



## wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 07:13 AM EDT

PDB ID : 9P7C / pdb\_00009p7c  
EMDB ID : EMD-71337  
Title : In situ human Hibernating class3 80S ribosome  
Authors : Wei, Z.; Yong, X.  
Deposited on : 2025-06-20  
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

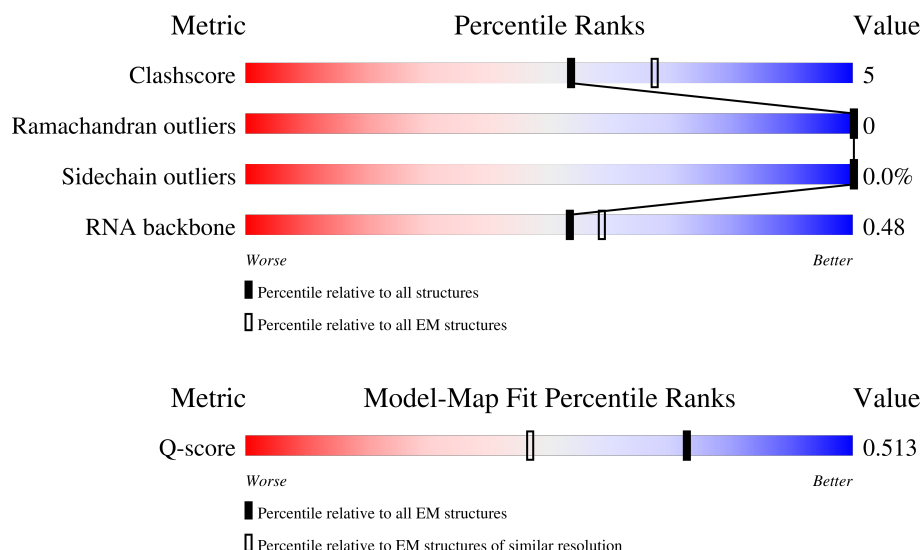
# 1 Overall quality at a glance

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.



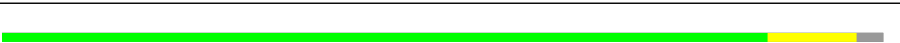
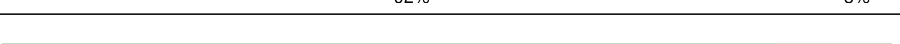
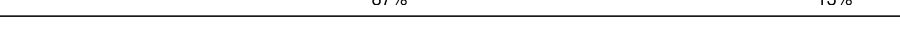
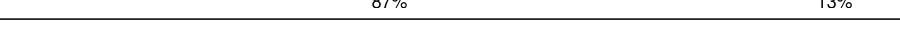
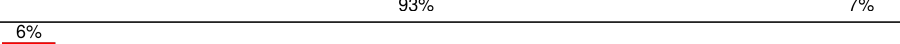
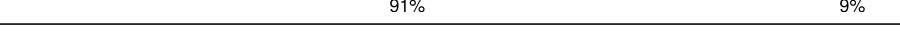
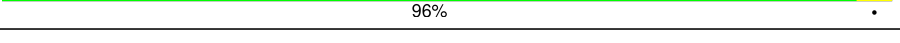
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 10754 ( 2.28 - 3.28 )                                    |

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   | CD    | 408    |                  |
| 2   | CI    | 31     |                  |
| 3   | L5    | 5070   |                  |

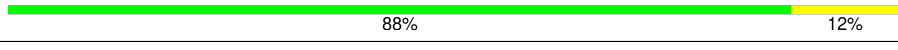
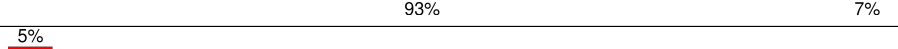
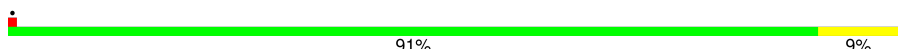
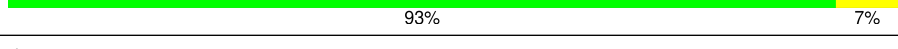
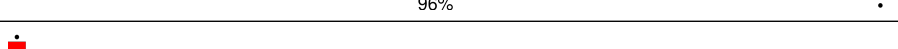
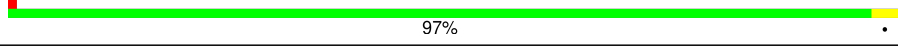
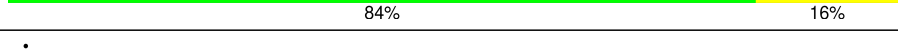
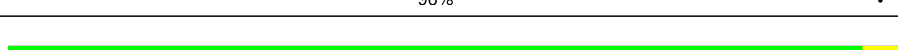
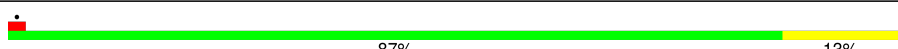
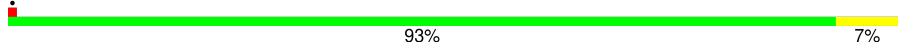
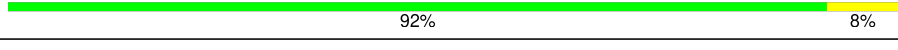
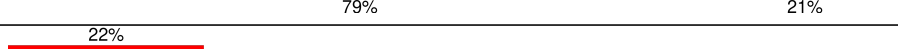
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | L7    | 120    |    |
| 5   | L8    | 156    |    |
| 6   | LA    | 248    |    |
| 7   | LB    | 402    |    |
| 8   | LC    | 368    |    |
| 9   | LD    | 293    |    |
| 10  | LE    | 250    |    |
| 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  | LR    | 187    |  |
| 23  | LS    | 175    |  |
| 24  | LT    | 159    |  |
| 25  | LU    | 101    |  |
| 26  | LV    | 131    |  |
| 27  | LW    | 124    |  |
| 28  | LX    | 120    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | LY    | 134    |    |
| 30  | LZ    | 135    |    |
| 31  | La    | 147    |    |
| 32  | Lb    | 121    |    |
| 33  | Lc    | 98     |    |
| 34  | Ld    | 107    |    |
| 35  | Le    | 128    |    |
| 36  | Lf    | 109    |    |
| 37  | Lg    | 114    |    |
| 38  | Lh    | 122    |   |
| 39  | Li    | 102    |  |
| 40  | Lj    | 86     |  |
| 41  | Lk    | 69     |  |
| 42  | Ll    | 50     |  |
| 43  | Lm    | 52     |  |
| 44  | Ln    | 24     |  |
| 45  | Lo    | 105    |  |
| 46  | Lp    | 91     |  |
| 47  | Lr    | 125    |  |
| 48  | Ls    | 196    |  |
| 49  | Lt    | 157    |  |
| 50  | SA    | 221    |  |
| 51  | SB    | 214    |  |
| 52  | SC    | 222    |  |
| 53  | SE    | 262    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | SG    | 237    |                  |
| 55  | SH    | 189    |                  |
| 56  | SI    | 206    |                  |
| 57  | SJ    | 185    |                  |
| 58  | SL    | 153    |                  |
| 59  | SN    | 150    |                  |
| 60  | SO    | 140    |                  |
| 61  | SV    | 83     |                  |
| 62  | SW    | 129    |                  |
| 63  | SX    | 141    |                  |
| 64  | SY    | 131    |                  |
| 65  | Sa    | 102    |                  |
| 66  | Sb    | 83     |                  |
| 67  | Se    | 58     |                  |
| 68  | S2    | 1740   |                  |
| 69  | SR    | 135    |                  |
| 70  | SD    | 227    |                  |
| 71  | SF    | 189    |                  |
| 72  | SK    | 98     |                  |
| 73  | SM    | 122    |                  |
| 74  | SP    | 121    |                  |
| 75  | SQ    | 144    |                  |
| 76  | SS    | 145    |                  |
| 77  | ST    | 143    |                  |
| 78  | SU    | 104    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 79  | SZ    | 75     |                  |
| 80  | Sc    | 64     |                  |
| 81  | Sd    | 55     |                  |
| 82  | Sf    | 67     |                  |
| 83  | Sg    | 313    |                  |
| 84  | Et    | 75     |                  |
| 85  | CB    | 856    |                  |
| 86  | CA    | 356    |                  |

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 228149 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 SERPINE1 mRNA-binding protein 1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1   | CD    | 55       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 440   | 263 | 87 | 90 |         |       |

- Molecule 2 is a protein called Transcription factor BTF3.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2   | CI    | 31       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 247   | 153 | 55 | 38 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 3   | L5    | 3655     | Total | C     | N     | O     | P    | 1       | 0     |
|     |       |          | 78444 | 34968 | 14346 | 25475 | 3655 |         |       |

- 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     |
|     |       |          | 3315  | 1481 | 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    | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1935  | 1242 | 368 | 321 | 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    | 205      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1658  | 1052 | 318 | 274 | 14 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | LJ    | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1362  | 861 | 254 | 241 | 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 L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | LR    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 971 | 336 | 250 | 9 |         |       |

- Molecule 23 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | LS    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1453  | 925 | 283 | 235 | 10 |         |       |

- Molecule 24 is a protein called 60S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | LT    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 25 is a protein called Heparin-binding protein HBp15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | LU    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 825   | 529 | 144 | 150 | 2 |         |       |

- Molecule 26 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | LV    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 618 | 184 | 172 | 5 |         |       |

- Molecule 27 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | LW    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 945   | 592 | 193 | 156 | 4 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L23a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | LX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 630 | 185 | 169 | 1 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | LY    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | LZ    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | La    | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 736 | 237 | 186 | 3 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | Lb    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 546 | 189 | 137 | 4 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | Lc    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 485 | 135 | 138 | 6 |         |       |

- Molecule 34 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Ld    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 560 | 171 | 155 | 2 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Le    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1053  | 667 | 216 | 165 | 5 |         |       |

- Molecule 36 is a protein called 60S ribosomal protein L35a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Lf    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 144 | 3 |         |       |

- Molecule 37 is a protein called 60S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | Lg    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | Lh    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 641 | 205 | 168 | 1 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Li    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 521 | 177 | 129 | 5 |         |       |

- Molecule 40 is a protein called 60S ribosomal protein L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Lj    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 705   | 434 | 155 | 111 | 5 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 41  | Lk    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

- Molecule 42 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | Ll    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 444   | 281 | 98 | 64 | 1 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | Lm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | Ln    | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L36a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Lo    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 542 | 175 | 139 | 6 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | Lp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Lr    | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1002  | 622 | 207 | 168 | 5 |         |       |

- 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 Large ribosomal subunit protein uL11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | Lt    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 998   | 626 | 180 | 189 | 3 |         |       |

- Molecule 50 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | SA    | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1741  | 1106 | 305 | 322 | 8 |         |       |

- Molecule 51 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51  | SB    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1738  | 1103 | 310 | 311 | 14 |         |       |

- Molecule 52 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | SC    | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1707  | 1104 | 293 | 300 | 10 |         |       |

- Molecule 53 is a protein called Small ribosomal subunit protein eS4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 53  | SE    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

- Molecule 54 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | SG    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 55 is a protein called Small ribosomal subunit protein eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | SH    | 186      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1497  | 956 | 274 | 266 | 1 |         |       |

- Molecule 56 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | SI    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

- Molecule 57 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | SJ    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 58 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | SL    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1247  | 793 | 234 | 214 | 6 |         |       |

- Molecule 59 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | SN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 60 is a protein called Small ribosomal subunit protein uS11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | SO    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1024  | 627 | 200 | 191 | 6 |         |       |

- Molecule 61 is a protein called Small ribosomal subunit protein eS21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | SV    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

- Molecule 62 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | SW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 63 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | SX    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | SY    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 673 | 209 | 178 | 5 |         |       |

- Molecule 65 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | Sa    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 512 | 171 | 133 | 5 |         |       |

- Molecule 66 is a protein called Small ribosomal subunit protein eS27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | Sb    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 67 is a protein called Small ribosomal subunit protein eS30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 67  | Se    | 58       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 459   | 284 | 100 | 74 | 1 |         |       |

- Molecule 68 is a RNA chain called 18S rRNA [Homo sapiens].

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 68  | S2    | 1740     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36952 | 16508 | 6600 | 12105 | 1739 |         |       |

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | SR    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1090  | 685 | 202 | 198 | 5 |         |       |

- Molecule 70 is a protein called Small ribosomal subunit protein uS3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 70  | SD    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |

- Molecule 71 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | SF    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 934 | 284 | 270 | 7 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | SK    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 539 | 148 | 134 | 6 |         |       |

- Molecule 73 is a protein called Small ribosomal subunit protein eS12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | SM    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 940   | 590 | 164 | 177 | 9 |         |       |

- Molecule 74 is a protein called Small ribosomal subunit protein uS19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | SP    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 623 | 185 | 170 | 7 |         |       |

- Molecule 75 is a protein called Small ribosomal subunit protein uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | SQ    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1142  | 726 | 216 | 197 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | SS    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 751 | 242 | 203 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | ST    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1112  | 697 | 214 | 198 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | SU    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 821   | 514 | 155 | 148 | 4 |         |       |

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | SZ    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 598   | 382 | 111 | 104 | 1 |         |       |

- Molecule 80 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 80  | Sc    | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 506   | 308 | 102 | 94 | 2 |         |       |

- Molecule 81 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 81  | Sd    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 82  | Sf    | 67       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 548   | 346 | 102 | 93 | 7 |         |       |

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 83  | Sg    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 84 is a RNA chain called E site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 84  | Et    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1593  | 712 | 281 | 526 | 74 |         |       |

- Molecule 85 is a protein called Elongation factor 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 85  | CB    | 846      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6605  | 4193 | 1136 | 1232 | 44 |         |       |

- Molecule 86 is a protein called Proliferation-associated protein 2G4.

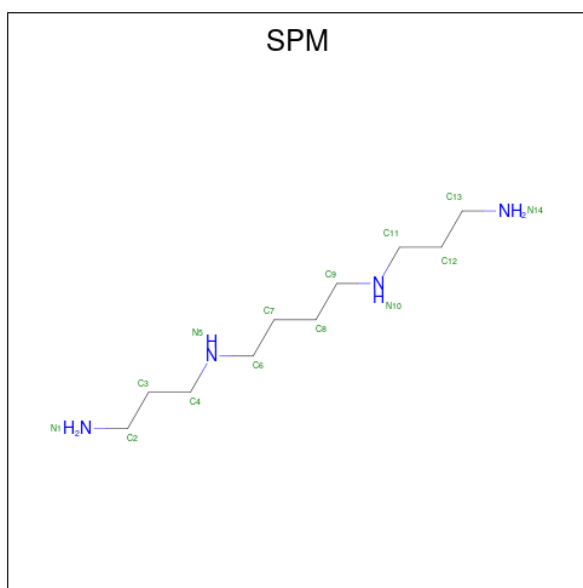
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 86  | CA    | 354      | Total | C    | N   | O   | S  | 4       | 0     |
|     |       |          | 2764  | 1744 | 475 | 528 | 17 |         |       |

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 87  | L5    | 177      | Total | Mg  | 0       |
|     |       |          | 177   | 177 |         |
| 87  | L7    | 3        | Total | Mg  | 0       |
|     |       |          | 3     | 3   |         |
| 87  | L8    | 5        | Total | Mg  | 0       |
|     |       |          | 5     | 5   |         |
| 87  | LA    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | LB    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | LI    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | LP    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | LV    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | Le    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | SG    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | S2    | 26       | Total | Mg  | 0       |
|     |       |          | 26    | 26  |         |

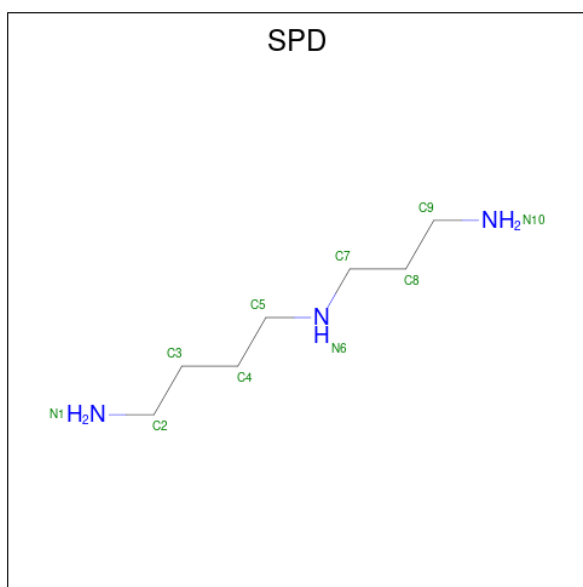
- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>) (labeled as "Ligand of

Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 88  | L5    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 88  | L5    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 88  | L5    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 88  | L5    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 88  | L5    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 88  | L5    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L5    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 89  | L8    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 90  | Lg    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

*Continued on next page...*

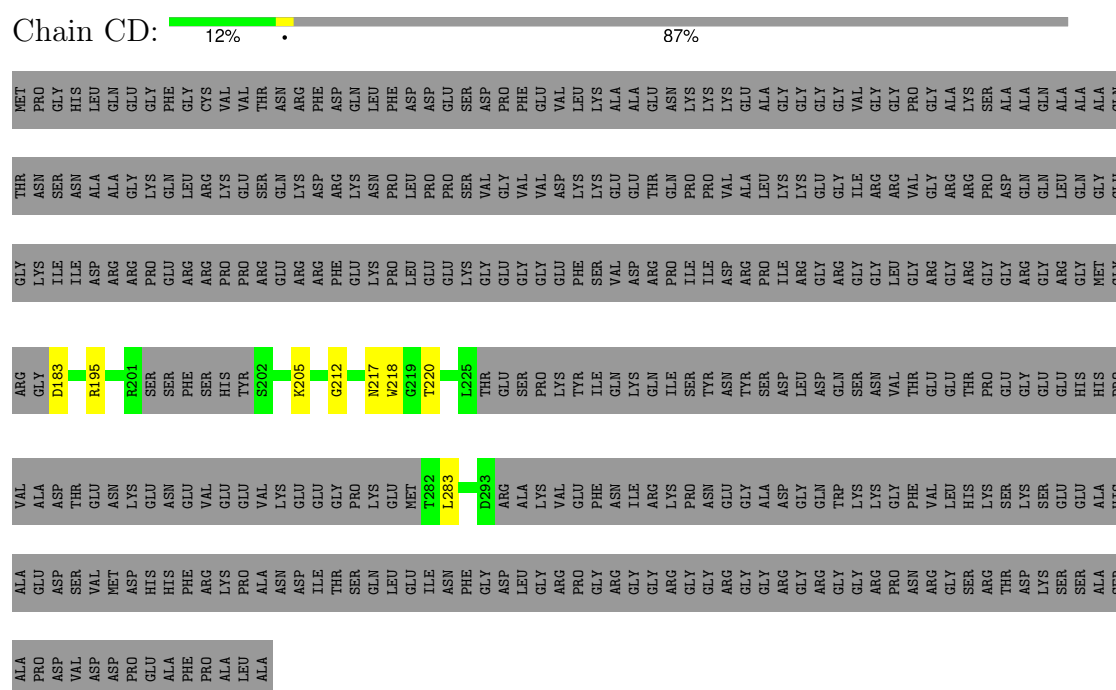
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 90  | Lj    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 90  | Lm    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 90  | Lo    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 90  | Lp    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 90  | Sa    | 1        | Total<br>1 | Zn<br>1 | 0       |

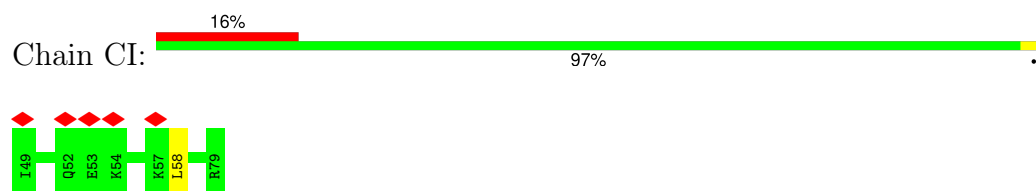
### 3 Residue-property plots

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.

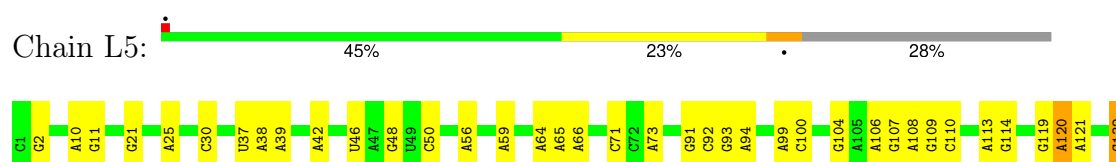
#### • Molecule 1: SERPINE1 mRNA-binding protein 1



#### • Molecule 2: Transcription factor BTF3



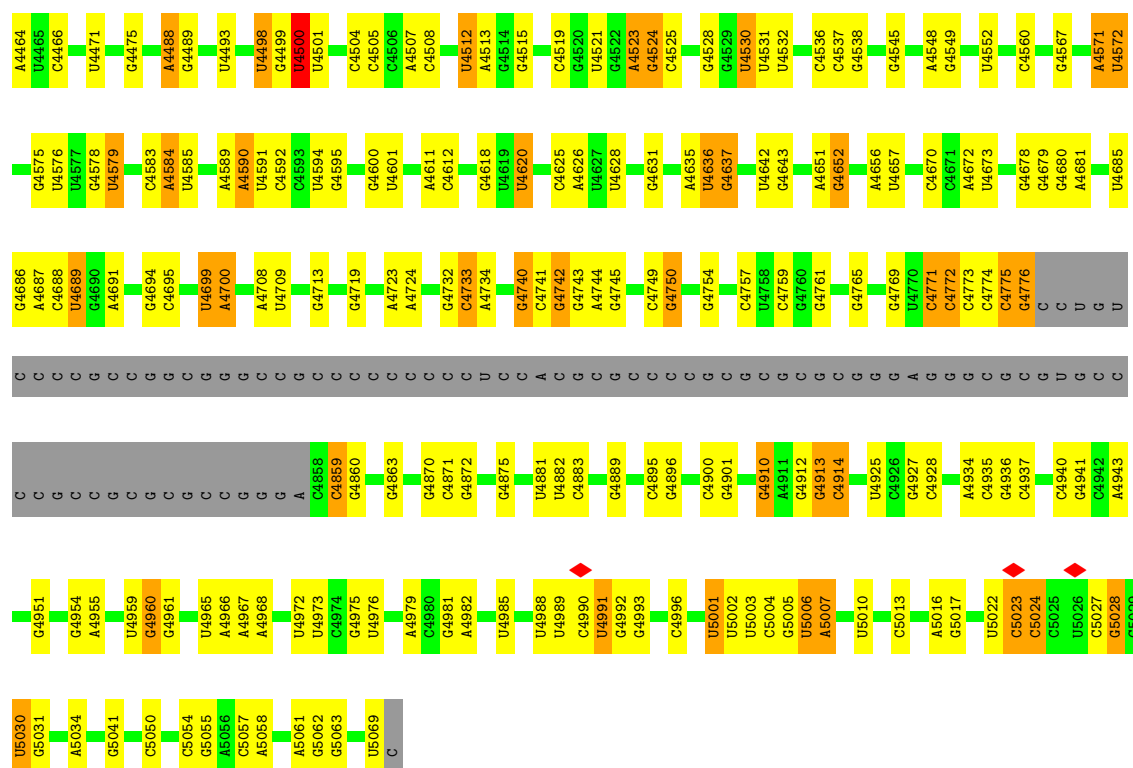
#### • Molecule 3: 28S rRNA





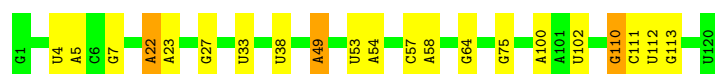






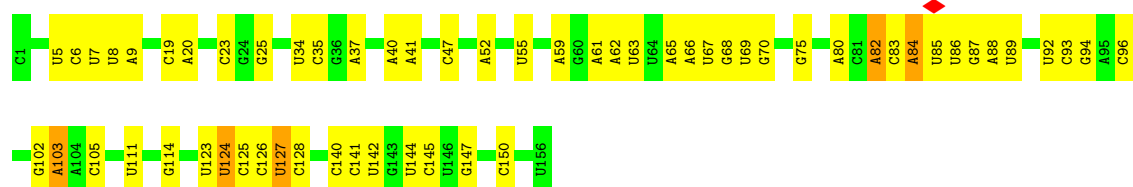
• Molecule 4: 5S rRNA

Chain L7: 82% 15%



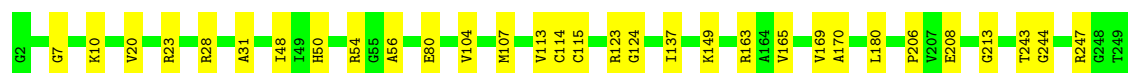
• Molecule 5: 5.8S rRNA

Chain L8: 62% 35%



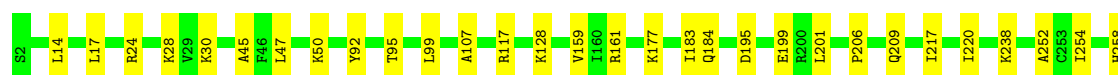
• Molecule 6: 60S ribosomal protein L8

Chain LA: 88% 12%

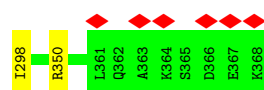


• Molecule 7: Large ribosomal subunit protein uL3

Chain LB: 88% 12%



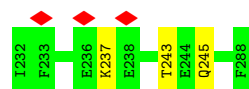
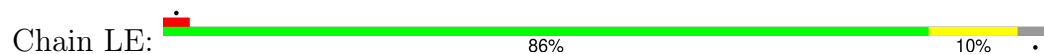
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



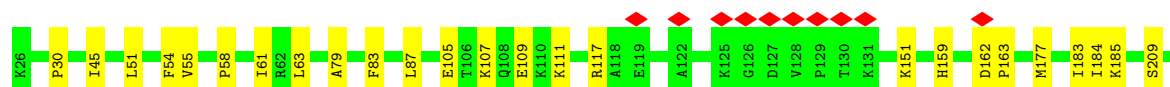
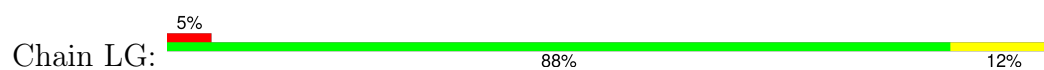
- Molecule 10: Large ribosomal subunit protein eL6

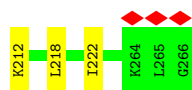


- Molecule 11: 60S ribosomal protein L7



- Molecule 12: 60S ribosomal protein L7a





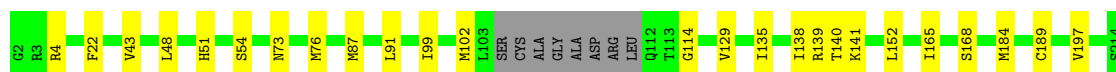
- Molecule 13: 60S ribosomal protein L9

Chain LH: 89% 11%



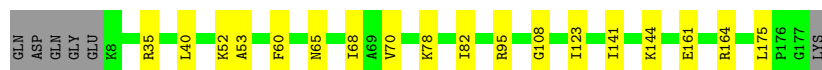
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 85% 12% .



