



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 05:51 AM EST

PDB ID : 6W6P  
EMDB ID : EMD-21562  
Title : MultiBody Refinement of 70S Ribosome from *Enterococcus faecalis*  
Authors : Jogl, G.; Khayat, R.  
Deposited on : 2020-03-17  
Resolution : 2.90 Å (reported)  
Based on initial models : 4YBB, 5LI0

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

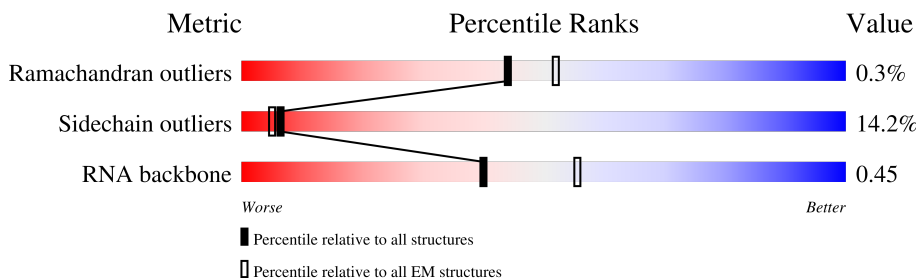
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |
| RNA backbone          | 4643                        | 859                         |

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   | a     | 1548   |                  |
| 2   | c     | 204    |                  |
| 3   | d     | 201    |                  |
| 4   | e     | 163    |                  |
| 5   | f     | 97     |                  |
| 6   | g     | 154    |                  |
| 7   | h     | 131    |                  |
| 8   | i     | 128    |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 9   | j     | 99     | <div> <div>42%</div> <div>90%</div> <div>10%</div> </div> |
| 10  | k     | 117    | <div> <div>40%</div> <div>88%</div> <div>12%</div> </div> |
| 11  | l     | 136    | <div> <div>10%</div> <div>79%</div> <div>20%</div> </div> |
| 12  | m     | 112    | <div> <div>42%</div> <div>86%</div> <div>12%</div> </div> |
| 13  | n     | 60     | <div> <div>98%</div> </div>                               |
| 14  | o     | 88     | <div> <div>14%</div> <div>83%</div> <div>16%</div> </div> |
| 15  | p     | 89     | <div> <div>6%</div> <div>88%</div> <div>12%</div> </div>  |
| 16  | q     | 83     | <div> <div>18%</div> <div>84%</div> <div>16%</div> </div> |
| 17  | r     | 66     | <div> <div>21%</div> <div>91%</div> <div>8%</div> </div>  |
| 18  | s     | 78     | <div> <div>12%</div> <div>82%</div> <div>17%</div> </div> |
| 19  | t     | 82     | <div> <div>13%</div> <div>88%</div> <div>12%</div> </div> |
| 20  | A     | 2908   | <div> <div>70%</div> <div>22%</div> <div>6%</div> </div>  |
| 21  | B     | 116    | <div> <div>6%</div> <div>66%</div> <div>33%</div> </div>  |
| 22  | C     | 275    | <div> <div>93%</div> <div>7%</div> </div>                 |
| 23  | D     | 207    | <div> <div>85%</div> <div>14%</div> </div>                |
| 24  | E     | 206    | <div> <div>85%</div> <div>15%</div> </div>                |
| 25  | F     | 177    | <div> <div>55%</div> <div>86%</div> <div>14%</div> </div> |
| 26  | G     | 176    | <div> <div>30%</div> <div>86%</div> <div>14%</div> </div> |
| 27  | K     | 145    | <div> <div>88%</div> <div>12%</div> </div>                |
| 28  | L     | 122    | <div> <div>89%</div> <div>11%</div> </div>                |
| 29  | M     | 146    | <div> <div>5%</div> <div>93%</div> <div>5%</div> </div>   |
| 30  | N     | 141    | <div> <div>10%</div> <div>89%</div> <div>11%</div> </div> |
| 31  | O     | 124    | <div> <div>6%</div> <div>86%</div> <div>14%</div> </div>  |
| 32  | P     | 117    | <div> <div>14%</div> <div>90%</div> <div>10%</div> </div> |
| 33  | Q     | 114    | <div> <div>88%</div> <div>12%</div> </div>                |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | R     | 118    |  93% 6%      |
| 35  | S     | 102    |  88% 12%     |
| 36  | T     | 112    |  87% 13%     |
| 37  | U     | 89     |  84% 15%     |
| 38  | V     | 101    |  29% 85% 15% |
| 39  | X     | 76     |  83% 17%     |
| 40  | Y     | 54     |  7% 80% 20%  |
| 41  | Z     | 61     |  10% 84% 16% |
| 42  | 0     | 58     |  91% 9%      |
| 43  | 2     | 56     |  88% 12%     |
| 44  | 3     | 49     |  12% 94% 6%  |
| 45  | 4     | 44     |  89% 11%   |
| 46  | 5     | 64     |  89% 11%   |
| 47  | 6     | 38     |  87% 13%   |

## 2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 133554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | a     | 1523     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32646 | 14564 | 5967 | 10592 | 1523 |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | c     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1610  | 1012 | 303 | 292 | 3 |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | d     | 201      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1620  | 1016 | 303 | 297 | 4 |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | e     | 163      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1204  | 759 | 222 | 221 | 2 |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | f     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 795   | 501 | 137 | 154 | 3 |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | g     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1229  | 765 | 236 | 222 | 6 |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | h     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1041  | 662 | 184 | 193 | 2 |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | i     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 990   | 615 | 197 | 177 | 1 |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | j     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 800   | 504 | 147 | 147 | 2 |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | k     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 863   | 533 | 165 | 161 | 4 |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | l     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1065  | 661 | 214 | 188 | 2 |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | m     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 870   | 531 | 178 | 160 | 1 |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 13  | n     | 60       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 492   | 310 | 100 | 77 | 5 |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | o     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 455 | 152 | 133 | 1 |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | p     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 448 | 131 | 127 | 2 |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | q     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 681   | 427 | 127 | 124 | 3 |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | r     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 537   | 343 | 99 | 94 | 1 |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | s     | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 634   | 410 | 113 | 109 | 2 |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | t     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 377 | 120 | 118 | 2 |         |       |

