |
| 31  | Lc    | 65  | MET  |
| 31  | Lc    | 69  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | Lc    | 87  | LYS  |
| 31  | Lc    | 91  | VAL  |
| 31  | Lc    | 92  | CYS  |
| 31  | Lc    | 98  | ASP  |
| 32  | Ld    | 26  | THR  |
| 32  | Ld    | 55  | LYS  |
| 32  | Ld    | 68  | LEU  |
| 32  | Ld    | 84  | ILE  |
| 32  | Ld    | 95  | ASP  |
| 32  | Ld    | 105 | LEU  |
| 32  | Ld    | 106 | VAL  |
| 33  | Le    | 26  | ASP  |
| 33  | Le    | 65  | LYS  |
| 33  | Le    | 76  | LYS  |
| 33  | Le    | 87  | VAL  |
| 33  | Le    | 102 | ASN  |
| 34  | Lf    | 25  | THR  |
| 34  | Lf    | 37  | ASP  |
| 34  | Lf    | 46  | ARG  |
| 35  | Lg    | 28  | ASN  |
| 35  | Lg    | 44  | SER  |
| 35  | Lg    | 53  | LEU  |
| 35  | Lg    | 63  | VAL  |
| 35  | Lg    | 73  | HIS  |
| 35  | Lg    | 75  | SER  |
| 36  | Lh    | 82  | ASP  |
| 36  | Lh    | 87  | LYS  |
| 36  | Lh    | 112 | ARG  |
| 37  | Li    | 4   | ARG  |
| 37  | Li    | 23  | LYS  |
| 37  | Li    | 42  | ASP  |
| 37  | Li    | 55  | ARG  |
| 38  | Lj    | 22  | CYS  |
| 38  | Lj    | 36  | LYS  |
| 38  | Lj    | 63  | ARG  |
| 39  | Lk    | 9   | LYS  |
| 39  | Lk    | 29  | LYS  |
| 39  | Lk    | 40  | ARG  |
| 39  | Lk    | 52  | LYS  |
| 39  | Lk    | 55  | LYS  |
| 39  | Lk    | 67  | LYS  |
| 40  | Ll    | 21  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | Ll    | 39  | SER  |
| 40  | Ll    | 51  | LEU  |
| 41  | Lm    | 81  | SER  |
| 41  | Lm    | 90  | ASN  |
| 42  | Ln    | 10  | MET  |
| 43  | Lo    | 15  | CYS  |
| 43  | Lo    | 31  | ASP  |
| 43  | Lo    | 36  | GLN  |
| 43  | Lo    | 69  | ARG  |
| 43  | Lo    | 71  | GLU  |
| 43  | Lo    | 74  | GLU  |
| 43  | Lo    | 77  | CYS  |
| 43  | Lo    | 97  | LYS  |
| 44  | Lp    | 84  | ARG  |
| 45  | Lr    | 14  | SER  |
| 45  | Lr    | 21  | ASN  |
| 45  | Lr    | 37  | SER  |
| 45  | Lr    | 49  | VAL  |
| 45  | Lr    | 51  | VAL  |
| 45  | Lr    | 58  | LYS  |
| 45  | Lr    | 60  | VAL  |
| 45  | Lr    | 62  | VAL  |
| 45  | Lr    | 63  | VAL  |
| 45  | Lr    | 80  | THR  |
| 45  | Lr    | 91  | SER  |
| 45  | Lr    | 96  | MET  |
| 45  | Lr    | 98  | ARG  |
| 45  | Lr    | 99  | LYS  |
| 45  | Lr    | 119 | ARG  |
| 45  | Lr    | 125 | MET  |
| 46  | Lz    | 3   | SER  |
| 46  | Lz    | 5   | VAL  |
| 46  | Lz    | 7   | ARG  |
| 46  | Lz    | 22  | GLN  |
| 46  | Lz    | 39  | LYS  |
| 46  | Lz    | 80  | VAL  |
| 46  | Lz    | 85  | MET  |
| 46  | Lz    | 110 | PHE  |
| 46  | Lz    | 122 | ARG  |
| 46  | Lz    | 148 | VAL  |
| 46  | Lz    | 156 | LYS  |
| 46  | Lz    | 161 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | Lz    | 173 | LYS  |
| 46  | Lz    | 210 | MET  |
| 47  | CA    | 21  | TYR  |
| 47  | CA    | 35  | LEU  |
| 47  | CA    | 51  | LYS  |
| 47  | CA    | 71  | LYS  |
| 47  | CA    | 93  | LYS  |
| 47  | CA    | 95  | ASP  |
| 47  | CA    | 134 | GLN  |
| 47  | CA    | 148 | LEU  |
| 47  | CA    | 185 | MET  |
| 47  | CA    | 191 | LYS  |
| 47  | CA    | 210 | LYS  |
| 47  | CA    | 221 | HIS  |
| 47  | CA    | 224 | TYR  |
| 47  | CA    | 243 | ARG  |
| 47  | CA    | 254 | GLN  |
| 47  | CA    | 274 | ASP  |
| 47  | CA    | 276 | MET  |
| 47  | CA    | 294 | VAL  |
| 47  | CA    | 295 | GLU  |
| 47  | CA    | 310 | GLU  |
| 47  | CA    | 331 | MET  |
| 47  | CA    | 342 | LEU  |
| 47  | CA    | 357 | LEU  |
| 48  | Ls    | 10  | LYS  |
| 48  | Ls    | 14  | PHE  |
| 48  | Ls    | 39  | GLN  |
| 48  | Ls    | 52  | VAL  |
| 48  | Ls    | 68  | HIS  |
| 48  | Ls    | 69  | LEU  |
| 48  | Ls    | 76  | GLU  |
| 48  | Ls    | 79  | LEU  |
| 48  | Ls    | 91  | THR  |
| 48  | Ls    | 99  | ARG  |
| 48  | Ls    | 105 | ASN  |
| 48  | Ls    | 107 | VAL  |
| 48  | Ls    | 146 | LYS  |
| 48  | Ls    | 149 | ARG  |
| 48  | Ls    | 153 | GLU  |
| 48  | Ls    | 173 | THR  |
| 48  | Ls    | 176 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | Ls    | 181 | SER  |
| 48  | Ls    | 183 | PHE  |
| 48  | Ls    | 185 | PHE  |
| 49  | Lt    | 44  | ASP  |
| 49  | Lt    | 45  | ASP  |
| 49  | Lt    | 61  | LYS  |
| 49  | Lt    | 63  | THR  |
| 49  | Lt    | 76  | SER  |
| 49  | Lt    | 104 | ILE  |
| 49  | Lt    | 114 | ARG  |
| 49  | Lt    | 116 | MET  |
| 49  | Lt    | 146 | ARG  |
| 50  | SD    | 4   | GLN  |
| 50  | SD    | 10  | LYS  |
| 50  | SD    | 34  | TYR  |
| 50  | SD    | 35  | SER  |
| 50  | SD    | 42  | THR  |
| 50  | SD    | 43  | PRO  |
| 50  | SD    | 46  | THR  |
| 50  | SD    | 47  | GLU  |
| 50  | SD    | 56  | GLN  |
| 50  | SD    | 67  | ARG  |
| 50  | SD    | 76  | ARG  |
| 50  | SD    | 81  | GLU  |
| 50  | SD    | 104 | SER  |
| 50  | SD    | 115 | VAL  |
| 50  | SD    | 125 | PHE  |
| 50  | SD    | 132 | LYS  |
| 50  | SD    | 142 | LEU  |
| 50  | SD    | 146 | ARG  |
| 50  | SD    | 148 | LYS  |
| 50  | SD    | 149 | SER  |
| 50  | SD    | 157 | MET  |
| 50  | SD    | 167 | TYR  |
| 50  | SD    | 170 | THR  |
| 50  | SD    | 173 | ARG  |
| 50  | SD    | 174 | HIS  |
| 50  | SD    | 189 | MET  |
| 50  | SD    | 192 | TRP  |
| 50  | SD    | 197 | LYS  |
| 50  | SD    | 209 | SER  |
| 51  | SF    | 27  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | SF    | 45  | TYR  |
| 51  | SF    | 72  | LEU  |
| 51  | SF    | 79  | HIS  |
| 51  | SF    | 85  | LYS  |
| 51  | SF    | 86  | LYS  |
| 51  | SF    | 94  | LYS  |
| 51  | SF    | 106 | GLU  |
| 51  | SF    | 125 | SER  |
| 51  | SF    | 142 | SER  |
| 51  | SF    | 165 | ASN  |
| 51  | SF    | 168 | THR  |
| 51  | SF    | 169 | ILE  |
| 51  | SF    | 192 | LYS  |
| 52  | SK    | 3   | MET  |
| 52  | SK    | 5   | LYS  |
| 52  | SK    | 7   | ASN  |
| 52  | SK    | 8   | ARG  |
| 52  | SK    | 50  | GLN  |
| 52  | SK    | 55  | ARG  |
| 52  | SK    | 65  | ARG  |
| 52  | SK    | 77  | GLN  |
| 52  | SK    | 84  | HIS  |
| 53  | SP    | 36  | LEU  |
| 53  | SP    | 55  | SER  |
| 53  | SP    | 58  | LYS  |
| 53  | SP    | 62  | LYS  |
| 53  | SP    | 66  | GLU  |
| 53  | SP    | 79  | HIS  |
| 53  | SP    | 97  | TYR  |
| 53  | SP    | 130 | ARG  |
| 54  | SQ    | 11  | GLN  |
| 54  | SQ    | 22  | VAL  |
| 54  | SQ    | 37  | ARG  |
| 54  | SQ    | 41  | MET  |
| 54  | SQ    | 47  | LEU  |
| 54  | SQ    | 52  | LEU  |
| 54  | SQ    | 57  | LEU  |
| 54  | SQ    | 78  | VAL  |
| 54  | SQ    | 100 | VAL  |
| 54  | SQ    | 106 | LYS  |
| 54  | SQ    | 109 | LYS  |
| 54  | SQ    | 112 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | SQ    | 125 | ARG  |
| 54  | SQ    | 140 | ARG  |
| 54  | SQ    | 142 | GLN  |
| 54  | SQ    | 145 | TYR  |
| 55  | SS    | 1   | MET  |
| 55  | SS    | 9   | PHE  |
| 55  | SS    | 18  | THR  |
| 55  | SS    | 24  | ARG  |
| 55  | SS    | 40  | TYR  |
| 55  | SS    | 49  | ASP  |
| 55  | SS    | 54  | LYS  |
| 55  | SS    | 58  | GLU  |
| 55  | SS    | 73  | ASN  |
| 55  | SS    | 77  | TYR  |
| 55  | SS    | 81  | ASP  |
| 55  | SS    | 83  | PHE  |
| 55  | SS    | 84  | LEU  |
| 55  | SS    | 89  | ASP  |
| 55  | SS    | 92  | ASP  |
| 55  | SS    | 97  | GLN  |
| 55  | SS    | 101 | ASN  |
| 55  | SS    | 106 | LYS  |
| 55  | SS    | 116 | LYS  |
| 56  | ST    | 29  | LYS  |
| 56  | ST    | 50  | GLU  |
| 56  | ST    | 56  | ARG  |
| 56  | ST    | 64  | LEU  |
| 56  | ST    | 94  | ARG  |
| 56  | ST    | 99  | VAL  |
| 56  | ST    | 102 | ARG  |
| 56  | ST    | 122 | LYS  |
| 56  | ST    | 126 | GLN  |
| 56  | ST    | 129 | ARG  |
| 56  | ST    | 131 | LEU  |
| 56  | ST    | 133 | ARG  |
| 57  | SU    | 18  | HIS  |
| 57  | SU    | 21  | ARG  |
| 57  | SU    | 23  | THR  |
| 57  | SU    | 26  | SER  |
| 57  | SU    | 41  | ARG  |
| 57  | SU    | 49  | LYS  |
| 57  | SU    | 82  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | Sc    | 7   | GLN  |
| 58  | Sc    | 10  | LYS  |
| 58  | Sc    | 17  | VAL  |
| 58  | Sc    | 18  | LEU  |
| 58  | Sc    | 21  | THR  |
| 58  | Sc    | 35  | MET  |
| 58  | Sc    | 36  | ASP  |
| 58  | Sc    | 37  | ASP  |
| 58  | Sc    | 40  | ARG  |
| 58  | Sc    | 55  | VAL  |
| 59  | Sd    | 4   | GLN  |
| 59  | Sd    | 6   | LEU  |
| 59  | Sd    | 8   | TRP  |
| 59  | Sd    | 18  | SER  |
| 60  | Sg    | 3   | GLU  |
| 60  | Sg    | 8   | ARG  |
| 60  | Sg    | 14  | HIS  |
| 60  | Sg    | 27  | PHE  |
| 60  | Sg    | 30  | MET  |
| 60  | Sg    | 32  | LEU  |
| 60  | Sg    | 37  | ASP  |
| 60  | Sg    | 42  | MET  |
| 60  | Sg    | 49  | GLU  |
| 60  | Sg    | 64  | HIS  |
| 60  | Sg    | 77  | PHE  |
| 60  | Sg    | 79  | LEU  |
| 60  | Sg    | 86  | THR  |
| 60  | Sg    | 107 | ASP  |
| 60  | Sg    | 113 | PHE  |
| 60  | Sg    | 125 | ARG  |
| 60  | Sg    | 134 | THR  |
| 60  | Sg    | 140 | TYR  |
| 60  | Sg    | 141 | THR  |
| 60  | Sg    | 155 | ARG  |
| 60  | Sg    | 173 | LEU  |
| 60  | Sg    | 231 | ASP  |
| 60  | Sg    | 236 | ILE  |
| 60  | Sg    | 241 | PHE  |
| 60  | Sg    | 245 | ARG  |
| 60  | Sg    | 247 | TRP  |
| 60  | Sg    | 249 | CYS  |
| 60  | Sg    | 252 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 60  | Sg    | 259 | TRP  |
| 60  | Sg    | 289 | LEU  |
| 60  | Sg    | 297 | THR  |
| 60  | Sg    | 303 | THR  |
| 60  | Sg    | 308 | ARG  |
| 60  | Sg    | 311 | GLN  |
| 61  | SM    | 22  | LEU  |
| 61  | SM    | 33  | ARG  |
| 61  | SM    | 45  | ARG  |
| 61  | SM    | 52  | LEU  |
| 61  | SM    | 60  | MET  |
| 61  | SM    | 61  | TYR  |
| 61  | SM    | 82  | ASN  |
| 61  | SM    | 83  | LYS  |
| 61  | SM    | 84  | LYS  |
| 61  | SM    | 93  | LYS  |
| 61  | SM    | 99  | LYS  |
| 61  | SM    | 112 | LYS  |
| 61  | SM    | 127 | TYR  |
| 62  | SZ    | 55  | TYR  |
| 62  | SZ    | 66  | LYS  |
| 62  | SZ    | 69  | THR  |
| 62  | SZ    | 77  | LEU  |
| 62  | SZ    | 113 | THR  |
| 63  | Sf    | 94  | LYS  |
| 63  | Sf    | 110 | GLU  |
| 63  | Sf    | 113 | LYS  |
| 63  | Sf    | 116 | ARG  |
| 63  | Sf    | 126 | CYS  |
| 63  | Sf    | 138 | ARG  |
| 64  | CD    | 185 | PHE  |
| 64  | CD    | 199 | SER  |
| 64  | CD    | 201 | ARG  |
| 64  | CD    | 205 | LYS  |
| 64  | CD    | 286 | TRP  |
| 65  | LW    | 12  | LYS  |
| 65  | LW    | 28  | VAL  |
| 65  | LW    | 47  | ARG  |
| 65  | LW    | 74  | ARG  |
| 65  | LW    | 78  | PHE  |
| 65  | LW    | 86  | SER  |
| 65  | LW    | 104 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 65  | LW    | 116 | LYS  |
| 66  | SE    | 57  | THR  |
| 66  | SE    | 62  | LYS  |
| 66  | SE    | 65  | CYS  |
| 66  | SE    | 66  | MET  |
| 66  | SE    | 71  | LYS  |
| 66  | SE    | 87  | MET  |
| 66  | SE    | 94  | LYS  |
| 66  | SE    | 121 | TYR  |
| 66  | SE    | 124 | CYS  |
| 66  | SE    | 136 | ILE  |
| 66  | SE    | 142 | HIS  |
| 66  | SE    | 172 | PHE  |
| 66  | SE    | 198 | ARG  |
| 66  | SE    | 201 | HIS  |
| 66  | SE    | 207 | VAL  |
| 66  | SE    | 208 | VAL  |
| 66  | SE    | 209 | HIS  |
| 66  | SE    | 211 | LYS  |
| 66  | SE    | 252 | ARG  |
| 66  | SE    | 259 | LYS  |
| 67  | SI    | 4   | SER  |
| 67  | SI    | 7   | ASN  |
| 67  | SI    | 74  | ARG  |
| 67  | SI    | 81  | VAL  |
| 67  | SI    | 110 | ARG  |
| 67  | SI    | 111 | GLN  |
| 67  | SI    | 117 | TYR  |
| 67  | SI    | 119 | LEU  |
| 67  | SI    | 129 | LEU  |
| 67  | SI    | 130 | THR  |
| 67  | SI    | 132 | GLU  |
| 67  | SI    | 140 | LYS  |
| 67  | SI    | 153 | LYS  |
| 67  | SI    | 168 | GLN  |
| 67  | SI    | 186 | ASP  |
| 67  | SI    | 197 | PHE  |
| 67  | SI    | 201 | LYS  |
| 68  | SL    | 5   | GLN  |
| 68  | SL    | 42  | LEU  |
| 68  | SL    | 55  | TYR  |
| 68  | SL    | 58  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 68  | SL    | 69  | ARG  |
| 68  | SL    | 73  | LEU  |
| 68  | SL    | 80  | MET  |
| 68  | SL    | 81  | LYS  |
| 68  | SL    | 84  | ARG  |
| 68  | SL    | 90  | ARG  |
| 68  | SL    | 92  | TYR  |
| 68  | SL    | 97  | ARG  |
| 68  | SL    | 109 | MET  |
| 68  | SL    | 116 | CYS  |
| 68  | SL    | 139 | ARG  |
| 68  | SL    | 141 | ASN  |
| 68  | SL    | 144 | LYS  |
| 68  | SL    | 147 | LYS  |
| 69  | SX    | 4   | CYS  |
| 69  | SX    | 26  | GLN  |
| 69  | SX    | 67  | ARG  |
| 69  | SX    | 72  | VAL  |
| 69  | SX    | 88  | ASP  |
| 69  | SX    | 105 | PHE  |
| 69  | SX    | 119 | ARG  |
| 69  | SX    | 138 | LYS  |
| 70  | SG    | 1   | MET  |
| 70  | SG    | 7   | PHE  |
| 70  | SG    | 14  | LYS  |
| 70  | SG    | 45  | TRP  |
| 70  | SG    | 48  | TYR  |
| 70  | SG    | 50  | VAL  |
| 70  | SG    | 68  | LEU  |
| 70  | SG    | 70  | HIS  |
| 70  | SG    | 77  | LEU  |
| 70  | SG    | 98  | ARG  |
| 70  | SG    | 105 | ASN  |
| 70  | SG    | 108 | VAL  |
| 70  | SG    | 114 | VAL  |
| 70  | SG    | 119 | LYS  |
| 70  | SG    | 131 | ARG  |
| 70  | SG    | 132 | ARG  |
| 70  | SG    | 133 | LEU  |
| 70  | SG    | 143 | LYS  |
| 70  | SG    | 151 | ASP  |
| 70  | SG    | 168 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 70  | SG    | 170 | ARG  |
| 70  | SG    | 195 | LYS  |
| 70  | SG    | 197 | GLN  |
| 70  | SG    | 202 | ASN  |
| 70  | SG    | 215 | LYS  |
| 70  | SG    | 217 | MET  |
| 70  | SG    | 224 | ARG  |
| 71  | SJ    | 7   | TRP  |
| 71  | SJ    | 10  | ARG  |
| 71  | SJ    | 12  | THR  |
| 71  | SJ    | 13  | TYR  |
| 71  | SJ    | 75  | ASN  |
| 71  | SJ    | 80  | ARG  |
| 71  | SJ    | 88  | ASP  |
| 71  | SJ    | 92  | MET  |
| 71  | SJ    | 103 | GLU  |
| 71  | SJ    | 115 | PHE  |
| 71  | SJ    | 121 | LYS  |
| 71  | SJ    | 125 | HIS  |
| 71  | SJ    | 137 | VAL  |
| 71  | SJ    | 141 | VAL  |
| 71  | SJ    | 142 | VAL  |
| 71  | SJ    | 155 | LYS  |
| 71  | SJ    | 158 | ASP  |
| 71  | SJ    | 159 | PHE  |
| 71  | SJ    | 173 | VAL  |
| 71  | SJ    | 180 | LYS  |
| 72  | SY    | 10  | ARG  |
| 72  | SY    | 16  | ARG  |
| 72  | SY    | 23  | MET  |
| 72  | SY    | 26  | ASP  |
| 72  | SY    | 35  | VAL  |
| 72  | SY    | 47  | MET  |
| 72  | SY    | 48  | TYR  |
| 72  | SY    | 51  | THR  |
| 72  | SY    | 72  | PHE  |
| 72  | SY    | 90  | ARG  |
| 72  | SY    | 94  | HIS  |
| 72  | SY    | 97  | TYR  |
| 72  | SY    | 98  | GLU  |
| 72  | SY    | 99  | LYS  |
| 72  | SY    | 101 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 72  | SY    | 110 | ARG  |
| 72  | SY    | 113 | ARG  |
| 72  | SY    | 118 | ARG  |
| 72  | SY    | 132 | LYS  |
| 73  | Se    | 25  | LYS  |
| 73  | Se    | 31  | ARG  |
| 73  | Se    | 39  | ASN  |
| 73  | Se    | 40  | ARG  |
| 73  | Se    | 41  | ARG  |
| 73  | Se    | 58  | ASN  |
| 74  | SA    | 17  | LYS  |
| 74  | SA    | 18  | PHE  |
| 74  | SA    | 23  | THR  |
| 74  | SA    | 25  | LEU  |
| 74  | SA    | 52  | LYS  |
| 74  | SA    | 57  | LYS  |
| 74  | SA    | 69  | GLU  |
| 74  | SA    | 74  | VAL  |
| 74  | SA    | 77  | ILE  |
| 74  | SA    | 138 | SER  |
| 74  | SA    | 144 | THR  |
| 74  | SA    | 177 | MET  |
| 74  | SA    | 198 | MET  |
| 74  | SA    | 203 | PHE  |
| 74  | SA    | 209 | GLU  |
| 75  | SB    | 23  | ASP  |
| 75  | SB    | 42  | ARG  |
| 75  | SB    | 47  | THR  |
| 75  | SB    | 50  | THR  |
| 75  | SB    | 51  | ARG  |
| 75  | SB    | 53  | GLN  |
| 75  | SB    | 62  | LEU  |
| 75  | SB    | 68  | GLU  |
| 75  | SB    | 94  | LYS  |
| 75  | SB    | 101 | HIS  |
| 75  | SB    | 103 | MET  |
| 75  | SB    | 108 | ASP  |
| 75  | SB    | 118 | GLN  |
| 75  | SB    | 134 | LEU  |
| 75  | SB    | 154 | SER  |
| 75  | SB    | 162 | ARG  |
| 75  | SB    | 165 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | SB    | 166 | LYS  |
| 75  | SB    | 174 | ARG  |
| 75  | SB    | 179 | ASN  |
| 75  | SB    | 182 | LYS  |
| 75  | SB    | 201 | CYS  |
| 75  | SB    | 202 | GLN  |
| 75  | SB    | 210 | VAL  |
| 75  | SB    | 217 | MET  |
| 75  | SB    | 220 | LYS  |
| 75  | SB    | 231 | LEU  |
| 75  | SB    | 232 | HIS  |
| 76  | SH    | 32  | MET  |
| 76  | SH    | 39  | GLN  |
| 76  | SH    | 57  | ARG  |
| 76  | SH    | 81  | ARG  |
| 76  | SH    | 86  | LYS  |
| 76  | SH    | 103 | LYS  |
| 76  | SH    | 119 | SER  |
| 76  | SH    | 122 | LEU  |
| 76  | SH    | 135 | PHE  |
| 76  | SH    | 138 | GLU  |
| 76  | SH    | 155 | LYS  |
| 76  | SH    | 174 | SER  |
| 76  | SH    | 177 | TYR  |
| 76  | SH    | 178 | LYS  |
| 76  | SH    | 179 | LYS  |
| 77  | SV    | 1   | MET  |
| 77  | SV    | 17  | CYS  |
| 77  | SV    | 21  | ASN  |
| 77  | SV    | 22  | ARG  |
| 77  | SV    | 33  | GLN  |
| 77  | SV    | 45  | ARG  |
| 77  | SV    | 50  | PHE  |
| 77  | SV    | 52  | THR  |
| 77  | SV    | 56  | CYS  |
| 77  | SV    | 71  | ARG  |
| 77  | SV    | 74  | LYS  |
| 78  | Sa    | 15  | ARG  |
| 78  | Sa    | 23  | CYS  |
| 78  | Sa    | 37  | LYS  |
| 78  | Sa    | 68  | TYR  |
| 78  | Sa    | 71  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | Sa    | 81  | SER  |
| 78  | Sa    | 100 | ARG  |
| 79  | SC    | 65  | LYS  |
| 79  | SC    | 76  | LYS  |
| 79  | SC    | 91  | SER  |
| 79  | SC    | 93  | ILE  |
| 79  | SC    | 102 | LEU  |
| 79  | SC    | 103 | LYS  |
| 79  | SC    | 112 | VAL  |
| 79  | SC    | 113 | GLN  |
| 79  | SC    | 161 | SER  |
| 79  | SC    | 163 | VAL  |
| 79  | SC    | 167 | ARG  |
| 79  | SC    | 172 | ASN  |
| 79  | SC    | 206 | SER  |
| 79  | SC    | 220 | ASP  |
| 79  | SC    | 221 | ASP  |
| 79  | SC    | 227 | ARG  |
| 79  | SC    | 236 | PHE  |
| 79  | SC    | 257 | LYS  |
| 79  | SC    | 262 | THR  |
| 79  | SC    | 263 | LYS  |
| 79  | SC    | 264 | SER  |
| 79  | SC    | 271 | ASP  |
| 79  | SC    | 275 | LYS  |
| 80  | SN    | 14  | SER  |
| 80  | SN    | 20  | ARG  |
| 80  | SN    | 30  | SER  |
| 80  | SN    | 45  | LEU  |
| 80  | SN    | 46  | THR  |
| 80  | SN    | 57  | SER  |
| 80  | SN    | 60  | VAL  |
| 80  | SN    | 64  | ARG  |
| 80  | SN    | 72  | LEU  |
| 80  | SN    | 77  | SER  |
| 80  | SN    | 89  | TYR  |
| 80  | SN    | 105 | ASN  |
| 80  | SN    | 109 | LYS  |
| 80  | SN    | 114 | ARG  |
| 80  | SN    | 121 | ARG  |
| 80  | SN    | 140 | LYS  |
| 81  | SO    | 14  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | SO    | 38  | ASN  |
| 81  | SO    | 43  | HIS  |
| 81  | SO    | 48  | SER  |
| 81  | SO    | 52  | THR  |
| 81  | SO    | 75  | MET  |
| 81  | SO    | 84  | ARG  |
| 81  | SO    | 122 | SER  |
| 81  | SO    | 124 | MET  |
| 81  | SO    | 140 | THR  |
| 82  | SW    | 13  | SER  |
| 82  | SW    | 14  | ILE  |
| 82  | SW    | 57  | ARG  |
| 82  | SW    | 70  | ASN  |
| 82  | SW    | 103 | VAL  |
| 82  | SW    | 104 | LEU  |
| 82  | SW    | 112 | ASP  |
| 82  | SW    | 115 | GLU  |
| 83  | Sb    | 6   | ASP  |
| 83  | Sb    | 11  | SER  |
| 83  | Sb    | 13  | GLU  |
| 83  | Sb    | 31  | TYR  |
| 83  | Sb    | 56  | CYS  |
| 83  | Sb    | 57  | VAL  |
| 83  | Sb    | 64  | CYS  |
| 83  | Sb    | 77  | CYS  |
| 83  | Sb    | 81  | ARG  |
| 83  | Sb    | 82  | LYS  |
| 83  | Sb    | 83  | GLN  |
| 84  | CB    | 4   | PHE  |
| 84  | CB    | 12  | ILE  |
| 84  | CB    | 13  | MET  |
| 84  | CB    | 16  | LYS  |
| 84  | CB    | 20  | ARG  |
| 84  | CB    | 23  | SER  |
| 84  | CB    | 30  | HIS  |
| 84  | CB    | 32  | LYS  |
| 84  | CB    | 38  | SER  |
| 84  | CB    | 42  | LYS  |
| 84  | CB    | 48  | SER  |
| 84  | CB    | 57  | THR  |
| 84  | CB    | 78  | PHE  |
| 84  | CB    | 81  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 84  | CB    | 82  | SER  |
| 84  | CB    | 90  | LYS  |
| 84  | CB    | 93  | LYS  |
| 84  | CB    | 98  | PHE  |
| 84  | CB    | 104 | ASP  |
| 84  | CB    | 109 | VAL  |
| 84  | CB    | 110 | ASP  |
| 84  | CB    | 122 | THR  |
| 84  | CB    | 137 | VAL  |
| 84  | CB    | 141 | THR  |
| 84  | CB    | 155 | LEU  |
| 84  | CB    | 200 | MET  |
| 84  | CB    | 209 | LEU  |
| 84  | CB    | 212 | VAL  |
| 84  | CB    | 214 | PHE  |
| 84  | CB    | 231 | MET  |
| 84  | CB    | 235 | LYS  |
| 84  | CB    | 249 | ARG  |
| 84  | CB    | 251 | LYS  |
| 84  | CB    | 274 | SER  |
| 84  | CB    | 275 | LYS  |
| 84  | CB    | 284 | LYS  |
| 84  | CB    | 295 | ASP  |
| 84  | CB    | 302 | ASP  |
| 84  | CB    | 322 | LYS  |
| 84  | CB    | 328 | LYS  |
| 84  | CB    | 329 | ASP  |
| 84  | CB    | 352 | GLN  |
| 84  | CB    | 373 | TYR  |
| 84  | CB    | 388 | CYS  |
| 84  | CB    | 397 | TYR  |
| 84  | CB    | 409 | ARG  |
| 84  | CB    | 428 | ARG  |
| 84  | CB    | 435 | THR  |
| 84  | CB    | 439 | LYS  |
| 84  | CB    | 448 | GLN  |
| 84  | CB    | 456 | ARG  |
| 84  | CB    | 457 | TYR  |
| 84  | CB    | 466 | CYS  |
| 84  | CB    | 476 | ASP  |
| 84  | CB    | 481 | LYS  |
| 84  | CB    | 505 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 84  | CB    | 516 | ASP  |
| 84  | CB    | 533 | MET  |
| 84  | CB    | 539 | GLU  |
| 84  | CB    | 553 | HIS  |
| 84  | CB    | 574 | ASP  |
| 84  | CB    | 587 | SER  |
| 84  | CB    | 598 | LYS  |
| 84  | CB    | 601 | ARG  |
| 84  | CB    | 625 | ARG  |
| 84  | CB    | 641 | TRP  |
| 84  | CB    | 652 | PHE  |
| 84  | CB    | 673 | ASN  |
| 84  | CB    | 707 | VAL  |
| 84  | CB    | 724 | THR  |
| 84  | CB    | 745 | TYR  |
| 84  | CB    | 766 | LYS  |
| 84  | CB    | 784 | VAL  |
| 84  | CB    | 799 | ASP  |
| 84  | CB    | 829 | SER  |
| 84  | CB    | 830 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | LA    | 162 | ASN  |
| 10  | LE    | 128 | HIS  |
| 14  | LI    | 203 | HIS  |
| 27  | LY    | 72  | GLN  |
| 29  | La    | 93  | ASN  |
| 31  | Lc    | 40  | GLN  |
| 46  | Lz    | 119 | GLN  |
| 46  | Lz    | 143 | ASN  |
| 47  | CA    | 83  | ASN  |
| 47  | CA    | 88  | HIS  |
| 48  | Ls    | 127 | ASN  |
| 49  | Lt    | 70  | GLN  |
| 51  | SF    | 107 | ASN  |
| 52  | SK    | 7   | ASN  |
| 54  | SQ    | 11  | GLN  |
| 54  | SQ    | 48  | GLN  |
| 56  | ST    | 105 | GLN  |
| 62  | SZ    | 64  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | SZ    | 103 | HIS  |
| 66  | SE    | 112 | HIS  |
| 68  | SL    | 5   | GLN  |
| 71  | SJ    | 111 | GLN  |
| 71  | SJ    | 177 | ASN  |
| 74  | SA    | 9   | GLN  |
| 76  | SH    | 91  | HIS  |
| 77  | SV    | 35  | ASN  |
| 79  | SC    | 272 | HIS  |
| 81  | SO    | 38  | ASN  |
| 82  | SW    | 90  | GLN  |
| 83  | Sb    | 51  | GLN  |
| 84  | CB    | 27  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2   | S2    | 1717/1869 (91%) | 467 (27%)         | 5 (0%)          |
| 3   | L5    | 3705/5070 (73%) | 877 (23%)         | 22 (0%)         |
| 4   | L7    | 119/120 (99%)   | 14 (11%)          | 0               |
| 5   | L8    | 155/156 (99%)   | 29 (18%)          | 0               |
| 85  | Et    | 73/75 (97%)     | 55 (75%)          | 0               |
| All | All   | 5769/7290 (79%) | 1442 (24%)        | 27 (0%)         |