- Molecule 15: 60S ribosomal protein L11

Chain LJ: 86% 10% .



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL: 91% 9%



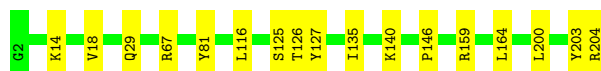
- Molecule 17: 60S ribosomal protein L14

Chain LM: 91% 9%



- Molecule 18: 60S ribosomal protein L15

Chain LN: 92% 8%



- Molecule 19: 60S ribosomal protein L13a

Chain LO: 87% 13%



- Molecule 20: 60S ribosomal protein L17

Chain LP: 87% 13%



- Molecule 21: 60S ribosomal protein L18

Chain LQ: 93% 7%



- Molecule 22: 60S ribosomal protein L19

Chain LR: 6% 91% 9%



- Molecule 23: 60S ribosomal protein L18a

Chain LS: 89% 11%



- Molecule 24: 60S ribosomal protein L21

Chain LT: 96% 4%



- Molecule 25: Heparin-binding protein HBp15

Chain LU: 83% 17%

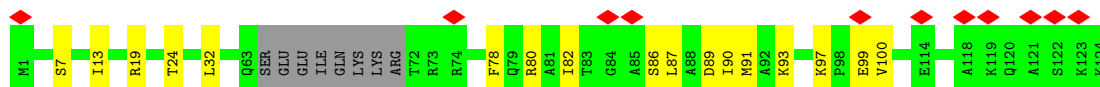
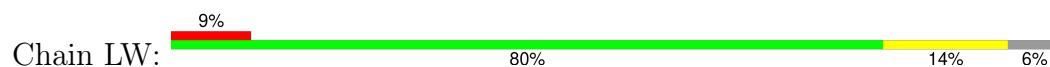


- Molecule 26: 60S ribosomal protein L23

Chain LV: 89% 11%



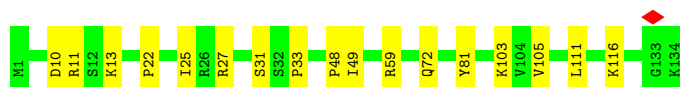
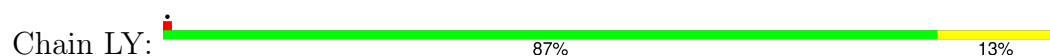
- Molecule 27: Ribosomal protein L24



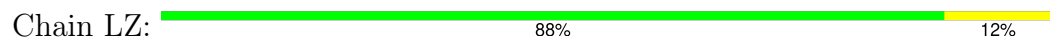
- Molecule 28: 60S ribosomal protein L23a



- Molecule 29: 60S ribosomal protein L26



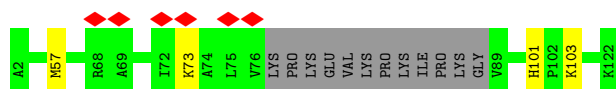
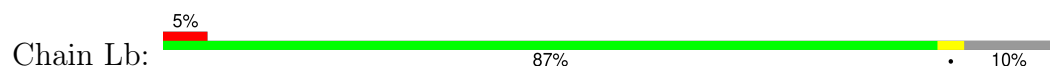
- Molecule 30: 60S ribosomal protein L27



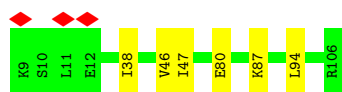
- Molecule 31: 60S ribosomal protein L27a



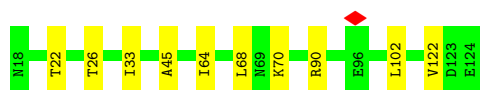
- Molecule 32: Large ribosomal subunit protein eL29



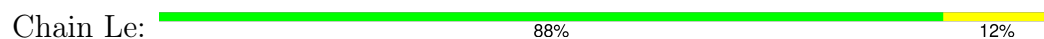
- Molecule 33: 60S ribosomal protein L30



- Molecule 34: 60S ribosomal protein L31



- Molecule 35: 60S ribosomal protein L32



- Molecule 36: 60S ribosomal protein L35a



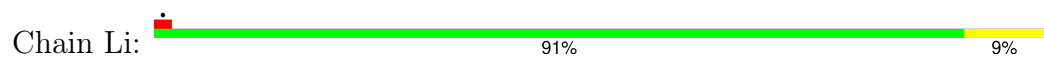
- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36



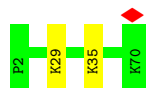
- Molecule 40: 60S ribosomal protein L37

Chain Lj:  91% 9%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  97%



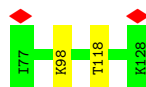
- Molecule 42: 60S ribosomal protein L39

Chain Ll:  84% 16%

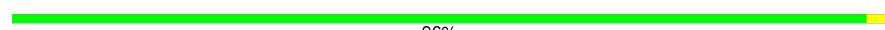


- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  96%



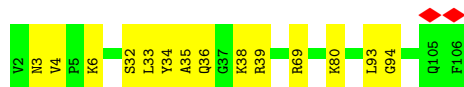
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  96%



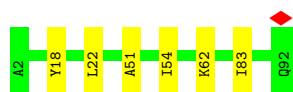
- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  87% 13%



- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  93% 7%



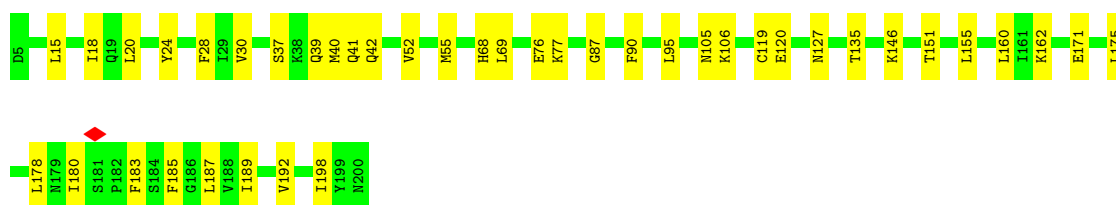
- Molecule 47: 60S ribosomal protein L28

Chain Lr: 92% 8%



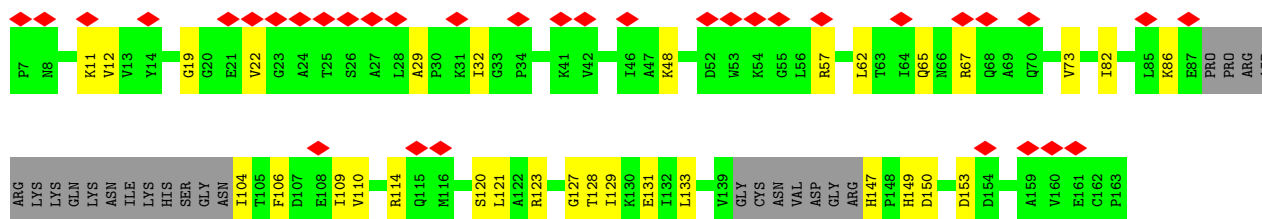
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls: 79% 21%



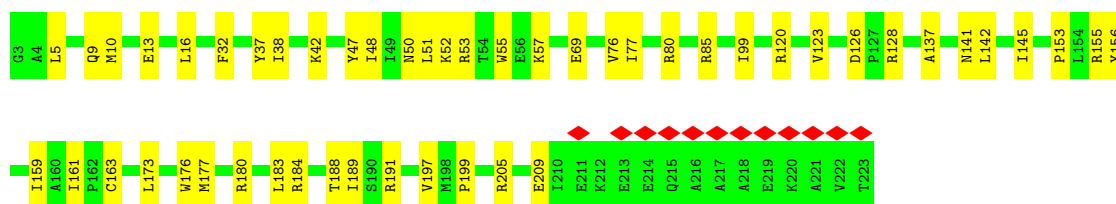
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt: 22% 66% 20% 15%



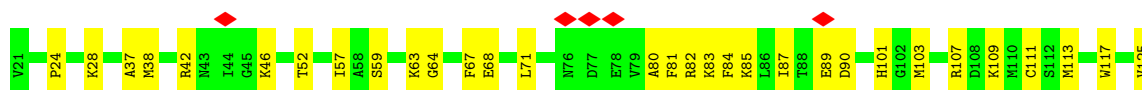
- Molecule 50: 40S ribosomal protein SA

Chain SA: 5% 77% 23%



- Molecule 51: 40S ribosomal protein S3a

Chain SB: 5% 71% 29%





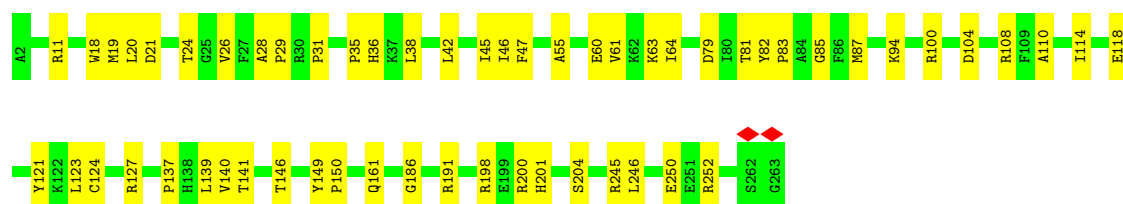
- Molecule 52: 40S ribosomal protein S2

Chain SC: 82% 17%



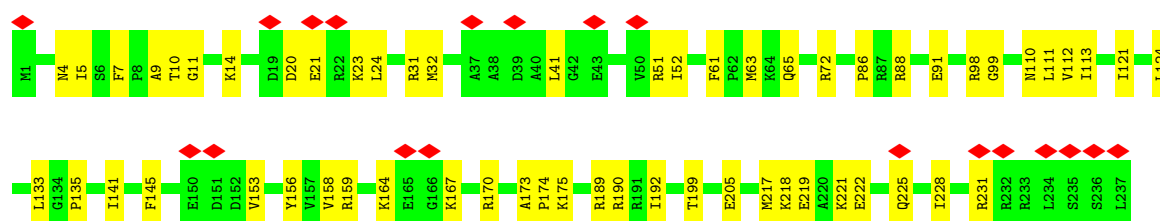
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE: 78% 22%



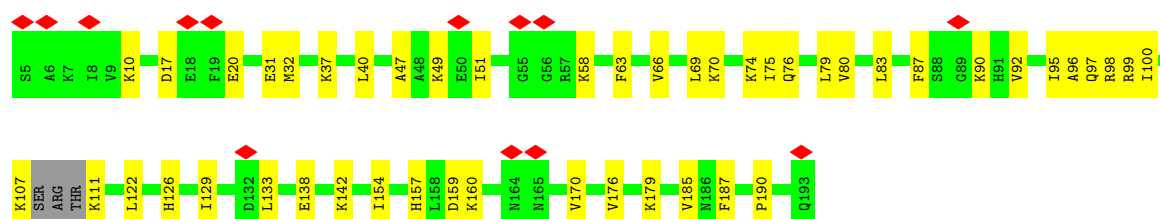
- Molecule 54: 40S ribosomal protein S6

Chain SG: 8% 76% 24%

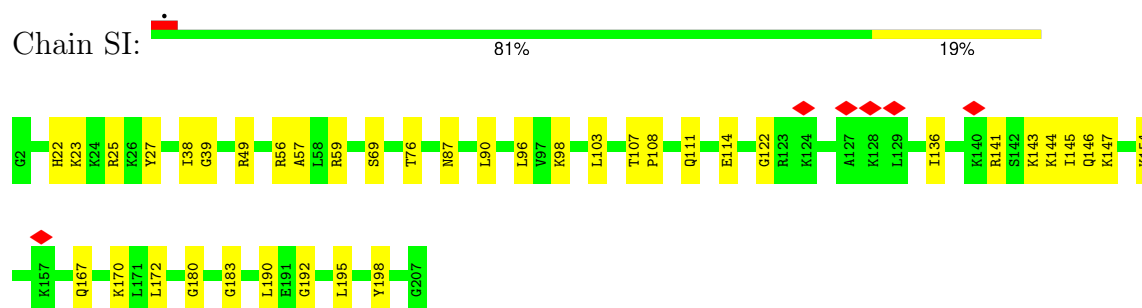


- Molecule 55: Small ribosomal subunit protein eS7

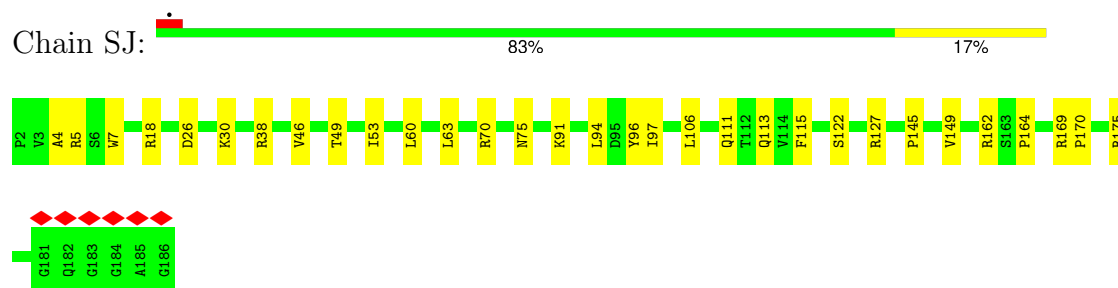
Chain SH: 7% 73% 25%



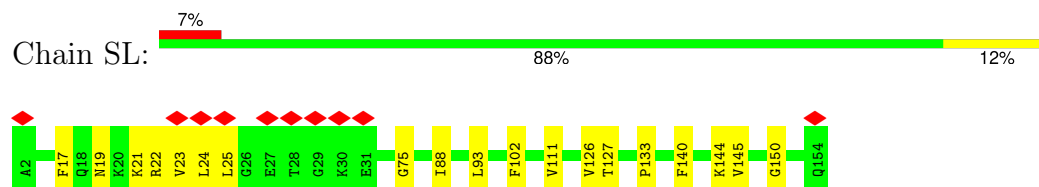
- Molecule 56: 40S ribosomal protein S8



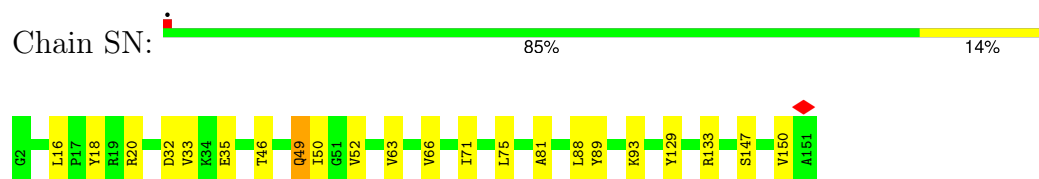
- Molecule 57: 40S ribosomal protein S9



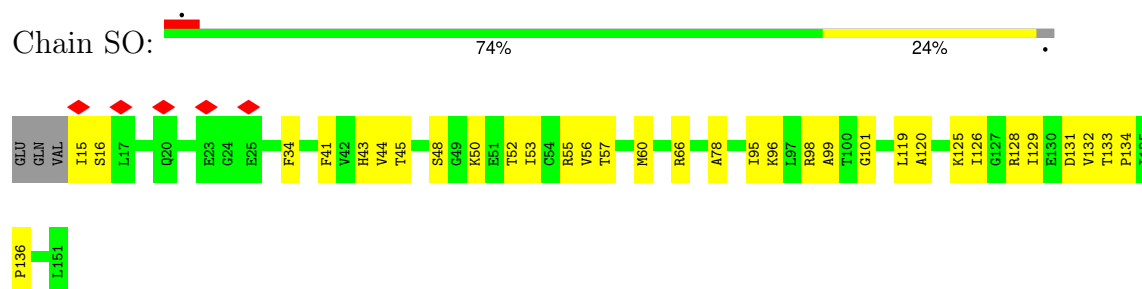
- Molecule 58: 40S ribosomal protein S11



- Molecule 59: 40S ribosomal protein S13



- Molecule 60: Small ribosomal subunit protein uS11



- Molecule 61: Small ribosomal subunit protein eS21

Chain SV:  83% 17%



- Molecule 62: 40S ribosomal protein S15a

Chain SW:  87% 13%



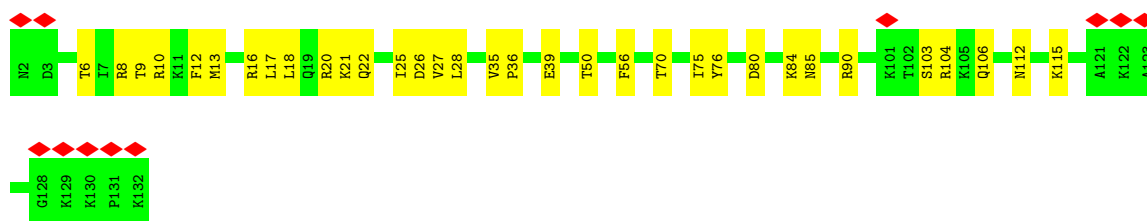
- Molecule 63: 40S ribosomal protein S23

Chain SX:  91% 9%



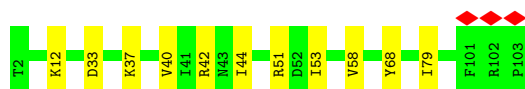
- Molecule 64: 40S ribosomal protein S24

Chain SY:  8% 75% 25%



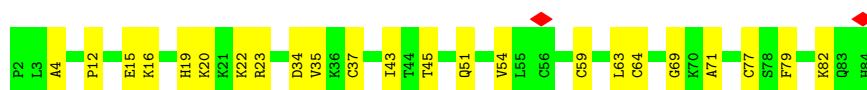
- Molecule 65: 40S ribosomal protein S26

Chain Sa:  89% 11%



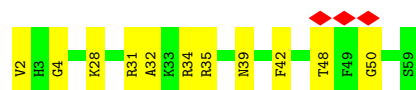
- Molecule 66: Small ribosomal subunit protein eS27

Chain Sb:  72% 28%



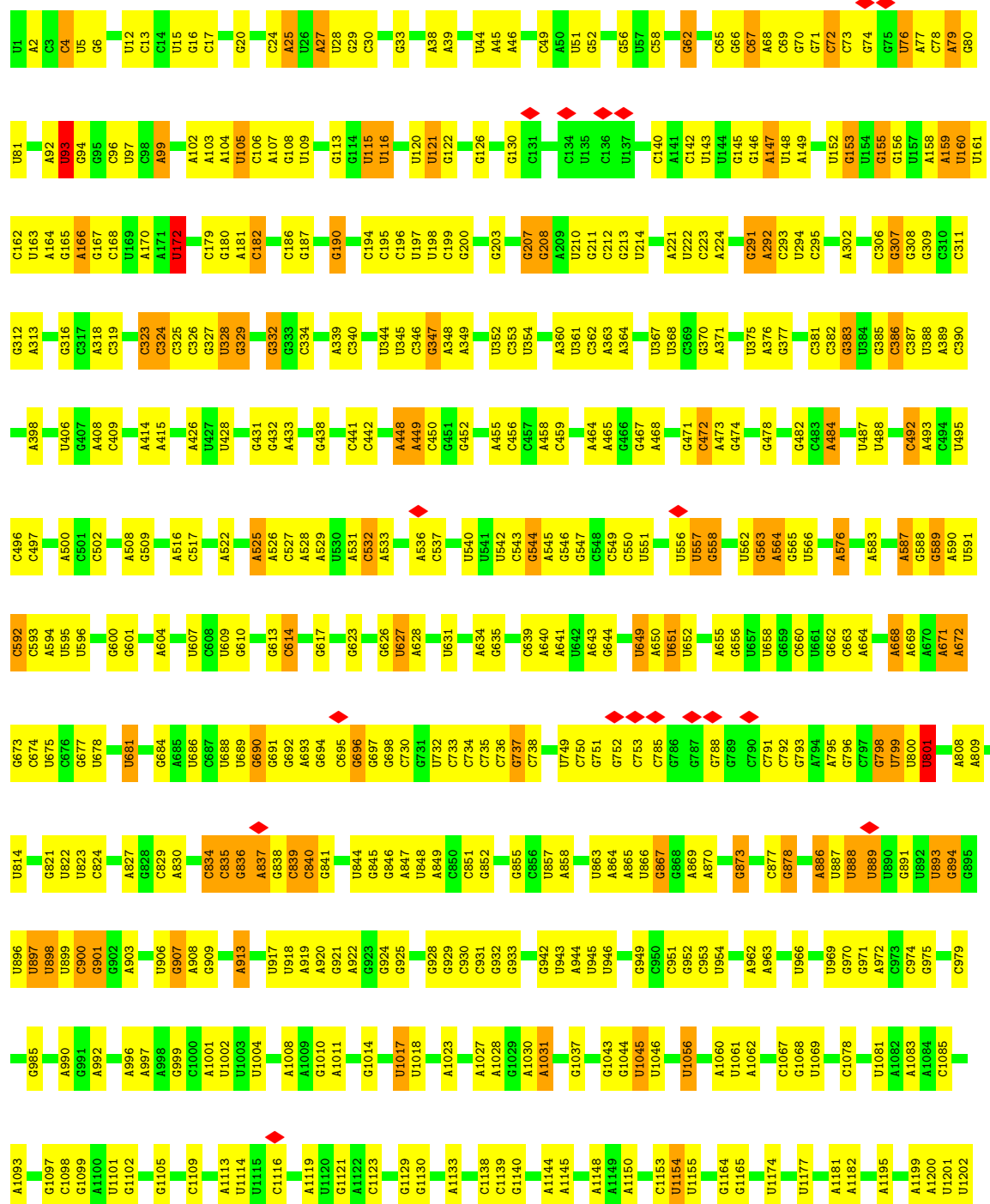
- Molecule 67: Small ribosomal subunit protein eS30

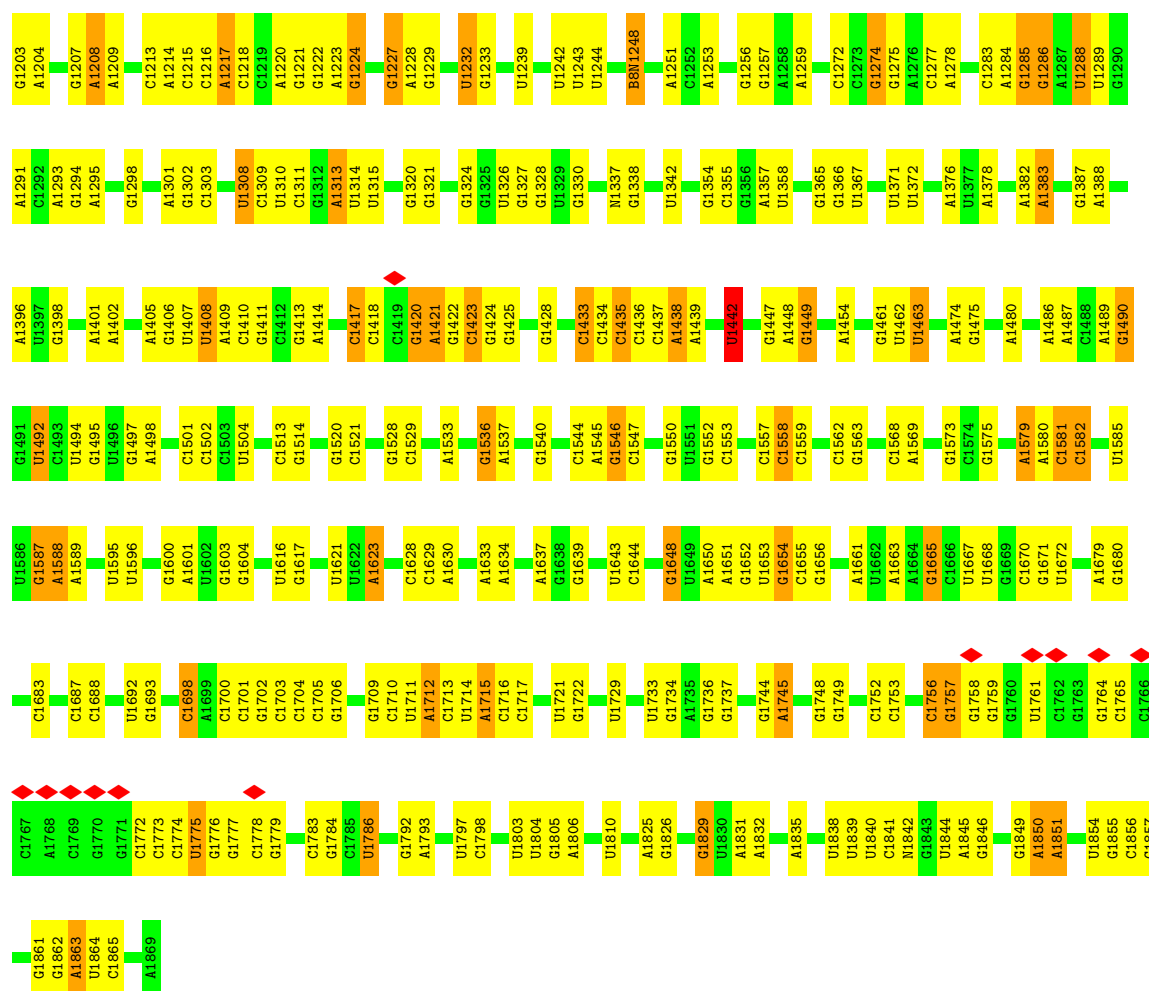
Chain Se:  5% 81% 19%



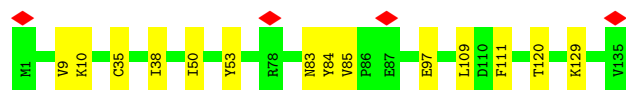
• Molecule 68: 18S rRNA [Homo sapiens]