- Molecule 20 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 20  | A     | 2739     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 58793 | 26244 | 10818 | 18992 | 2739 |         |       |

- Molecule 21 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 21  | B     | 116      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2480  | 1106 | 444 | 814 | 116 |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | C     | 275      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2115  | 1311 | 416 | 381 | 7 |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | D     | 207      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1579  | 994 | 292 | 289 | 4 |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | E     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1574  | 984 | 290 | 298 | 2 |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | F     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1392  | 887 | 239 | 260 | 6 |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | G     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1345  | 842 | 244 | 255 | 4 |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | K     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1130  | 714 | 205 | 207 | 4 |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L14.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | L     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 922   | 574 | 176 | 170 | 2 |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | M     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1095  | 677 | 212 | 205 | 1 |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | N     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1118  | 710 | 216 | 185 | 7 |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | O     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 991   | 612 | 191 | 185 | 3 |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | P     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 899   | 556 | 175 | 167 | 1 |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 33  | Q     | 114      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 924   | 582 | 185 | 157 |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | R     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 602 | 184 | 160 | 4 |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | S     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 500 | 139 | 143 | 2 |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | T     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 849   | 532 | 156 | 159 | 2 |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | U     | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 720   | 458 | 127 | 132 | 3 |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | V     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 763   | 486 | 135 | 140 | 2 |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39  | X     | 76       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 572   | 351 | 109 | 112 |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | Y     | 54       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 425   | 265 | 86 | 72 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| Y     | 51      | ALA      | THR    | conflict | UNP A0A1B4XRZ8 |

- Molecule 41 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | Z     | 61       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 504   | 314 | 94 | 95 | 1 |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 42  | 0     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 435   | 271 | 81 | 82 | 1 |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 43  | 2     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 262 | 88 | 73 | 6 |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | 3     | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 253 | 86 | 76 | 4 |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 45  | 4     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 374   | 227 | 91 | 54 | 2 |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 46  | 5     | 64       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 522   | 320 | 122 | 78 | 2 |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47  | 6     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 304   | 188 | 66 | 44 | 6 |         |       |

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 48  | n     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 48  | 2     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 48  | 3     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 48  | 6     | 1        | Total<br>1 | Zn<br>1 | 0       |

### 3 Residue-property plots

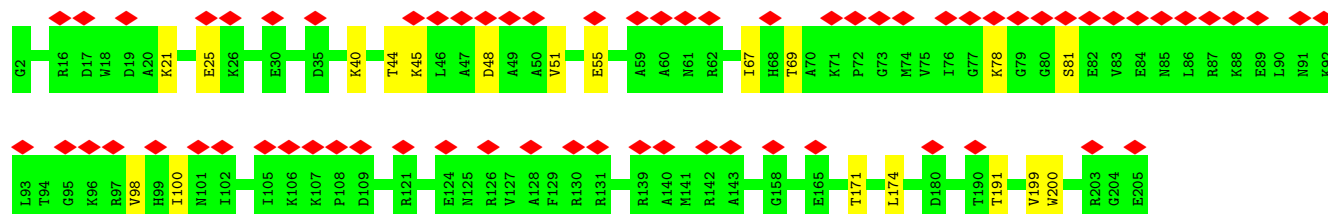
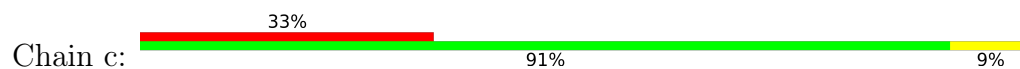
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

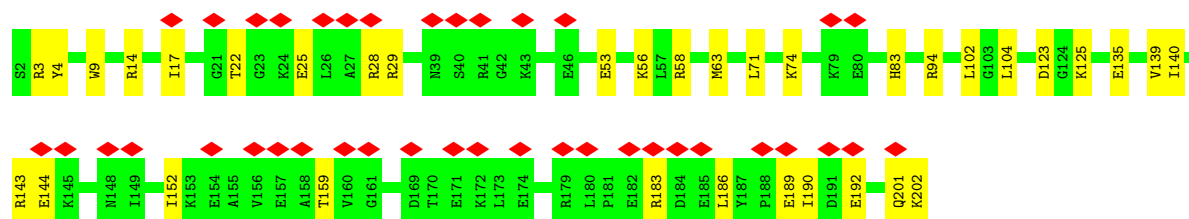
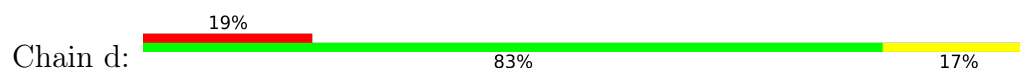




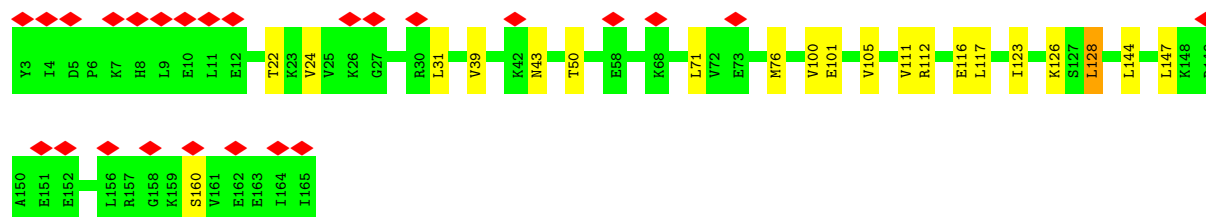
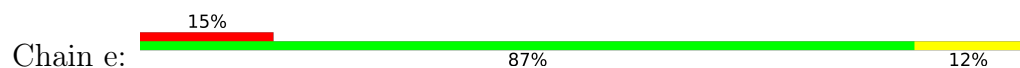
• Molecule 2: 30S ribosomal protein S3