All (1442) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 4   | C    |
| 2   | S2    | 13  | C    |
| 2   | S2    | 14  | C    |
| 2   | S2    | 17  | C    |
| 2   | S2    | 23  | G    |
| 2   | S2    | 24  | C    |
| 2   | S2    | 25  | A    |
| 2   | S2    | 33  | G    |
| 2   | S2    | 42  | A    |
| 2   | S2    | 44  | U    |
| 2   | S2    | 45  | A    |
| 2   | S2    | 46  | A    |
| 2   | S2    | 56  | G    |
| 2   | S2    | 58  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 59  | U    |
| 2   | S2    | 62  | G    |
| 2   | S2    | 64  | A    |
| 2   | S2    | 65  | C    |
| 2   | S2    | 66  | G    |
| 2   | S2    | 67  | C    |
| 2   | S2    | 68  | A    |
| 2   | S2    | 72  | C    |
| 2   | S2    | 73  | C    |
| 2   | S2    | 74  | G    |
| 2   | S2    | 76  | U    |
| 2   | S2    | 79  | A    |
| 2   | S2    | 92  | A    |
| 2   | S2    | 103 | A    |
| 2   | S2    | 110 | U    |
| 2   | S2    | 113 | G    |
| 2   | S2    | 114 | G    |
| 2   | S2    | 115 | U    |
| 2   | S2    | 116 | U    |
| 2   | S2    | 126 | G    |
| 2   | S2    | 129 | C    |
| 2   | S2    | 130 | G    |
| 2   | S2    | 139 | C    |
| 2   | S2    | 142 | C    |
| 2   | S2    | 143 | U    |
| 2   | S2    | 149 | A    |
| 2   | S2    | 155 | G    |
| 2   | S2    | 158 | A    |
| 2   | S2    | 160 | U    |
| 2   | S2    | 161 | U    |
| 2   | S2    | 162 | C    |
| 2   | S2    | 163 | U    |
| 2   | S2    | 168 | C    |
| 2   | S2    | 170 | A    |
| 2   | S2    | 175 | A    |
| 2   | S2    | 182 | C    |
| 2   | S2    | 184 | G    |
| 2   | S2    | 190 | G    |
| 2   | S2    | 192 | C    |
| 2   | S2    | 196 | C    |
| 2   | S2    | 197 | U    |
| 2   | S2    | 198 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 200 | G    |
| 2   | S2    | 202 | G    |
| 2   | S2    | 203 | G    |
| 2   | S2    | 204 | G    |
| 2   | S2    | 206 | G    |
| 2   | S2    | 207 | G    |
| 2   | S2    | 208 | G    |
| 2   | S2    | 209 | A    |
| 2   | S2    | 211 | G    |
| 2   | S2    | 212 | C    |
| 2   | S2    | 213 | G    |
| 2   | S2    | 214 | U    |
| 2   | S2    | 291 | G    |
| 2   | S2    | 292 | A    |
| 2   | S2    | 295 | C    |
| 2   | S2    | 298 | G    |
| 2   | S2    | 301 | A    |
| 2   | S2    | 303 | C    |
| 2   | S2    | 305 | U    |
| 2   | S2    | 306 | C    |
| 2   | S2    | 307 | G    |
| 2   | S2    | 308 | G    |
| 2   | S2    | 309 | G    |
| 2   | S2    | 310 | C    |
| 2   | S2    | 311 | C    |
| 2   | S2    | 312 | G    |
| 2   | S2    | 317 | C    |
| 2   | S2    | 318 | A    |
| 2   | S2    | 319 | C    |
| 2   | S2    | 323 | C    |
| 2   | S2    | 324 | C    |
| 2   | S2    | 325 | C    |
| 2   | S2    | 326 | C    |
| 2   | S2    | 328 | U    |
| 2   | S2    | 329 | G    |
| 2   | S2    | 332 | G    |
| 2   | S2    | 338 | G    |
| 2   | S2    | 339 | A    |
| 2   | S2    | 340 | C    |
| 2   | S2    | 347 | G    |
| 2   | S2    | 360 | A    |
| 2   | S2    | 361 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 362 | C    |
| 2   | S2    | 364 | A    |
| 2   | S2    | 368 | U    |
| 2   | S2    | 370 | G    |
| 2   | S2    | 373 | G    |
| 2   | S2    | 375 | U    |
| 2   | S2    | 385 | G    |
| 2   | S2    | 386 | C    |
| 2   | S2    | 408 | A    |
| 2   | S2    | 409 | C    |
| 2   | S2    | 421 | G    |
| 2   | S2    | 426 | A    |
| 2   | S2    | 437 | G    |
| 2   | S2    | 442 | C    |
| 2   | S2    | 448 | A    |
| 2   | S2    | 449 | A    |
| 2   | S2    | 450 | C    |
| 2   | S2    | 452 | G    |
| 2   | S2    | 464 | A    |
| 2   | S2    | 465 | A    |
| 2   | S2    | 466 | G    |
| 2   | S2    | 471 | G    |
| 2   | S2    | 472 | C    |
| 2   | S2    | 473 | A    |
| 2   | S2    | 474 | G    |
| 2   | S2    | 476 | A    |
| 2   | S2    | 482 | G    |
| 2   | S2    | 487 | U    |
| 2   | S2    | 488 | U    |
| 2   | S2    | 492 | C    |
| 2   | S2    | 493 | A    |
| 2   | S2    | 496 | C    |
| 2   | S2    | 500 | A    |
| 2   | S2    | 502 | C    |
| 2   | S2    | 516 | A    |
| 2   | S2    | 517 | C    |
| 2   | S2    | 525 | A    |
| 2   | S2    | 528 | A    |
| 2   | S2    | 530 | U    |
| 2   | S2    | 531 | A    |
| 2   | S2    | 532 | C    |
| 2   | S2    | 533 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 536 | A    |
| 2   | S2    | 537 | C    |
| 2   | S2    | 538 | U    |
| 2   | S2    | 540 | U    |
| 2   | S2    | 541 | U    |
| 2   | S2    | 542 | U    |
| 2   | S2    | 546 | G    |
| 2   | S2    | 547 | G    |
| 2   | S2    | 549 | C    |
| 2   | S2    | 557 | U    |
| 2   | S2    | 558 | G    |
| 2   | S2    | 559 | G    |
| 2   | S2    | 560 | A    |
| 2   | S2    | 563 | G    |
| 2   | S2    | 564 | A    |
| 2   | S2    | 566 | U    |
| 2   | S2    | 569 | A    |
| 2   | S2    | 583 | A    |
| 2   | S2    | 587 | A    |
| 2   | S2    | 589 | G    |
| 2   | S2    | 590 | A    |
| 2   | S2    | 591 | U    |
| 2   | S2    | 593 | C    |
| 2   | S2    | 594 | A    |
| 2   | S2    | 604 | A    |
| 2   | S2    | 606 | G    |
| 2   | S2    | 607 | U    |
| 2   | S2    | 612 | U    |
| 2   | S2    | 614 | C    |
| 2   | S2    | 623 | G    |
| 2   | S2    | 628 | A    |
| 2   | S2    | 629 | A    |
| 2   | S2    | 631 | U    |
| 2   | S2    | 643 | A    |
| 2   | S2    | 644 | G    |
| 2   | S2    | 655 | A    |
| 2   | S2    | 660 | C    |
| 2   | S2    | 664 | A    |
| 2   | S2    | 668 | A    |
| 2   | S2    | 669 | A    |
| 2   | S2    | 671 | A    |
| 2   | S2    | 672 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 673 | G    |
| 2   | S2    | 678 | U    |
| 2   | S2    | 683 | G    |
| 2   | S2    | 684 | G    |
| 2   | S2    | 688 | U    |
| 2   | S2    | 689 | U    |
| 2   | S2    | 692 | G    |
| 2   | S2    | 693 | A    |
| 2   | S2    | 695 | C    |
| 2   | S2    | 696 | G    |
| 2   | S2    | 697 | G    |
| 2   | S2    | 698 | G    |
| 2   | S2    | 732 | U    |
| 2   | S2    | 733 | C    |
| 2   | S2    | 734 | C    |
| 2   | S2    | 736 | C    |
| 2   | S2    | 738 | C    |
| 2   | S2    | 749 | U    |
| 2   | S2    | 750 | C    |
| 2   | S2    | 751 | G    |
| 2   | S2    | 752 | G    |
| 2   | S2    | 753 | C    |
| 2   | S2    | 788 | G    |
| 2   | S2    | 789 | G    |
| 2   | S2    | 791 | C    |
| 2   | S2    | 792 | C    |
| 2   | S2    | 793 | G    |
| 2   | S2    | 794 | A    |
| 2   | S2    | 798 | G    |
| 2   | S2    | 799 | U    |
| 2   | S2    | 801 | U    |
| 2   | S2    | 821 | G    |
| 2   | S2    | 822 | U    |
| 2   | S2    | 823 | U    |
| 2   | S2    | 824 | C    |
| 2   | S2    | 827 | A    |
| 2   | S2    | 830 | A    |
| 2   | S2    | 833 | C    |
| 2   | S2    | 834 | C    |
| 2   | S2    | 835 | C    |
| 2   | S2    | 836 | G    |
| 2   | S2    | 837 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S2    | 838 | G    |
| 2   | S2    | 839 | C    |
| 2   | S2    | 840 | C    |
| 2   | S2    | 842 | C    |
| 2   | S2    | 844 | U    |
| 2   | S2    | 847 | A    |
| 2   | S2    | 859 | G    |
| 2   | S2    | 869 | A    |
| 2   | S2    | 870 | A    |
| 2   | S2    | 873 | G    |
| 2   | S2    | 874 | G    |
| 2   | S2    | 877 | C    |
| 2   | S2    | 881 | G    |
| 2   | S2    | 882 | U    |
| 2   | S2    | 888 | U    |
| 2   | S2    | 889 | U    |
| 2   | S2    | 890 | U    |
| 2   | S2    | 891 | G    |
| 2   | S2    | 892 | U    |
| 2   | S2    | 893 | U    |
| 2   | S2    | 896 | U    |
| 2   | S2    | 897 | U    |
| 2   | S2    | 898 | U    |
| 2   | S2    | 899 | U    |
| 2   | S2    | 900 | C    |
| 2   | S2    | 901 | G    |
| 2   | S2    | 903 | A    |
| 2   | S2    | 904 | A    |
| 2   | S2    | 913 | A    |
| 2   | S2    | 919 | A    |
| 2   | S2    | 920 | A    |
| 2   | S2    | 922 | A    |
| 2   | S2    | 925 | G    |
| 2   | S2    | 933 | G    |
| 2   | S2    | 934 | G    |
| 2   | S2    | 949 | G    |
| 2   | S2    | 954 | U    |
| 2   | S2    | 955 | A    |
| 2   | S2    | 956 | G    |
| 2   | S2    | 963 | A    |
| 2   | S2    | 970 | G    |
| 2   | S2    | 971 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 972  | A    |
| 2   | S2    | 978  | G    |
| 2   | S2    | 980  | A    |
| 2   | S2    | 988  | C    |
| 2   | S2    | 989  | C    |
| 2   | S2    | 990  | A    |
| 2   | S2    | 992  | A    |
| 2   | S2    | 999  | G    |
| 2   | S2    | 1001 | A    |
| 2   | S2    | 1008 | A    |
| 2   | S2    | 1017 | U    |
| 2   | S2    | 1023 | A    |
| 2   | S2    | 1027 | A    |
| 2   | S2    | 1033 | G    |
| 2   | S2    | 1042 | A    |
| 2   | S2    | 1045 | U    |
| 2   | S2    | 1047 | C    |
| 2   | S2    | 1060 | A    |
| 2   | S2    | 1061 | U    |
| 2   | S2    | 1062 | A    |
| 2   | S2    | 1067 | C    |
| 2   | S2    | 1083 | A    |
| 2   | S2    | 1085 | C    |
| 2   | S2    | 1088 | U    |
| 2   | S2    | 1109 | C    |
| 2   | S2    | 1113 | A    |
| 2   | S2    | 1114 | U    |
| 2   | S2    | 1115 | U    |
| 2   | S2    | 1116 | C    |
| 2   | S2    | 1118 | C    |
| 2   | S2    | 1119 | A    |
| 2   | S2    | 1121 | G    |
| 2   | S2    | 1126 | G    |
| 2   | S2    | 1133 | A    |
| 2   | S2    | 1138 | C    |
| 2   | S2    | 1148 | A    |
| 2   | S2    | 1153 | C    |
| 2   | S2    | 1154 | U    |
| 2   | S2    | 1155 | U    |
| 2   | S2    | 1195 | A    |
| 2   | S2    | 1207 | G    |
| 2   | S2    | 1208 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 1215 | C    |
| 2   | S2    | 1216 | C    |
| 2   | S2    | 1217 | A    |
| 2   | S2    | 1220 | A    |
| 2   | S2    | 1224 | G    |
| 2   | S2    | 1227 | G    |
| 2   | S2    | 1242 | U    |
| 2   | S2    | 1243 | U    |
| 2   | S2    | 1251 | A    |
| 2   | S2    | 1253 | A    |
| 2   | S2    | 1256 | G    |
| 2   | S2    | 1257 | G    |
| 2   | S2    | 1259 | A    |
| 2   | S2    | 1264 | C    |
| 2   | S2    | 1274 | G    |
| 2   | S2    | 1275 | G    |
| 2   | S2    | 1283 | C    |
| 2   | S2    | 1284 | A    |
| 2   | S2    | 1286 | G    |
| 2   | S2    | 1293 | A    |
| 2   | S2    | 1294 | G    |
| 2   | S2    | 1295 | A    |
| 2   | S2    | 1301 | A    |
| 2   | S2    | 1302 | G    |
| 2   | S2    | 1303 | C    |
| 2   | S2    | 1308 | U    |
| 2   | S2    | 1322 | G    |
| 2   | S2    | 1342 | U    |
| 2   | S2    | 1348 | G    |
| 2   | S2    | 1364 | U    |
| 2   | S2    | 1371 | U    |
| 2   | S2    | 1372 | U    |
| 2   | S2    | 1373 | C    |
| 2   | S2    | 1376 | A    |
| 2   | S2    | 1378 | A    |
| 2   | S2    | 1396 | A    |
| 2   | S2    | 1401 | A    |
| 2   | S2    | 1402 | A    |
| 2   | S2    | 1408 | U    |
| 2   | S2    | 1411 | G    |
| 2   | S2    | 1414 | A    |
| 2   | S2    | 1415 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 1419 | C    |
| 2   | S2    | 1420 | G    |
| 2   | S2    | 1421 | A    |
| 2   | S2    | 1422 | G    |
| 2   | S2    | 1423 | C    |
| 2   | S2    | 1424 | G    |
| 2   | S2    | 1428 | G    |
| 2   | S2    | 1431 | G    |
| 2   | S2    | 1433 | C    |
| 2   | S2    | 1434 | C    |
| 2   | S2    | 1435 | C    |
| 2   | S2    | 1436 | C    |
| 2   | S2    | 1438 | A    |
| 2   | S2    | 1442 | U    |
| 2   | S2    | 1449 | G    |
| 2   | S2    | 1454 | A    |
| 2   | S2    | 1458 | G    |
| 2   | S2    | 1462 | U    |
| 2   | S2    | 1463 | U    |
| 2   | S2    | 1478 | U    |
| 2   | S2    | 1479 | G    |
| 2   | S2    | 1486 | A    |
| 2   | S2    | 1488 | C    |
| 2   | S2    | 1489 | A    |
| 2   | S2    | 1490 | G    |
| 2   | S2    | 1494 | U    |
| 2   | S2    | 1495 | G    |
| 2   | S2    | 1497 | G    |
| 2   | S2    | 1498 | A    |
| 2   | S2    | 1508 | A    |
| 2   | S2    | 1521 | C    |
| 2   | S2    | 1533 | A    |
| 2   | S2    | 1535 | U    |
| 2   | S2    | 1536 | G    |
| 2   | S2    | 1537 | A    |
| 2   | S2    | 1544 | C    |
| 2   | S2    | 1552 | G    |
| 2   | S2    | 1556 | A    |
| 2   | S2    | 1570 | G    |
| 2   | S2    | 1574 | C    |
| 2   | S2    | 1579 | A    |
| 2   | S2    | 1580 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 1581 | C    |
| 2   | S2    | 1582 | C    |
| 2   | S2    | 1584 | G    |
| 2   | S2    | 1585 | U    |
| 2   | S2    | 1586 | U    |
| 2   | S2    | 1587 | G    |
| 2   | S2    | 1588 | A    |
| 2   | S2    | 1599 | U    |
| 2   | S2    | 1601 | A    |
| 2   | S2    | 1603 | G    |
| 2   | S2    | 1606 | G    |
| 2   | S2    | 1621 | U    |
| 2   | S2    | 1623 | A    |
| 2   | S2    | 1629 | C    |
| 2   | S2    | 1633 | A    |
| 2   | S2    | 1634 | A    |
| 2   | S2    | 1637 | A    |
| 2   | S2    | 1638 | G    |
| 2   | S2    | 1639 | G    |
| 2   | S2    | 1640 | A    |
| 2   | S2    | 1648 | G    |
| 2   | S2    | 1654 | G    |
| 2   | S2    | 1663 | A    |
| 2   | S2    | 1665 | G    |
| 2   | S2    | 1671 | G    |
| 2   | S2    | 1696 | C    |
| 2   | S2    | 1699 | A    |
| 2   | S2    | 1712 | A    |
| 2   | S2    | 1715 | A    |
| 2   | S2    | 1722 | G    |
| 2   | S2    | 1729 | U    |
| 2   | S2    | 1742 | C    |
| 2   | S2    | 1743 | G    |
| 2   | S2    | 1744 | G    |
| 2   | S2    | 1745 | A    |
| 2   | S2    | 1752 | C    |
| 2   | S2    | 1753 | C    |
| 2   | S2    | 1754 | G    |
| 2   | S2    | 1755 | C    |
| 2   | S2    | 1756 | C    |
| 2   | S2    | 1757 | G    |
| 2   | S2    | 1758 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 1759 | G    |
| 2   | S2    | 1761 | U    |
| 2   | S2    | 1772 | C    |
| 2   | S2    | 1773 | C    |
| 2   | S2    | 1774 | C    |
| 2   | S2    | 1777 | G    |
| 2   | S2    | 1780 | G    |
| 2   | S2    | 1782 | G    |
| 2   | S2    | 1783 | C    |
| 2   | S2    | 1784 | G    |
| 2   | S2    | 1785 | C    |
| 2   | S2    | 1787 | G    |
| 2   | S2    | 1798 | C    |
| 2   | S2    | 1806 | A    |
| 2   | S2    | 1809 | A    |
| 2   | S2    | 1810 | U    |
| 2   | S2    | 1812 | U    |
| 2   | S2    | 1813 | A    |
| 2   | S2    | 1822 | A    |
| 2   | S2    | 1823 | A    |
| 2   | S2    | 1825 | A    |
| 2   | S2    | 1826 | G    |
| 2   | S2    | 1829 | G    |
| 2   | S2    | 1831 | A    |
| 2   | S2    | 1835 | A    |
| 2   | S2    | 1838 | U    |
| 2   | S2    | 1849 | G    |
| 2   | S2    | 1851 | A    |
| 2   | S2    | 1852 | C    |
| 2   | S2    | 1861 | G    |
| 2   | S2    | 1862 | G    |
| 2   | S2    | 1863 | A    |
| 2   | S2    | 1865 | C    |
| 3   | L5    | 2    | G    |
| 3   | L5    | 25   | A    |
| 3   | L5    | 26   | C    |
| 3   | L5    | 30   | C    |
| 3   | L5    | 39   | A    |
| 3   | L5    | 42   | A    |
| 3   | L5    | 48   | G    |
| 3   | L5    | 56   | A    |
| 3   | L5    | 59   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 64  | A    |
| 3   | L5    | 65  | A    |
| 3   | L5    | 66  | A    |
| 3   | L5    | 69  | A    |
| 3   | L5    | 73  | A    |
| 3   | L5    | 74  | G    |