Chain S2: 54% 38% 8%





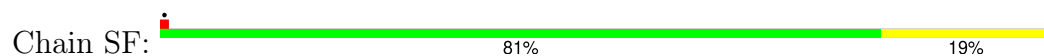
- Molecule 69: Small ribosomal subunit protein eS17

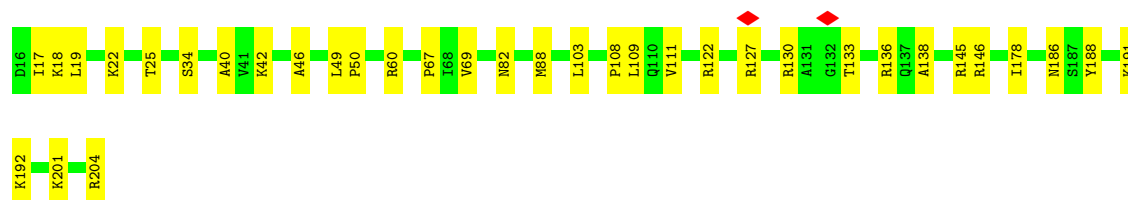


- Molecule 70: Small ribosomal subunit protein uS3

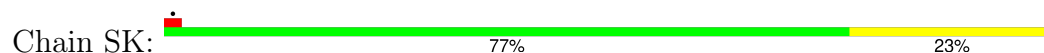


- Molecule 71: 40S ribosomal protein S5

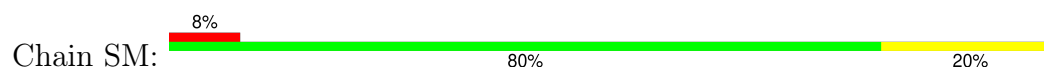




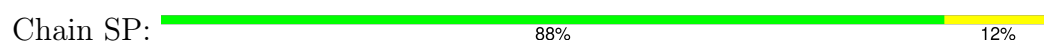
- Molecule 72: 40S ribosomal protein S10



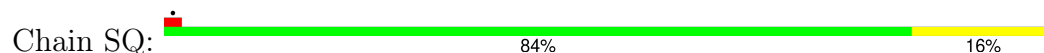
- Molecule 73: Small ribosomal subunit protein eS12



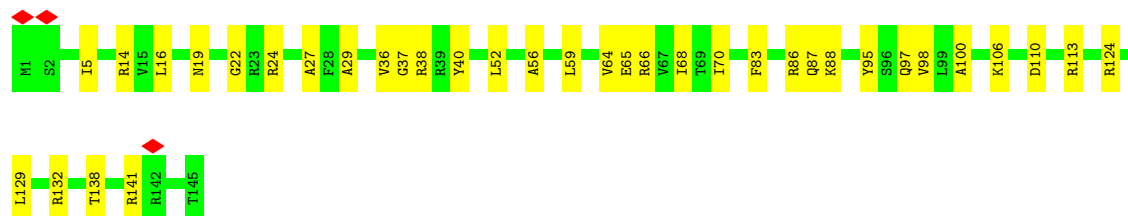
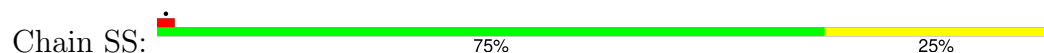
- Molecule 74: Small ribosomal subunit protein uS19



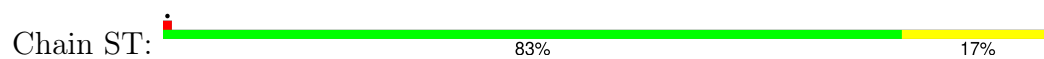
- Molecule 75: Small ribosomal subunit protein uS9



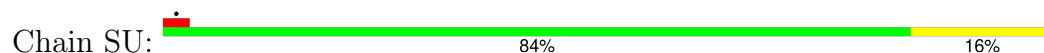
- Molecule 76: 40S ribosomal protein S18



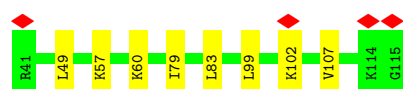
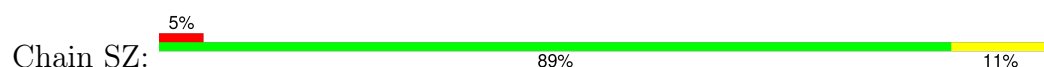
- Molecule 77: 40S ribosomal protein S19



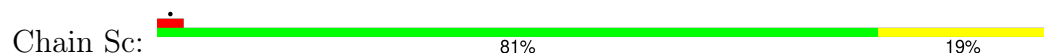
- Molecule 78: 40S ribosomal protein S20



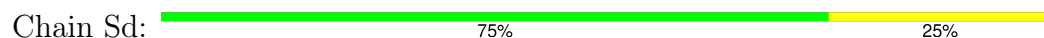
- Molecule 79: Small ribosomal subunit protein eS25



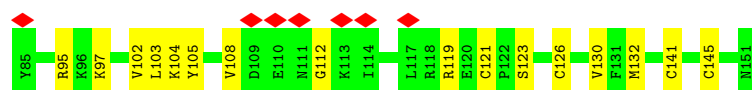
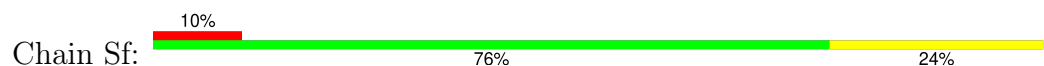
- Molecule 80: 40S ribosomal protein S28



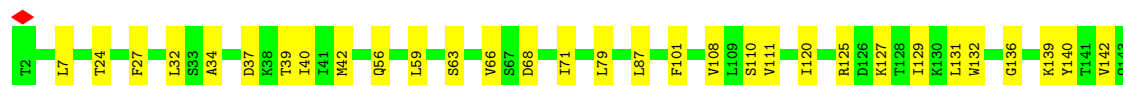
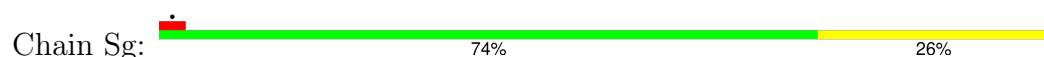
- Molecule 81: 40S ribosomal protein S29

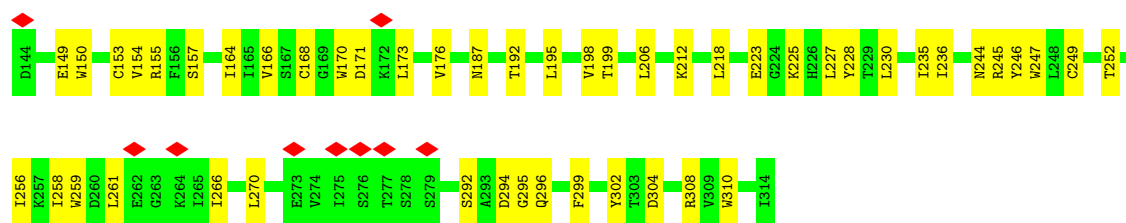


- Molecule 82: Ubiquitin-40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1

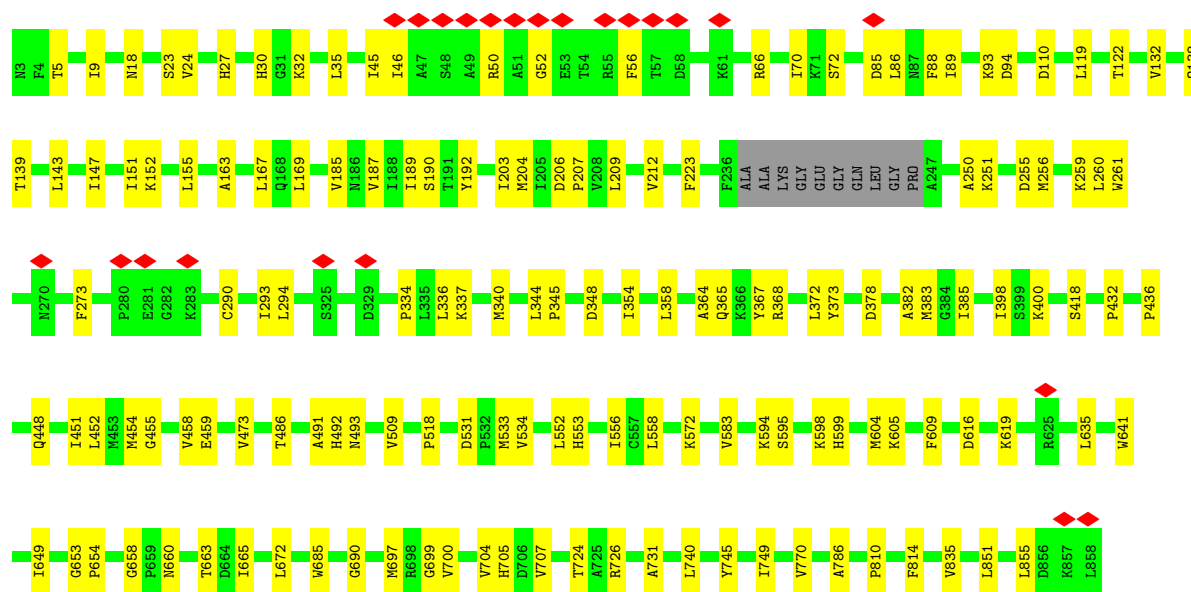
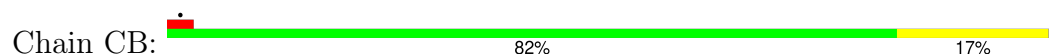




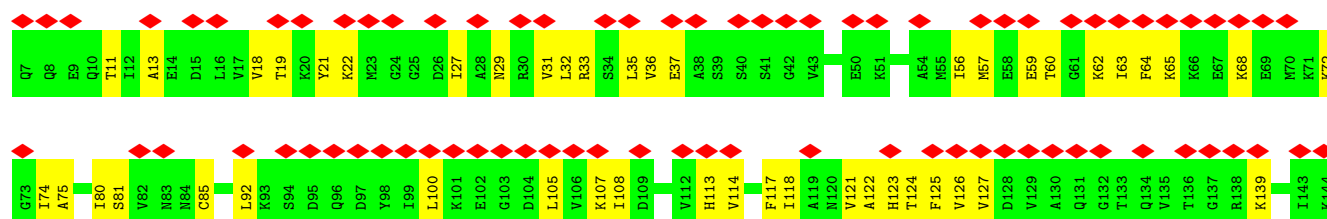
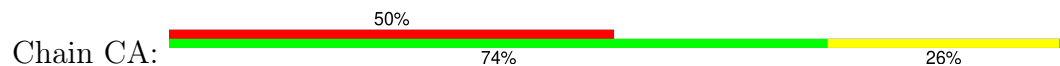
• Molecule 84: E site tRNA

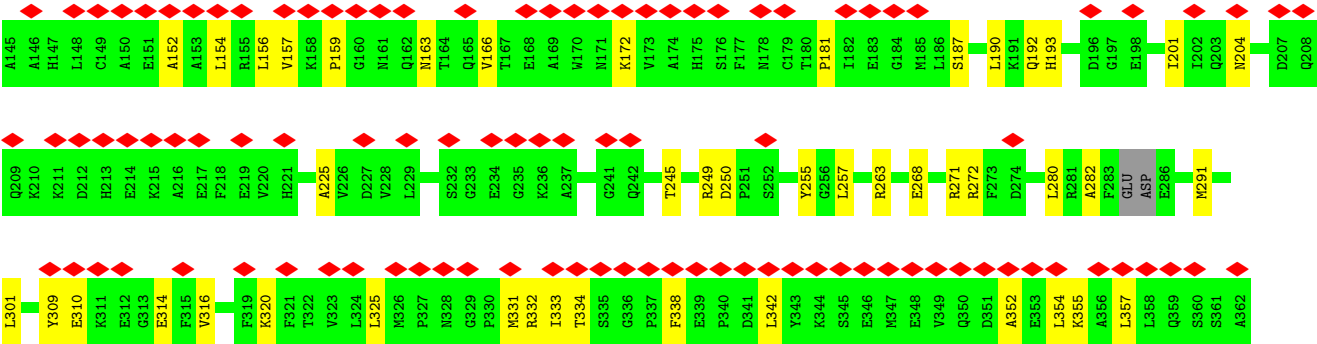


• Molecule 85: Elongation factor 2



• Molecule 86: Proliferation-associated protein 2G4





## 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 TECNAI F30            | 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                    | 0.270                     | Depositor |
| Minimum map value                    | -0.084                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.009                     | Depositor |
| Recommended contour level            | 0.025                     | 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: B8N, PSU, UR3, 1MA, OMU, OMC, G7M, 6MZ, ZN, SPM, 4AC, UY1, MG, SPD, A2M, MA6, 5MC, OMG