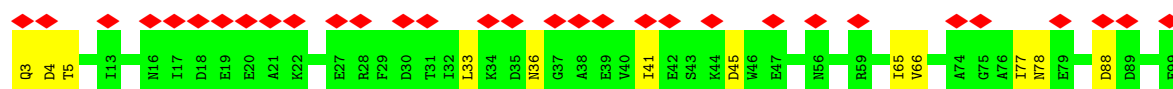
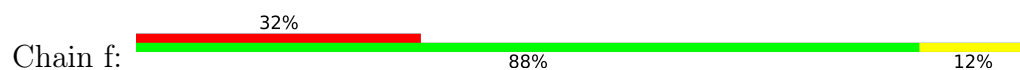
• Molecule 3: 30S ribosomal protein S4



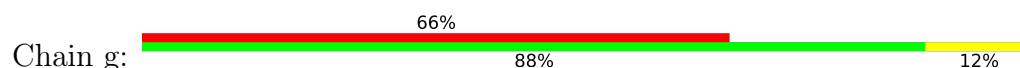
• Molecule 4: 30S ribosomal protein S5

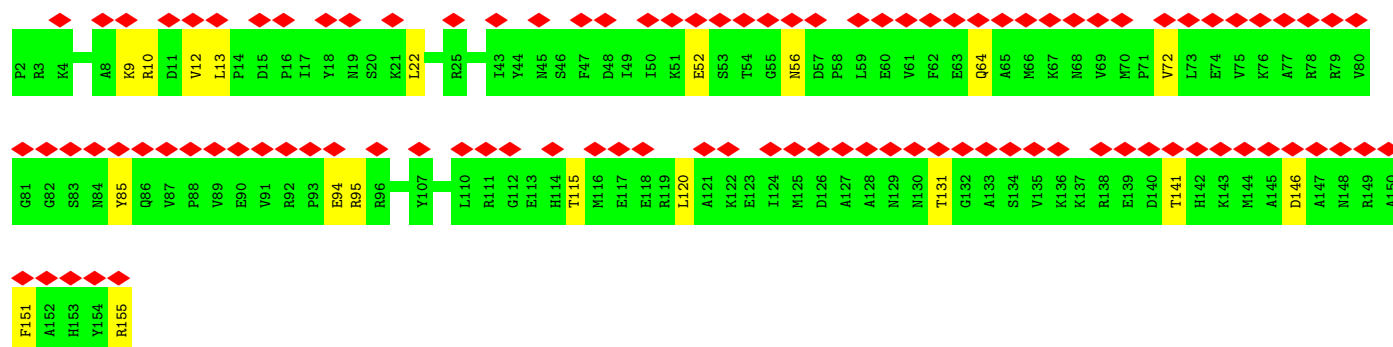


• Molecule 5: 30S ribosomal protein S6

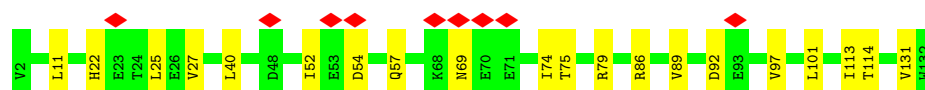
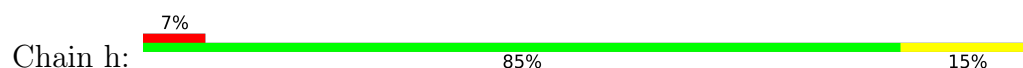


• Molecule 6: 30S ribosomal protein S7

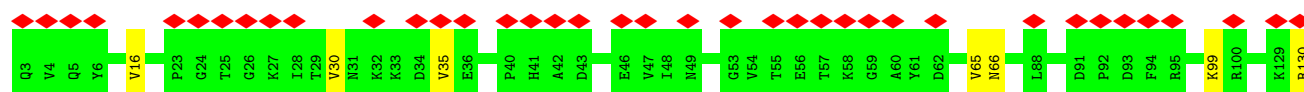




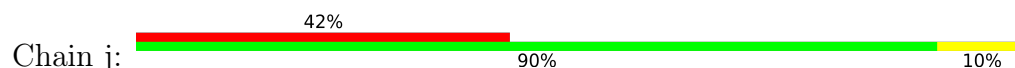
- Molecule 7: 30S ribosomal protein S8



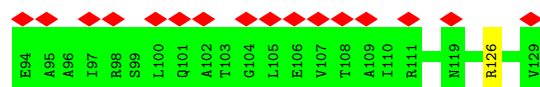
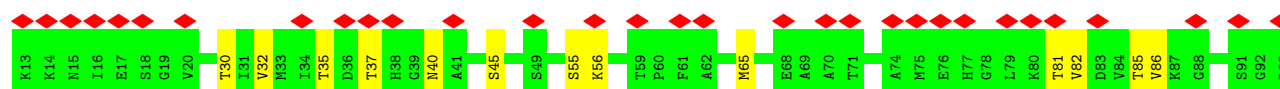
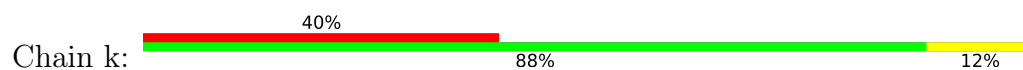
- Molecule 8: 30S ribosomal protein S9



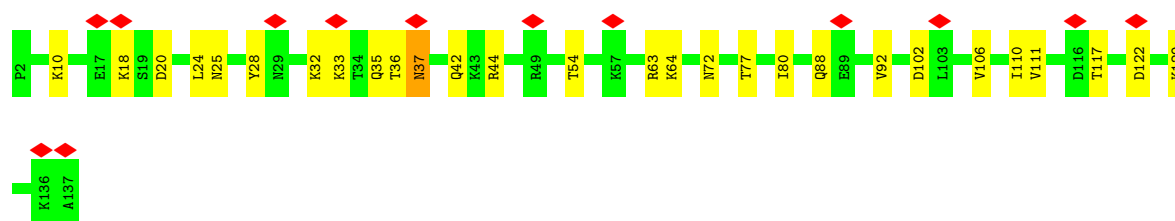
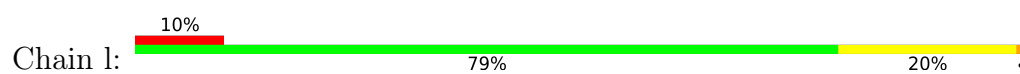
- Molecule 9: 30S ribosomal protein S10