| 3   | L5    | 91  | G    |
| 3   | L5    | 98  | A    |
| 3   | L5    | 104 | G    |
| 3   | L5    | 108 | A    |
| 3   | L5    | 109 | G    |
| 3   | L5    | 110 | C    |
| 3   | L5    | 119 | G    |
| 3   | L5    | 120 | A    |
| 3   | L5    | 132 | G    |
| 3   | L5    | 133 | C    |
| 3   | L5    | 134 | G    |
| 3   | L5    | 135 | G    |
| 3   | L5    | 145 | G    |
| 3   | L5    | 152 | U    |
| 3   | L5    | 159 | C    |
| 3   | L5    | 165 | A    |
| 3   | L5    | 172 | C    |
| 3   | L5    | 183 | C    |
| 3   | L5    | 184 | U    |
| 3   | L5    | 185 | C    |
| 3   | L5    | 188 | G    |
| 3   | L5    | 189 | G    |
| 3   | L5    | 200 | U    |
| 3   | L5    | 209 | U    |
| 3   | L5    | 216 | C    |
| 3   | L5    | 218 | A    |
| 3   | L5    | 220 | C    |
| 3   | L5    | 234 | G    |
| 3   | L5    | 237 | G    |
| 3   | L5    | 255 | C    |
| 3   | L5    | 256 | G    |
| 3   | L5    | 261 | G    |
| 3   | L5    | 263 | G    |
| 3   | L5    | 264 | C    |
| 3   | L5    | 265 | C    |
| 3   | L5    | 266 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 267 | G    |
| 3   | L5    | 269 | G    |
| 3   | L5    | 275 | C    |
| 3   | L5    | 280 | G    |
| 3   | L5    | 297 | U    |
| 3   | L5    | 306 | A    |
| 3   | L5    | 315 | G    |
| 3   | L5    | 316 | U    |
| 3   | L5    | 326 | C    |
| 3   | L5    | 340 | C    |
| 3   | L5    | 350 | C    |
| 3   | L5    | 373 | G    |
| 3   | L5    | 385 | A    |
| 3   | L5    | 387 | G    |
| 3   | L5    | 388 | A    |
| 3   | L5    | 396 | A    |
| 3   | L5    | 407 | A    |
| 3   | L5    | 409 | G    |
| 3   | L5    | 410 | A    |
| 3   | L5    | 411 | G    |
| 3   | L5    | 412 | G    |
| 3   | L5    | 415 | G    |
| 3   | L5    | 431 | G    |
| 3   | L5    | 432 | U    |
| 3   | L5    | 440 | U    |
| 3   | L5    | 449 | C    |
| 3   | L5    | 450 | G    |
| 3   | L5    | 452 | A    |
| 3   | L5    | 453 | G    |
| 3   | L5    | 454 | U    |
| 3   | L5    | 456 | C    |
| 3   | L5    | 457 | G    |
| 3   | L5    | 465 | G    |
| 3   | L5    | 467 | U    |
| 3   | L5    | 468 | U    |
| 3   | L5    | 472 | C    |
| 3   | L5    | 484 | U    |
| 3   | L5    | 485 | C    |
| 3   | L5    | 486 | C    |
| 3   | L5    | 489 | C    |
| 3   | L5    | 493 | G    |
| 3   | L5    | 494 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 497 | G    |
| 3   | L5    | 498 | C    |
| 3   | L5    | 499 | G    |
| 3   | L5    | 500 | G    |
| 3   | L5    | 501 | C    |
| 3   | L5    | 502 | C    |
| 3   | L5    | 503 | C    |
| 3   | L5    | 504 | G    |
| 3   | L5    | 505 | G    |
| 3   | L5    | 509 | A    |
| 3   | L5    | 510 | U    |
| 3   | L5    | 512 | U    |
| 3   | L5    | 513 | U    |
| 3   | L5    | 514 | U    |
| 3   | L5    | 516 | C    |
| 3   | L5    | 518 | G    |
| 3   | L5    | 643 | C    |
| 3   | L5    | 644 | G    |
| 3   | L5    | 645 | G    |
| 3   | L5    | 646 | G    |
| 3   | L5    | 653 | U    |
| 3   | L5    | 654 | C    |
| 3   | L5    | 656 | C    |
| 3   | L5    | 657 | C    |
| 3   | L5    | 659 | G    |
| 3   | L5    | 665 | C    |
| 3   | L5    | 666 | G    |
| 3   | L5    | 667 | A    |
| 3   | L5    | 668 | C    |
| 3   | L5    | 669 | C    |
| 3   | L5    | 672 | C    |
| 3   | L5    | 673 | C    |
| 3   | L5    | 685 | C    |
| 3   | L5    | 686 | A    |
| 3   | L5    | 687 | U    |
| 3   | L5    | 696 | C    |
| 3   | L5    | 703 | G    |
| 3   | L5    | 704 | C    |
| 3   | L5    | 706 | C    |
| 3   | L5    | 708 | G    |
| 3   | L5    | 730 | G    |
| 3   | L5    | 731 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 738 | C    |
| 3   | L5    | 739 | G    |
| 3   | L5    | 742 | G    |
| 3   | L5    | 753 | C    |
| 3   | L5    | 758 | G    |
| 3   | L5    | 759 | G    |
| 3   | L5    | 904 | C    |
| 3   | L5    | 905 | C    |
| 3   | L5    | 906 | C    |
| 3   | L5    | 907 | C    |
| 3   | L5    | 910 | G    |
| 3   | L5    | 911 | U    |
| 3   | L5    | 912 | G    |
| 3   | L5    | 913 | U    |
| 3   | L5    | 914 | U    |
| 3   | L5    | 915 | A    |
| 3   | L5    | 917 | A    |
| 3   | L5    | 918 | G    |
| 3   | L5    | 923 | C    |
| 3   | L5    | 924 | C    |
| 3   | L5    | 926 | G    |
| 3   | L5    | 932 | A    |
| 3   | L5    | 933 | G    |
| 3   | L5    | 935 | A    |
| 3   | L5    | 936 | C    |
| 3   | L5    | 937 | U    |
| 3   | L5    | 944 | A    |
| 3   | L5    | 945 | U    |
| 3   | L5    | 959 | G    |
| 3   | L5    | 960 | A    |
| 3   | L5    | 961 | G    |
| 3   | L5    | 962 | C    |
| 3   | L5    | 965 | G    |
| 3   | L5    | 966 | A    |
| 3   | L5    | 967 | C    |
| 3   | L5    | 968 | C    |
| 3   | L5    | 969 | C    |
| 3   | L5    | 970 | G    |
| 3   | L5    | 977 | C    |
| 3   | L5    | 982 | U    |
| 3   | L5    | 985 | C    |
| 3   | L5    | 989 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 990  | C    |
| 3   | L5    | 992  | C    |
| 3   | L5    | 993  | G    |
| 3   | L5    | 995  | C    |
| 3   | L5    | 1048 | G    |
| 3   | L5    | 1049 | C    |
| 3   | L5    | 1050 | C    |
| 3   | L5    | 1051 | G    |
| 3   | L5    | 1070 | G    |
| 3   | L5    | 1071 | C    |
| 3   | L5    | 1072 | C    |
| 3   | L5    | 1075 | G    |
| 3   | L5    | 1082 | C    |
| 3   | L5    | 1083 | U    |
| 3   | L5    | 1094 | G    |
| 3   | L5    | 1095 | A    |
| 3   | L5    | 1168 | G    |
| 3   | L5    | 1171 | G    |
| 3   | L5    | 1172 | C    |
| 3   | L5    | 1173 | G    |
| 3   | L5    | 1174 | G    |
| 3   | L5    | 1179 | U    |
| 3   | L5    | 1180 | C    |
| 3   | L5    | 1182 | C    |
| 3   | L5    | 1183 | C    |
| 3   | L5    | 1198 | G    |
| 3   | L5    | 1202 | C    |
| 3   | L5    | 1203 | G    |
| 3   | L5    | 1204 | C    |
| 3   | L5    | 1205 | G    |
| 3   | L5    | 1210 | C    |
| 3   | L5    | 1211 | G    |
| 3   | L5    | 1214 | C    |
| 3   | L5    | 1215 | C    |
| 3   | L5    | 1217 | G    |
| 3   | L5    | 1218 | G    |
| 3   | L5    | 1219 | G    |
| 3   | L5    | 1222 | A    |
| 3   | L5    | 1235 | G    |
| 3   | L5    | 1241 | C    |
| 3   | L5    | 1242 | G    |
| 3   | L5    | 1246 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1253 | G    |
| 3   | L5    | 1254 | A    |
| 3   | L5    | 1257 | A    |
| 3   | L5    | 1258 | G    |
| 3   | L5    | 1261 | G    |
| 3   | L5    | 1266 | G    |
| 3   | L5    | 1267 | C    |
| 3   | L5    | 1269 | G    |
| 3   | L5    | 1270 | A    |
| 3   | L5    | 1271 | G    |
| 3   | L5    | 1272 | C    |
| 3   | L5    | 1273 | G    |
| 3   | L5    | 1274 | A    |
| 3   | L5    | 1275 | G    |
| 3   | L5    | 1280 | C    |
| 3   | L5    | 1284 | G    |
| 3   | L5    | 1285 | U    |
| 3   | L5    | 1287 | G    |
| 3   | L5    | 1293 | G    |
| 3   | L5    | 1294 | A    |
| 3   | L5    | 1295 | C    |
| 3   | L5    | 1301 | C    |
| 3   | L5    | 1312 | A    |
| 3   | L5    | 1314 | C    |
| 3   | L5    | 1326 | A    |
| 3   | L5    | 1337 | A    |
| 3   | L5    | 1354 | A    |
| 3   | L5    | 1358 | G    |
| 3   | L5    | 1359 | G    |
| 3   | L5    | 1365 | C    |
| 3   | L5    | 1367 | C    |
| 3   | L5    | 1370 | G    |
| 3   | L5    | 1387 | A    |
| 3   | L5    | 1394 | G    |
| 3   | L5    | 1397 | A    |
| 3   | L5    | 1404 | G    |
| 3   | L5    | 1405 | C    |
| 3   | L5    | 1407 | C    |
| 3   | L5    | 1409 | C    |
| 3   | L5    | 1410 | U    |
| 3   | L5    | 1411 | C    |
| 3   | L5    | 1414 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1415 | G    |
| 3   | L5    | 1417 | C    |
| 3   | L5    | 1418 | C    |
| 3   | L5    | 1420 | A    |
| 3   | L5    | 1435 | G    |
| 3   | L5    | 1437 | C    |
| 3   | L5    | 1439 | C    |
| 3   | L5    | 1443 | A    |
| 3   | L5    | 1444 | G    |
| 3   | L5    | 1446 | C    |
| 3   | L5    | 1447 | C    |
| 3   | L5    | 1482 | G    |
| 3   | L5    | 1483 | C    |
| 3   | L5    | 1497 | A    |
| 3   | L5    | 1498 | G    |
| 3   | L5    | 1502 | G    |
| 3   | L5    | 1516 | G    |
| 3   | L5    | 1517 | G    |
| 3   | L5    | 1518 | A    |
| 3   | L5    | 1525 | A    |
| 3   | L5    | 1534 | A    |
| 3   | L5    | 1547 | A    |
| 3   | L5    | 1562 | G    |
| 3   | L5    | 1566 | C    |
| 3   | L5    | 1578 | U    |
| 3   | L5    | 1591 | U    |
| 3   | L5    | 1596 | U    |
| 3   | L5    | 1621 | A    |
| 3   | L5    | 1624 | G    |
| 3   | L5    | 1625 | G    |
| 3   | L5    | 1631 | A    |
| 3   | L5    | 1633 | G    |
| 3   | L5    | 1634 | A    |
| 3   | L5    | 1638 | A    |
| 3   | L5    | 1640 | C    |
| 3   | L5    | 1641 | G    |
| 3   | L5    | 1642 | A    |
| 3   | L5    | 1654 | G    |
| 3   | L5    | 1661 | C    |
| 3   | L5    | 1663 | C    |
| 3   | L5    | 1676 | C    |
| 3   | L5    | 1677 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1678 | C    |
| 3   | L5    | 1681 | G    |
| 3   | L5    | 1685 | G    |
| 3   | L5    | 1694 | C    |
| 3   | L5    | 1699 | A    |
| 3   | L5    | 1700 | G    |
| 3   | L5    | 1703 | C    |
| 3   | L5    | 1704 | C    |
| 3   | L5    | 1705 | G    |
| 3   | L5    | 1707 | C    |
| 3   | L5    | 1718 | C    |
| 3   | L5    | 1734 | G    |
| 3   | L5    | 1740 | C    |
| 3   | L5    | 1741 | G    |
| 3   | L5    | 1742 | A    |
| 3   | L5    | 1750 | G    |
| 3   | L5    | 1753 | G    |
| 3   | L5    | 1757 | U    |
| 3   | L5    | 1758 | G    |
| 3   | L5    | 1760 | G    |
| 3   | L5    | 1761 | G    |
| 3   | L5    | 1762 | C    |
| 3   | L5    | 1763 | C    |
| 3   | L5    | 1764 | G    |
| 3   | L5    | 1765 | A    |
| 3   | L5    | 1766 | A    |
| 3   | L5    | 1768 | C    |
| 3   | L5    | 1769 | G    |
| 3   | L5    | 1770 | A    |
| 3   | L5    | 1787 | A    |
| 3   | L5    | 1804 | A    |
| 3   | L5    | 1806 | G    |
| 3   | L5    | 1810 | G    |
| 3   | L5    | 1820 | C    |
| 3   | L5    | 1821 | G    |
| 3   | L5    | 1822 | U    |
| 3   | L5    | 1834 | U    |
| 3   | L5    | 1836 | G    |
| 3   | L5    | 1837 | A    |
| 3   | L5    | 1842 | G    |
| 3   | L5    | 1843 | A    |
| 3   | L5    | 1855 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 1869 | G    |
| 3   | L5    | 1882 | U    |
| 3   | L5    | 1893 | C    |
| 3   | L5    | 1897 | A    |
| 3   | L5    | 1898 | C    |
| 3   | L5    | 1917 | A    |
| 3   | L5    | 1918 | U    |
| 3   | L5    | 1919 | G    |
| 3   | L5    | 1920 | C    |
| 3   | L5    | 1921 | C    |
| 3   | L5    | 1922 | G    |
| 3   | L5    | 1925 | G    |
| 3   | L5    | 1931 | C    |
| 3   | L5    | 1932 | A    |
| 3   | L5    | 1940 | G    |
| 3   | L5    | 1948 | G    |
| 3   | L5    | 1951 | G    |
| 3   | L5    | 1959 | U    |
| 3   | L5    | 1961 | G    |
| 3   | L5    | 1962 | A    |
| 3   | L5    | 1974 | U    |
| 3   | L5    | 1975 | G    |
| 3   | L5    | 1978 | C    |
| 3   | L5    | 1980 | U    |
| 3   | L5    | 1981 | G    |
| 3   | L5    | 1982 | G    |
| 3   | L5    | 1984 | A    |
| 3   | L5    | 1985 | G    |
| 3   | L5    | 1986 | U    |
| 3   | L5    | 1991 | A    |
| 3   | L5    | 1992 | U    |
| 3   | L5    | 1993 | C    |
| 3   | L5    | 1997 | U    |
| 3   | L5    | 1998 | A    |
| 3   | L5    | 2001 | G    |
| 3   | L5    | 2002 | A    |
| 3   | L5    | 2011 | C    |
| 3   | L5    | 2016 | C    |
| 3   | L5    | 2017 | A    |
| 3   | L5    | 2018 | C    |
| 3   | L5    | 2024 | G    |
| 3   | L5    | 2026 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2033 | A    |
| 3   | L5    | 2034 | G    |
| 3   | L5    | 2046 | G    |
| 3   | L5    | 2048 | U    |
| 3   | L5    | 2055 | G    |
| 3   | L5    | 2056 | G    |
| 3   | L5    | 2069 | A    |
| 3   | L5    | 2084 | C    |
| 3   | L5    | 2085 | G    |
| 3   | L5    | 2092 | G    |
| 3   | L5    | 2093 | A    |
| 3   | L5    | 2095 | A    |
| 3   | L5    | 2096 | G    |
| 3   | L5    | 2097 | U    |
| 3   | L5    | 2098 | G    |
| 3   | L5    | 2101 | C    |
| 3   | L5    | 2102 | G    |
| 3   | L5    | 2103 | G    |
| 3   | L5    | 2106 | G    |
| 3   | L5    | 2107 | C    |
| 3   | L5    | 2108 | G    |
| 3   | L5    | 2110 | C    |
| 3   | L5    | 2111 | G    |
| 3   | L5    | 2112 | G    |
| 3   | L5    | 2250 | C    |
| 3   | L5    | 2252 | G    |
| 3   | L5    | 2253 | A    |
| 3   | L5    | 2255 | C    |
| 3   | L5    | 2256 | C    |
| 3   | L5    | 2257 | C    |
| 3   | L5    | 2258 | C    |
| 3   | L5    | 2259 | G    |
| 3   | L5    | 2260 | C    |
| 3   | L5    | 2263 | A    |
| 3   | L5    | 2289 | C    |
| 3   | L5    | 2300 | A    |
| 3   | L5    | 2301 | G    |
| 3   | L5    | 2306 | G    |
| 3   | L5    | 2313 | A    |
| 3   | L5    | 2331 | G    |
| 3   | L5    | 2332 | A    |
| 3   | L5    | 2333 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2344 | U    |
| 3   | L5    | 2345 | G    |
| 3   | L5    | 2348 | G    |
| 3   | L5    | 2351 | C    |
| 3   | L5    | 2360 | A    |
| 3   | L5    | 2364 | G    |
| 3   | L5    | 2382 | A    |
| 3   | L5    | 2383 | C    |
| 3   | L5    | 2395 | A    |
| 3   | L5    | 2397 | G    |
| 3   | L5    | 2402 | G    |
| 3   | L5    | 2412 | A    |
| 3   | L5    | 2417 | A    |
| 3   | L5    | 2421 | G    |
| 3   | L5    | 2425 | U    |
| 3   | L5    | 2441 | C    |
| 3   | L5    | 2450 | G    |
| 3   | L5    | 2453 | A    |
| 3   | L5    | 2464 | C    |
| 3   | L5    | 2465 | C    |
| 3   | L5    | 2471 | G    |
| 3   | L5    | 2474 | G    |
| 3   | L5    | 2475 | G    |
| 3   | L5    | 2478 | C    |
| 3   | L5    | 2479 | G    |
| 3   | L5    | 2483 | G    |
| 3   | L5    | 2484 | A    |
| 3   | L5    | 2485 | U    |
| 3   | L5    | 2486 | G    |
| 3   | L5    | 2487 | G    |
| 3   | L5    | 2488 | C    |
| 3   | L5    | 2489 | C    |
| 3   | L5    | 2490 | U    |
| 3   | L5    | 2491 | C    |
| 3   | L5    | 2494 | U    |
| 3   | L5    | 2503 | G    |
| 3   | L5    | 2504 | C    |
| 3   | L5    | 2505 | C    |
| 3   | L5    | 2506 | G    |
| 3   | L5    | 2513 | A    |
| 3   | L5    | 2519 | U    |
| 3   | L5    | 2520 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2537 | A    |
| 3   | L5    | 2544 | G    |
| 3   | L5    | 2546 | G    |
| 3   | L5    | 2547 | G    |
| 3   | L5    | 2554 | U    |
| 3   | L5    | 2555 | G    |
| 3   | L5    | 2560 | C    |
| 3   | L5    | 2565 | A    |
| 3   | L5    | 2567 | G    |
| 3   | L5    | 2568 | C    |
| 3   | L5    | 2573 | A    |
| 3   | L5    | 2583 | C    |
| 3   | L5    | 2586 | G    |
| 3   | L5    | 2587 | A    |
| 3   | L5    | 2589 | C    |
| 3   | L5    | 2618 | G    |
| 3   | L5    | 2627 | C    |
| 3   | L5    | 2652 | G    |
| 3   | L5    | 2653 | C    |
| 3   | L5    | 2662 | G    |
| 3   | L5    | 2664 | G    |
| 3   | L5    | 2669 | C    |
| 3   | L5    | 2675 | G    |
| 3   | L5    | 2676 | A    |
| 3   | L5    | 2687 | U    |
| 3   | L5    | 2694 | G    |