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   | CD    | 0.17         | 0/447       | 0.32        | 0/592       |
| 2   | CI    | 0.13         | 0/247       | 0.30        | 0/323       |
| 3   | L5    | 0.35         | 0/85098     | 0.33        | 0/132762    |
| 4   | L7    | 0.34         | 0/2861      | 0.28        | 0/4459      |
| 5   | L8    | 0.35         | 0/3631      | 0.30        | 0/5657      |
| 6   | LA    | 0.34         | 0/1936      | 0.38        | 0/2596      |
| 7   | LB    | 0.31         | 0/3306      | 0.35        | 0/4424      |
| 8   | LC    | 0.32         | 0/2981      | 0.34        | 0/4002      |
| 9   | LD    | 0.27         | 0/2428      | 0.32        | 0/3252      |
| 10  | LE    | 0.25         | 0/1973      | 0.34        | 0/2645      |
| 11  | LF    | 0.33         | 0/1905      | 0.32        | 0/2539      |
| 12  | LG    | 0.27         | 0/1960      | 0.36        | 0/2637      |
| 13  | LH    | 0.29         | 0/1537      | 0.34        | 0/2066      |
| 14  | LI    | 0.29         | 0/1697      | 0.31        | 0/2266      |
| 15  | LJ    | 0.23         | 0/1385      | 0.33        | 0/1852      |
| 16  | LL    | 0.29         | 0/1732      | 0.32        | 0/2315      |
| 17  | LM    | 0.29         | 0/1161      | 0.32        | 0/1554      |
| 18  | LN    | 0.35         | 0/1746      | 0.35        | 0/2338      |
| 19  | LO    | 0.32         | 0/1682      | 0.34        | 0/2250      |
| 20  | LP    | 0.32         | 0/1268      | 0.35        | 0/1701      |
| 21  | LQ    | 0.33         | 0/1537      | 0.36        | 0/2052      |
| 22  | LR    | 0.27         | 0/1582      | 0.29        | 0/2091      |
| 23  | LS    | 0.33         | 0/1493      | 0.35        | 0/2003      |
| 24  | LT    | 0.30         | 0/1326      | 0.30        | 0/1770      |
| 25  | LU    | 0.23         | 0/839       | 0.33        | 0/1126      |
| 26  | LV    | 0.31         | 0/993       | 0.35        | 0/1332      |
| 27  | LW    | 0.24         | 0/959       | 0.31        | 0/1270      |
| 28  | LX    | 0.28         | 0/1002      | 0.30        | 0/1345      |
| 29  | LY    | 0.29         | 0/1132      | 0.31        | 0/1504      |
| 30  | LZ    | 0.27         | 0/1130      | 0.36        | 0/1507      |
| 31  | La    | 0.32         | 0/1191      | 0.30        | 0/1591      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 32  | Lb    | 0.26         | 0/889   | 0.36        | 0/1175  |
| 33  | Lc    | 0.27         | 0/774   | 0.36        | 0/1038  |
| 34  | Ld    | 0.30         | 0/903   | 0.34        | 0/1216  |
| 35  | Le    | 0.34         | 0/1071  | 0.32        | 0/1429  |
| 36  | Lf    | 0.35         | 0/895   | 0.39        | 0/1198  |
| 37  | Lg    | 0.29         | 0/916   | 0.33        | 0/1220  |
| 38  | Lh    | 0.27         | 0/1023  | 0.33        | 0/1351  |
| 39  | Li    | 0.25         | 0/843   | 0.30        | 0/1115  |
| 40  | Lj    | 0.35         | 0/720   | 0.39        | 0/952   |
| 41  | Lk    | 0.23         | 0/575   | 0.27        | 0/761   |
| 42  | Ll    | 0.32         | 0/454   | 0.34        | 0/599   |
| 43  | Lm    | 0.28         | 0/435   | 0.34        | 0/575   |
| 44  | Ln    | 0.25         | 0/231   | 0.25        | 0/294   |
| 45  | Lo    | 0.29         | 0/876   | 0.34        | 0/1156  |
| 46  | Lp    | 0.31         | 0/718   | 0.31        | 0/953   |
| 47  | Lr    | 0.32         | 0/1017  | 0.35        | 0/1364  |
| 48  | Ls    | 0.16         | 0/1519  | 0.33        | 0/2052  |
| 49  | Lt    | 0.20         | 0/1009  | 0.49        | 0/1363  |
| 50  | SA    | 0.20         | 0/1778  | 0.33        | 0/2416  |
| 51  | SB    | 0.18         | 0/1765  | 0.33        | 0/2362  |
| 52  | SC    | 0.22         | 0/1744  | 0.36        | 0/2357  |
| 53  | SE    | 0.19         | 0/2118  | 0.33        | 0/2849  |
| 54  | SG    | 0.16         | 0/1946  | 0.36        | 0/2590  |
| 55  | SH    | 0.18         | 0/1519  | 0.40        | 0/2033  |
| 56  | SI    | 0.20         | 0/1715  | 0.34        | 0/2287  |
| 57  | SJ    | 0.20         | 0/1550  | 0.34        | 0/2069  |
| 58  | SL    | 0.21         | 0/1268  | 0.32        | 0/1696  |
| 59  | SN    | 0.20         | 0/1232  | 0.30        | 0/1656  |
| 60  | SO    | 0.19         | 0/1037  | 0.38        | 0/1391  |
| 61  | SV    | 0.19         | 0/643   | 0.30        | 0/860   |
| 62  | SW    | 0.23         | 0/1051  | 0.33        | 0/1406  |
| 63  | SX    | 0.24         | 0/1116  | 0.39        | 0/1490  |
| 64  | SY    | 0.16         | 0/1083  | 0.31        | 0/1438  |
| 65  | Sa    | 0.23         | 0/836   | 0.34        | 0/1121  |
| 66  | Sb    | 0.17         | 0/665   | 0.34        | 0/891   |
| 67  | Se    | 0.18         | 0/465   | 0.35        | 0/612   |
| 68  | S2    | 0.26         | 0/39756 | 0.30        | 0/61939 |
| 69  | SR    | 0.19         | 0/1105  | 0.39        | 0/1484  |
| 70  | SD    | 0.20         | 0/1793  | 0.32        | 0/2414  |
| 71  | SF    | 0.18         | 0/1516  | 0.35        | 0/2037  |
| 72  | SK    | 0.19         | 0/851   | 0.38        | 0/1147  |
| 73  | SM    | 0.16         | 0/950   | 0.40        | 0/1275  |
| 74  | SP    | 0.20         | 0/1003  | 0.33        | 0/1342  |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 75  | SQ    | 0.20         | 0/1160   | 0.36        | 0/1553   |
| 76  | SS    | 0.17         | 0/1216   | 0.30        | 0/1628   |
| 77  | ST    | 0.19         | 0/1131   | 0.33        | 0/1515   |
| 78  | SU    | 0.20         | 0/831    | 0.35        | 0/1115   |
| 79  | SZ    | 0.19         | 0/604    | 0.39        | 0/810    |
| 80  | Sc    | 0.17         | 0/508    | 0.31        | 0/680    |
| 81  | Sd    | 0.22         | 0/470    | 0.33        | 0/623    |
| 82  | Sf    | 0.17         | 0/560    | 0.47        | 0/745    |
| 83  | Sg    | 0.16         | 0/2493   | 0.35        | 0/3394   |
| 84  | Et    | 0.20         | 0/1778   | 0.39        | 0/2767   |
| 85  | CB    | 0.19         | 0/6734   | 0.34        | 0/9094   |
| 86  | CA    | 0.14         | 0/2810   | 0.36        | 0/3780   |
| All | All   | 0.29         | 0/239833 | 0.33        | 0/350498 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CD    | 440   | 0        | 402      | 7       | 0            |
| 2   | CI    | 247   | 0        | 283      | 1       | 0            |
| 3   | L5    | 78444 | 0        | 39719    | 535     | 0            |
| 4   | L7    | 2561  | 0        | 1295     | 9       | 0            |
| 5   | L8    | 3315  | 0        | 1685     | 26      | 0            |
| 6   | LA    | 1898  | 0        | 1993     | 23      | 0            |
| 7   | LB    | 3238  | 0        | 3376     | 34      | 0            |
| 8   | LC    | 2927  | 0        | 3104     | 24      | 0            |
| 9   | LD    | 2382  | 0        | 2410     | 20      | 0            |
| 10  | LE    | 1935  | 0        | 2096     | 18      | 0            |
| 11  | LF    | 1870  | 0        | 1996     | 15      | 0            |
| 12  | LG    | 1927  | 0        | 2074     | 18      | 0            |
| 13  | LH    | 1518  | 0        | 1601     | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | LI    | 1658  | 0        | 1697     | 15      | 0            |
| 15  | LJ    | 1362  | 0        | 1399     | 10      | 0            |
| 16  | LL    | 1701  | 0        | 1818     | 19      | 0            |
| 17  | LM    | 1138  | 0        | 1204     | 7       | 0            |
| 18  | LN    | 1701  | 0        | 1749     | 15      | 0            |
| 19  | LO    | 1650  | 0        | 1794     | 15      | 0            |
| 20  | LP    | 1242  | 0        | 1269     | 13      | 0            |
| 21  | LQ    | 1513  | 0        | 1628     | 11      | 0            |
| 22  | LR    | 1566  | 0        | 1729     | 15      | 0            |
| 23  | LS    | 1453  | 0        | 1490     | 11      | 0            |
| 24  | LT    | 1298  | 0        | 1366     | 5       | 0            |
| 25  | LU    | 825   | 0        | 850      | 10      | 0            |
| 26  | LV    | 979   | 0        | 1039     | 9       | 0            |
| 27  | LW    | 945   | 0        | 1003     | 13      | 0            |
| 28  | LX    | 985   | 0        | 1066     | 6       | 0            |
| 29  | LY    | 1115  | 0        | 1205     | 10      | 0            |
| 30  | LZ    | 1107  | 0        | 1182     | 10      | 0            |
| 31  | La    | 1162  | 0        | 1213     | 7       | 0            |
| 32  | Lb    | 876   | 0        | 948      | 3       | 0            |
| 33  | Lc    | 764   | 0        | 804      | 4       | 0            |
| 34  | Ld    | 888   | 0        | 930      | 6       | 0            |
| 35  | Le    | 1053  | 0        | 1147     | 9       | 0            |
| 36  | Lf    | 876   | 0        | 912      | 4       | 0            |
| 37  | Lg    | 906   | 0        | 998      | 4       | 0            |
| 38  | Lh    | 1015  | 0        | 1148     | 11      | 0            |
| 39  | Li    | 832   | 0        | 917      | 7       | 0            |
| 40  | Lj    | 705   | 0        | 737      | 6       | 0            |
| 41  | Lk    | 569   | 0        | 637      | 2       | 0            |
| 42  | Ll    | 444   | 0        | 483      | 5       | 0            |
| 43  | Lm    | 429   | 0        | 465      | 1       | 0            |
| 44  | Ln    | 230   | 0        | 276      | 1       | 0            |
| 45  | Lo    | 862   | 0        | 929      | 8       | 0            |
| 46  | Lp    | 708   | 0        | 756      | 5       | 0            |
| 47  | Lr    | 1002  | 0        | 1068     | 7       | 0            |
| 48  | Ls    | 1496  | 0        | 1540     | 25      | 0            |
| 49  | Lt    | 998   | 0        | 1032     | 23      | 0            |
| 50  | SA    | 1741  | 0        | 1746     | 35      | 0            |
| 51  | SB    | 1738  | 0        | 1809     | 43      | 0            |
| 52  | SC    | 1707  | 0        | 1791     | 29      | 0            |
| 53  | SE    | 2076  | 0        | 2177     | 41      | 0            |
| 54  | SG    | 1923  | 0        | 2089     | 48      | 0            |
| 55  | SH    | 1497  | 0        | 1590     | 29      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56  | SI    | 1686  | 0        | 1772     | 27      | 0            |
| 57  | SJ    | 1525  | 0        | 1640     | 23      | 0            |
| 58  | SL    | 1247  | 0        | 1323     | 16      | 0            |
| 59  | SN    | 1208  | 0        | 1294     | 14      | 0            |
| 60  | SO    | 1024  | 0        | 1050     | 25      | 0            |
| 61  | SV    | 636   | 0        | 637      | 9       | 0            |
| 62  | SW    | 1034  | 0        | 1080     | 16      | 0            |
| 63  | SX    | 1098  | 0        | 1167     | 9       | 0            |
| 64  | SY    | 1065  | 0        | 1142     | 24      | 0            |
| 65  | Sa    | 821   | 0        | 870      | 10      | 0            |
| 66  | Sb    | 651   | 0        | 669      | 16      | 0            |
| 67  | Se    | 459   | 0        | 503      | 10      | 0            |
| 68  | S2    | 36952 | 0        | 18678    | 425     | 0            |
| 69  | SR    | 1090  | 0        | 1149     | 11      | 0            |
| 70  | SD    | 1765  | 0        | 1865     | 18      | 0            |
| 71  | SF    | 1495  | 0        | 1549     | 24      | 0            |
| 72  | SK    | 827   | 0        | 854      | 19      | 0            |
| 73  | SM    | 940   | 0        | 965      | 16      | 0            |
| 74  | SP    | 985   | 0        | 1031     | 11      | 0            |
| 75  | SQ    | 1142  | 0        | 1213     | 17      | 0            |
| 76  | SS    | 1198  | 0        | 1261     | 23      | 0            |
| 77  | ST    | 1112  | 0        | 1146     | 16      | 0            |
| 78  | SU    | 821   | 0        | 883      | 11      | 0            |
| 79  | SZ    | 598   | 0        | 656      | 6       | 0            |
| 80  | Sc    | 506   | 0        | 536      | 10      | 0            |
| 81  | Sd    | 459   | 0        | 449      | 8       | 0            |
| 82  | Sf    | 548   | 0        | 551      | 13      | 0            |
| 83  | Sg    | 2436  | 0        | 2391     | 51      | 0            |
| 84  | Et    | 1593  | 0        | 810      | 26      | 0            |
| 85  | CB    | 6605  | 0        | 6679     | 89      | 0            |
| 86  | CA    | 2764  | 0        | 2779     | 60      | 0            |
| 87  | L5    | 177   | 0        | 0        | 0       | 0            |
| 87  | L7    | 3     | 0        | 0        | 0       | 0            |
| 87  | L8    | 5     | 0        | 0        | 0       | 0            |
| 87  | LA    | 1     | 0        | 0        | 0       | 0            |
| 87  | LB    | 1     | 0        | 0        | 0       | 0            |
| 87  | LI    | 1     | 0        | 0        | 0       | 0            |
| 87  | LP    | 1     | 0        | 0        | 0       | 0            |
| 87  | LV    | 1     | 0        | 0        | 0       | 0            |
| 87  | Le    | 1     | 0        | 0        | 0       | 0            |
| 87  | S2    | 26    | 0        | 0        | 0       | 0            |
| 87  | SG    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 88  | L5    | 98     | 0        | 182      | 5       | 0            |
| 89  | L5    | 90     | 0        | 171      | 2       | 0            |
| 89  | L8    | 10     | 0        | 19       | 0       | 0            |
| 90  | Lg    | 1      | 0        | 0        | 0       | 0            |
| 90  | Lj    | 1      | 0        | 0        | 0       | 0            |
| 90  | Lm    | 1      | 0        | 0        | 0       | 0            |
| 90  | Lo    | 1      | 0        | 0        | 0       | 0            |
| 90  | Lp    | 1      | 0        | 0        | 0       | 0            |
| 90  | Sa    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 228149 | 0        | 172628   | 2072    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2072 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 84:Et:26:A:H62   | 84:Et:44:G:N2    | 1.48                     | 1.12              |
| 84:Et:26:A:N6    | 84:Et:44:G:H21   | 1.50                     | 1.10              |
| 68:S2:70:G:H21   | 68:S2:79:A:H62   | 1.08                     | 0.95              |
| 68:S2:1417:C:H42 | 68:S2:1422:G:H22 | 1.02                     | 0.93              |
| 68:S2:1748:G:H1  | 68:S2:1786:U:H3  | 1.19                     | 0.87              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed     | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|--------------|----------|---------|----------|-------------|-----|
| 1   | CD    | 51/408 (12%) | 49 (96%) | 2 (4%)  | 0        | 100         | 100 |
| 2   | CI    | 29/31 (94%)  | 28 (97%) | 1 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 6   | LA    | 246/248 (99%)  | 238 (97%) | 8 (3%)  | 0        | 100         | 100 |
| 7   | LB    | 400/402 (100%) | 387 (97%) | 13 (3%) | 0        | 100         | 100 |
| 8   | LC    | 366/368 (100%) | 354 (97%) | 12 (3%) | 0        | 100         | 100 |
| 9   | LD    | 291/293 (99%)  | 281 (97%) | 10 (3%) | 0        | 100         | 100 |
| 10  | LE    | 236/250 (94%)  | 224 (95%) | 12 (5%) | 0        | 100         | 100 |
| 11  | LF    | 223/225 (99%)  | 216 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 12  | LG    | 239/241 (99%)  | 229 (96%) | 10 (4%) | 0        | 100         | 100 |
| 13  | LH    | 188/190 (99%)  | 181 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 14  | LI    | 201/213 (94%)  | 197 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 15  | LJ    | 168/176 (96%)  | 164 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 16  | LL    | 208/210 (99%)  | 200 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 17  | LM    | 137/139 (99%)  | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 18  | LN    | 201/203 (99%)  | 197 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 19  | LO    | 199/201 (99%)  | 196 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 20  | LP    | 151/153 (99%)  | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 21  | LQ    | 185/187 (99%)  | 181 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 22  | LR    | 185/187 (99%)  | 181 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 23  | LS    | 173/175 (99%)  | 168 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 24  | LT    | 157/159 (99%)  | 151 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 25  | LU    | 99/101 (98%)   | 93 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 26  | LV    | 129/131 (98%)  | 123 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 27  | LW    | 112/124 (90%)  | 111 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 28  | LX    | 118/120 (98%)  | 117 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 29  | LY    | 132/134 (98%)  | 128 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 30  | LZ    | 133/135 (98%)  | 125 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 31  | La    | 145/147 (99%)  | 138 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 32  | Lb    | 105/121 (87%)  | 101 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 33  | Lc    | 96/98 (98%)    | 93 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 34  | Ld    | 105/107 (98%)  | 103 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 35  | Le    | 126/128 (98%)  | 124 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 36  | Lf    | 107/109 (98%)  | 105 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 37  | Lg    | 112/114 (98%) | 112 (100%) | 0        | 0        | 100         | 100 |
| 38  | Lh    | 120/122 (98%) | 117 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 39  | Li    | 100/102 (98%) | 96 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 40  | Lj    | 84/86 (98%)   | 82 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 41  | Lk    | 67/69 (97%)   | 67 (100%)  | 0        | 0        | 100         | 100 |
| 42  | Ll    | 48/50 (96%)   | 45 (94%)   | 3 (6%)   | 0        | 100         | 100 |
| 43  | Lm    | 50/52 (96%)   | 50 (100%)  | 0        | 0        | 100         | 100 |
| 44  | Ln    | 22/24 (92%)   | 22 (100%)  | 0        | 0        | 100         | 100 |
| 45  | Lo    | 103/105 (98%) | 95 (92%)   | 8 (8%)   | 0        | 100         | 100 |
| 46  | Lp    | 89/91 (98%)   | 87 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 47  | Lr    | 123/125 (98%) | 119 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 48  | Ls    | 194/196 (99%) | 184 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 49  | Lt    | 128/157 (82%) | 105 (82%)  | 23 (18%) | 0        | 100         | 100 |
| 50  | SA    | 219/221 (99%) | 210 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 51  | SB    | 212/214 (99%) | 207 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 52  | SC    | 218/222 (98%) | 211 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 53  | SE    | 260/262 (99%) | 248 (95%)  | 12 (5%)  | 0        | 100         | 100 |
| 54  | SG    | 235/237 (99%) | 218 (93%)  | 17 (7%)  | 0        | 100         | 100 |
| 55  | SH    | 182/189 (96%) | 163 (90%)  | 19 (10%) | 0        | 100         | 100 |
| 56  | SI    | 204/206 (99%) | 195 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 57  | SJ    | 183/185 (99%) | 171 (93%)  | 12 (7%)  | 0        | 100         | 100 |
| 58  | SL    | 151/153 (99%) | 141 (93%)  | 10 (7%)  | 0        | 100         | 100 |
| 59  | SN    | 148/150 (99%) | 146 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 60  | SO    | 135/140 (96%) | 127 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 61  | SV    | 81/83 (98%)   | 76 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 62  | SW    | 127/129 (98%) | 124 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 63  | SX    | 139/141 (99%) | 132 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 64  | SY    | 129/131 (98%) | 124 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 65  | Sa    | 100/102 (98%) | 97 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 66  | Sb    | 81/83 (98%)   | 74 (91%)   | 7 (9%)   | 0        | 100         | 100 |
| 67  | Se    | 56/58 (97%)   | 53 (95%)   | 3 (5%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 69  | SR    | 133/135 (98%)     | 128 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 70  | SD    | 225/227 (99%)     | 220 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 71  | SF    | 187/189 (99%)     | 177 (95%)   | 10 (5%)  | 0        | 100         | 100 |
| 72  | SK    | 96/98 (98%)       | 91 (95%)    | 5 (5%)   | 0        | 100         | 100 |
| 73  | SM    | 120/122 (98%)     | 113 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 74  | SP    | 119/121 (98%)     | 117 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 75  | SQ    | 142/144 (99%)     | 137 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 76  | SS    | 143/145 (99%)     | 136 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 77  | ST    | 141/143 (99%)     | 139 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 78  | SU    | 102/104 (98%)     | 98 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 79  | SZ    | 73/75 (97%)       | 68 (93%)    | 5 (7%)   | 0        | 100         | 100 |
| 80  | Sc    | 62/64 (97%)       | 60 (97%)    | 2 (3%)   | 0        | 100         | 100 |
| 81  | Sd    | 53/55 (96%)       | 52 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 82  | Sf    | 65/67 (97%)       | 58 (89%)    | 7 (11%)  | 0        | 100         | 100 |
| 83  | Sg    | 311/313 (99%)     | 285 (92%)   | 26 (8%)  | 0        | 100         | 100 |
| 85  | CB    | 842/856 (98%)     | 814 (97%)   | 28 (3%)  | 0        | 100         | 100 |
| 86  | CA    | 350/356 (98%)     | 335 (96%)   | 15 (4%)  | 0        | 100         | 100 |
| All | All   | 12905/13527 (95%) | 12389 (96%) | 516 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | CD    | 46/328 (14%)   | 46 (100%)  | 0        | 100         | 100 |
| 2   | CI    | 25/25 (100%)   | 25 (100%)  | 0        | 100         | 100 |
| 6   | LA    | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 7   | LB    | 348/348 (100%) | 348 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 8   | LC    | 306/306 (100%) | 306 (100%) | 0        | 100         | 100 |
| 9   | LD    | 246/247 (100%) | 246 (100%) | 0        | 100         | 100 |
| 10  | LE    | 212/222 (96%)  | 212 (100%) | 0        | 100         | 100 |
| 11  | LF    | 194/194 (100%) | 194 (100%) | 0        | 100         | 100 |
| 12  | LG    | 203/205 (99%)  | 203 (100%) | 0        | 100         | 100 |
| 13  | LH    | 169/169 (100%) | 169 (100%) | 0        | 100         | 100 |
| 14  | LI    | 175/180 (97%)  | 175 (100%) | 0        | 100         | 100 |
| 15  | LJ    | 143/148 (97%)  | 143 (100%) | 0        | 100         | 100 |
| 16  | LL    | 176/176 (100%) | 175 (99%)  | 1 (1%)   | 78          | 91  |
| 17  | LM    | 118/118 (100%) | 118 (100%) | 0        | 100         | 100 |
| 18  | LN    | 171/171 (100%) | 171 (100%) | 0        | 100         | 100 |
| 19  | LO    | 173/173 (100%) | 173 (100%) | 0        | 100         | 100 |
| 20  | LP    | 134/134 (100%) | 134 (100%) | 0        | 100         | 100 |
| 21  | LQ    | 164/164 (100%) | 164 (100%) | 0        | 100         | 100 |
| 22  | LR    | 166/166 (100%) | 166 (100%) | 0        | 100         | 100 |
| 23  | LS    | 156/156 (100%) | 156 (100%) | 0        | 100         | 100 |
| 24  | LT    | 139/139 (100%) | 139 (100%) | 0        | 100         | 100 |
| 25  | LU    | 91/91 (100%)   | 91 (100%)  | 0        | 100         | 100 |
| 26  | LV    | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 27  | LW    | 95/103 (92%)   | 95 (100%)  | 0        | 100         | 100 |
| 28  | LX    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 29  | LY    | 124/124 (100%) | 124 (100%) | 0        | 100         | 100 |
| 30  | LZ    | 117/117 (100%) | 117 (100%) | 0        | 100         | 100 |
| 31  | La    | 120/120 (100%) | 120 (100%) | 0        | 100         | 100 |
| 32  | Lb    | 88/101 (87%)   | 88 (100%)  | 0        | 100         | 100 |
| 33  | Lc    | 83/83 (100%)   | 83 (100%)  | 0        | 100         | 100 |
| 34  | Ld    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 35  | Le    | 114/114 (100%) | 114 (100%) | 0        | 100         | 100 |
| 36  | Lf    | 88/88 (100%)   | 88 (100%)  | 0        | 100         | 100 |
| 37  | Lg    | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 38  | Lh    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 39  | Li    | 86/86 (100%)   | 86 (100%)  | 0        | 100         | 100 |
| 40  | Lj    | 73/73 (100%)   | 73 (100%)  | 0        | 100         | 100 |
| 41  | Lk    | 64/64 (100%)   | 64 (100%)  | 0        | 100         | 100 |
| 42  | Ll    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 43  | Lm    | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 44  | Ln    | 23/23 (100%)   | 23 (100%)  | 0        | 100         | 100 |
| 45  | Lo    | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 46  | Lp    | 74/74 (100%)   | 73 (99%)   | 1 (1%)   | 59          | 82  |
| 47  | Lr    | 109/109 (100%) | 109 (100%) | 0        | 100         | 100 |
| 48  | Ls    | 162/164 (99%)  | 162 (100%) | 0        | 100         | 100 |
| 49  | Lt    | 107/130 (82%)  | 107 (100%) | 0        | 100         | 100 |
| 50  | SA    | 183/183 (100%) | 183 (100%) | 0        | 100         | 100 |
| 51  | SB    | 195/195 (100%) | 195 (100%) | 0        | 100         | 100 |
| 52  | SC    | 186/188 (99%)  | 186 (100%) | 0        | 100         | 100 |
| 53  | SE    | 224/224 (100%) | 224 (100%) | 0        | 100         | 100 |
| 54  | SG    | 207/207 (100%) | 207 (100%) | 0        | 100         | 100 |
| 55  | SH    | 166/169 (98%)  | 166 (100%) | 0        | 100         | 100 |
| 56  | SI    | 178/178 (100%) | 178 (100%) | 0        | 100         | 100 |
| 57  | SJ    | 161/161 (100%) | 160 (99%)  | 1 (1%)   | 78          | 91  |
| 58  | SL    | 137/137 (100%) | 137 (100%) | 0        | 100         | 100 |
| 59  | SN    | 130/130 (100%) | 129 (99%)  | 1 (1%)   | 73          | 89  |
| 60  | SO    | 107/110 (97%)  | 107 (100%) | 0        | 100         | 100 |
| 61  | SV    | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 62  | SW    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 63  | SX    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 64  | SY    | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 65  | Sa    | 89/89 (100%)   | 89 (100%)  | 0        | 100         | 100 |
| 66  | Sb    | 75/75 (100%)   | 75 (100%)  | 0        | 100         | 100 |
| 67  | Se    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 69  | SR    | 122/122 (100%) | 122 (100%) | 0        | 100         | 100 |
| 70  | SD    | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 71  | SF    | 159/159 (100%)    | 159 (100%)   | 0        | 100         | 100 |
| 72  | SK    | 89/89 (100%)      | 89 (100%)    | 0        | 100         | 100 |
| 73  | SM    | 102/104 (98%)     | 102 (100%)   | 0        | 100         | 100 |
| 74  | SP    | 107/107 (100%)    | 107 (100%)   | 0        | 100         | 100 |
| 75  | SQ    | 119/119 (100%)    | 119 (100%)   | 0        | 100         | 100 |
| 76  | SS    | 126/126 (100%)    | 126 (100%)   | 0        | 100         | 100 |
| 77  | ST    | 113/113 (100%)    | 113 (100%)   | 0        | 100         | 100 |
| 78  | SU    | 94/94 (100%)      | 94 (100%)    | 0        | 100         | 100 |
| 79  | SZ    | 66/66 (100%)      | 66 (100%)    | 0        | 100         | 100 |
| 80  | Sc    | 57/57 (100%)      | 57 (100%)    | 0        | 100         | 100 |
| 81  | Sd    | 48/48 (100%)      | 48 (100%)    | 0        | 100         | 100 |
| 82  | Sf    | 60/60 (100%)      | 60 (100%)    | 0        | 100         | 100 |
| 83  | Sg    | 272/272 (100%)    | 272 (100%)   | 0        | 100         | 100 |
| 85  | CB    | 722/728 (99%)     | 722 (100%)   | 0        | 100         | 100 |
| 86  | CA    | 303/305 (99%)     | 303 (100%)   | 0        | 100         | 100 |
| All | All   | 11213/11582 (97%) | 11209 (100%) | 4 (0%)   | 100         | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | LL    | 59  | VAL  |
| 46  | Lp    | 83  | ILE  |
| 57  | SJ    | 53  | ILE  |
| 59  | SN    | 49  | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | SH    | 76  | GLN  |
| 67  | Se    | 58  | ASN  |
| 56  | SI    | 87  | ASN  |
| 59  | SN    | 49  | GLN  |
| 71  | SF    | 114 | ASN  |

### 5.3.3 RNA

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 3   | L5    | 3643/5070 (71%) | 765 (20%)         | 17 (0%)         |
| 4   | L7    | 119/120 (99%)   | 11 (9%)           | 0               |
| 5   | L8    | 155/156 (99%)   | 27 (17%)          | 0               |
| 68  | S2    | 1715/1740 (98%) | 390 (22%)         | 3 (0%)          |
| 84  | Et    | 73/75 (97%)     | 29 (39%)          | 0               |
| All | All   | 5705/7161 (79%) | 1222 (21%)        | 20 (0%)         |

5 of 1222 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L5    | 2   | G    |
| 3   | L5    | 25  | A    |
| 3   | L5    | 30  | C    |
| 3   | L5    | 39  | A    |
| 3   | L5    | 42  | A    |