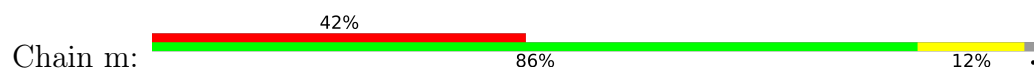
- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12



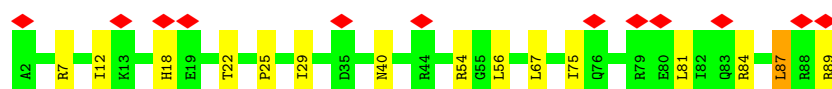
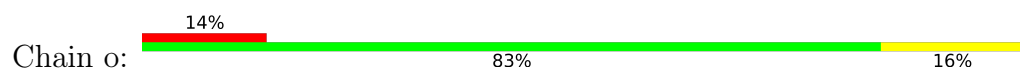
- Molecule 12: 30S ribosomal protein S13



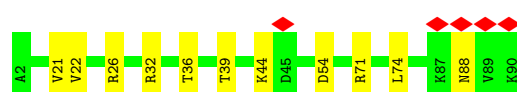
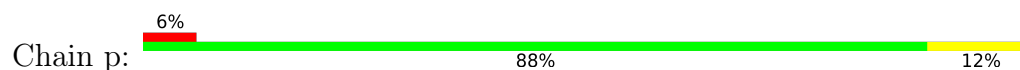
- Molecule 13: 30S ribosomal protein S14 type Z



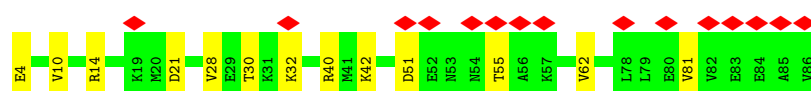
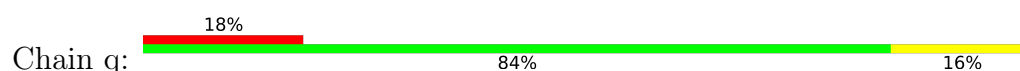
- Molecule 14: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S16

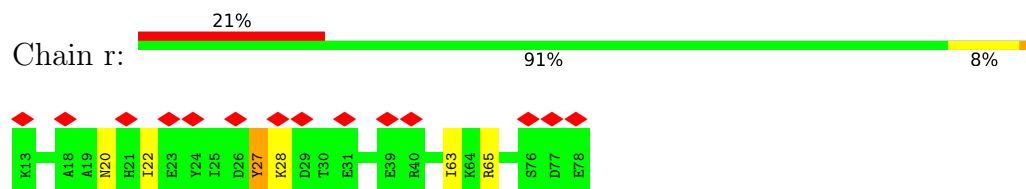


- Molecule 16: 30S ribosomal protein S17

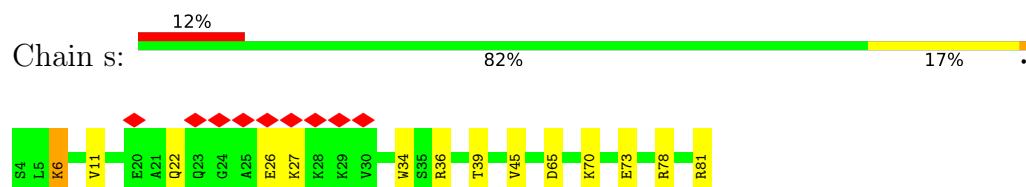




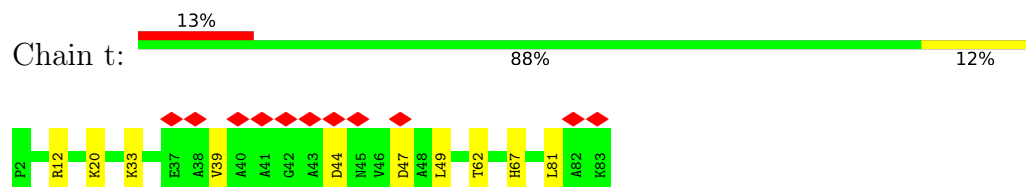
- Molecule 17: 30S ribosomal protein S18



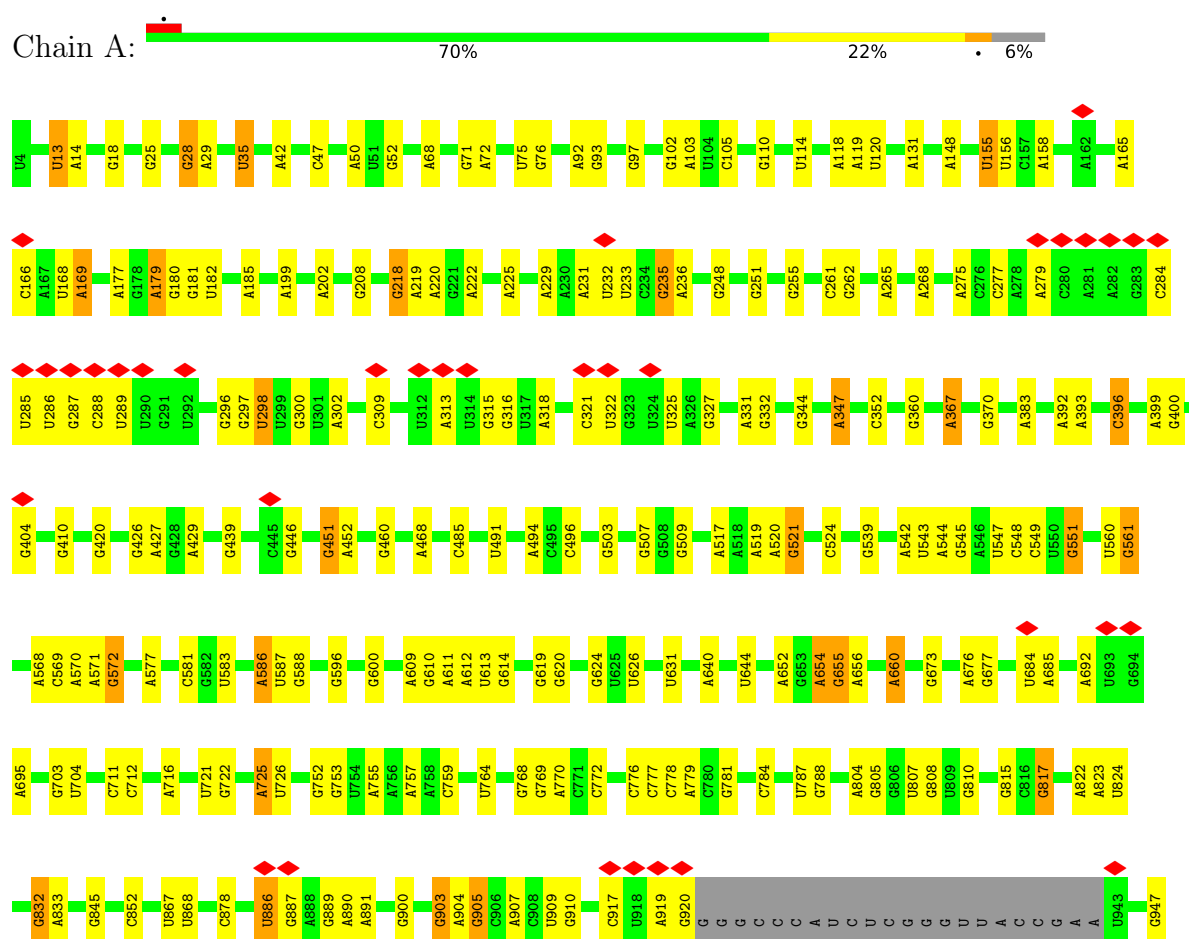
- Molecule 18: 30S ribosomal protein S19