| 3   | L5    | 2695 | A    |
| 3   | L5    | 2696 | A    |
| 3   | L5    | 2703 | G    |
| 3   | L5    | 2707 | U    |
| 3   | L5    | 2708 | U    |
| 3   | L5    | 2710 | C    |
| 3   | L5    | 2711 | G    |
| 3   | L5    | 2712 | G    |
| 3   | L5    | 2721 | G    |
| 3   | L5    | 2724 | G    |
| 3   | L5    | 2726 | G    |
| 3   | L5    | 2739 | C    |
| 3   | L5    | 2742 | G    |
| 3   | L5    | 2743 | A    |
| 3   | L5    | 2746 | A    |
| 3   | L5    | 2761 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 2763 | U    |
| 3   | L5    | 2764 | A    |
| 3   | L5    | 2769 | U    |
| 3   | L5    | 2770 | C    |
| 3   | L5    | 2787 | A    |
| 3   | L5    | 2788 | U    |
| 3   | L5    | 2790 | U    |
| 3   | L5    | 2806 | A    |
| 3   | L5    | 2826 | U    |
| 3   | L5    | 2827 | G    |
| 3   | L5    | 2838 | G    |
| 3   | L5    | 2846 | G    |
| 3   | L5    | 2848 | G    |
| 3   | L5    | 2855 | G    |
| 3   | L5    | 2867 | C    |
| 3   | L5    | 2877 | G    |
| 3   | L5    | 2892 | C    |
| 3   | L5    | 2894 | A    |
| 3   | L5    | 2895 | A    |
| 3   | L5    | 2899 | C    |
| 3   | L5    | 2900 | U    |
| 3   | L5    | 2902 | G    |
| 3   | L5    | 2903 | G    |
| 3   | L5    | 2904 | U    |
| 3   | L5    | 2905 | C    |
| 3   | L5    | 2906 | G    |
| 3   | L5    | 2908 | U    |
| 3   | L5    | 3586 | G    |
| 3   | L5    | 3588 | C    |
| 3   | L5    | 3590 | G    |
| 3   | L5    | 3591 | C    |
| 3   | L5    | 3594 | C    |
| 3   | L5    | 3595 | U    |
| 3   | L5    | 3596 | A    |
| 3   | L5    | 3597 | G    |
| 3   | L5    | 3599 | A    |
| 3   | L5    | 3605 | C    |
| 3   | L5    | 3615 | G    |
| 3   | L5    | 3618 | C    |
| 3   | L5    | 3626 | G    |
| 3   | L5    | 3630 | A    |
| 3   | L5    | 3635 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 3644 | U    |
| 3   | L5    | 3646 | A    |
| 3   | L5    | 3648 | A    |
| 3   | L5    | 3662 | A    |
| 3   | L5    | 3664 | G    |
| 3   | L5    | 3670 | C    |
| 3   | L5    | 3673 | C    |
| 3   | L5    | 3674 | G    |
| 3   | L5    | 3685 | C    |
| 3   | L5    | 3710 | G    |
| 3   | L5    | 3711 | A    |
| 3   | L5    | 3713 | U    |
| 3   | L5    | 3714 | G    |
| 3   | L5    | 3726 | A    |
| 3   | L5    | 3727 | A    |
| 3   | L5    | 3739 | C    |
| 3   | L5    | 3748 | A    |
| 3   | L5    | 3750 | G    |
| 3   | L5    | 3756 | A    |
| 3   | L5    | 3759 | A    |
| 3   | L5    | 3766 | A    |
| 3   | L5    | 3769 | C    |
| 3   | L5    | 3773 | U    |
| 3   | L5    | 3774 | A    |
| 3   | L5    | 3776 | G    |
| 3   | L5    | 3777 | G    |
| 3   | L5    | 3783 | A    |
| 3   | L5    | 3784 | A    |
| 3   | L5    | 3786 | U    |
| 3   | L5    | 3788 | C    |
| 3   | L5    | 3802 | U    |
| 3   | L5    | 3810 | C    |
| 3   | L5    | 3811 | G    |
| 3   | L5    | 3812 | C    |
| 3   | L5    | 3814 | U    |
| 3   | L5    | 3817 | A    |
| 3   | L5    | 3818 | U    |
| 3   | L5    | 3819 | G    |
| 3   | L5    | 3823 | G    |
| 3   | L5    | 3824 | A    |
| 3   | L5    | 3838 | U    |
| 3   | L5    | 3839 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 3840 | U    |
| 3   | L5    | 3841 | C    |
| 3   | L5    | 3867 | A    |
| 3   | L5    | 3868 | G    |
| 3   | L5    | 3877 | A    |
| 3   | L5    | 3878 | C    |
| 3   | L5    | 3879 | G    |
| 3   | L5    | 3880 | G    |
| 3   | L5    | 3885 | G    |
| 3   | L5    | 3887 | C    |
| 3   | L5    | 3890 | A    |
| 3   | L5    | 3892 | U    |
| 3   | L5    | 3897 | G    |
| 3   | L5    | 3901 | A    |
| 3   | L5    | 3906 | A    |
| 3   | L5    | 3907 | G    |
| 3   | L5    | 3908 | A    |
| 3   | L5    | 3915 | U    |
| 3   | L5    | 3922 | G    |
| 3   | L5    | 3930 | U    |
| 3   | L5    | 3938 | G    |
| 3   | L5    | 3939 | G    |
| 3   | L5    | 3942 | A    |
| 3   | L5    | 3943 | A    |
| 3   | L5    | 3944 | G    |
| 3   | L5    | 3947 | A    |
| 3   | L5    | 3948 | C    |
| 3   | L5    | 3949 | A    |
| 3   | L5    | 3950 | U    |
| 3   | L5    | 3951 | G    |
| 3   | L5    | 3953 | G    |
| 3   | L5    | 3955 | G    |
| 3   | L5    | 3956 | G    |
| 3   | L5    | 3957 | U    |
| 3   | L5    | 3959 | U    |
| 3   | L5    | 3960 | A    |
| 3   | L5    | 3961 | G    |
| 3   | L5    | 3962 | A    |
| 3   | L5    | 3963 | A    |
| 3   | L5    | 3964 | U    |
| 3   | L5    | 3965 | A    |
| 3   | L5    | 3966 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 3968 | U    |
| 3   | L5    | 3969 | G    |
| 3   | L5    | 3970 | G    |
| 3   | L5    | 3972 | A    |
| 3   | L5    | 3973 | G    |
| 3   | L5    | 3974 | G    |
| 3   | L5    | 3977 | C    |
| 3   | L5    | 4034 | G    |
| 3   | L5    | 4038 | C    |
| 3   | L5    | 4039 | G    |
| 3   | L5    | 4041 | C    |
| 3   | L5    | 4042 | G    |
| 3   | L5    | 4043 | G    |
| 3   | L5    | 4044 | U    |
| 3   | L5    | 4045 | G    |
| 3   | L5    | 4046 | A    |
| 3   | L5    | 4047 | A    |
| 3   | L5    | 4048 | A    |
| 3   | L5    | 4049 | U    |
| 3   | L5    | 4050 | A    |
| 3   | L5    | 4051 | C    |
| 3   | L5    | 4052 | C    |
| 3   | L5    | 4053 | A    |
| 3   | L5    | 4054 | C    |
| 3   | L5    | 4055 | U    |
| 3   | L5    | 4056 | A    |
| 3   | L5    | 4057 | C    |
| 3   | L5    | 4058 | U    |
| 3   | L5    | 4059 | C    |
| 3   | L5    | 4060 | U    |
| 3   | L5    | 4061 | G    |
| 3   | L5    | 4062 | A    |
| 3   | L5    | 4063 | U    |
| 3   | L5    | 4064 | C    |
| 3   | L5    | 4065 | G    |
| 3   | L5    | 4067 | U    |
| 3   | L5    | 4068 | U    |
| 3   | L5    | 4069 | U    |
| 3   | L5    | 4076 | G    |
| 3   | L5    | 4084 | G    |
| 3   | L5    | 4093 | G    |
| 3   | L5    | 4096 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4097 | G    |
| 3   | L5    | 4098 | A    |
| 3   | L5    | 4099 | G    |
| 3   | L5    | 4100 | C    |
| 3   | L5    | 4101 | C    |
| 3   | L5    | 4102 | C    |
| 3   | L5    | 4103 | C    |
| 3   | L5    | 4104 | G    |
| 3   | L5    | 4108 | G    |
| 3   | L5    | 4111 | U    |
| 3   | L5    | 4112 | C    |
| 3   | L5    | 4114 | C    |
| 3   | L5    | 4115 | G    |
| 3   | L5    | 4116 | C    |
| 3   | L5    | 4117 | U    |
| 3   | L5    | 4119 | C    |
| 3   | L5    | 4127 | A    |
| 3   | L5    | 4133 | C    |
| 3   | L5    | 4134 | C    |
| 3   | L5    | 4138 | C    |
| 3   | L5    | 4140 | C    |
| 3   | L5    | 4141 | G    |
| 3   | L5    | 4142 | C    |
| 3   | L5    | 4143 | G    |
| 3   | L5    | 4144 | C    |
| 3   | L5    | 4146 | G    |
| 3   | L5    | 4149 | C    |
| 3   | L5    | 4160 | C    |
| 3   | L5    | 4162 | C    |
| 3   | L5    | 4163 | U    |
| 3   | L5    | 4170 | A    |
| 3   | L5    | 4183 | G    |
| 3   | L5    | 4184 | G    |
| 3   | L5    | 4191 | G    |
| 3   | L5    | 4196 | G    |
| 3   | L5    | 4197 | G    |
| 3   | L5    | 4201 | G    |
| 3   | L5    | 4203 | A    |
| 3   | L5    | 4222 | G    |
| 3   | L5    | 4225 | G    |
| 3   | L5    | 4228 | G    |
| 3   | L5    | 4229 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4232 | U    |
| 3   | L5    | 4233 | A    |
| 3   | L5    | 4234 | A    |
| 3   | L5    | 4237 | C    |
| 3   | L5    | 4249 | G    |
| 3   | L5    | 4251 | A    |
| 3   | L5    | 4254 | G    |
| 3   | L5    | 4255 | A    |
| 3   | L5    | 4257 | A    |
| 3   | L5    | 4258 | C    |
| 3   | L5    | 4265 | U    |
| 3   | L5    | 4268 | A    |
| 3   | L5    | 4273 | A    |
| 3   | L5    | 4291 | G    |
| 3   | L5    | 4296 | U    |
| 3   | L5    | 4297 | G    |
| 3   | L5    | 4304 | A    |
| 3   | L5    | 4305 | G    |
| 3   | L5    | 4306 | U    |
| 3   | L5    | 4313 | A    |
| 3   | L5    | 4314 | C    |
| 3   | L5    | 4319 | C    |
| 3   | L5    | 4330 | G    |
| 3   | L5    | 4332 | C    |
| 3   | L5    | 4339 | A    |
| 3   | L5    | 4349 | C    |
| 3   | L5    | 4371 | G    |
| 3   | L5    | 4373 | G    |
| 3   | L5    | 4376 | A    |
| 3   | L5    | 4377 | G    |
| 3   | L5    | 4378 | A    |
| 3   | L5    | 4380 | A    |
| 3   | L5    | 4387 | C    |
| 3   | L5    | 4391 | G    |
| 3   | L5    | 4394 | A    |
| 3   | L5    | 4420 | U    |
| 3   | L5    | 4421 | C    |
| 3   | L5    | 4422 | A    |
| 3   | L5    | 4438 | U    |
| 3   | L5    | 4448 | G    |
| 3   | L5    | 4449 | A    |
| 3   | L5    | 4453 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4464 | A    |
| 3   | L5    | 4466 | C    |
| 3   | L5    | 4475 | G    |
| 3   | L5    | 4488 | A    |
| 3   | L5    | 4500 | U    |
| 3   | L5    | 4512 | U    |
| 3   | L5    | 4513 | A    |
| 3   | L5    | 4515 | G    |
| 3   | L5    | 4519 | C    |
| 3   | L5    | 4524 | G    |
| 3   | L5    | 4525 | C    |
| 3   | L5    | 4528 | G    |
| 3   | L5    | 4545 | G    |
| 3   | L5    | 4548 | A    |
| 3   | L5    | 4549 | G    |
| 3   | L5    | 4560 | C    |
| 3   | L5    | 4567 | G    |
| 3   | L5    | 4573 | G    |
| 3   | L5    | 4575 | G    |
| 3   | L5    | 4583 | C    |
| 3   | L5    | 4584 | A    |
| 3   | L5    | 4589 | A    |
| 3   | L5    | 4590 | A    |
| 3   | L5    | 4600 | G    |
| 3   | L5    | 4601 | U    |
| 3   | L5    | 4617 | G    |
| 3   | L5    | 4627 | U    |
| 3   | L5    | 4635 | A    |
| 3   | L5    | 4636 | U    |
| 3   | L5    | 4637 | G    |
| 3   | L5    | 4648 | A    |
| 3   | L5    | 4652 | G    |
| 3   | L5    | 4656 | A    |
| 3   | L5    | 4657 | U    |
| 3   | L5    | 4659 | G    |
| 3   | L5    | 4670 | C    |
| 3   | L5    | 4672 | A    |
| 3   | L5    | 4679 | G    |
| 3   | L5    | 4694 | G    |
| 3   | L5    | 4695 | C    |
| 3   | L5    | 4700 | A    |
| 3   | L5    | 4708 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4709 | U    |
| 3   | L5    | 4719 | G    |
| 3   | L5    | 4733 | C    |
| 3   | L5    | 4734 | A    |
| 3   | L5    | 4741 | C    |
| 3   | L5    | 4742 | G    |
| 3   | L5    | 4745 | G    |
| 3   | L5    | 4754 | G    |
| 3   | L5    | 4757 | C    |
| 3   | L5    | 4759 | C    |
| 3   | L5    | 4761 | G    |
| 3   | L5    | 4765 | G    |
| 3   | L5    | 4771 | C    |
| 3   | L5    | 4772 | C    |
| 3   | L5    | 4773 | C    |
| 3   | L5    | 4775 | C    |
| 3   | L5    | 4776 | G    |
| 3   | L5    | 4859 | C    |
| 3   | L5    | 4860 | G    |
| 3   | L5    | 4863 | G    |
| 3   | L5    | 4870 | G    |
| 3   | L5    | 4871 | C    |
| 3   | L5    | 4875 | G    |
| 3   | L5    | 4880 | C    |
| 3   | L5    | 4882 | U    |
| 3   | L5    | 4883 | C    |
| 3   | L5    | 4889 | G    |
| 3   | L5    | 4895 | C    |
| 3   | L5    | 4896 | G    |
| 3   | L5    | 4900 | C    |
| 3   | L5    | 4901 | G    |
| 3   | L5    | 4902 | C    |
| 3   | L5    | 4910 | G    |
| 3   | L5    | 4912 | G    |
| 3   | L5    | 4914 | C    |
| 3   | L5    | 4922 | C    |
| 3   | L5    | 4923 | C    |
| 3   | L5    | 4925 | U    |
| 3   | L5    | 4926 | C    |
| 3   | L5    | 4927 | G    |
| 3   | L5    | 4928 | C    |
| 3   | L5    | 4940 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4941 | G    |
| 3   | L5    | 4943 | A    |
| 3   | L5    | 4951 | G    |
| 3   | L5    | 4960 | G    |
| 3   | L5    | 4976 | U    |
| 3   | L5    | 4988 | U    |
| 3   | L5    | 4989 | U    |
| 3   | L5    | 4990 | C    |
| 3   | L5    | 4991 | U    |
| 3   | L5    | 5007 | A    |
| 3   | L5    | 5009 | G    |
| 3   | L5    | 5013 | C    |
| 3   | L5    | 5014 | A    |
| 3   | L5    | 5017 | G    |
| 3   | L5    | 5023 | C    |
| 3   | L5    | 5024 | C    |
| 3   | L5    | 5027 | C    |
| 3   | L5    | 5028 | G    |
| 3   | L5    | 5029 | C    |
| 3   | L5    | 5030 | U    |
| 3   | L5    | 5031 | G    |
| 3   | L5    | 5034 | A    |
| 3   | L5    | 5041 | G    |
| 3   | L5    | 5050 | C    |
| 3   | L5    | 5054 | C    |
| 3   | L5    | 5055 | G    |
| 3   | L5    | 5061 | A    |
| 3   | L5    | 5069 | U    |
| 4   | L7    | 2    | U    |
| 4   | L7    | 4    | U    |
| 4   | L7    | 5    | A    |
| 4   | L7    | 7    | G    |
| 4   | L7    | 22   | A    |
| 4   | L7    | 24   | C    |
| 4   | L7    | 33   | U    |
| 4   | L7    | 38   | U    |
| 4   | L7    | 53   | U    |
| 4   | L7    | 54   | A    |
| 4   | L7    | 63   | C    |
| 4   | L7    | 64   | G    |
| 4   | L7    | 100  | A    |
| 4   | L7    | 110  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L8    | 25  | G    |
| 5   | L8    | 34  | U    |
| 5   | L8    | 35  | C    |
| 5   | L8    | 48  | A    |
| 5   | L8    | 52  | A    |
| 5   | L8    | 59  | A    |
| 5   | L8    | 60  | G    |
| 5   | L8    | 62  | A    |
| 5   | L8    | 63  | U    |
| 5   | L8    | 68  | G    |
| 5   | L8    | 82  | A    |
| 5   | L8    | 84  | A    |
| 5   | L8    | 85  | U    |
| 5   | L8    | 86  | U    |
| 5   | L8    | 87  | G    |
| 5   | L8    | 94  | G    |
| 5   | L8    | 103 | A    |
| 5   | L8    | 105 | C    |
| 5   | L8    | 110 | U    |
| 5   | L8    | 111 | U    |
| 5   | L8    | 114 | G    |
| 5   | L8    | 123 | U    |
| 5   | L8    | 124 | U    |
| 5   | L8    | 125 | C    |
| 5   | L8    | 126 | C    |
| 5   | L8    | 127 | U    |
| 5   | L8    | 147 | G    |
| 5   | L8    | 151 | G    |
| 5   | L8    | 156 | U    |
| 85  | Et    | 3   | C    |
| 85  | Et    | 4   | C    |
| 85  | Et    | 5   | G    |
| 85  | Et    | 6   | G    |
| 85  | Et    | 7   | A    |
| 85  | Et    | 8   | U    |
| 85  | Et    | 9   | A    |
| 85  | Et    | 10  | G    |
| 85  | Et    | 11  | C    |
| 85  | Et    | 13  | C    |
| 85  | Et    | 14  | A    |
| 85  | Et    | 15  | G    |
| 85  | Et    | 19  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 85  | Et    | 20  | U    |
| 85  | Et    | 21  | A    |
| 85  | Et    | 22  | G    |
| 85  | Et    | 24  | G    |
| 85  | Et    | 25  | C    |
| 85  | Et    | 26  | A    |
| 85  | Et    | 27  | U    |
| 85  | Et    | 29  | A    |
| 85  | Et    | 30  | G    |
| 85  | Et    | 31  | A    |
| 85  | Et    | 34  | U    |
| 85  | Et    | 35  | U    |
| 85  | Et    | 37  | A    |
| 85  | Et    | 38  | A    |
| 85  | Et    | 40  | C    |
| 85  | Et    | 41  | U    |
| 85  | Et    | 42  | G    |
| 85  | Et    | 45  | G    |
| 85  | Et    | 46  | G    |
| 85  | Et    | 47  | U    |
| 85  | Et    | 48  | C    |
| 85  | Et    | 49  | C    |
| 85  | Et    | 50  | A    |
| 85  | Et    | 52  | G    |
| 85  | Et    | 53  | G    |
| 85  | Et    | 54  | U    |
| 85  | Et    | 55  | U    |
| 85  | Et    | 58  | A    |
| 85  | Et    | 59  | G    |
| 85  | Et    | 60  | U    |
| 85  | Et    | 61  | C    |
| 85  | Et    | 63  | C    |
| 85  | Et    | 64  | U    |
| 85  | Et    | 65  | G    |
| 85  | Et    | 67  | U    |
| 85  | Et    | 68  | C    |
| 85  | Et    | 69  | G    |
| 85  | Et    | 70  | G    |
| 85  | Et    | 71  | G    |
| 85  | Et    | 72  | C    |
| 85  | Et    | 73  | G    |
| 85  | Et    | 76  | A    |