5 of 20 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | L5    | 4600 | G    |
| 68  | S2    | 291  | G    |
| 68  | S2    | 688  | U    |
| 68  | S2    | 563  | G    |
| 3   | L5    | 1698 | C    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | OMC  | L5    | 4456 | 3    | 19,22,23     | 0.74 | 0           | 25,31,34    | 0.65 | 0           |
| 68  | OMG  | S2    | 1490 | 68   | 23,26,27     | 0.53 | 0           | 32,38,41    | 0.44 | 0           |
| 3   | A2M  | L5    | 2787 | 3    | 22,25,26     | 1.16 | 1 (4%)      | 30,36,39    | 1.50 | 7 (23%)     |
| 3   | OMC  | L5    | 2861 | 3    | 19,22,23     | 0.67 | 0           | 25,31,34    | 0.80 | 1 (4%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMG  | L5    | 3627 | 3    | 23,26,27     | 0.62 | 0        | 32,38,41    | 0.61 | 0        |
| 3   | PSU  | L5    | 1782 | 3    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.93 | 4 (19%)  |
| 3   | OMG  | L5    | 4494 | 3    | 23,26,27     | 0.59 | 0        | 32,38,41    | 0.49 | 0        |
| 68  | PSU  | S2    | 649  | 68   | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | OMG  | L5    | 4196 | 3    | 23,26,27     | 0.56 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | OMC  | L5    | 4536 | 3    | 19,22,23     | 0.70 | 0        | 25,31,34    | 0.71 | 0        |
| 3   | OMC  | L5    | 3869 | 3    | 19,22,23     | 0.71 | 0        | 25,31,34    | 0.63 | 0        |
| 3   | A2M  | L5    | 4523 | 87,3 | 22,25,26     | 1.28 | 2 (9%)   | 30,36,39    | 1.57 | 8 (26%)  |
| 3   | PSU  | L5    | 4628 | 3    | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.98 | 4 (19%)  |
| 3   | OMG  | L5    | 4618 | 3    | 23,26,27     | 0.64 | 0        | 32,38,41    | 0.51 | 0        |
| 68  | PSU  | S2    | 866  | 68   | 18,21,22     | 1.14 | 1 (5%)   | 21,30,33    | 2.01 | 5 (23%)  |
| 68  | OMC  | S2    | 1391 | 68   | 19,22,23     | 0.59 | 0        | 25,31,34    | 0.69 | 0        |
| 68  | PSU  | S2    | 1174 | 68   | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 1.91 | 4 (19%)  |
| 68  | PSU  | S2    | 863  | 68   | 18,21,22     | 1.12 | 1 (5%)   | 21,30,33    | 1.96 | 4 (19%)  |
| 3   | OMC  | L5    | 2365 | 3    | 19,22,23     | 0.66 | 0        | 25,31,34    | 0.60 | 0        |
| 68  | PSU  | S2    | 93   | 68   | 18,21,22     | 1.05 | 1 (5%)   | 21,30,33    | 1.78 | 4 (19%)  |
| 3   | OMG  | L5    | 4370 | 3    | 23,26,27     | 0.60 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | A2M  | L5    | 2363 | 87,3 | 22,25,26     | 1.27 | 3 (13%)  | 30,36,39    | 1.56 | 9 (30%)  |
| 3   | PSU  | L5    | 4973 | 3    | 18,21,22     | 1.05 | 2 (11%)  | 21,30,33    | 1.93 | 4 (19%)  |
| 68  | A2M  | S2    | 166  | 68   | 22,25,26     | 1.25 | 1 (4%)   | 30,36,39    | 1.60 | 7 (23%)  |
| 68  | OMC  | S2    | 1703 | 68   | 19,22,23     | 0.57 | 0        | 25,31,34    | 0.63 | 0        |
| 3   | A2M  | L5    | 398  | 3    | 22,25,26     | 1.21 | 2 (9%)   | 30,36,39    | 1.58 | 7 (23%)  |
| 3   | OMG  | L5    | 3744 | 3    | 23,26,27     | 0.60 | 0        | 32,38,41    | 0.49 | 0        |
| 3   | 1MA  | L5    | 1322 | 87,3 | 21,25,26     | 0.66 | 0        | 30,37,40    | 0.82 | 2 (6%)   |
| 3   | PSU  | L5    | 4296 | 3    | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 2.06 | 5 (23%)  |
| 3   | OMG  | L5    | 2424 | 3    | 23,26,27     | 0.58 | 0        | 32,38,41    | 0.43 | 0        |
| 3   | OMG  | L5    | 1625 | 3    | 23,26,27     | 0.58 | 0        | 32,38,41    | 0.49 | 0        |
| 68  | A2M  | S2    | 27   | 68   | 22,25,26     | 1.23 | 1 (4%)   | 30,36,39    | 1.50 | 8 (26%)  |
| 68  | OMG  | S2    | 601  | 68   | 23,26,27     | 0.55 | 0        | 32,38,41    | 0.44 | 0        |
| 68  | OMU  | S2    | 1442 | 68   | 19,22,23     | 3.32 | 7 (36%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 3   | OMU  | L5    | 4306 | 3    | 19,22,23     | 3.18 | 7 (36%)  | 25,31,34    | 1.76 | 4 (16%)  |
| 3   | PSU  | L5    | 4579 | 3    | 18,21,22     | 1.05 | 2 (11%)  | 21,30,33    | 1.99 | 4 (19%)  |
| 3   | PSU  | L5    | 4353 | 3    | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 1.94 | 4 (19%)  |
| 3   | OMC  | L5    | 2422 | 87,3 | 19,22,23     | 0.70 | 0        | 25,31,34    | 0.75 | 1 (4%)   |
| 3   | PSU  | L5    | 4532 | 3    | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.98 | 4 (19%)  |
| 68  | PSU  | S2    | 1046 | 68   | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.85 | 4 (19%)  |
| 3   | PSU  | L5    | 4293 | 3    | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.92 | 4 (19%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L5    | 3822 | 3    | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 2.01 | 6 (28%)  |
| 68  | OMU  | S2    | 172  | 68   | 19,22,23     | 3.32 | 7 (36%)  | 25,31,34    | 1.74 | 5 (20%)  |
| 3   | PSU  | L5    | 4431 | 3    | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.93 | 4 (19%)  |
| 68  | PSU  | S2    | 1081 | 68   | 18,21,22     | 1.04 | 1 (5%)   | 21,30,33    | 1.89 | 4 (19%)  |
| 3   | A2M  | L5    | 3867 | 3    | 22,25,26     | 1.36 | 2 (9%)   | 30,36,39    | 1.53 | 9 (30%)  |
| 68  | PSU  | S2    | 109  | 68   | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.92 | 4 (19%)  |
| 68  | PSU  | S2    | 681  | 68   | 18,21,22     | 1.00 | 2 (11%)  | 21,30,33    | 1.89 | 4 (19%)  |
| 68  | PSU  | S2    | 1367 | 68   | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 1.95 | 5 (23%)  |
| 3   | OMG  | L5    | 3899 | 3    | 23,26,27     | 0.67 | 0        | 32,38,41    | 0.49 | 0        |
| 3   | PSU  | L5    | 4299 | 3    | 18,21,22     | 1.04 | 2 (11%)  | 21,30,33    | 1.82 | 4 (19%)  |
| 3   | PSU  | L5    | 3920 | 87,3 | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.99 | 6 (28%)  |
| 3   | UR3  | L5    | 4530 | 3    | 19,22,23     | 2.64 | 7 (36%)  | 26,32,35    | 1.64 | 4 (15%)  |
| 68  | OMU  | S2    | 354  | 68   | 19,22,23     | 3.25 | 7 (36%)  | 25,31,34    | 1.81 | 5 (20%)  |
| 3   | PSU  | L5    | 2632 | 3    | 18,21,22     | 1.04 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 68  | B8N  | S2    | 1248 | 68   | 25,29,30     | 3.21 | 6 (24%)  | 28,42,45    | 1.96 | 8 (28%)  |
| 68  | OMU  | S2    | 1288 | 68   | 19,22,23     | 3.32 | 7 (36%)  | 25,31,34    | 1.73 | 5 (20%)  |
| 3   | 6MZ  | L5    | 4220 | 3    | 22,25,26     | 2.94 | 6 (27%)  | 29,36,39    | 2.39 | 10 (34%) |
| 68  | OMC  | S2    | 462  | 68   | 19,22,23     | 0.52 | 0        | 25,31,34    | 0.64 | 0        |
| 3   | A2M  | L5    | 1524 | 3    | 22,25,26     | 1.33 | 3 (13%)  | 30,36,39    | 1.51 | 8 (26%)  |
| 68  | OMC  | S2    | 517  | 68   | 19,22,23     | 0.59 | 0        | 25,31,34    | 0.74 | 0        |
| 3   | OMC  | L5    | 2804 | 3    | 19,22,23     | 0.67 | 0        | 25,31,34    | 0.61 | 0        |
| 68  | OMG  | S2    | 1328 | 68   | 23,26,27     | 0.52 | 0        | 32,38,41    | 0.44 | 0        |
| 3   | OMC  | L5    | 2824 | 3    | 19,22,23     | 0.66 | 0        | 25,31,34    | 0.80 | 1 (4%)   |
| 68  | OMG  | S2    | 644  | 68   | 23,26,27     | 0.52 | 0        | 32,38,41    | 0.49 | 0        |
| 68  | PSU  | S2    | 406  | 68   | 18,21,22     | 1.11 | 2 (11%)  | 21,30,33    | 1.92 | 4 (19%)  |
| 68  | PSU  | S2    | 814  | 68   | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | OMC  | L5    | 3701 | 3    | 19,22,23     | 0.62 | 0        | 25,31,34    | 0.58 | 0        |
| 3   | PSU  | L5    | 4521 | 87,3 | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 2.07 | 5 (23%)  |
| 3   | PSU  | L5    | 1536 | 3    | 18,21,22     | 1.07 | 2 (11%)  | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | PSU  | L5    | 4552 | 3    | 18,21,22     | 1.12 | 2 (11%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 3   | PSU  | L5    | 1862 | 3    | 18,21,22     | 1.04 | 1 (5%)   | 21,30,33    | 1.92 | 4 (19%)  |
| 3   | OMG  | L5    | 1316 | 3    | 23,26,27     | 0.75 | 0        | 32,38,41    | 0.60 | 0        |
| 68  | OMU  | S2    | 428  | 68   | 19,22,23     | 3.31 | 7 (36%)  | 25,31,34    | 1.80 | 5 (20%)  |
| 3   | A2M  | L5    | 3785 | 87,3 | 22,25,26     | 1.20 | 1 (4%)   | 30,36,39    | 1.57 | 9 (30%)  |
| 3   | A2M  | L5    | 1326 | 3    | 22,25,26     | 1.24 | 2 (9%)   | 30,36,39    | 1.48 | 8 (26%)  |
| 3   | PSU  | L5    | 4636 | 3    | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 2.09 | 6 (28%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PSU  | L5    | 5001 | 3    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.97 | 5 (23%)  |
| 3   | OMC  | L5    | 3841 | 3    | 19,22,23     | 0.70 | 0        | 25,31,34    | 0.52 | 0        |
| 3   | PSU  | L5    | 4689 | 3    | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 1.91 | 4 (19%)  |
| 68  | PSU  | S2    | 686  | 68   | 18,21,22     | 1.09 | 1 (5%)   | 21,30,33    | 1.93 | 4 (19%)  |
| 3   | PSU  | L5    | 4442 | 3    | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.96 | 5 (23%)  |
| 68  | PSU  | S2    | 1244 | 68   | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.94 | 4 (19%)  |
| 3   | OMG  | L5    | 2876 | 3    | 23,26,27     | 0.57 | 0        | 32,38,41    | 0.53 | 0        |
| 3   | A2M  | L5    | 1323 | 3    | 22,25,26     | 1.31 | 3 (13%)  | 30,36,39    | 1.61 | 9 (30%)  |
| 3   | PSU  | L5    | 1683 | 3    | 18,21,22     | 1.04 | 2 (11%)  | 21,30,33    | 2.00 | 4 (19%)  |
| 3   | PSU  | L5    | 3851 | 3    | 18,21,22     | 1.05 | 2 (11%)  | 21,30,33    | 1.92 | 4 (19%)  |
| 3   | PSU  | L5    | 4500 | 3    | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 2.08 | 5 (23%)  |
| 3   | OMU  | L5    | 4227 | 3    | 19,22,23     | 3.15 | 7 (36%)  | 25,31,34    | 1.84 | 4 (16%)  |
| 3   | PSU  | L5    | 3853 | 87,3 | 18,21,22     | 1.03 | 1 (5%)   | 21,30,33    | 1.87 | 4 (19%)  |
| 3   | A2M  | L5    | 3718 | 3    | 22,25,26     | 1.19 | 2 (9%)   | 30,36,39    | 1.59 | 8 (26%)  |
| 3   | A2M  | L5    | 2401 | 3    | 22,25,26     | 1.21 | 2 (9%)   | 30,36,39    | 1.54 | 7 (23%)  |
| 3   | OMC  | L5    | 3808 | 87,3 | 19,22,23     | 0.73 | 1 (5%)   | 25,31,34    | 0.88 | 2 (8%)   |
| 3   | PSU  | L5    | 3884 | 3    | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 1.96 | 4 (19%)  |
| 3   | PSU  | L5    | 3695 | 3    | 18,21,22     | 1.05 | 2 (11%)  | 21,30,33    | 1.97 | 4 (19%)  |
| 68  | 4AC  | S2    | 1337 | 68   | 21,24,25     | 0.41 | 0        | 28,34,37    | 0.58 | 0        |
| 3   | PSU  | L5    | 4361 | 3    | 18,21,22     | 1.00 | 1 (5%)   | 21,30,33    | 1.89 | 4 (19%)  |
| 68  | PSU  | S2    | 1056 | 68   | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.93 | 4 (19%)  |
| 3   | PSU  | L5    | 4403 | 3    | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 1.99 | 6 (28%)  |
| 3   | 5MC  | L5    | 4447 | 3    | 19,22,23     | 1.03 | 2 (10%)  | 26,32,35    | 0.80 | 0        |
| 3   | OMC  | L5    | 2351 | 87,3 | 19,22,23     | 0.73 | 1 (5%)   | 25,31,34    | 0.86 | 1 (4%)   |
| 68  | OMC  | S2    | 174  | 68   | 19,22,23     | 0.55 | 0        | 25,31,34    | 0.68 | 0        |
| 68  | PSU  | S2    | 1004 | 68   | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.91 | 4 (19%)  |
| 3   | PSU  | L5    | 3844 | 3    | 18,21,22     | 1.14 | 1 (5%)   | 21,30,33    | 1.88 | 4 (19%)  |
| 68  | OMG  | S2    | 867  | 68   | 23,26,27     | 0.54 | 0        | 32,38,41    | 0.48 | 0        |
| 3   | PSU  | L5    | 1582 | 3    | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 2.02 | 4 (19%)  |
| 68  | A2M  | S2    | 1031 | 68   | 22,25,26     | 1.16 | 1 (4%)   | 30,36,39    | 1.55 | 7 (23%)  |
| 3   | A2M  | L5    | 4571 | 3    | 22,25,26     | 1.42 | 3 (13%)  | 30,36,39    | 1.66 | 8 (26%)  |
| 68  | A2M  | S2    | 159  | 68   | 22,25,26     | 1.25 | 1 (4%)   | 30,36,39    | 1.61 | 7 (23%)  |
| 68  | PSU  | S2    | 1045 | 68   | 18,21,22     | 1.15 | 1 (5%)   | 21,30,33    | 1.89 | 4 (19%)  |
| 68  | PSU  | S2    | 1232 | 68   | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.98 | 5 (23%)  |
| 3   | OMC  | L5    | 3887 | 3    | 19,22,23     | 0.62 | 0        | 25,31,34    | 0.66 | 0        |
| 68  | PSU  | S2    | 1177 | 68   | 18,21,22     | 1.10 | 2 (11%)  | 21,30,33    | 1.99 | 4 (19%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | OMG  | L5    | 2364 | 87,3  | 23,26,27     | 0.62 | 0        | 32,38,41    | 0.44 | 0        |
| 68  | MA6  | S2    | 1851 | 68    | 23,26,27     | 1.29 | 3 (13%)  | 33,38,41    | 3.38 | 12 (36%) |
| 3   | A2M  | L5    | 3825 | 3     | 22,25,26     | 1.25 | 2 (9%)   | 30,36,39    | 1.56 | 7 (23%)  |
| 3   | PSU  | L5    | 1744 | 87,3  | 18,21,22     | 1.05 | 2 (11%)  | 21,30,33    | 1.95 | 4 (19%)  |
| 5   | OMG  | L8    | 75   | 5     | 23,26,27     | 0.58 | 0        | 32,38,41    | 0.46 | 0        |
| 3   | OMG  | L5    | 1522 | 3     | 23,26,27     | 0.62 | 0        | 32,38,41    | 0.62 | 0        |
| 5   | PSU  | L8    | 55   | 5     | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 1.85 | 4 (19%)  |
| 3   | OMG  | L5    | 4637 | 3     | 23,26,27     | 0.59 | 0        | 32,38,41    | 0.48 | 0        |
| 3   | OMU  | L5    | 2837 | 3     | 19,22,23     | 3.21 | 7 (36%)  | 25,31,34    | 1.92 | 5 (20%)  |
| 68  | PSU  | S2    | 801  | 68    | 18,21,22     | 1.16 | 1 (5%)   | 21,30,33    | 1.78 | 4 (19%)  |
| 3   | A2M  | L5    | 1871 | 87,3  | 22,25,26     | 1.36 | 3 (13%)  | 30,36,39    | 1.64 | 8 (26%)  |
| 68  | G7M  | S2    | 1639 | 84,68 | 23,26,27     | 2.66 | 9 (39%)  | 34,39,42    | 2.58 | 11 (32%) |
| 3   | PSU  | L5    | 4972 | 3     | 18,21,22     | 1.06 | 1 (5%)   | 21,30,33    | 1.94 | 4 (19%)  |
| 68  | OMG  | S2    | 683  | 68    | 23,26,27     | 0.54 | 0        | 32,38,41    | 0.47 | 0        |
| 3   | PSU  | L5    | 1860 | 3     | 18,21,22     | 1.07 | 2 (11%)  | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | A2M  | L5    | 400  | 3     | 22,25,26     | 1.26 | 2 (9%)   | 30,36,39    | 1.56 | 9 (30%)  |
| 68  | PSU  | S2    | 105  | 68    | 18,21,22     | 1.03 | 1 (5%)   | 21,30,33    | 1.98 | 5 (23%)  |
| 68  | 6MZ  | S2    | 1832 | 87,68 | 22,25,26     | 3.04 | 5 (22%)  | 29,36,39    | 2.21 | 10 (34%) |
| 3   | PSU  | L5    | 4312 | 3     | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.81 | 4 (19%)  |
| 68  | OMU  | S2    | 627  | 68    | 19,22,23     | 3.30 | 7 (36%)  | 25,31,34    | 1.84 | 5 (20%)  |
| 3   | A2M  | L5    | 3830 | 3     | 22,25,26     | 1.23 | 1 (4%)   | 30,36,39    | 1.57 | 6 (20%)  |
| 3   | PSU  | L5    | 4673 | 3     | 18,21,22     | 1.04 | 2 (11%)  | 21,30,33    | 1.86 | 4 (19%)  |
| 3   | PSU  | L5    | 4493 | 3     | 18,21,22     | 1.07 | 1 (5%)   | 21,30,33    | 1.87 | 4 (19%)  |
| 3   | A2M  | L5    | 4590 | 3     | 22,25,26     | 1.27 | 3 (13%)  | 30,36,39    | 1.57 | 6 (20%)  |
| 68  | A2M  | S2    | 576  | 68    | 22,25,26     | 1.19 | 1 (4%)   | 30,36,39    | 1.53 | 5 (16%)  |
| 3   | PSU  | L5    | 2839 | 3     | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 1.93 | 4 (19%)  |
| 3   | PSU  | L5    | 1792 | 3     | 18,21,22     | 1.01 | 1 (5%)   | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | PSU  | L5    | 3639 | 3     | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 1.97 | 4 (19%)  |
| 3   | OMG  | L5    | 4499 | 3     | 23,26,27     | 0.60 | 0        | 32,38,41    | 0.50 | 0        |
| 68  | OMU  | S2    | 799  | 68    | 19,22,23     | 3.40 | 7 (36%)  | 25,31,34    | 1.89 | 5 (20%)  |
| 3   | OMG  | L5    | 4623 | 3     | 23,26,27     | 0.64 | 0        | 32,38,41    | 0.58 | 0        |
| 3   | OMU  | L5    | 4620 | 3     | 19,22,23     | 3.10 | 7 (36%)  | 25,31,34    | 1.78 | 5 (20%)  |
| 68  | 4AC  | S2    | 1842 | 68    | 21,24,25     | 0.41 | 0        | 28,34,37    | 0.46 | 0        |
| 3   | 5MC  | L5    | 3782 | 87,3  | 19,22,23     | 0.79 | 0        | 26,32,35    | 0.83 | 1 (3%)   |
| 3   | OMG  | L5    | 4228 | 3     | 23,26,27     | 0.61 | 0        | 32,38,41    | 0.61 | 0        |
| 68  | OMU  | S2    | 1326 | 68    | 19,22,23     | 3.26 | 7 (36%)  | 25,31,34    | 1.85 | 5 (20%)  |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 68  | OMU  | S2    | 121  | 68    | 19,22,23     | 3.22 | 7 (36%)  | 25,31,34    | 1.59 | 4 (16%)  |
| 3   | PSU  | L5    | 1677 | 3     | 18,21,22     | 1.15 | 2 (11%)  | 21,30,33    | 2.12 | 6 (28%)  |
| 68  | A2M  | S2    | 468  | 68    | 22,25,26     | 1.21 | 1 (4%)   | 30,36,39    | 1.57 | 8 (26%)  |
| 3   | OMG  | L5    | 4392 | 3     | 23,26,27     | 0.65 | 0        | 32,38,41    | 0.49 | 0        |
| 68  | A2M  | S2    | 484  | 68    | 22,25,26     | 1.20 | 2 (9%)   | 30,36,39    | 1.46 | 7 (23%)  |
| 68  | PSU  | S2    | 966  | 87,68 | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.87 | 4 (19%)  |
| 68  | A2M  | S2    | 1383 | 68    | 22,25,26     | 1.16 | 1 (4%)   | 30,36,39    | 1.58 | 7 (23%)  |
| 68  | PSU  | S2    | 651  | 68    | 18,21,22     | 1.10 | 1 (5%)   | 21,30,33    | 1.96 | 4 (19%)  |
| 3   | A2M  | L5    | 1534 | 87,3  | 22,25,26     | 1.21 | 2 (9%)   | 30,36,39    | 1.42 | 7 (23%)  |
| 3   | OMU  | L5    | 4498 | 3     | 19,22,23     | 3.18 | 7 (36%)  | 25,31,34    | 1.96 | 5 (20%)  |
| 3   | OMC  | L5    | 1340 | 3     | 19,22,23     | 0.72 | 0        | 25,31,34    | 0.76 | 0        |
| 3   | A2M  | L5    | 2815 | 3     | 22,25,26     | 1.21 | 2 (9%)   | 30,36,39    | 1.51 | 9 (30%)  |
| 68  | OMU  | S2    | 116  | 68    | 19,22,23     | 3.31 | 7 (36%)  | 25,31,34    | 1.74 | 5 (20%)  |
| 3   | UY1  | L5    | 3818 | 3     | 19,22,23     | 4.76 | 9 (47%)  | 21,31,34    | 1.94 | 5 (23%)  |
| 68  | OMG  | S2    | 436  | 68    | 23,26,27     | 0.54 | 0        | 32,38,41    | 0.53 | 0        |
| 68  | OMC  | S2    | 1272 | 68    | 19,22,23     | 0.57 | 0        | 25,31,34    | 0.78 | 1 (4%)   |
| 68  | A2M  | S2    | 99   | 87,68 | 22,25,26     | 1.19 | 1 (4%)   | 30,36,39    | 1.64 | 8 (26%)  |
| 3   | PSU  | L5    | 4471 | 3     | 18,21,22     | 1.11 | 2 (11%)  | 21,30,33    | 1.94 | 4 (19%)  |
| 68  | A2M  | S2    | 668  | 87,68 | 22,25,26     | 1.37 | 2 (9%)   | 30,36,39    | 1.64 | 8 (26%)  |
| 3   | PSU  | L5    | 4457 | 3     | 18,21,22     | 1.09 | 3 (16%)  | 21,30,33    | 2.06 | 4 (19%)  |
| 3   | PSU  | L5    | 3637 | 3     | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 2.06 | 5 (23%)  |
| 68  | OMG  | S2    | 509  | 68    | 23,26,27     | 0.52 | 0        | 32,38,41    | 0.49 | 0        |
| 5   | PSU  | L8    | 69   | 5     | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.99 | 5 (23%)  |
| 3   | OMG  | L5    | 3792 | 3     | 23,26,27     | 0.60 | 0        | 32,38,41    | 0.53 | 0        |
| 3   | OMU  | L5    | 3925 | 3     | 19,22,23     | 3.13 | 7 (36%)  | 25,31,34    | 1.84 | 5 (20%)  |
| 3   | PSU  | L5    | 1781 | 3     | 18,21,22     | 1.06 | 2 (11%)  | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | PSU  | L5    | 4576 | 3     | 18,21,22     | 1.09 | 2 (11%)  | 21,30,33    | 1.88 | 4 (19%)  |
| 3   | PSU  | L5    | 5010 | 3     | 18,21,22     | 1.08 | 2 (11%)  | 21,30,33    | 1.89 | 4 (19%)  |
| 68  | MA6  | S2    | 1850 | 68    | 23,26,27     | 1.27 | 2 (8%)   | 33,38,41    | 3.38 | 11 (33%) |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | OMC  | L5    | 4456 | 3    | -       | 0/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 68  | OMG  | S2    | 1490 | 68   | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L5    | 2787 | 3    | -       | 5/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L5    | 2861 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | OMG  | L5    | 3627 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 1782 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 4494 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 68  | PSU  | S2    | 649  | 68   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 4196 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMC  | L5    | 4536 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | OMC  | L5    | 3869 | 3    | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L5    | 4523 | 87,3 | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 4628 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 4618 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 68  | PSU  | S2    | 866  | 68   | -       | 0/7/25/26 | 0/2/2/2 |
| 68  | OMC  | S2    | 1391 | 68   | -       | 0/9/27/28 | 0/2/2/2 |
| 68  | PSU  | S2    | 1174 | 68   | -       | 0/7/25/26 | 0/2/2/2 |
| 68  | PSU  | S2    | 863  | 68   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L5    | 2365 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 68  | PSU  | S2    | 93   | 68   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 4370 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | A2M  | L5    | 2363 | 87,3 | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | PSU  | L5    | 4973 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 68  | A2M  | S2    | 166  | 68   | -       | 1/9/27/28 | 0/3/3/3 |
| 68  | OMC  | S2    | 1703 | 68   | -       | 1/9/27/28 | 0/2/2/2 |
| 3   | A2M  | L5    | 398  | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L5    | 3744 | 3    | -       | 0/9/27/28 | 0/3/3/3 |
| 3   | 1MA  | L5    | 1322 | 87,3 | -       | 2/7/25/26 | 0/3/3/3 |
| 3   | PSU  | L5    | 4296 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMG  | L5    | 2424 | 3    | -       | 1/9/27/28 | 0/3/3/3 |
| 3   | OMG  | L5    | 1625 | 3    | -       | 2/9/27/28 | 0/3/3/3 |
| 68  | A2M  | S2    | 27   | 68   | -       | 1/9/27/28 | 0/3/3/3 |
| 68  | OMG  | S2    | 601  | 68   | -       | 1/9/27/28 | 0/3/3/3 |
| 68  | OMU  | S2    | 1442 | 68   | -       | 3/9/27/28 | 0/2/2/2 |
| 3   | OMU  | L5    | 4306 | 3    | -       | 0/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L5    | 4579 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4353 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | OMC  | L5    | 2422 | 87,3 | -       | 2/9/27/28 | 0/2/2/2 |
| 3   | PSU  | L5    | 4532 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 68  | PSU  | S2    | 1046 | 68   | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 4293 | 3    | -       | 0/7/25/26 | 0/2/2/2 |
| 3   | PSU  | L5    | 3822 | 3    | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 68  | OMU  | S2    | 172  | 68   | -       | 6/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4431 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 1081 | 68   | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 3867 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 68  | PSU  | S2    | 109  | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 681  | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 1367 | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 3899 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4299 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3920 | 87,3 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | UR3  | L5    | 4530 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | OMU  | S2    | 354  | 68   | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 2632 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 68  | B8N  | S2    | 1248 | 68   | -       | 6/16/34/35 | 0/2/2/2 |
| 68  | OMU  | S2    | 1288 | 68   | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | 6MZ  | L5    | 4220 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | OMC  | S2    | 462  | 68   | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L5    | 1524 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 68  | OMC  | S2    | 517  | 68   | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | OMC  | L5    | 2804 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 68  | OMG  | S2    | 1328 | 68   | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 2824 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 68  | OMG  | S2    | 644  | 68   | -       | 3/9/27/28  | 0/3/3/3 |
| 68  | PSU  | S2    | 406  | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 814  | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 3701 | 3    | -       | 6/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4521 | 87,3 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 1536 | 3    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4552 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 1862 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 1316 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | OMU  | S2    | 428  | 68   | -       | 6/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L5    | 3785 | 87,3 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 1326 | 3    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4636 | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 5001 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 3841 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 4689 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 686  | 68   | -       | 0/7/25/26  | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | PSU  | L5    | 4442 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 1244 | 68   | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 2876 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 1323 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 1683 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3851 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4500 | 3    | -       | 3/7/25/26  | 0/2/2/2 |
| 3   | OMU  | L5    | 4227 | 3    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 3853 | 87,3 | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 3718 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 2401 | 3    | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMC  | L5    | 3808 | 87,3 | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 3884 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3695 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | 4AC  | S2    | 1337 | 68   | -       | 0/11/29/30 | 0/2/2/2 |
| 3   | PSU  | L5    | 4361 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 1056 | 68   | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4403 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | 5MC  | L5    | 4447 | 3    | -       | 4/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 2351 | 87,3 | -       | 1/9/27/28  | 0/2/2/2 |
| 68  | OMC  | S2    | 174  | 68   | -       | 0/9/27/28  | 0/2/2/2 |
| 68  | PSU  | S2    | 1004 | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3844 | 3    | -       | 1/7/25/26  | 0/2/2/2 |
| 68  | OMG  | S2    | 867  | 68   | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 1582 | 3    | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | A2M  | S2    | 1031 | 68   | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | A2M  | L5    | 4571 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | A2M  | S2    | 159  | 68   | -       | 1/9/27/28  | 0/3/3/3 |
| 68  | PSU  | S2    | 1045 | 68   | -       | 2/7/25/26  | 0/2/2/2 |
| 68  | PSU  | S2    | 1232 | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMC  | L5    | 3887 | 3    | -       | 1/9/27/28  | 0/2/2/2 |
| 68  | PSU  | S2    | 1177 | 68   | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 2364 | 87,3 | -       | 2/9/27/28  | 0/3/3/3 |
| 68  | MA6  | S2    | 1851 | 68   | -       | 1/11/29/30 | 0/3/3/3 |
| 3   | A2M  | L5    | 3825 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 1744 | 87,3 | -       | 0/7/25/26  | 0/2/2/2 |
| 5   | OMG  | L8    | 75   | 5    | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 1522 | 3    | -       | 0/9/27/28  | 0/3/3/3 |
| 5   | PSU  | L8    | 55   | 5    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 4637 | 3    | -       | 3/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 3   | OMU  | L5    | 2837 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 68  | PSU  | S2    | 801  | 68    | -       | 2/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 1871 | 87,3  | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | G7M  | S2    | 1639 | 84,68 | -       | 0/7/25/26  | 0/3/3/3 |
| 3   | PSU  | L5    | 4972 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | OMG  | S2    | 683  | 68    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 1860 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 400  | 3     | -       | 1/9/27/28  | 0/3/3/3 |
| 68  | PSU  | S2    | 105  | 68    | -       | 1/7/25/26  | 0/2/2/2 |
| 68  | 6MZ  | S2    | 1832 | 87,68 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4312 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | OMU  | S2    | 627  | 68    | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L5    | 3830 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4673 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4493 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 4590 | 3     | -       | 4/9/27/28  | 0/3/3/3 |
| 68  | A2M  | S2    | 576  | 68    | -       | 3/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 2839 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 1792 | 3     | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3639 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 4499 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | OMU  | S2    | 799  | 68    | -       | 2/9/27/28  | 0/2/2/2 |
| 3   | OMG  | L5    | 4623 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMU  | L5    | 4620 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 68  | 4AC  | S2    | 1842 | 68    | -       | 0/11/29/30 | 0/2/2/2 |
| 3   | 5MC  | L5    | 3782 | 87,3  | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 4228 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 68  | OMU  | S2    | 1326 | 68    | -       | 0/9/27/28  | 0/2/2/2 |
| 68  | OMU  | S2    | 121  | 68    | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 1677 | 3     | -       | 1/7/25/26  | 0/2/2/2 |
| 68  | A2M  | S2    | 468  | 68    | -       | 0/9/27/28  | 0/3/3/3 |
| 3   | OMG  | L5    | 4392 | 3     | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | A2M  | S2    | 484  | 68    | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | PSU  | S2    | 966  | 87,68 | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | A2M  | S2    | 1383 | 68    | -       | 1/9/27/28  | 0/3/3/3 |
| 68  | PSU  | S2    | 651  | 68    | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | A2M  | L5    | 1534 | 87,3  | -       | 1/9/27/28  | 0/3/3/3 |
| 3   | OMU  | L5    | 4498 | 3     | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | OMC  | L5    | 1340 | 3     | -       | 1/9/27/28  | 0/2/2/2 |
| 3   | A2M  | L5    | 2815 | 3     | -       | 2/9/27/28  | 0/3/3/3 |