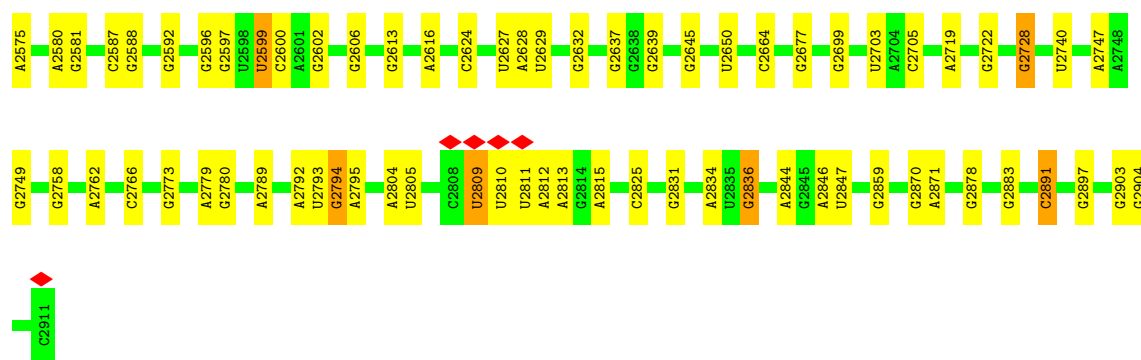
- Molecule 19: 30S ribosomal protein S20



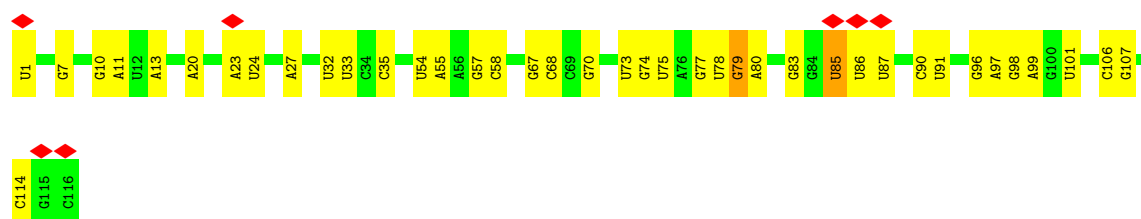
- Molecule 20: 23S rRNA







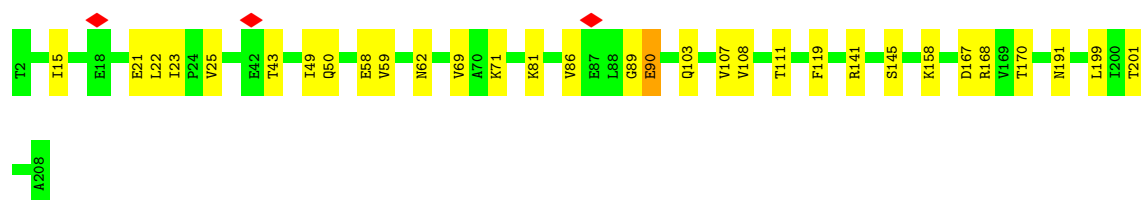
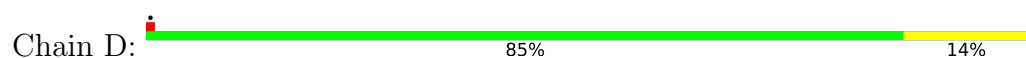
• Molecule 21: 5S rRNA



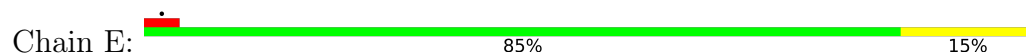
• Molecule 22: 50S ribosomal protein L2



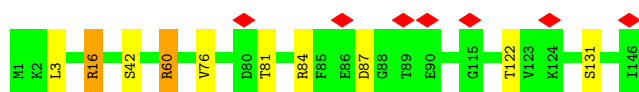
• Molecule 23: 50S ribosomal protein L3



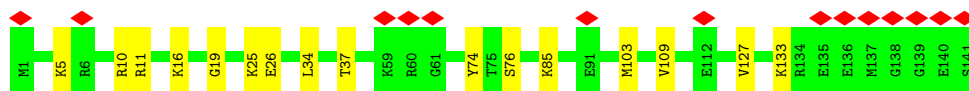
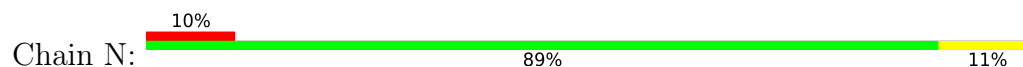
• Molecule 24: 50S ribosomal protein L4