All (27) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | S2    | 291  | G    |
| 2   | S2    | 420  | G    |
| 2   | S2    | 563  | G    |
| 2   | S2    | 688  | U    |
| 2   | S2    | 1434 | C    |
| 3   | L5    | 265  | C    |
| 3   | L5    | 406  | C    |
| 3   | L5    | 493  | G    |
| 3   | L5    | 914  | U    |
| 3   | L5    | 1082 | C    |
| 3   | L5    | 1590 | C    |
| 3   | L5    | 1633 | G    |
| 3   | L5    | 1977 | C    |
| 3   | L5    | 2033 | A    |
| 3   | L5    | 2416 | G    |
| 3   | L5    | 2485 | U    |
| 3   | L5    | 2675 | G    |
| 3   | L5    | 2760 | G    |
| 3   | L5    | 2786 | C    |
| 3   | L5    | 3614 | G    |
| 3   | L5    | 3673 | C    |
| 3   | L5    | 3948 | C    |
| 3   | L5    | 4055 | U    |
| 3   | L5    | 4061 | G    |
| 3   | L5    | 4600 | G    |
| 3   | L5    | 4699 | U    |
| 3   | L5    | 4913 | G    |

## 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 261 ligands modelled in this entry, 261 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 64  | CD    | 1                |
| 49  | Lt    | 1                |
| 85  | Et    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | CD    | 225:LEU   | C      | 282:THR   | N      | 57.40        |
| 1     | Lt    | 87:GLU    | C      | 104:ILE   | N      | 8.75         |
| 1     | Et    | 16:C      | O3'    | 18:U      | P      | 5.31         |