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| Mol | Type | Chain | Res  | Link  | Chirals | Torsions   | Rings   |
|-----|------|-------|------|-------|---------|------------|---------|
| 68  | OMU  | S2    | 116  | 68    | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | UY1  | L5    | 3818 | 3     | -       | 3/9/27/28  | 0/2/2/2 |
| 68  | OMG  | S2    | 436  | 68    | -       | 0/9/27/28  | 0/3/3/3 |
| 68  | OMC  | S2    | 1272 | 68    | -       | 0/9/27/28  | 0/2/2/2 |
| 68  | A2M  | S2    | 99   | 87,68 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4471 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | A2M  | S2    | 668  | 87,68 | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | PSU  | L5    | 4457 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 3637 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | OMG  | S2    | 509  | 68    | -       | 0/9/27/28  | 0/3/3/3 |
| 5   | PSU  | L8    | 69   | 5     | -       | 1/7/25/26  | 0/2/2/2 |
| 3   | OMG  | L5    | 3792 | 3     | -       | 2/9/27/28  | 0/3/3/3 |
| 3   | OMU  | L5    | 3925 | 3     | -       | 0/9/27/28  | 0/2/2/2 |
| 3   | PSU  | L5    | 1781 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 4576 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 3   | PSU  | L5    | 5010 | 3     | -       | 0/7/25/26  | 0/2/2/2 |
| 68  | MA6  | S2    | 1850 | 68    | -       | 0/11/29/30 | 0/3/3/3 |

The worst 5 of 330 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 68  | S2    | 1832 | 6MZ  | C6-N6 | 12.63 | 1.48        | 1.34     |
| 3   | L5    | 3818 | UY1  | C6-C5 | 12.21 | 1.48        | 1.35     |
| 3   | L5    | 4220 | 6MZ  | C6-N6 | 11.80 | 1.47        | 1.34     |
| 3   | L5    | 3818 | UY1  | C2-N1 | 11.47 | 1.51        | 1.36     |
| 68  | S2    | 799  | OMU  | C2-N1 | 8.70  | 1.52        | 1.38     |

The worst 5 of 688 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 68  | S2    | 1850 | MA6  | N1-C6-N6  | -12.18 | 102.02      | 116.86   |
| 68  | S2    | 1851 | MA6  | N1-C6-N6  | -11.97 | 102.27      | 116.86   |
| 68  | S2    | 1850 | MA6  | C5-C6-N6  | 8.04   | 138.05      | 125.33   |
| 68  | S2    | 1851 | MA6  | C5-C6-N6  | 7.98   | 137.97      | 125.33   |
| 68  | S2    | 1639 | G7M  | C1'-N9-C4 | 7.40   | 148.35      | 126.49   |

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | L5    | 400 | A2M  | C1'-C2'-O2'-CM' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | L5    | 1326 | A2M  | O4'-C4'-C5'-O5' |
| 3   | L5    | 1340 | OMC  | C1'-C2'-O2'-CM2 |
| 3   | L5    | 1625 | OMG  | O4'-C4'-C5'-O5' |
| 3   | L5    | 2364 | OMG  | O4'-C4'-C5'-O5' |

There are no ring outliers.

67 monomers are involved in 94 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 68  | S2    | 1490 | OMG  | 1       | 0            |
| 3   | L5    | 2861 | OMC  | 1       | 0            |
| 68  | S2    | 649  | PSU  | 1       | 0            |
| 3   | L5    | 4196 | OMG  | 1       | 0            |
| 3   | L5    | 4536 | OMC  | 1       | 0            |
| 3   | L5    | 4523 | A2M  | 1       | 0            |
| 3   | L5    | 4618 | OMG  | 1       | 0            |
| 68  | S2    | 93   | PSU  | 1       | 0            |
| 3   | L5    | 2363 | A2M  | 1       | 0            |
| 68  | S2    | 166  | A2M  | 3       | 0            |
| 68  | S2    | 1703 | OMC  | 2       | 0            |
| 3   | L5    | 2424 | OMG  | 1       | 0            |
| 3   | L5    | 1625 | OMG  | 1       | 0            |
| 68  | S2    | 27   | A2M  | 1       | 0            |
| 68  | S2    | 601  | OMG  | 2       | 0            |
| 68  | S2    | 1442 | OMU  | 1       | 0            |
| 3   | L5    | 4579 | PSU  | 1       | 0            |
| 68  | S2    | 172  | OMU  | 2       | 0            |
| 3   | L5    | 3867 | A2M  | 3       | 0            |
| 68  | S2    | 681  | PSU  | 1       | 0            |
| 3   | L5    | 3920 | PSU  | 1       | 0            |
| 3   | L5    | 4530 | UR3  | 1       | 0            |
| 68  | S2    | 1288 | OMU  | 2       | 0            |
| 3   | L5    | 4220 | 6MZ  | 3       | 0            |
| 68  | S2    | 517  | OMC  | 1       | 0            |
| 68  | S2    | 1328 | OMG  | 1       | 0            |
| 3   | L5    | 2824 | OMC  | 1       | 0            |
| 3   | L5    | 1316 | OMG  | 1       | 0            |
| 3   | L5    | 1326 | A2M  | 1       | 0            |
| 3   | L5    | 5001 | PSU  | 1       | 0            |
| 3   | L5    | 3841 | OMC  | 1       | 0            |
| 3   | L5    | 4689 | PSU  | 1       | 0            |
| 3   | L5    | 1683 | PSU  | 1       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | L5    | 3851 | PSU  | 1       | 0            |
| 3   | L5    | 4500 | PSU  | 1       | 0            |
| 3   | L5    | 4227 | OMU  | 1       | 0            |
| 3   | L5    | 3718 | A2M  | 2       | 0            |
| 68  | S2    | 1337 | 4AC  | 2       | 0            |
| 3   | L5    | 4447 | 5MC  | 2       | 0            |
| 3   | L5    | 2351 | OMC  | 2       | 0            |
| 68  | S2    | 867  | OMG  | 1       | 0            |
| 68  | S2    | 1031 | A2M  | 3       | 0            |
| 3   | L5    | 4571 | A2M  | 2       | 0            |
| 68  | S2    | 159  | A2M  | 3       | 0            |
| 68  | S2    | 1232 | PSU  | 2       | 0            |
| 3   | L5    | 4637 | OMG  | 1       | 0            |
| 68  | S2    | 801  | PSU  | 1       | 0            |
| 3   | L5    | 1871 | A2M  | 1       | 0            |
| 3   | L5    | 400  | A2M  | 1       | 0            |
| 3   | L5    | 2839 | PSU  | 1       | 0            |
| 3   | L5    | 4499 | OMG  | 1       | 0            |
| 3   | L5    | 4620 | OMU  | 1       | 0            |
| 68  | S2    | 1842 | 4AC  | 1       | 0            |
| 68  | S2    | 121  | OMU  | 2       | 0            |
| 3   | L5    | 4392 | OMG  | 2       | 0            |
| 68  | S2    | 484  | A2M  | 1       | 0            |
| 68  | S2    | 1383 | A2M  | 2       | 0            |
| 68  | S2    | 651  | PSU  | 1       | 0            |
| 3   | L5    | 1534 | A2M  | 2       | 0            |
| 3   | L5    | 4498 | OMU  | 1       | 0            |
| 3   | L5    | 1340 | OMC  | 2       | 0            |
| 68  | S2    | 116  | OMU  | 2       | 0            |
| 68  | S2    | 99   | A2M  | 2       | 0            |
| 3   | L5    | 4457 | PSU  | 1       | 0            |
| 68  | S2    | 509  | OMG  | 2       | 0            |
| 3   | L5    | 1781 | PSU  | 1       | 0            |
| 68  | S2    | 1850 | MA6  | 2       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 241 ligands modelled in this entry, 224 are monoatomic - leaving 17 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 89  | SPD  | L5    | 5284 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.81 | 0           |
| 88  | SPM  | L5    | 5258 | -    | 13,13,13     | 0.37 | 0           | 12,12,12    | 0.96 | 0           |
| 89  | SPD  | L5    | 5288 | -    | 9,9,9        | 0.32 | 0           | 8,8,8       | 0.89 | 0           |
| 88  | SPM  | L5    | 5266 | -    | 13,13,13     | 0.35 | 0           | 12,12,12    | 0.94 | 0           |
| 89  | SPD  | L5    | 5289 | -    | 9,9,9        | 0.34 | 0           | 8,8,8       | 0.80 | 0           |
| 89  | SPD  | L5    | 5282 | -    | 9,9,9        | 0.31 | 0           | 8,8,8       | 0.80 | 0           |
| 89  | SPD  | L5    | 5286 | -    | 9,9,9        | 0.30 | 0           | 8,8,8       | 0.80 | 0           |
| 88  | SPM  | L5    | 5290 | -    | 13,13,13     | 0.36 | 0           | 12,12,12    | 0.84 | 0           |
| 89  | SPD  | L5    | 5291 | -    | 9,9,9        | 0.35 | 0           | 8,8,8       | 0.91 | 0           |
| 88  | SPM  | L5    | 5292 | -    | 13,13,13     | 0.36 | 0           | 12,12,12    | 0.82 | 0           |
| 88  | SPM  | L5    | 5262 | -    | 13,13,13     | 0.35 | 0           | 12,12,12    | 0.99 | 0           |
| 89  | SPD  | L5    | 5260 | -    | 9,9,9        | 0.33 | 0           | 8,8,8       | 1.08 | 0           |
| 89  | SPD  | L5    | 5283 | -    | 9,9,9        | 0.31 | 0           | 8,8,8       | 0.90 | 0           |
| 89  | SPD  | L5    | 5285 | -    | 9,9,9        | 0.34 | 0           | 8,8,8       | 0.87 | 0           |
| 89  | SPD  | L8    | 202  | -    | 9,9,9        | 0.31 | 0           | 8,8,8       | 0.86 | 0           |
| 88  | SPM  | L5    | 5263 | -    | 13,13,13     | 0.38 | 0           | 12,12,12    | 1.13 | 0           |
| 88  | SPM  | L5    | 5287 | -    | 13,13,13     | 0.38 | 0           | 12,12,12    | 0.99 | 0           |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 89  | SPD  | L5    | 5284 | -    | -       | 0/7/7/7    | -     |
| 88  | SPM  | L5    | 5258 | -    | -       | 5/11/11/11 | -     |
| 89  | SPD  | L5    | 5288 | -    | -       | 1/7/7/7    | -     |
| 88  | SPM  | L5    | 5266 | -    | -       | 4/11/11/11 | -     |
| 89  | SPD  | L5    | 5289 | -    | -       | 5/7/7/7    | -     |
| 89  | SPD  | L5    | 5282 | -    | -       | 0/7/7/7    | -     |
| 89  | SPD  | L5    | 5286 | -    | -       | 3/7/7/7    | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings |
|-----|------|-------|------|------|---------|------------|-------|
| 88  | SPM  | L5    | 5290 | -    | -       | 4/11/11/11 | -     |
| 89  | SPD  | L5    | 5291 | -    | -       | 1/7/7/7    | -     |
| 88  | SPM  | L5    | 5292 | -    | -       | 4/11/11/11 | -     |
| 88  | SPM  | L5    | 5262 | -    | -       | 3/11/11/11 | -     |
| 89  | SPD  | L5    | 5260 | -    | -       | 1/7/7/7    | -     |
| 89  | SPD  | L5    | 5283 | -    | -       | 2/7/7/7    | -     |
| 89  | SPD  | L5    | 5285 | -    | -       | 2/7/7/7    | -     |
| 89  | SPD  | L8    | 202  | -    | -       | 2/7/7/7    | -     |
| 88  | SPM  | L5    | 5263 | -    | -       | 2/11/11/11 | -     |
| 88  | SPM  | L5    | 5287 | -    | -       | 4/11/11/11 | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 88  | L5    | 5290 | SPM  | N10-C11-C12-C13 |
| 88  | L5    | 5262 | SPM  | N5-C6-C7-C8     |
| 88  | L5    | 5263 | SPM  | C2-C3-C4-N5     |
| 89  | L5    | 5285 | SPD  | C3-C4-C5-N6     |
| 88  | L5    | 5262 | SPM  | N10-C11-C12-C13 |

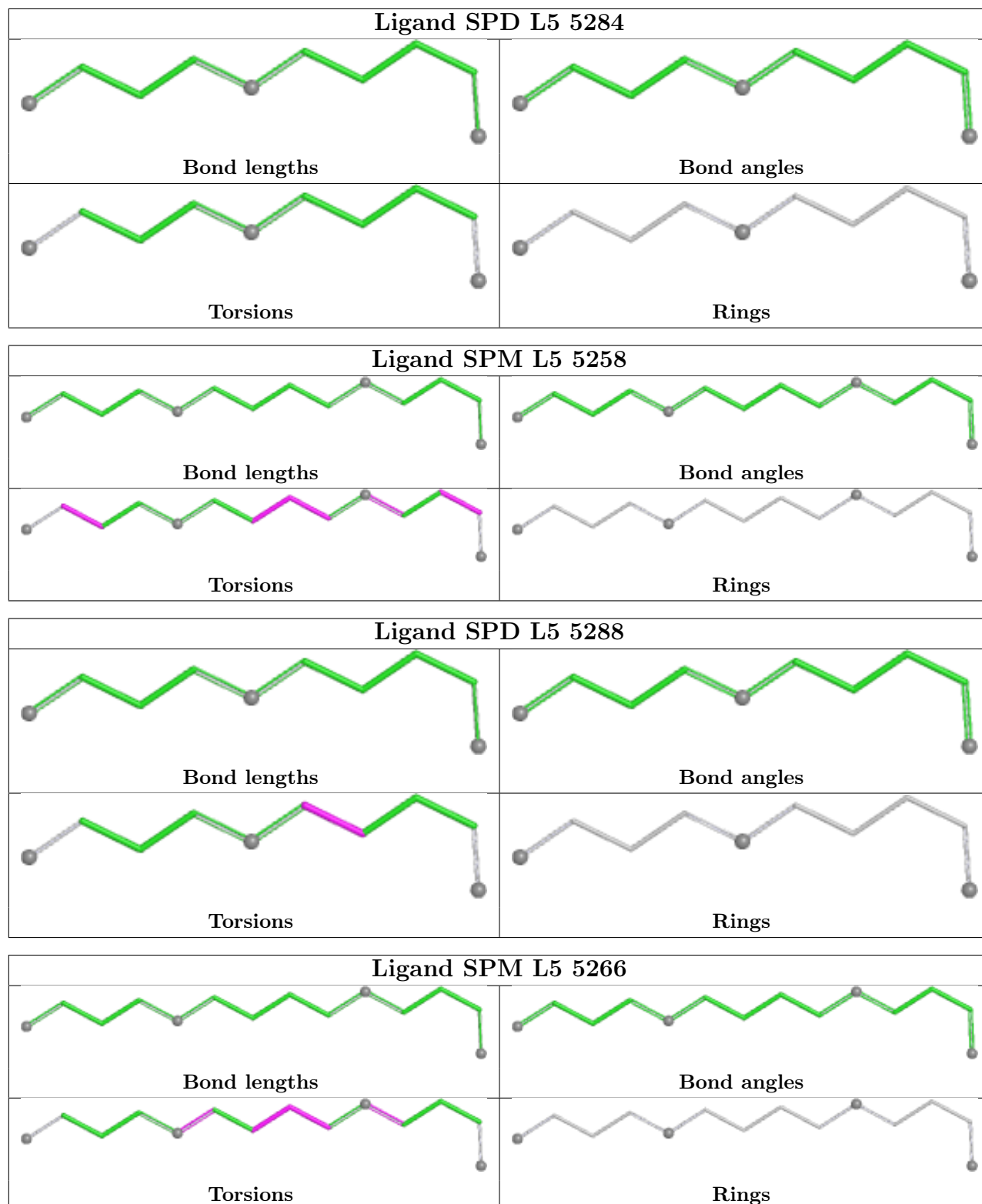
There are no ring outliers.

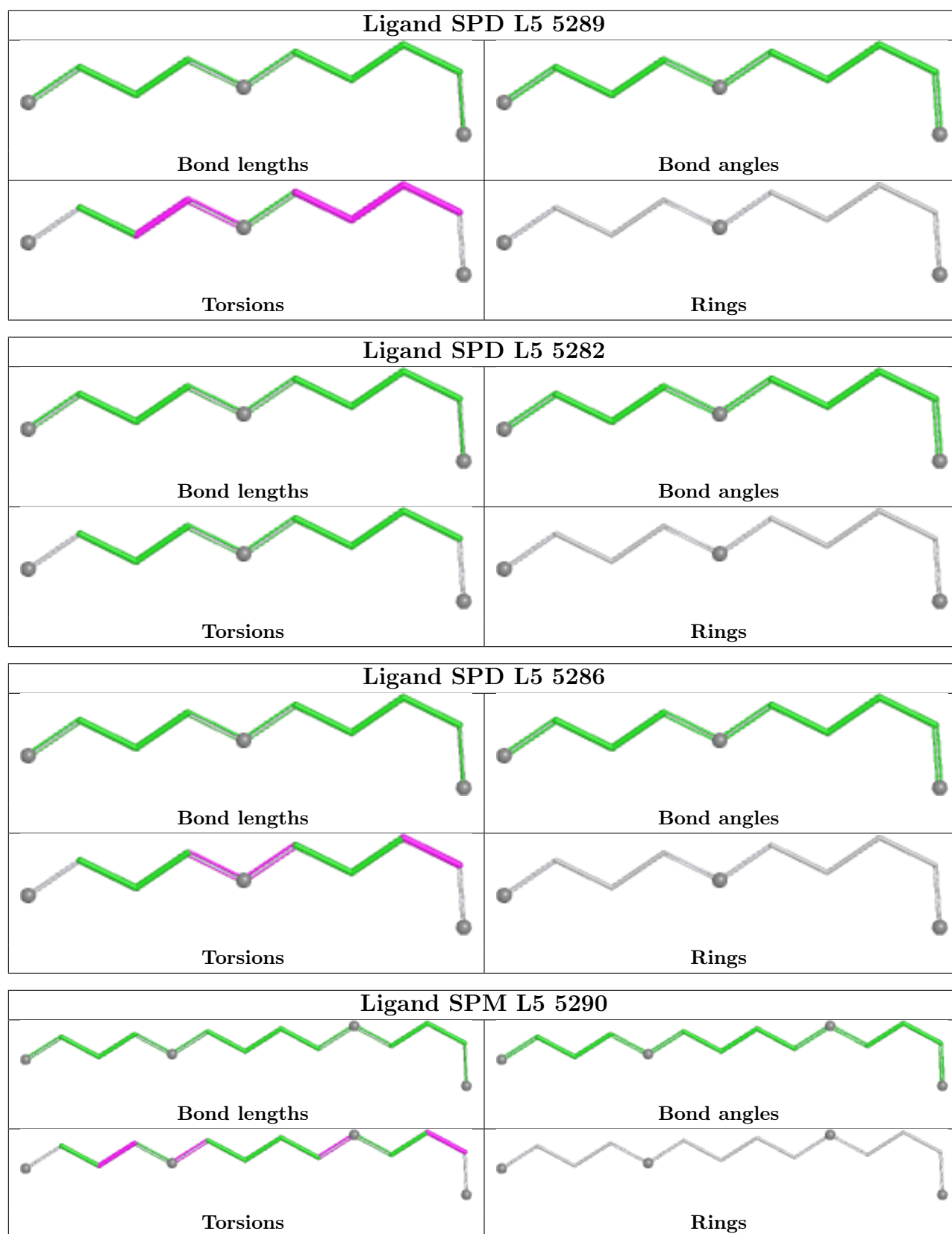
4 monomers are involved in 7 short contacts:

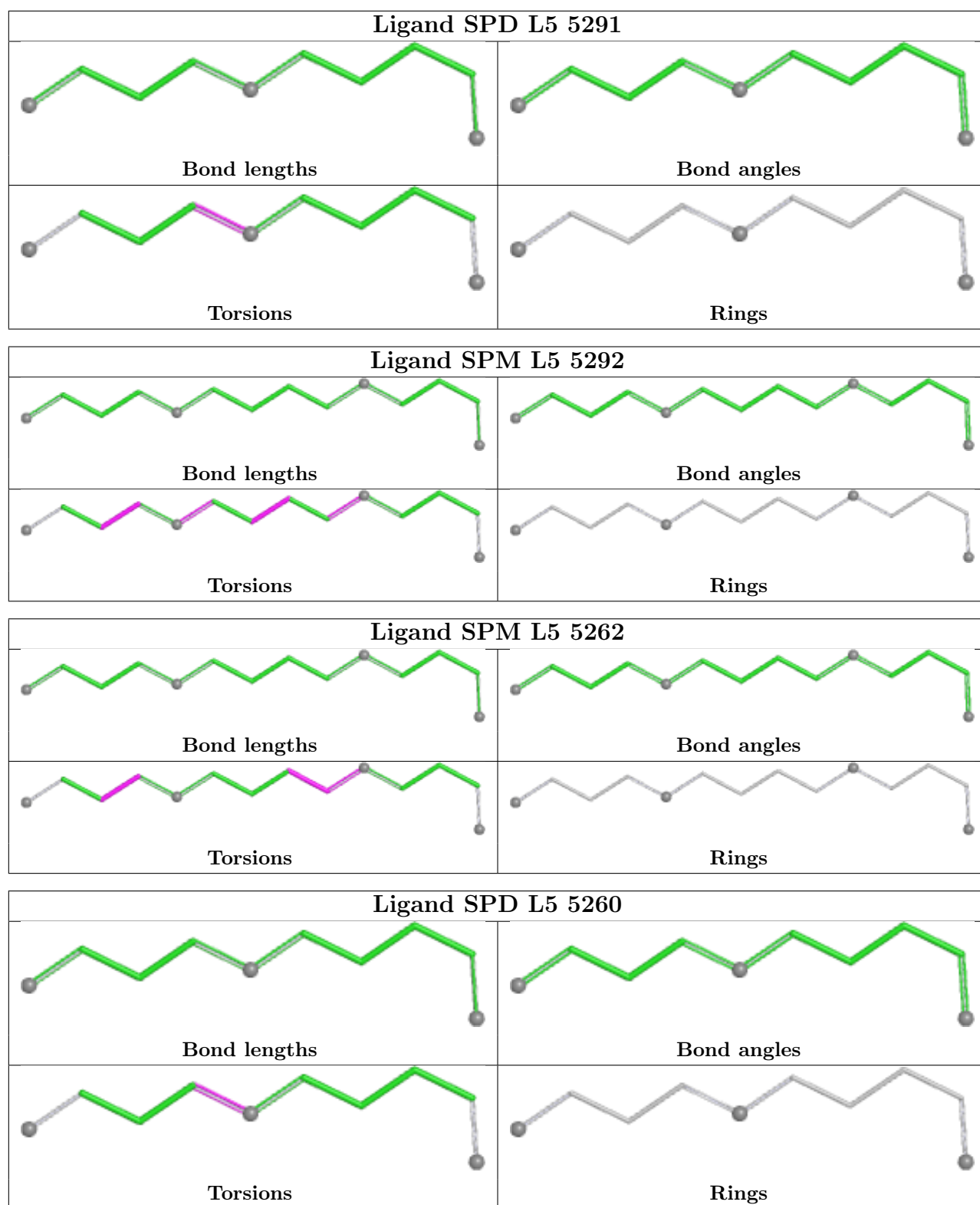
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 89  | L5    | 5288 | SPD  | 1       | 0            |
| 89  | L5    | 5282 | SPD  | 1       | 0            |
| 88  | L5    | 5292 | SPM  | 3       | 0            |
| 88  | L5    | 5287 | SPM  | 2       | 0            |