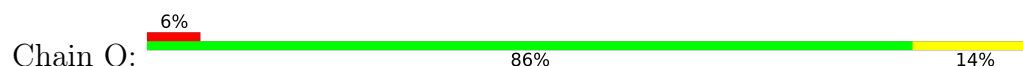




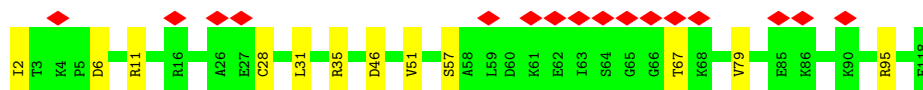
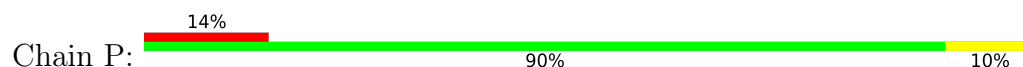
- Molecule 30: 50S ribosomal protein L16



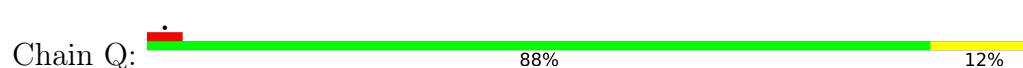
- Molecule 31: 50S ribosomal protein L17



- Molecule 32: 50S ribosomal protein L18



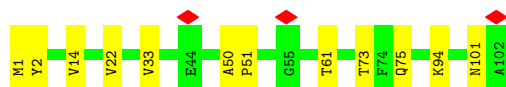
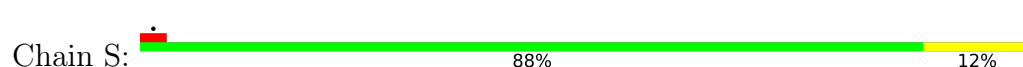
- Molecule 33: 50S ribosomal protein L19



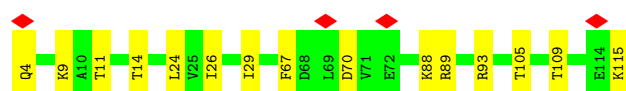
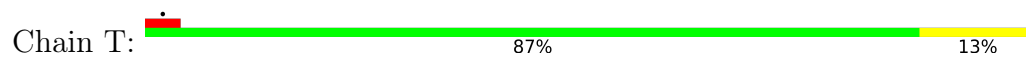
- Molecule 34: 50S ribosomal protein L20



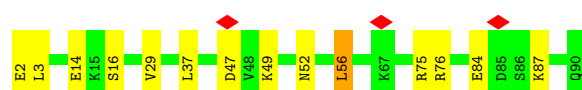
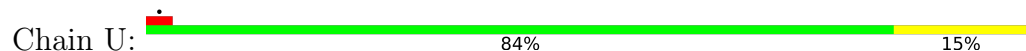
- Molecule 35: 50S ribosomal protein L21



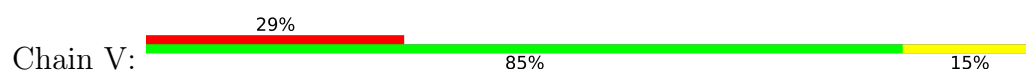
- Molecule 36: 50S ribosomal protein L22



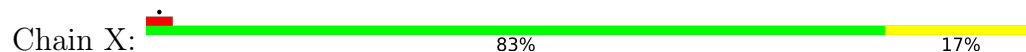
- Molecule 37: 50S ribosomal protein L23



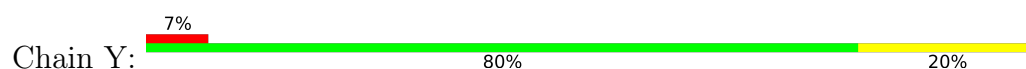
- Molecule 38: 50S ribosomal protein L24



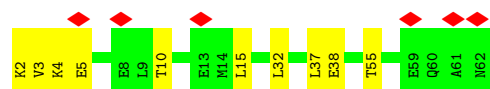
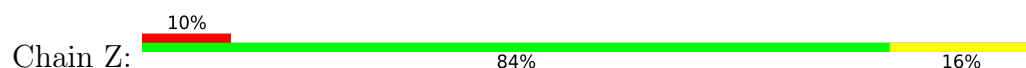
- Molecule 39: 50S ribosomal protein L27



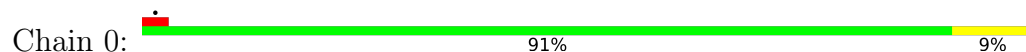
- Molecule 40: 50S ribosomal protein L28




- Molecule 41: 50S ribosomal protein L29



- Molecule 42: 50S ribosomal protein L30



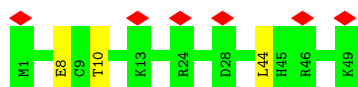
- Molecule 43: 50S ribosomal protein L32

Chain 2:  88% 12%




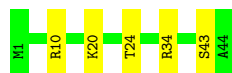
- Molecule 44: 50S ribosomal protein L33

Chain 3:  12% 94% 6%




- Molecule 45: 50S ribosomal protein L34

Chain 4:  89% 11%



- Molecule 46: 50S ribosomal protein L35

Chain 5:  89% 11%



- Molecule 47: 50S ribosomal protein L36

Chain 6:  87% 13%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 335675                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k)              | Depositor |
| Maximum map value                    | 0.226                                   | Depositor |
| Minimum map value                    | -0.019                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.035                                   | Depositor |
| Map size (Å)                         | 482.68, 482.68, 482.68                  | wwPDB     |
| Map dimensions                       | 440, 440, 440                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.097, 1.097, 1.097                     | Depositor |