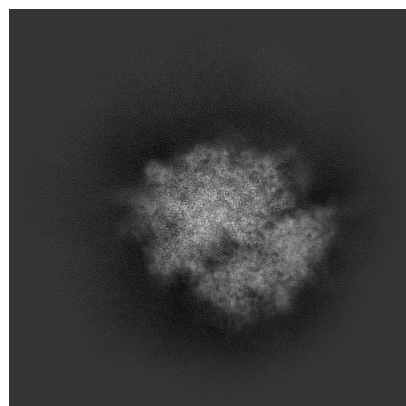
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44039. These allow visual inspection of the internal detail of the map and identification of artifacts.

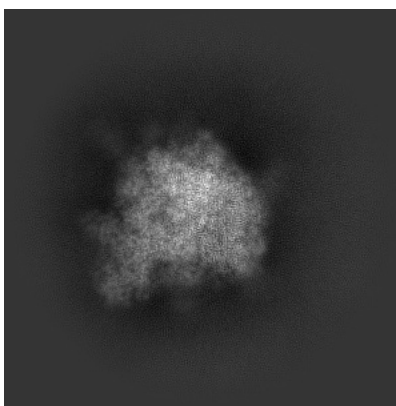
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

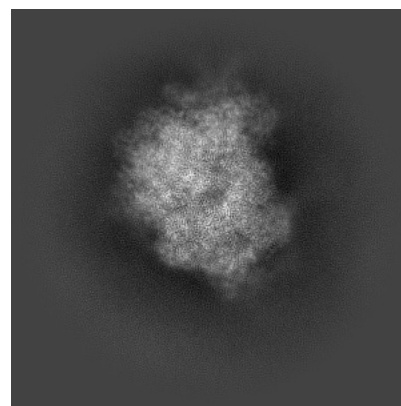
#### 6.1.1 Primary map



X

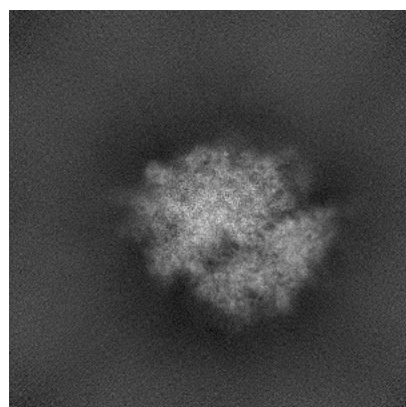


Y

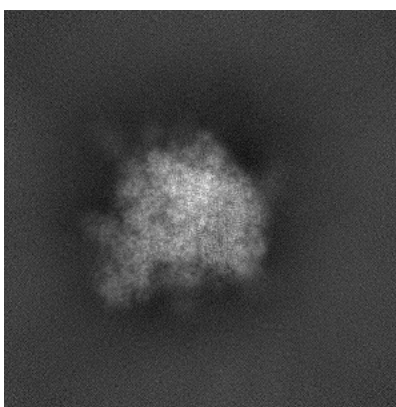


Z

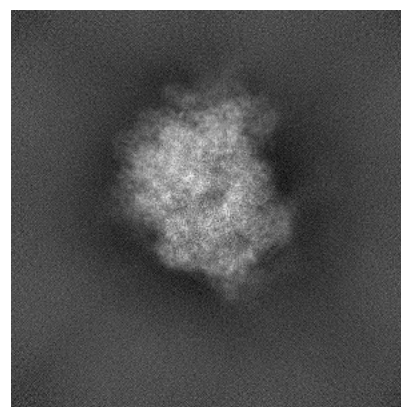
#### 6.1.2 Raw map



X



Y



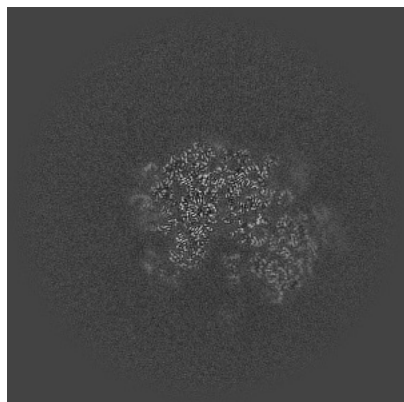
Z

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

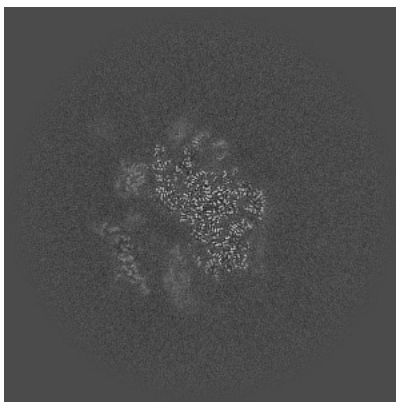


## 6.2 Central slices [i](#)

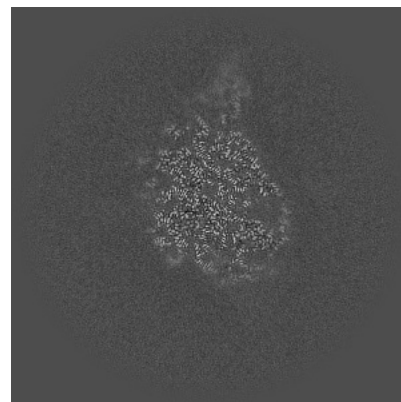
### 6.2.1 Primary map



X Index: 256

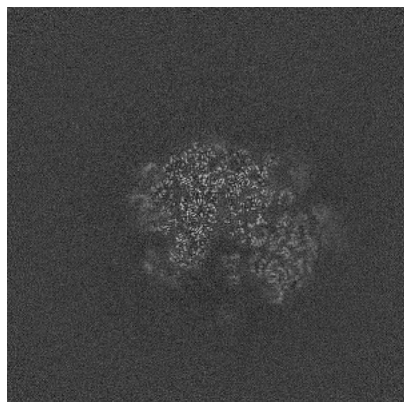


Y Index: 256

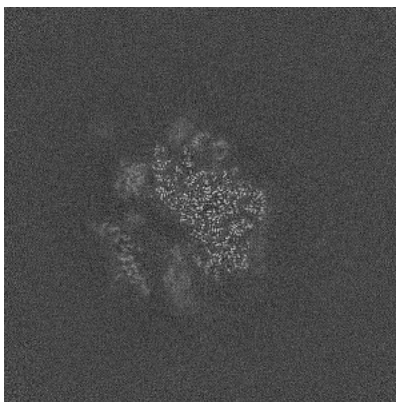


Z Index: 256

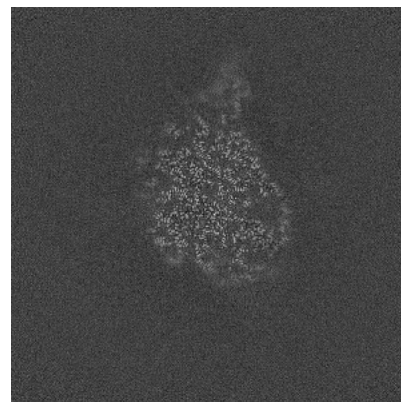
### 6.2.2 Raw map



X Index: 256



Y Index: 256

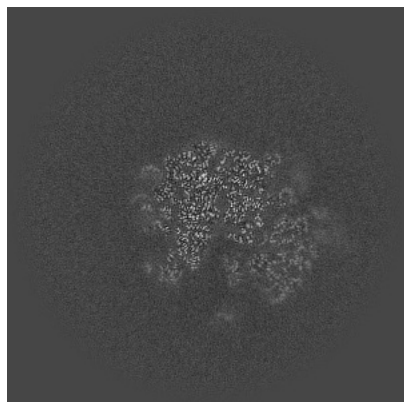


Z Index: 256

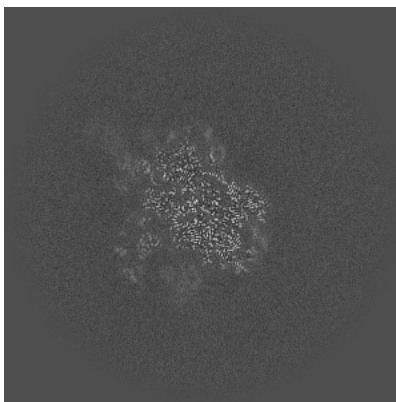
The images above show central slices of the map in three orthogonal directions.

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

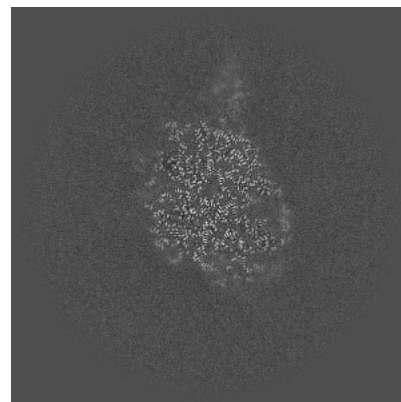
### 6.3.1 Primary map



X Index: 253

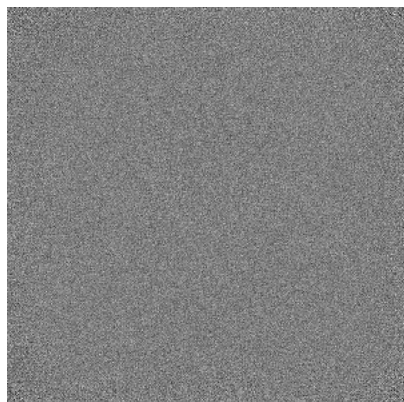


Y Index: 243

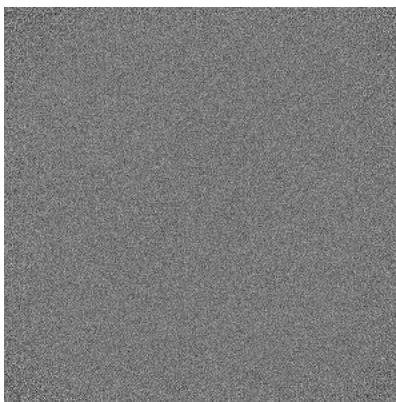


Z Index: 258

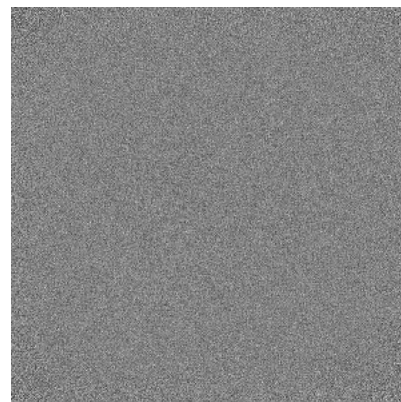
### 6.3.2 Raw map



X Index: 0



Y Index: 0

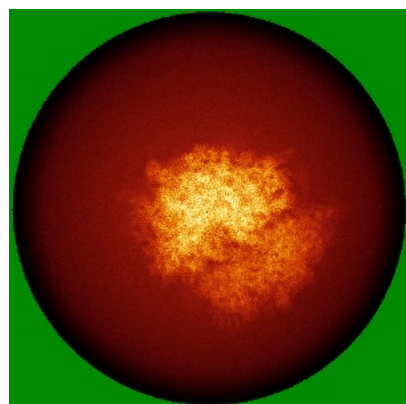


Z Index: 0

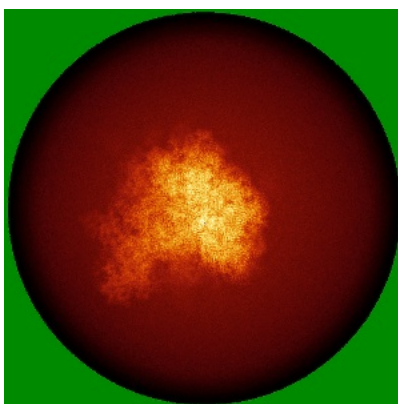
The images above show the largest variance slices of the map in three orthogonal directions.