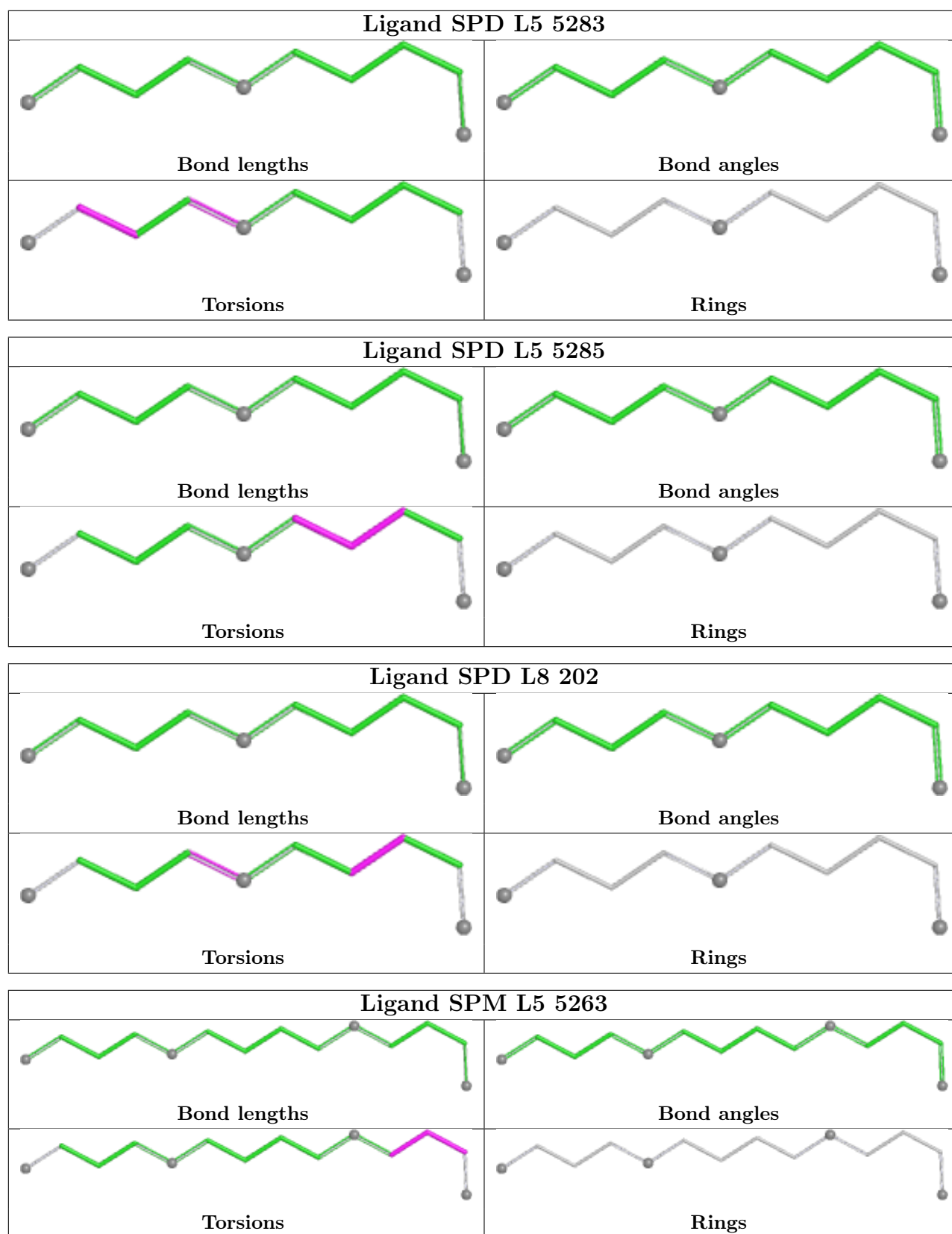
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

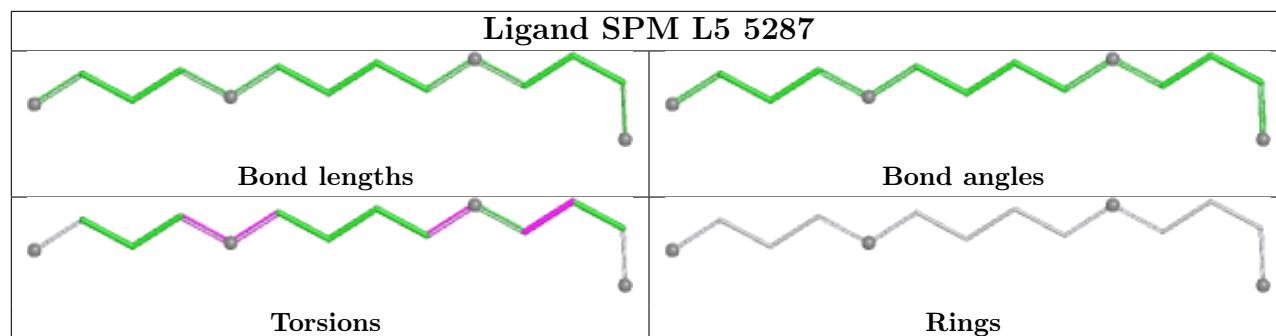
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 68  | S2    | 5                |
| 84  | Et    | 1                |

The worst 5 of 6 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | S2    | 753:C     | O3'    | 785:C     | P      | 28.96        |
| 1     | S2    | 698:G     | O3'    | 730:C     | P      | 14.10        |
| 1     | S2    | 739:C     | O3'    | 746:C     | P      | 13.38        |
| 1     | S2    | 225:G     | O3'    | 287:U     | P      | 7.80         |
| 1     | Et    | 16:C      | O3'    | 18:U      | P      | 7.35         |

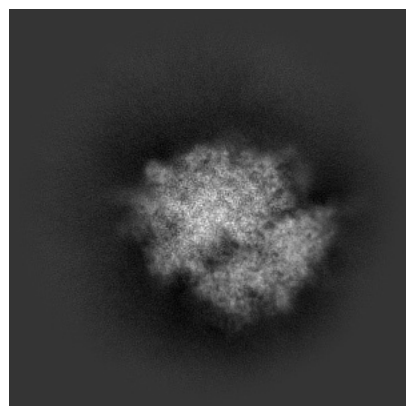
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71337. These allow visual inspection of the internal detail of the map and identification of artifacts.

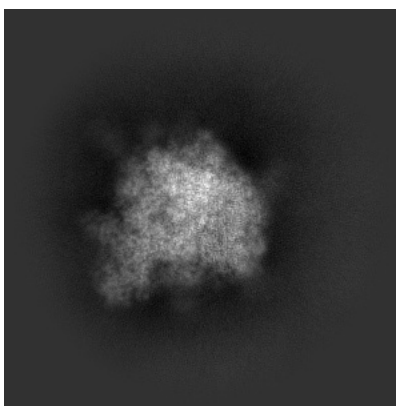
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

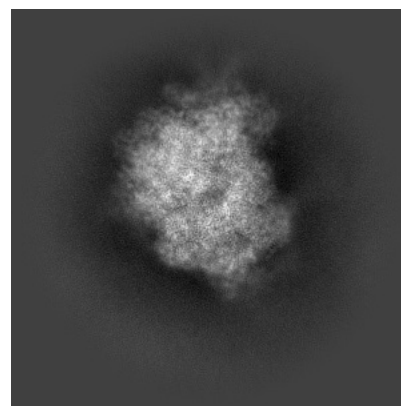
#### 6.1.1 Primary map



X

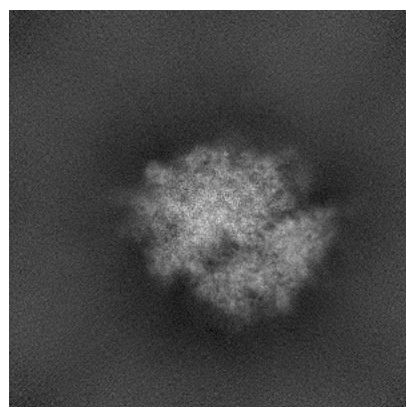


Y

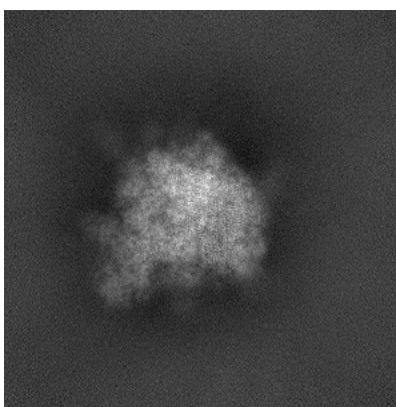


Z

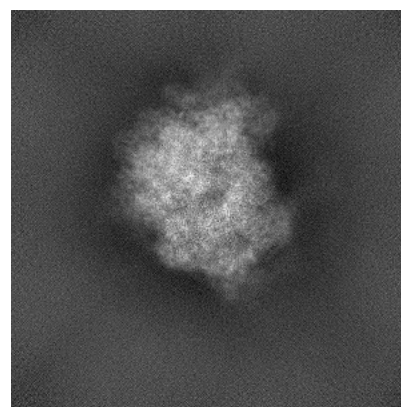
#### 6.1.2 Raw map



X



Y

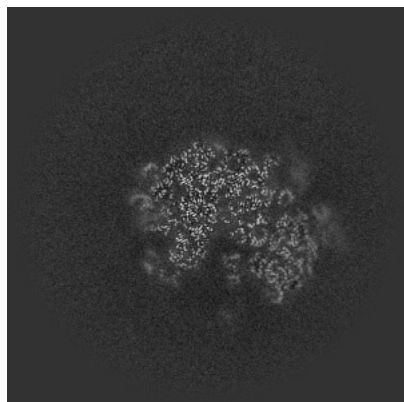


Z

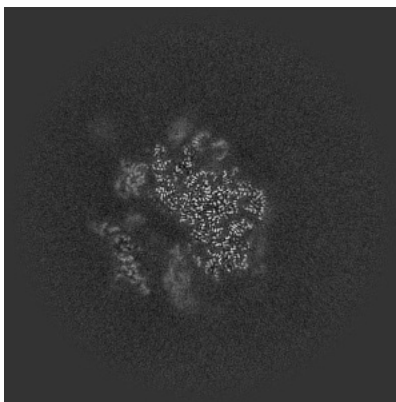
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

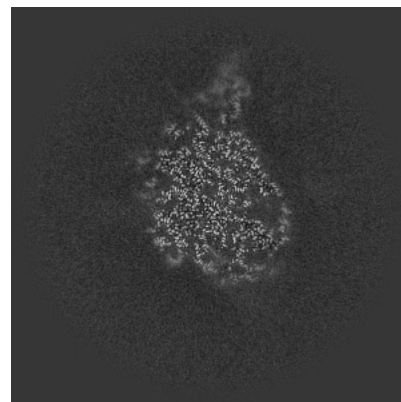
### 6.2.1 Primary map



X Index: 256

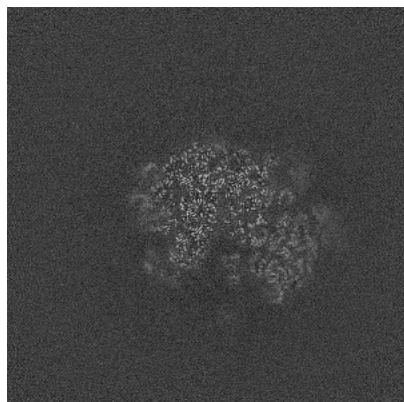


Y Index: 256

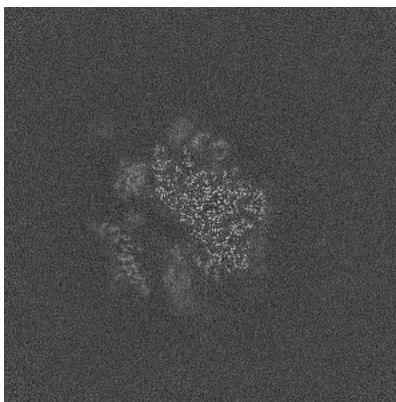


Z Index: 256

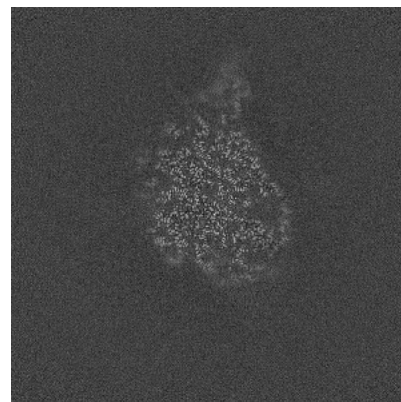
### 6.2.2 Raw map



X Index: 256



Y Index: 256

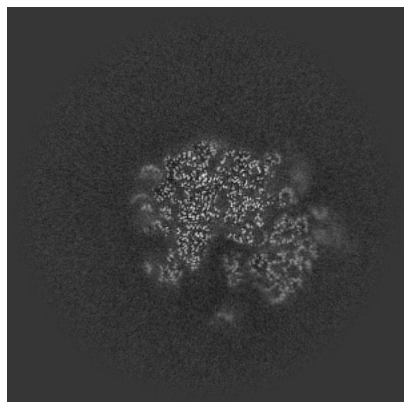


Z Index: 256

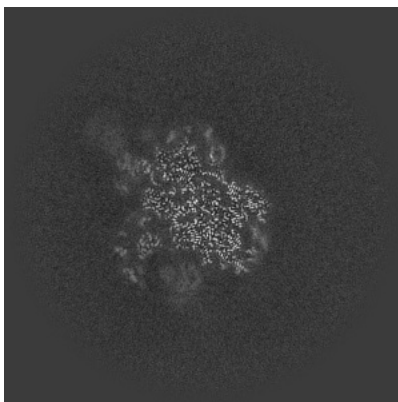
The images above show central slices of the map in three orthogonal directions.

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

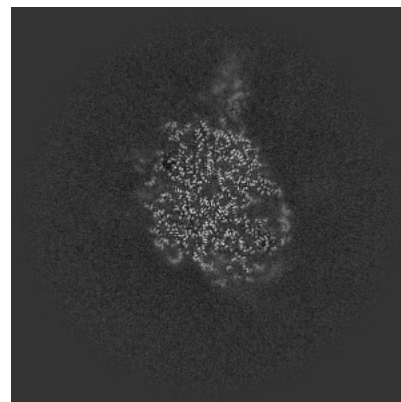
### 6.3.1 Primary map



X Index: 253

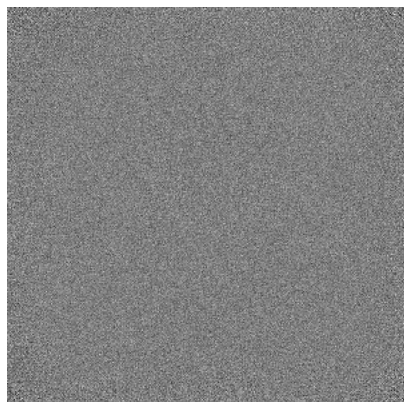


Y Index: 243

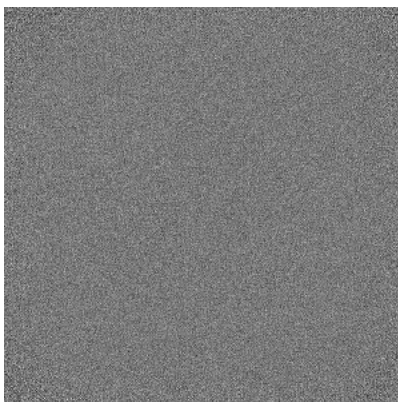


Z Index: 258

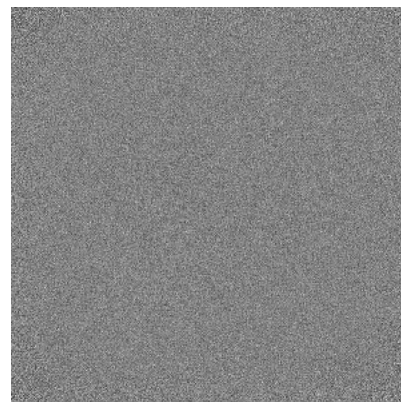
### 6.3.2 Raw map



X Index: 0



Y Index: 0

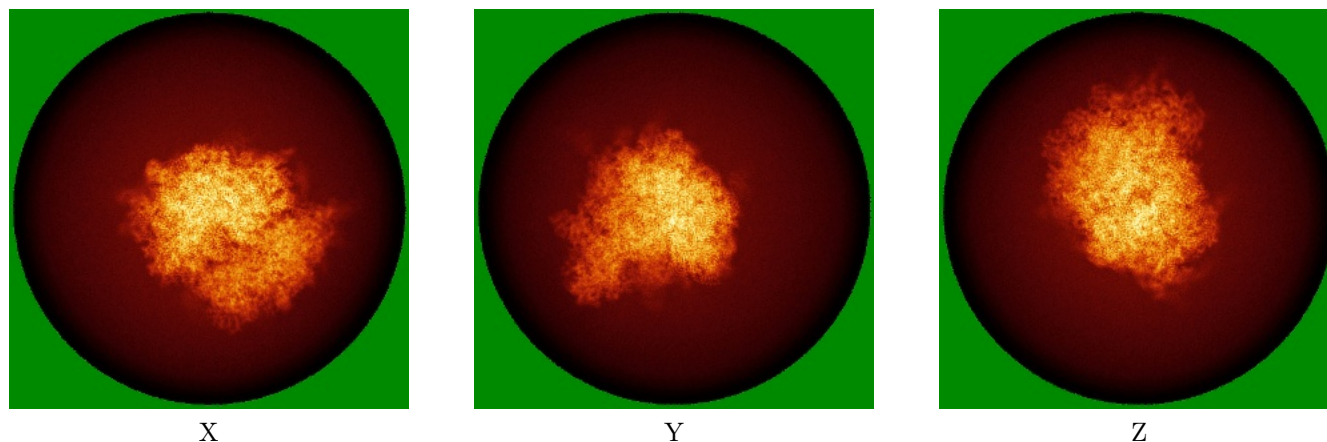


Z Index: 0

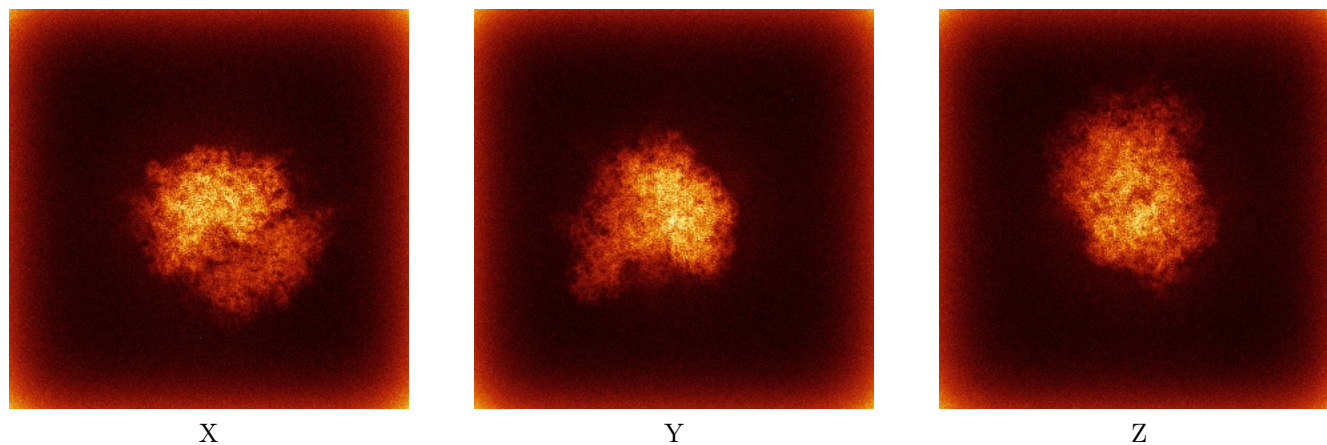
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



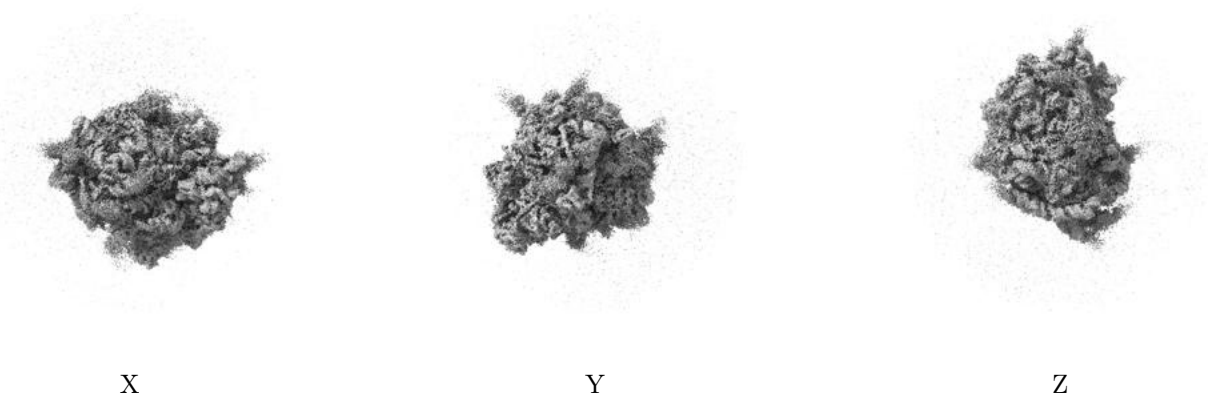
### 6.4.2 Raw map



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

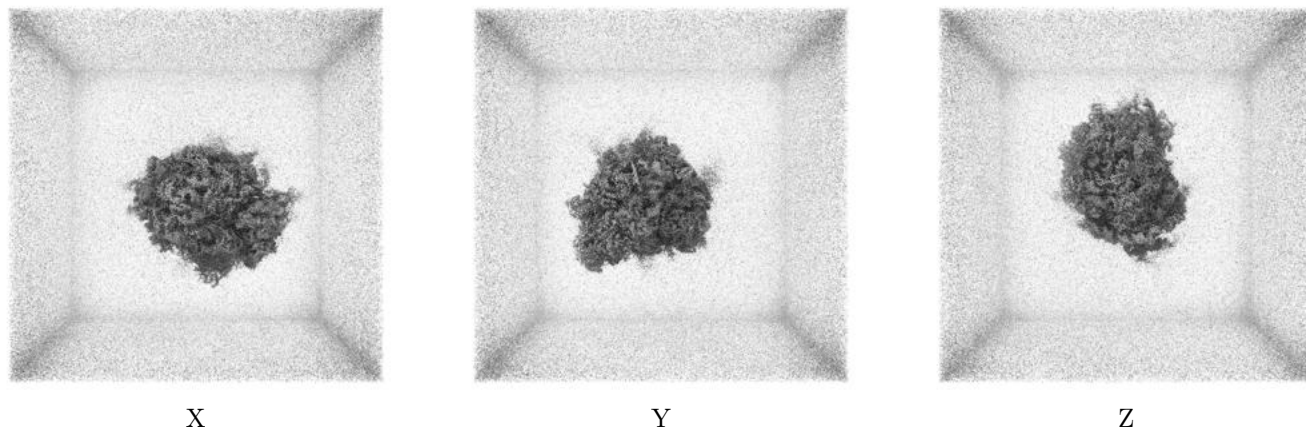
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

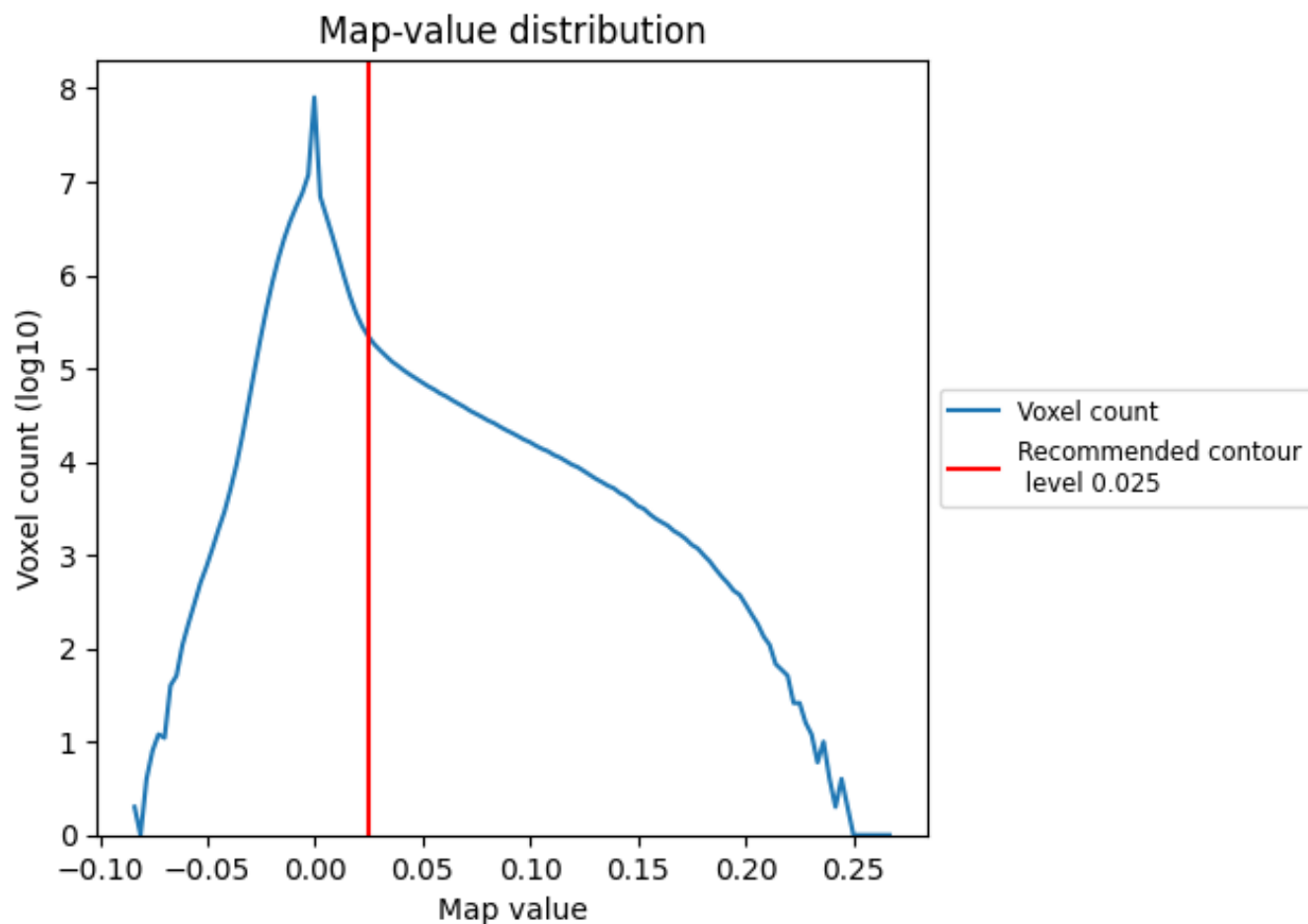
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