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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   | a     | 0.99         | 1/36547 (0.0%)  | 1.05        | 56/57003 (0.1%)   |
| 2   | c     | 0.36         | 0/1635          | 0.49        | 0/2197            |
| 3   | d     | 0.44         | 0/1650          | 0.58        | 0/2217            |
| 4   | e     | 0.41         | 0/1217          | 0.56        | 1/1641 (0.1%)     |
| 5   | f     | 0.38         | 0/807           | 0.52        | 0/1087            |
| 6   | g     | 0.33         | 0/1249          | 0.47        | 0/1682            |
| 7   | h     | 0.48         | 0/1054          | 0.57        | 0/1417            |
| 8   | i     | 0.41         | 0/1003          | 0.51        | 0/1343            |
| 9   | j     | 0.36         | 0/812           | 0.57        | 0/1093            |
| 10  | k     | 0.34         | 0/878           | 0.56        | 0/1185            |
| 11  | l     | 0.49         | 0/1082          | 0.61        | 0/1453            |
| 12  | m     | 0.36         | 0/875           | 0.56        | 0/1173            |
| 13  | n     | 0.42         | 0/504           | 0.49        | 0/669             |
| 14  | o     | 0.44         | 0/751           | 0.58        | 1/1001 (0.1%)     |
| 15  | p     | 0.54         | 0/720           | 0.58        | 0/966             |
| 16  | q     | 0.47         | 0/689           | 0.58        | 0/920             |
| 17  | r     | 0.44         | 0/544           | 0.54        | 0/728             |
| 18  | s     | 0.45         | 0/650           | 0.53        | 0/872             |
| 19  | t     | 0.39         | 0/620           | 0.54        | 0/829             |
| 20  | A     | 1.21         | 32/65858 (0.0%) | 1.30        | 435/102721 (0.4%) |
| 21  | B     | 0.97         | 1/2773 (0.0%)   | 1.23        | 23/4320 (0.5%)    |
| 22  | C     | 0.55         | 0/2150          | 0.68        | 0/2892            |
| 23  | D     | 0.54         | 0/1601          | 0.67        | 0/2150            |
| 24  | E     | 0.52         | 0/1596          | 0.63        | 0/2159            |
| 25  | F     | 0.36         | 0/1411          | 0.58        | 1/1897 (0.1%)     |
| 26  | G     | 0.39         | 0/1365          | 0.57        | 0/1839            |
| 27  | K     | 0.53         | 0/1151          | 0.68        | 2/1554 (0.1%)     |
| 28  | L     | 0.51         | 0/929           | 0.65        | 1/1247 (0.1%)     |
| 29  | M     | 0.52         | 1/1105 (0.1%)   | 0.64        | 0/1474            |
| 30  | N     | 0.49         | 0/1141          | 0.61        | 0/1519            |
| 31  | O     | 0.55         | 0/1000          | 0.71        | 1/1341 (0.1%)     |
| 32  | P     | 0.47         | 0/908           | 0.64        | 0/1216            |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 33  | Q     | 0.56         | 0/938            | 0.63        | 0/1262            |
| 34  | R     | 0.59         | 0/963            | 0.64        | 2/1280 (0.2%)     |
| 35  | S     | 0.54         | 0/796            | 0.62        | 0/1068            |
| 36  | T     | 0.49         | 0/858            | 0.64        | 1/1157 (0.1%)     |
| 37  | U     | 0.50         | 0/727            | 0.65        | 1/972 (0.1%)      |
| 38  | V     | 0.46         | 0/772            | 0.63        | 0/1035            |
| 39  | X     | 0.56         | 0/578            | 0.61        | 0/773             |
| 40  | Y     | 0.57         | 1/431 (0.2%)     | 0.60        | 0/574             |
| 41  | Z     | 0.42         | 0/505            | 0.57        | 0/672             |
| 42  | 0     | 0.47         | 0/437            | 0.63        | 0/589             |
| 43  | 2     | 0.55         | 0/436            | 0.63        | 0/578             |
| 44  | 3     | 0.46         | 0/423            | 0.60        | 0/563             |
| 45  | 4     | 0.48         | 0/377            | 0.61        | 0/491             |
| 46  | 5     | 0.43         | 0/528            | 0.62        | 0/689             |
| 47  | 6     | 0.47         | 0/309            | 0.67        | 0/409             |
| All | All   | 1.00         | 36/145353 (0.0%) | 1.10        | 525/217917 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | h     | 0                   | 1                   |
| 11  | l     | 0                   | 1                   |
| 18  | s     | 0                   | 1                   |
| 23  | D     | 0                   | 1                   |
| 30  | N     | 0                   | 2                   |
| 31  | O     | 0                   | 2                   |
| 35  | S     | 0                   | 1                   |
| 36  | T     | 0                   | 1                   |
| 38  | V     | 0                   | 1                   |
| All | All   | 0                   | 11                  |