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

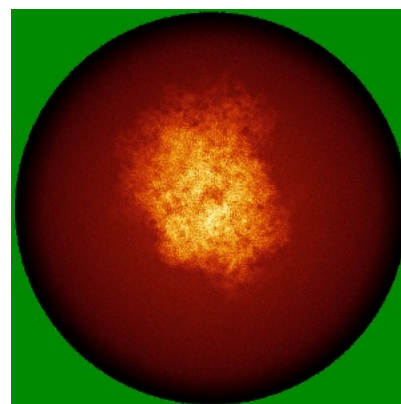
### 6.4.1 Primary map



X

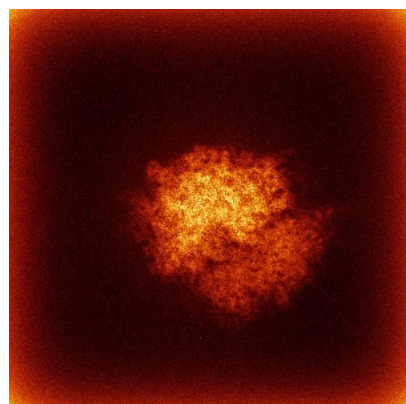


Y

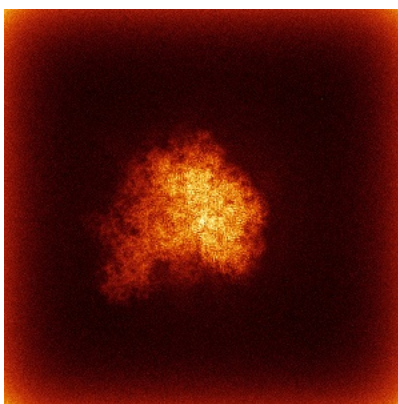


Z

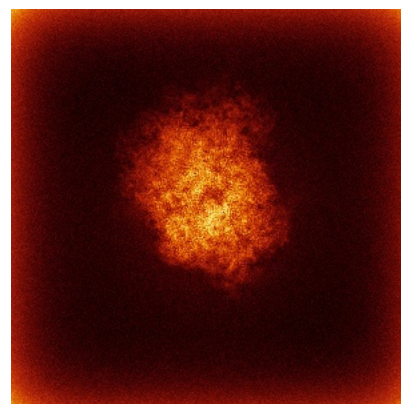
### 6.4.2 Raw map



X



Y



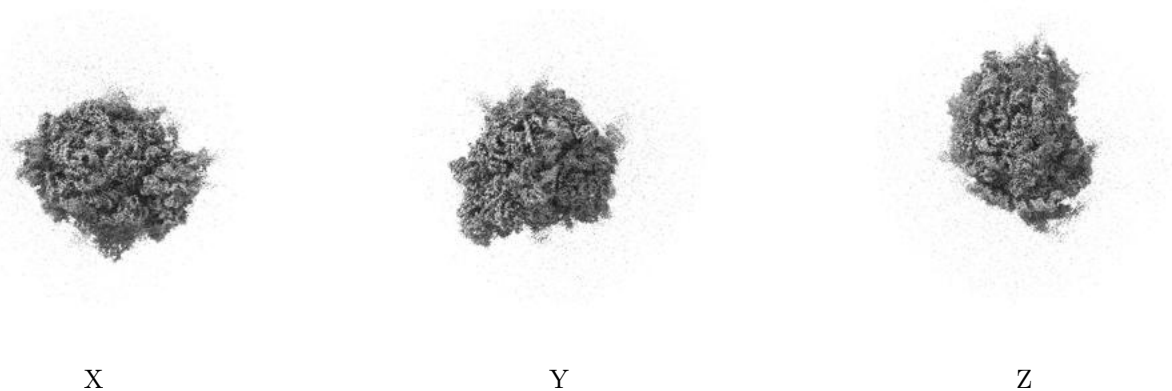
Z

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



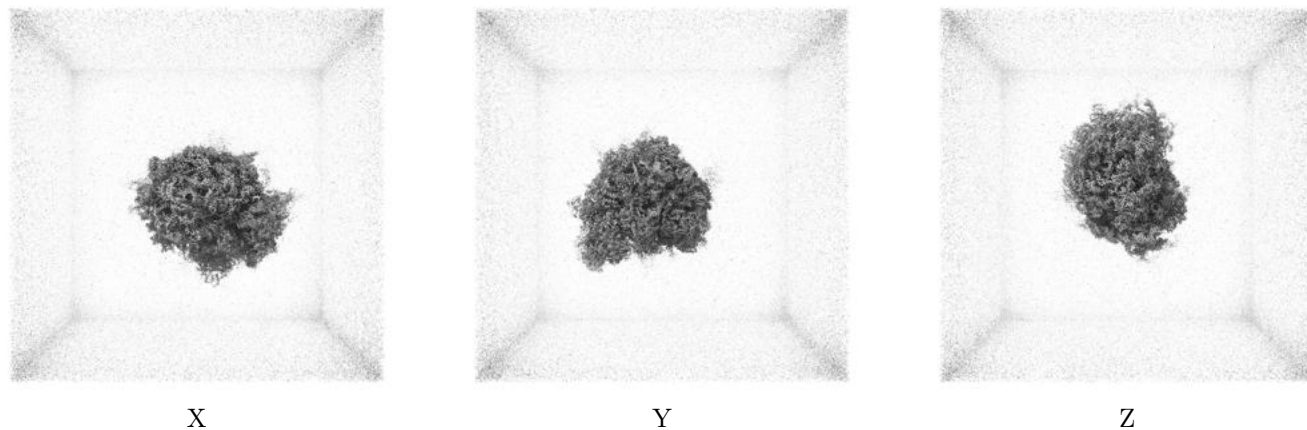
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

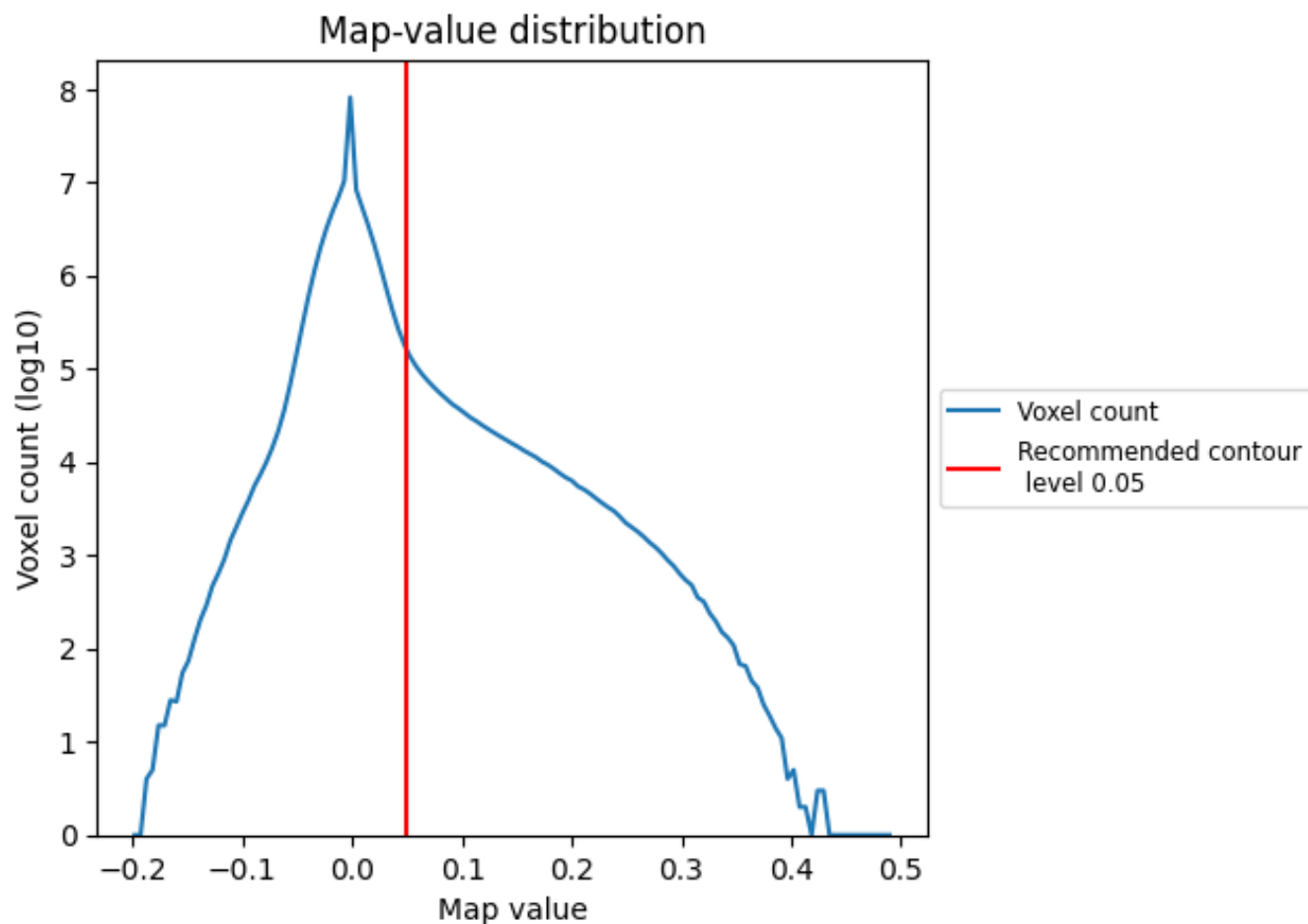
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

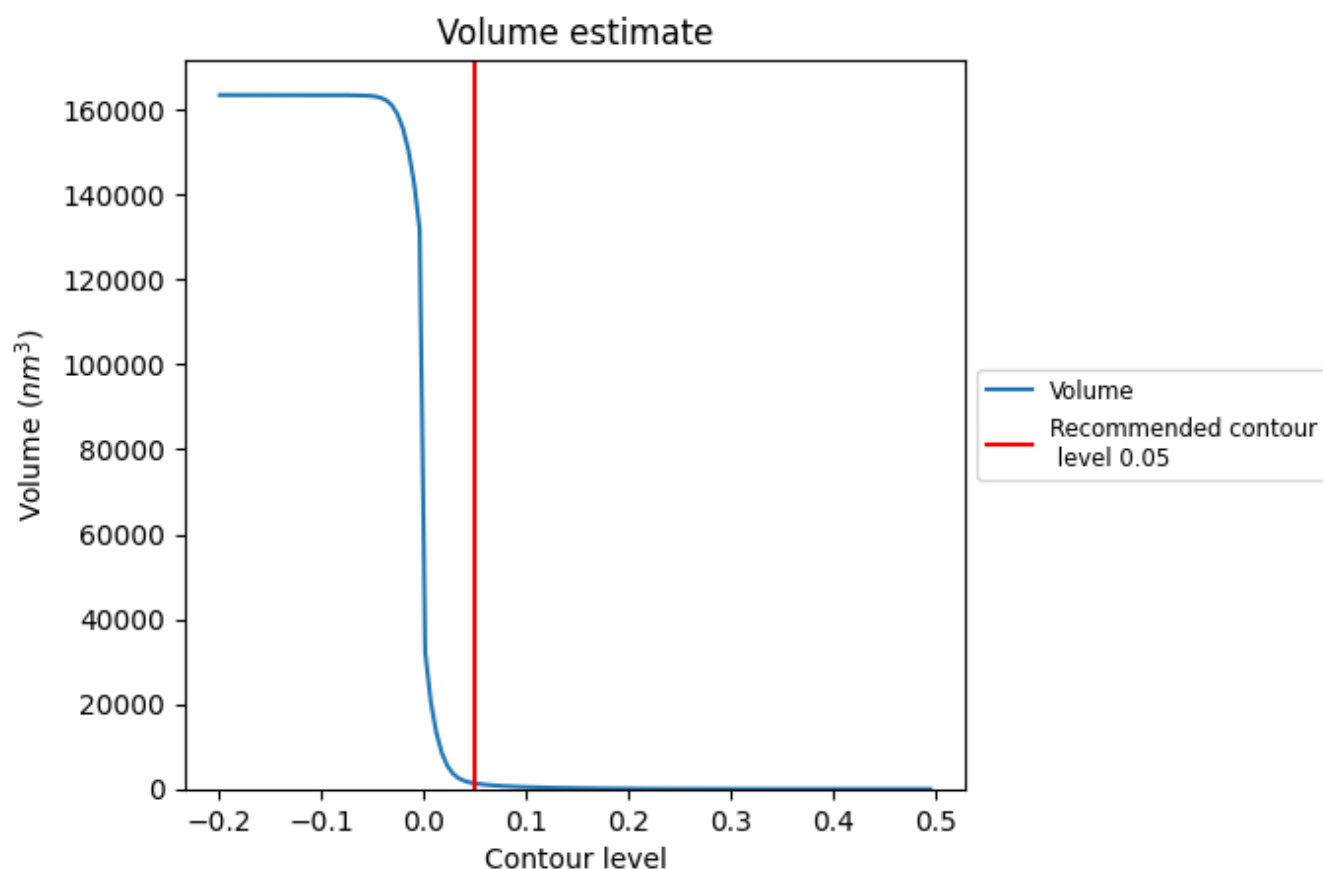
This section contains the results of statistical analysis of the map.

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



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

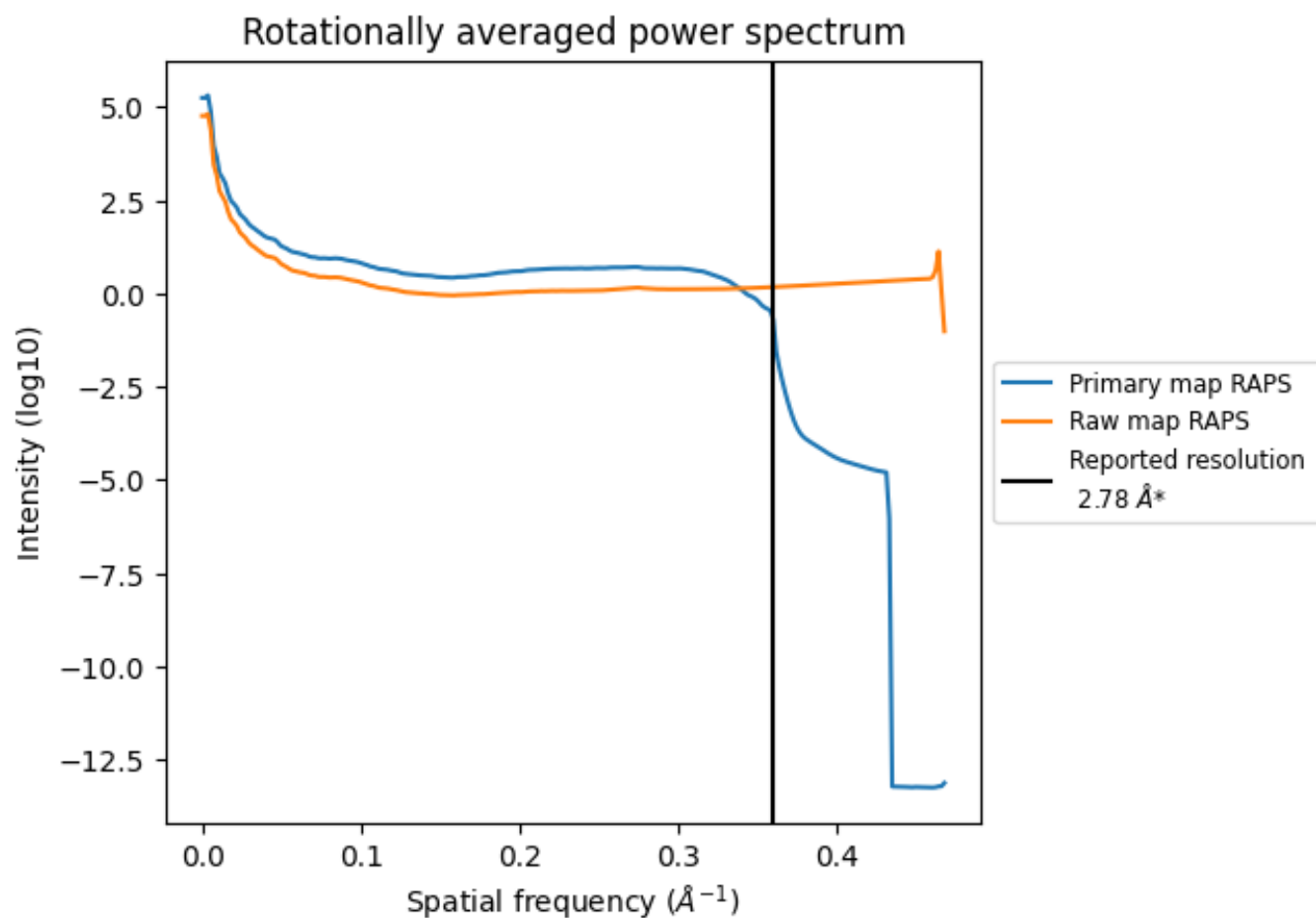
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1337  $\text{nm}^3$ ; this corresponds to an approximate mass of 1207 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