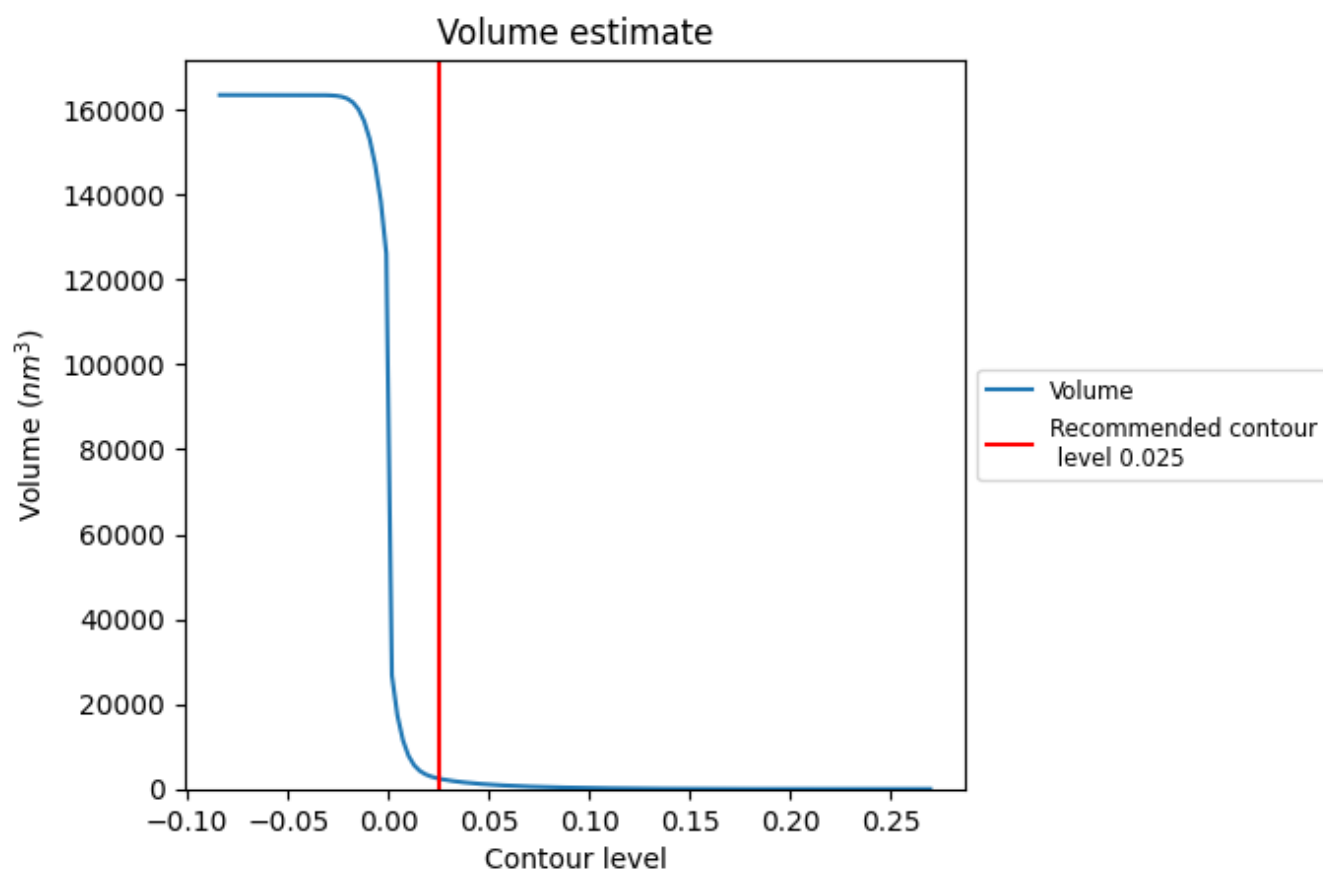
This section contains the results of statistical analysis of the map.

### 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.

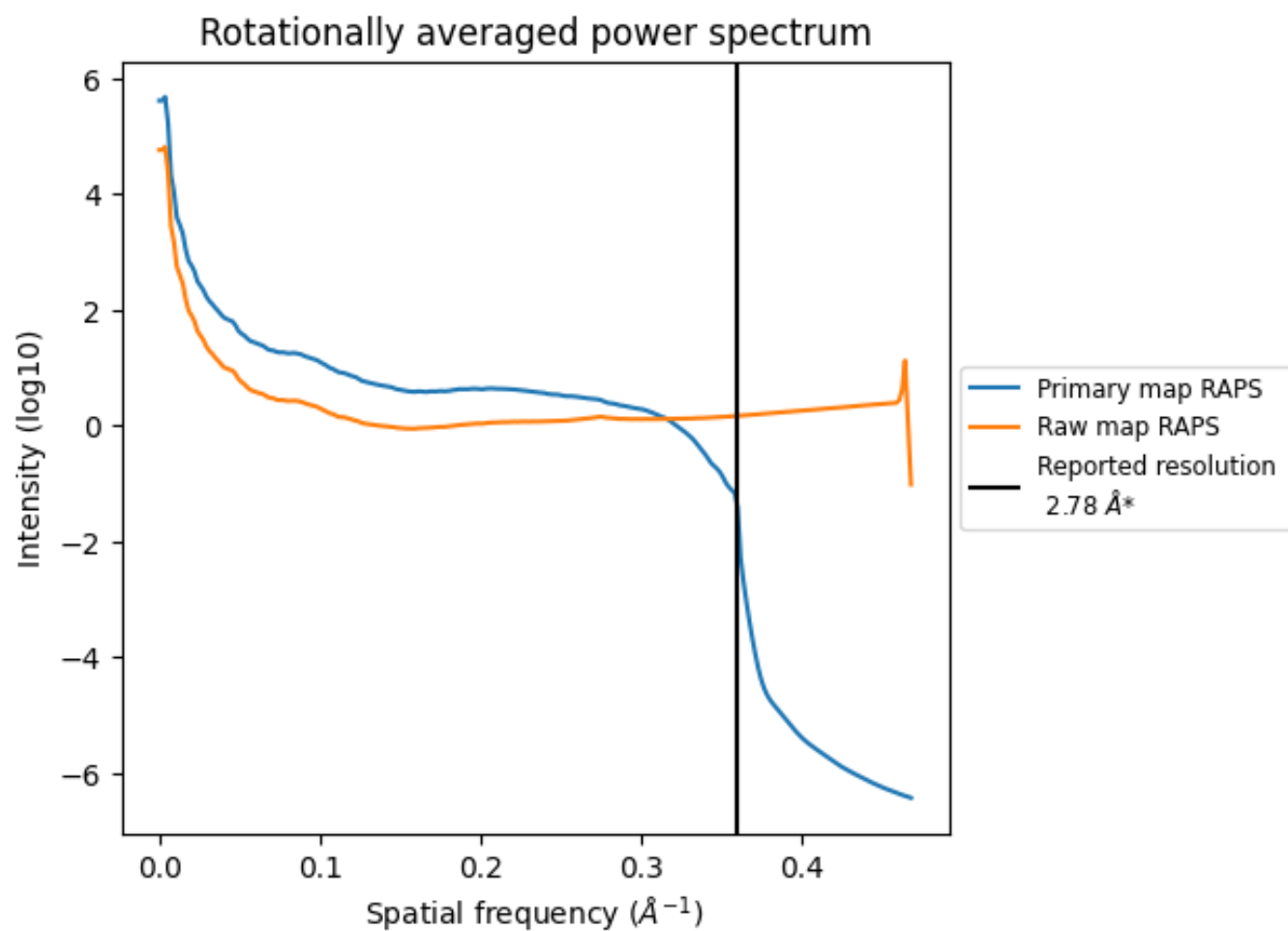
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2467  $\text{nm}^3$ ; this corresponds to an approximate mass of 2229 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 ⓘ

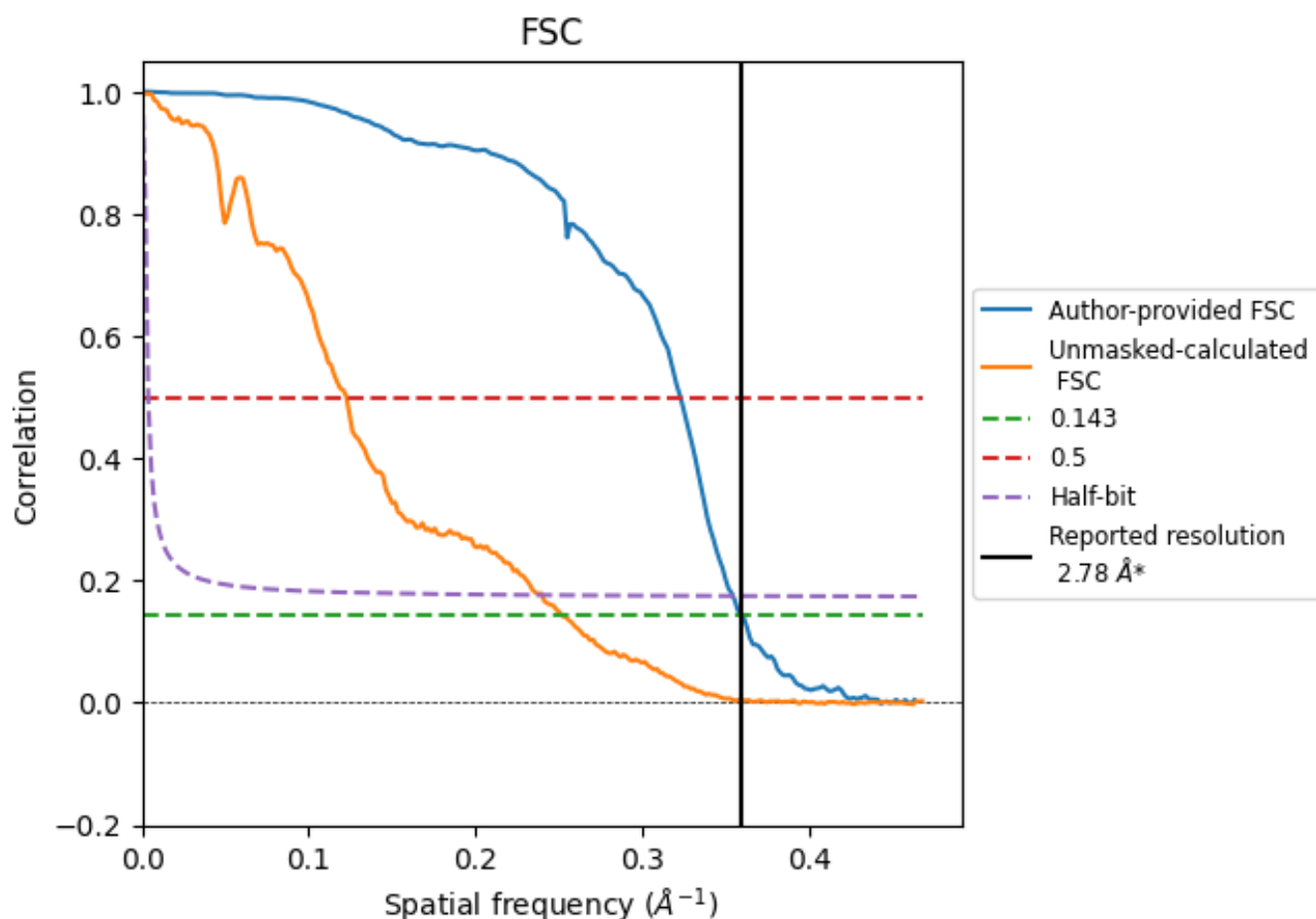


\*Reported resolution corresponds to spatial frequency of 0.360  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

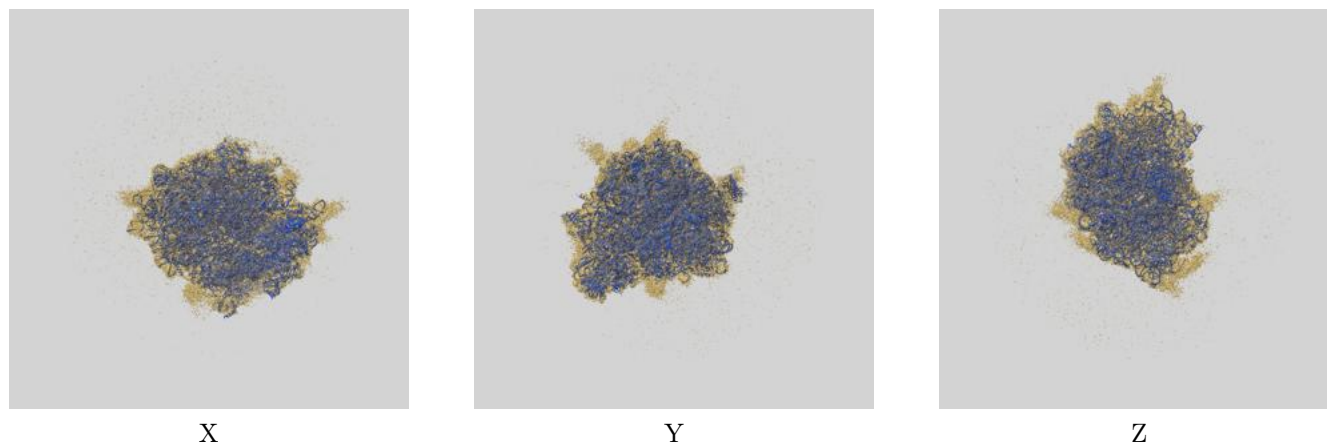
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.78                               | -    | -        |
| 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](#)

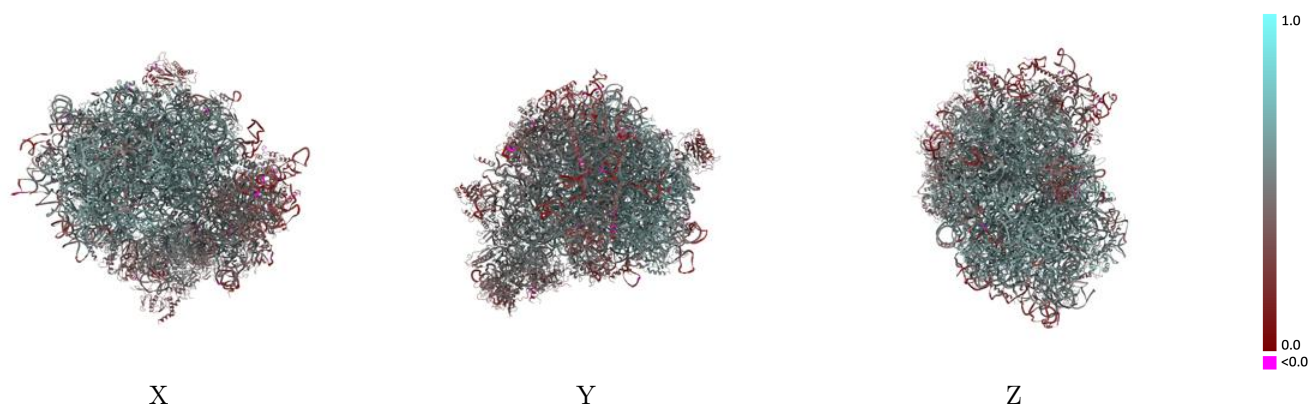
This section contains information regarding the fit between EMDB map EMD-71337 and PDB model 9P7C. Per-residue inclusion information can be found in section [3](#) on page [23](#).

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



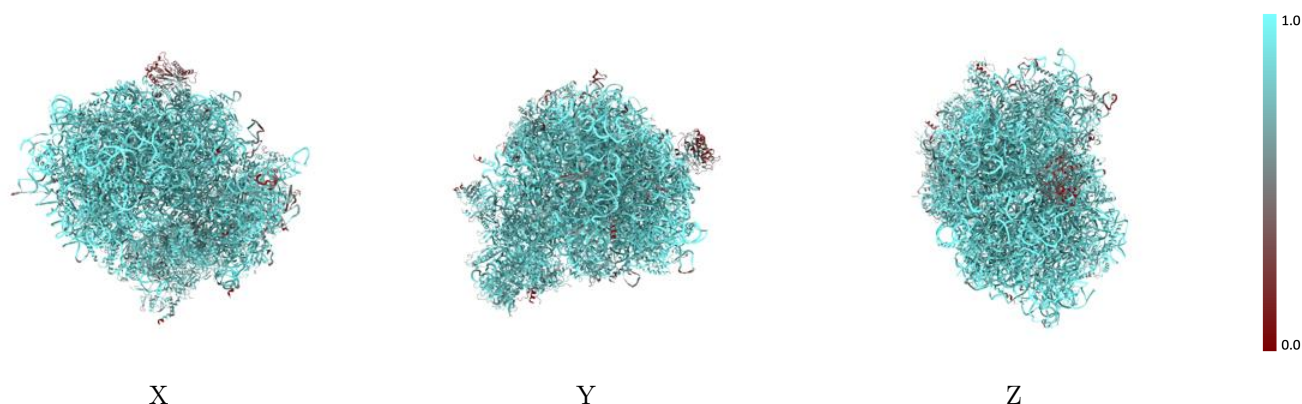
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



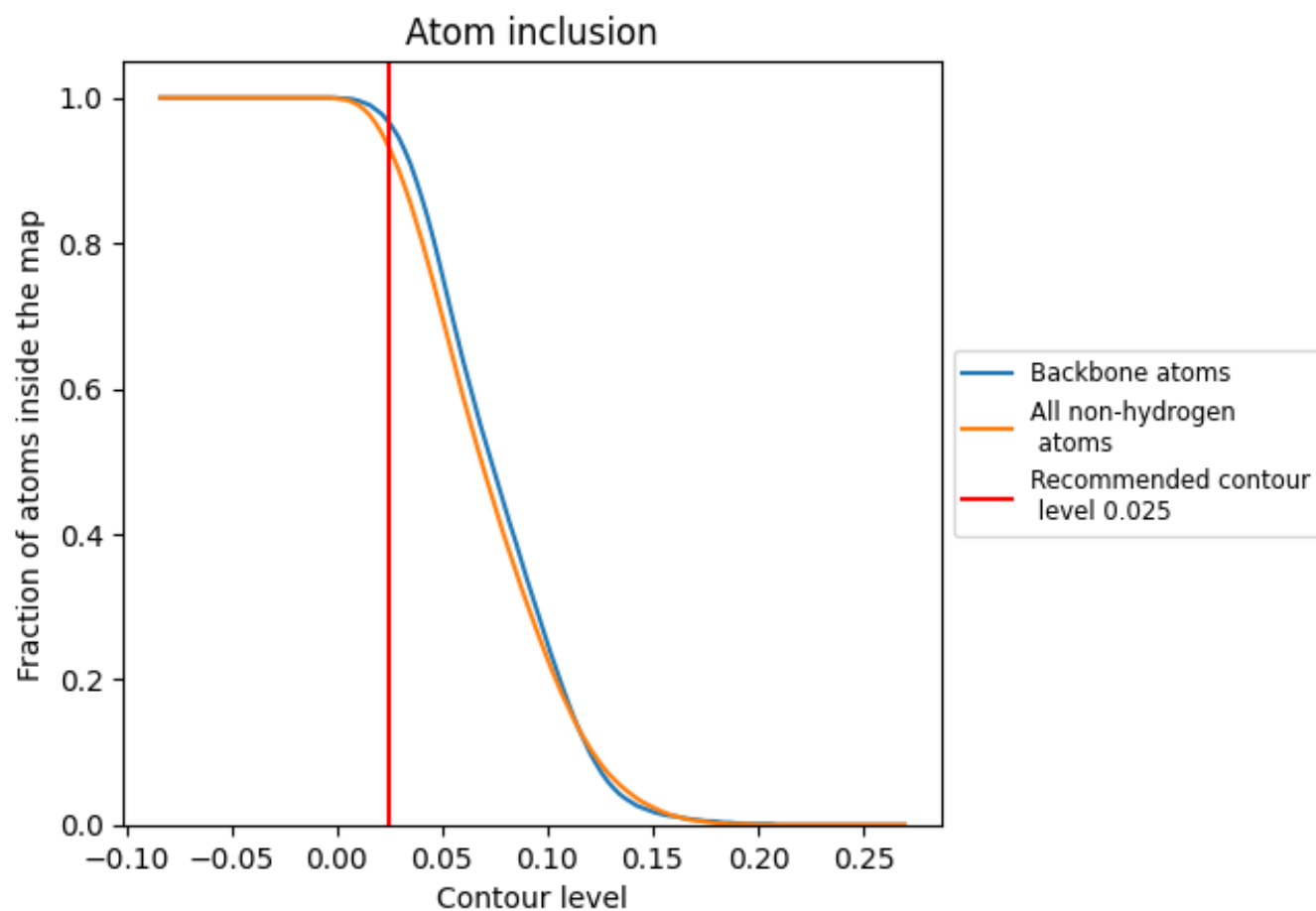
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9300   |  0.5130   |
| CA    |  0.4220   |  0.3300   |
| CB    |  0.8160   |  0.4580   |
| CD    |  0.8530   |  0.4530   |
| CI    |  0.6570   |  0.4460   |
| Et    |  0.8780   |  0.4030   |
| L5    |  0.9760   |  0.5450   |
| L7    |  0.9960   |  0.5850   |
| L8    |  0.9880   |  0.5690   |
| LA    |  0.9850   |  0.6080   |
| LB    |  0.9510   |  0.5890   |
| LC    |  0.9600   |  0.5880   |
| LD    |  0.9490   |  0.5600   |
| LE    |  0.9190   |  0.5430   |
| LF    |  0.9730  |  0.5890  |
| LG    |  0.8970 |  0.5410 |
| LH    |  0.9470 |  0.5780 |
| LI    |  0.9580 |  0.5920 |
| LJ    |  0.8940 |  0.5340 |
| LL    |  0.9270 |  0.5630 |
| LM    |  0.9650 |  0.5790 |
| LN    |  0.9930 |  0.6140 |
| LO    |  0.9720 |  0.5930 |
| LP    |  0.9600 |  0.5990 |
| LQ    |  0.9790 |  0.6060 |
| LR    |  0.9050 |  0.5290 |
| LS    |  0.9770 |  0.5990 |
| LT    |  0.9450 |  0.5760 |
| LU    |  0.9160 |  0.5140 |
| LV    |  0.9640 |  0.5950 |
| LW    |  0.8050 |  0.4400 |
| LX    |  0.9470 |  0.5680 |
| LY    |  0.9530 |  0.5760 |
| LZ    |  0.9620 |  0.5640 |
| La    |  0.9770 |  0.6080 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Lb    |  0.9040   |  0.5290   |
| Lc    |  0.9180   |  0.5420   |
| Ld    |  0.9430   |  0.5770   |
| Le    |  0.9800   |  0.6060   |
| Lf    |  0.9830   |  0.6070   |
| Lg    |  0.9510   |  0.5800   |
| Lh    |  0.9450   |  0.5700   |
| Li    |  0.9460   |  0.5640   |
| Lj    |  0.9900   |  0.6020   |
| Lk    |  0.9070   |  0.5350   |
| Ll    |  0.9840   |  0.5900   |
| Lm    |  0.9520   |  0.5910   |
| Ln    |  0.9470   |  0.5770   |
| Lo    |  0.9440   |  0.5850   |
| Lp    |  0.9520   |  0.5890   |
| Lr    |  0.9750   |  0.5920   |
| Ls    |  0.8370   |  0.4100   |
| Lt    |  0.6050  |  0.2490  |
| S2    |  0.9630 |  0.4660 |
| SA    |  0.8410 |  0.4470 |
| SB    |  0.7970 |  0.4050 |
| SC    |  0.9250 |  0.5140 |
| SD    |  0.8510 |  0.4630 |
| SE    |  0.8970 |  0.4650 |
| SF    |  0.8230 |  0.4320 |
| SG    |  0.7700 |  0.3180 |
| SH    |  0.7780 |  0.3650 |
| SI    |  0.8620 |  0.4530 |
| SJ    |  0.8980 |  0.4720 |
| SK    |  0.8520 |  0.4430 |
| SL    |  0.8630 |  0.4860 |
| SM    |  0.6890 |  0.3090 |
| SN    |  0.8870 |  0.4870 |
| SO    |  0.8450 |  0.4380 |
| SP    |  0.8670 |  0.4760 |
| SQ    |  0.8520 |  0.4400 |
| SR    |  0.8230 |  0.4250 |
| SS    |  0.8240 |  0.4450 |
| ST    |  0.8730 |  0.4430 |
| SU    |  0.8380 |  0.4430 |
| SV    |  0.8780 |  0.4700 |
| SW    |  0.9290 |  0.5140 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| SX    |  0.8990 |  0.5270 |
| SY    |  0.8060 |  0.3830 |
| SZ    |  0.7560 |  0.3900 |
| Sa    |  0.8820 |  0.4920 |
| Sb    |  0.8390 |  0.4370 |
| Sc    |  0.7980 |  0.4310 |
| Sd    |  0.9360 |  0.5200 |
| Se    |  0.8240 |  0.4500 |
| Sf    |  0.7360 |  0.3330 |
| Sg    |  0.8030 |  0.3750 |