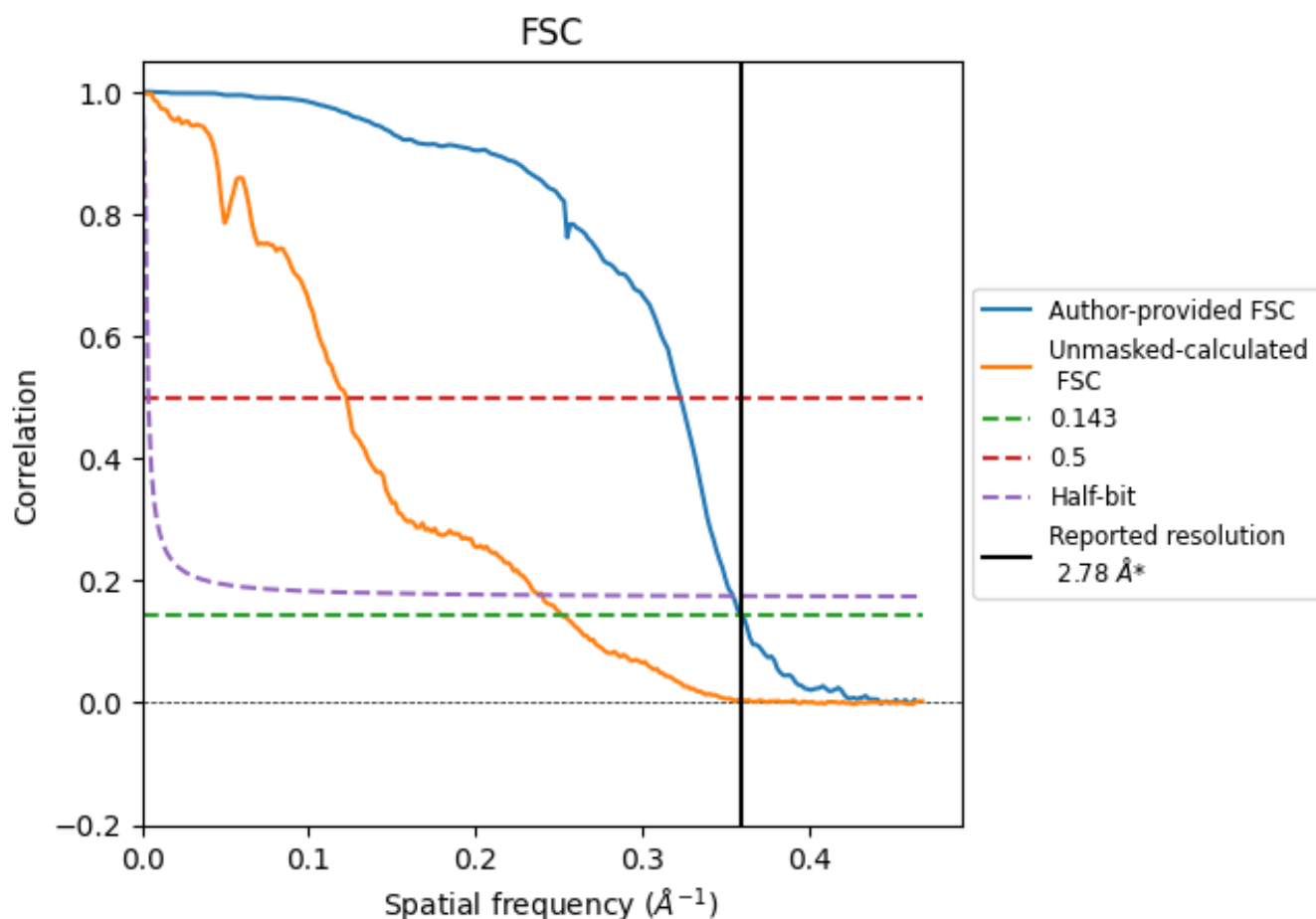


\*Reported resolution corresponds to spatial frequency of 0.360  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.360 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

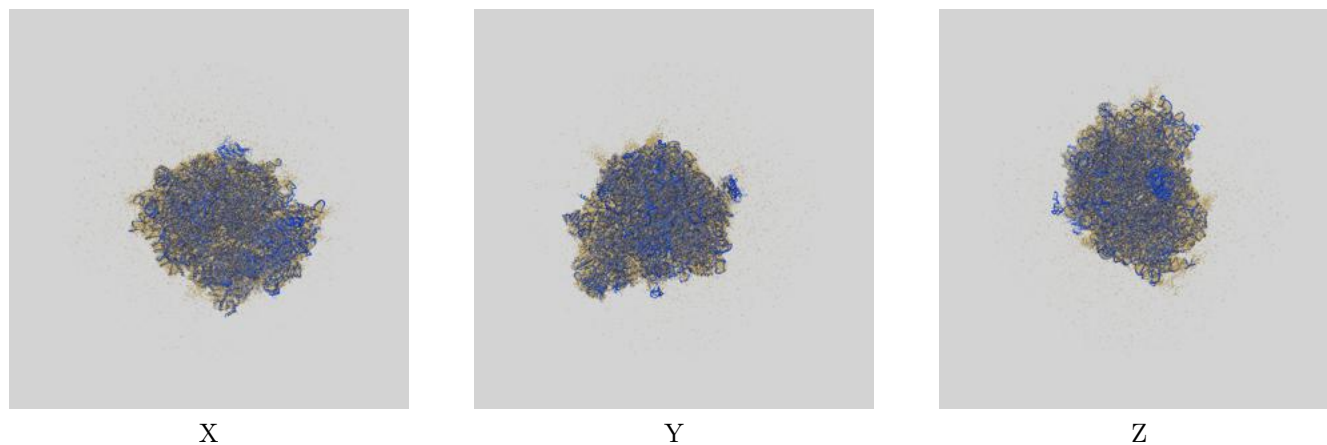
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.78                               | -    | -        |
| Author-provided FSC curve | 2.78                               | 3.10 | 2.82     |
| Unmasked-calculated*      | 3.97                               | 8.16 | 4.17     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 2.78 by more than 10 %

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

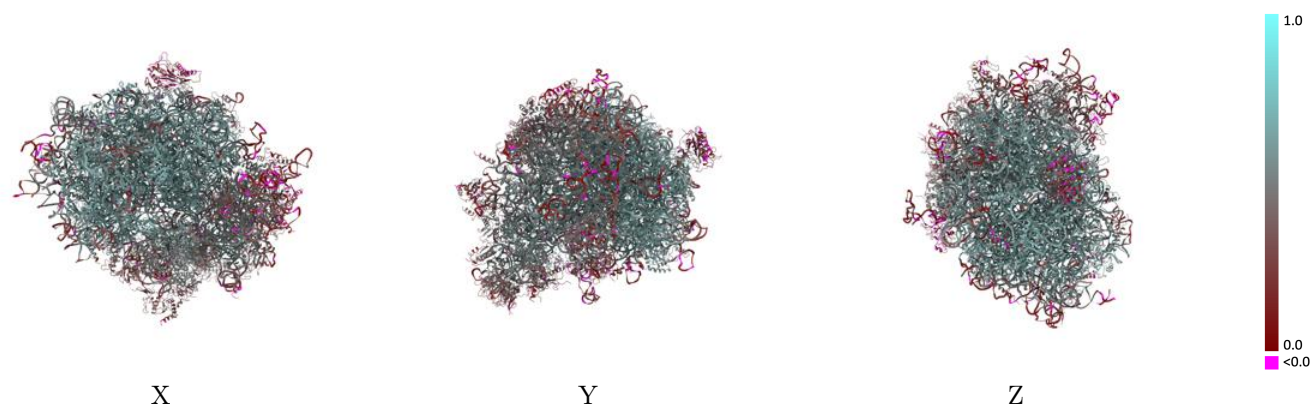
This section contains information regarding the fit between EMDB map EMD-44039 and PDB model 9B0F. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



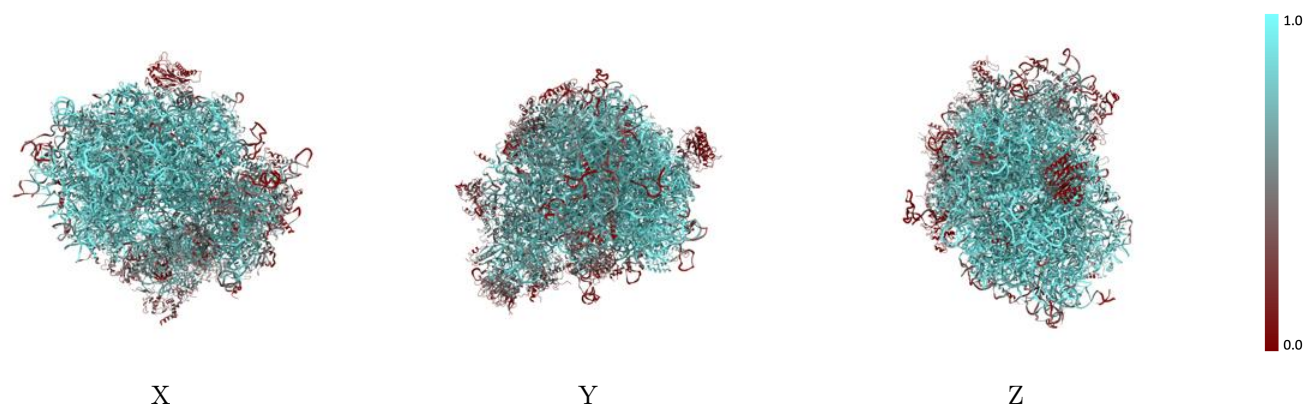
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



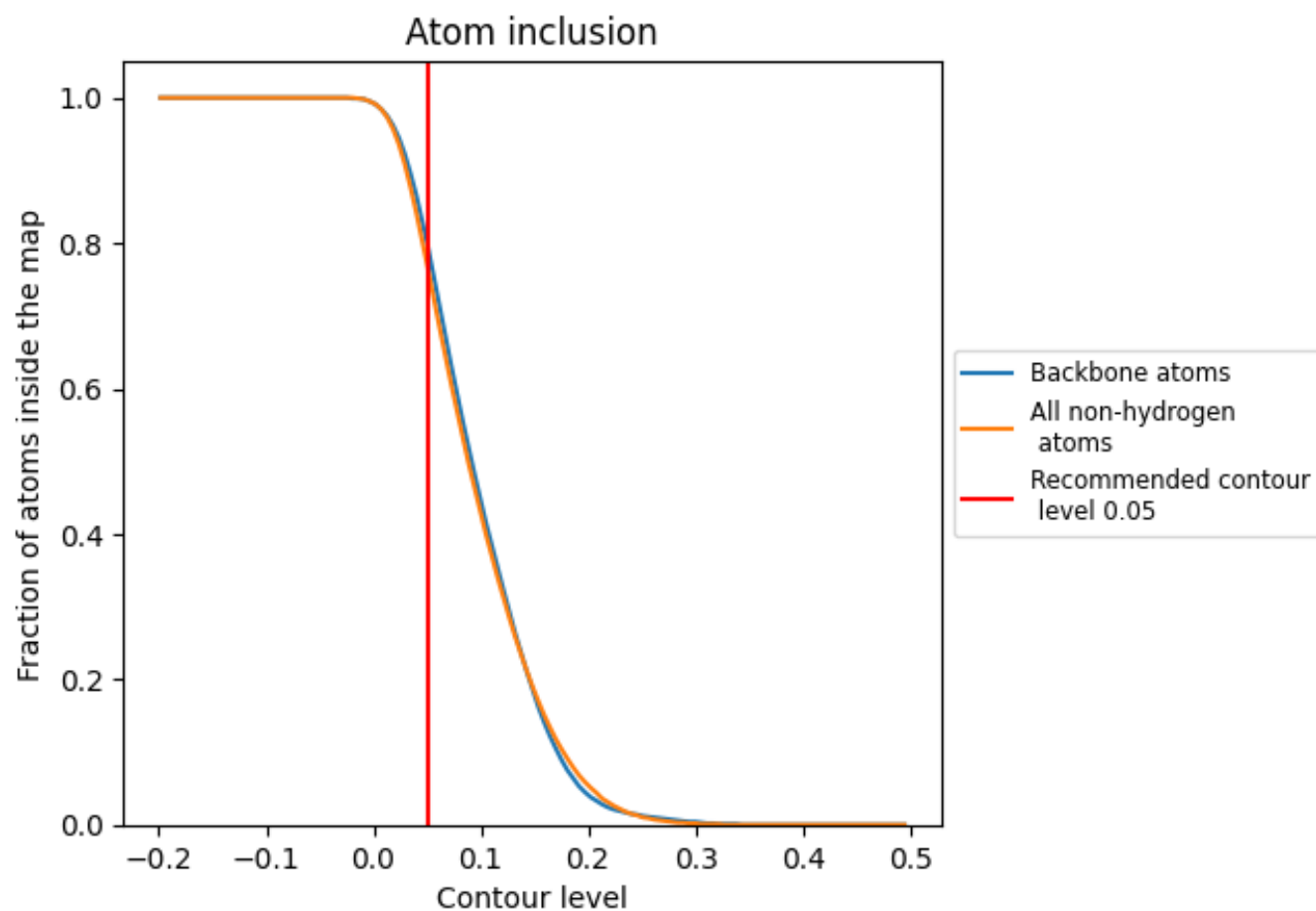
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7710   |  0.5060   |
| CA    |  0.1210   |  0.2390   |
| CB    |  0.5370   |  0.4600   |
| CD    |  0.5560   |  0.4260   |
| Et    |  0.2860   |  0.1280   |
| L5    |  0.8640   |  0.5390   |
| L7    |  0.9700   |  0.6060   |
| L8    |  0.9130   |  0.5780   |
| LA    |  0.9360   |  0.6180   |
| LB    |  0.8900   |  0.6000   |
| LC    |  0.8990   |  0.6000   |
| LD    |  0.8280   |  0.5640   |
| LE    |  0.7830   |  0.5340   |
| LF    |  0.9190   |  0.6090   |
| LG    |  0.7710  |  0.5440  |
| LH    |  0.8620 |  0.5860 |
| LI    |  0.8990 |  0.6080 |
| LJ    |  0.7040 |  0.4980 |
| LL    |  0.8420 |  0.5730 |
| LM    |  0.8920 |  0.5910 |
| LN    |  0.9730 |  0.6330 |
| LO    |  0.9330 |  0.6170 |
| LP    |  0.9100 |  0.6190 |
| LQ    |  0.9410 |  0.6280 |
| LR    |  0.7920 |  0.5500 |
| LS    |  0.9340 |  0.6170 |
| LT    |  0.8700 |  0.5870 |
| LU    |  0.7010 |  0.4780 |
| LV    |  0.9040 |  0.6130 |
| LW    |  0.5590 |  0.4080 |
| LX    |  0.8540 |  0.5920 |
| LY    |  0.8900 |  0.6010 |
| LZ    |  0.8540 |  0.5850 |
| La    |  0.9260 |  0.6240 |
| Lb    |  0.7540 |  0.5320 |





















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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| Lc    |  0.8300   |  0.5580   |
| Ld    |  0.8590   |  0.5900   |
| Le    |  0.9410   |  0.6240   |
| Lf    |  0.9480   |  0.6230   |
| Lg    |  0.8750   |  0.5930   |
| Lh    |  0.8650   |  0.5930   |
| Li    |  0.8420   |  0.5800   |
| Lj    |  0.9450   |  0.6220   |
| Lk    |  0.7380   |  0.5400   |
| Ll    |  0.9170   |  0.6120   |
| Lm    |  0.8940   |  0.6030   |
| Ln    |  0.8470   |  0.6040   |
| Lo    |  0.8650   |  0.5950   |
| Lp    |  0.8850   |  0.6070   |
| Lr    |  0.9150   |  0.6020   |
| Ls    |  0.4300   |  0.3790   |
| Lt    |  0.1790   |  0.2200   |
| Lz    |  0.0200   |  0.1060   |
| S2    |  0.8040   |  0.4660   |
| SA    |  0.5910  |  0.4480  |
| SB    |  0.4710 |  0.3730 |
| SC    |  0.7260 |  0.5230 |
| SD    |  0.5950 |  0.4620 |
| SE    |  0.6110 |  0.4630 |
| SF    |  0.5260 |  0.4080 |
| SG    |  0.3840 |  0.2970 |
| SH    |  0.3910 |  0.3360 |
| SI    |  0.6080 |  0.4570 |
| SJ    |  0.6760 |  0.4860 |
| SK    |  0.6000 |  0.4470 |
| SL    |  0.6760 |  0.4820 |
| SM    |  0.2480 |  0.2830 |
| SN    |  0.6630 |  0.4910 |
| SO    |  0.5580 |  0.4210 |
| SP    |  0.5990 |  0.4670 |
| SQ    |  0.5780 |  0.4270 |
| SS    |  0.5510 |  0.4310 |
| ST    |  0.5890 |  0.4440 |
| SU    |  0.5570 |  0.4070 |
| SV    |  0.6160 |  0.4540 |
| SW    |  0.7560 |  0.5260 |
| SX    |  0.7600 |  0.5470 |

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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| SY    |  0.4710 |  0.3540 |
| SZ    |  0.3720 |  0.3280 |
| Sa    |  0.6770 |  0.4890 |
| Sb    |  0.5150 |  0.4020 |
| Sc    |  0.3830 |  0.3300 |
| Sd    |  0.7800 |  0.5220 |
| Se    |  0.5610 |  0.4360 |
| Sf    |  0.2550 |  0.2660 |
| Sg    |  0.3670 |  0.3560 |