All (36) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 20  | A     | 903  | G    | C6-N1 | -11.86 | 1.31        | 1.39     |
| 21  | B     | 1    | U    | OP3-P | -10.45 | 1.48        | 1.61     |
| 20  | A     | 769  | G    | N9-C4 | -8.64  | 1.31        | 1.38     |
| 20  | A     | 1492 | G    | N9-C4 | -8.09  | 1.31        | 1.38     |
| 20  | A     | 956  | C    | N3-C4 | -7.24  | 1.28        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 20  | A     | 2836 | G    | N9-C4 | -7.18 | 1.32        | 1.38     |
| 40  | Y     | 19   | SER  | CA-CB | -7.15 | 1.42        | 1.52     |
| 20  | A     | 956  | C    | C4-N4 | -7.06 | 1.27        | 1.33     |
| 29  | M     | 60   | ARG  | C-N   | -6.82 | 1.18        | 1.34     |
| 20  | A     | 2444 | A    | N9-C4 | -6.65 | 1.33        | 1.37     |
| 20  | A     | 2044 | A    | N3-C4 | -6.53 | 1.30        | 1.34     |
| 20  | A     | 769  | G    | C2-N3 | -6.40 | 1.27        | 1.32     |
| 20  | A     | 1490 | A    | N9-C4 | -6.38 | 1.34        | 1.37     |
| 20  | A     | 769  | G    | N3-C4 | -6.37 | 1.30        | 1.35     |
| 20  | A     | 660  | A    | N9-C4 | -6.22 | 1.34        | 1.37     |
| 20  | A     | 660  | A    | N3-C4 | -6.11 | 1.31        | 1.34     |
| 20  | A     | 509  | G    | N9-C4 | -5.91 | 1.33        | 1.38     |
| 20  | A     | 1288 | A    | N3-C4 | -5.89 | 1.31        | 1.34     |
| 20  | A     | 2287 | A    | N3-C4 | -5.86 | 1.31        | 1.34     |
| 20  | A     | 903  | G    | C6-O6 | -5.83 | 1.19        | 1.24     |
| 20  | A     | 1571 | G    | N3-C4 | -5.73 | 1.31        | 1.35     |
| 20  | A     | 1337 | A    | N9-C4 | -5.54 | 1.34        | 1.37     |
| 20  | A     | 2606 | G    | C8-N7 | -5.46 | 1.27        | 1.30     |
| 20  | A     | 2007 | U    | C2-N3 | -5.27 | 1.34        | 1.37     |
| 20  | A     | 660  | A    | C5-C6 | -5.26 | 1.36        | 1.41     |
| 1   | a     | 183  | G    | N9-C4 | -5.25 | 1.33        | 1.38     |
| 20  | A     | 2728 | G    | C8-N7 | -5.21 | 1.27        | 1.30     |
| 20  | A     | 539  | G    | N9-C4 | -5.21 | 1.33        | 1.38     |
| 20  | A     | 275  | A    | N9-C4 | -5.18 | 1.34        | 1.37     |
| 20  | A     | 2444 | A    | N3-C4 | -5.18 | 1.31        | 1.34     |
| 20  | A     | 903  | G    | C5-C6 | -5.17 | 1.37        | 1.42     |
| 20  | A     | 1592 | G    | N9-C4 | -5.13 | 1.33        | 1.38     |
| 20  | A     | 1506 | A    | N9-C4 | -5.11 | 1.34        | 1.37     |
| 20  | A     | 2836 | G    | N3-C4 | -5.08 | 1.31        | 1.35     |
| 20  | A     | 1404 | G    | C6-N1 | -5.07 | 1.36        | 1.39     |
| 20  | A     | 2006 | G    | C8-N7 | -5.00 | 1.27        | 1.30     |

All (525) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 20  | A     | 956  | C    | N3-C4-N4 | -30.89 | 96.38       | 118.00   |
| 20  | A     | 956  | C    | C5-C4-N4 | 25.47  | 138.03      | 120.20   |
| 20  | A     | 903  | G    | N1-C6-O6 | -24.12 | 105.42      | 119.90   |
| 20  | A     | 903  | G    | C5-C6-O6 | 22.01  | 141.81      | 128.60   |
| 20  | A     | 1591 | A    | N1-C6-N6 | -15.79 | 109.12      | 118.60   |
| 20  | A     | 769  | G    | N3-C4-N9 | -14.07 | 117.56      | 126.00   |
| 20  | A     | 769  | G    | N3-C4-C5 | 13.80  | 135.50      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 20  | A     | 1492 | G    | N3-C4-C5   | 13.01  | 135.10      | 128.60   |
| 20  | A     | 2287 | A    | N7-C8-N9   | 12.67  | 120.14      | 113.80   |
| 20  | A     | 769  | G    | C2-N3-C4   | -12.50 | 105.65      | 111.90   |
| 1   | a     | 35   | G    | O5'-P-OP1  | -12.49 | 94.45       | 105.70   |
| 20  | A     | 1492 | G    | N3-C4-N9   | -12.02 | 118.79      | 126.00   |
| 20  | A     | 2287 | A    | C8-N9-C4   | -10.74 | 101.50      | 105.80   |
| 21  | B     | 85   | U    | C5-C6-N1   | 10.49  | 127.94      | 122.70   |
| 20  | A     | 903  | G    | C4-C5-N7   | 10.31  | 114.92      | 110.80   |
| 20  | A     | 2836 | G    | N3-C4-C5   | 10.05  | 133.62      | 128.60   |
| 20  | A     | 2836 | G    | N3-C4-N9   | -9.96  | 120.03      | 126.00   |
| 20  | A     | 903  | G    | C4-N9-C1'  | 9.85   | 139.30      | 126.50   |
| 20  | A     | 903  | G    | C8-N9-C1'  | -9.71  | 114.38      | 127.00   |
| 20  | A     | 956  | C    | C4-C5-C6   | -9.64  | 112.58      | 117.40   |
| 20  | A     | 1591 | A    | C2-N3-C4   | 9.62   | 115.41      | 110.60   |
| 20  | A     | 2287 | A    | C5-N7-C8   | -9.53  | 99.14       | 103.90   |
| 20  | A     | 2420 | C    | O5'-P-OP2  | -9.48  | 97.16       | 105.70   |
| 20  | A     | 769  | G    | N3-C2-N2   | -9.29  | 113.40      | 119.90   |
| 20  | A     | 1505 | C    | N3-C2-O2   | -9.22  | 115.44      | 121.90   |
| 20  | A     | 956  | C    | N3-C4-C5   | 9.19   | 125.58      | 121.90   |
| 20  | A     | 1592 | G    | N3-C4-C5   | 9.15   | 133.18      | 128.60   |
| 20  | A     | 1551 | U    | C2-N1-C1'  | 9.11   | 128.63      | 117.70   |
| 20  | A     | 903  | G    | N9-C4-C5   | -9.05  | 101.78      | 105.40   |
| 20  | A     | 1288 | A    | C2-N3-C4   | -8.96  | 106.12      | 110.60   |
| 20  | A     | 1167 | A    | C8-N9-C4   | -8.94  | 102.22      | 105.80   |
| 20  | A     | 2836 | G    | C5-N7-C8   | -8.90  | 99.85       | 104.30   |
| 20  | A     | 2454 | C    | O4'-C1'-N1 | 8.86   | 115.29      | 108.20   |
| 20  | A     | 655  | G    | C8-N9-C4   | 8.84   | 109.94      | 106.40   |
| 20  | A     | 551  | G    | O4'-C1'-N9 | 8.80   | 115.24      | 108.20   |
| 20  | A     | 2287 | A    | C2-N3-C4   | -8.56  | 106.32      | 110.60   |
| 20  | A     | 2836 | G    | C2-N3-C4   | -8.49  | 107.66      | 111.90   |
| 20  | A     | 1592 | G    | N3-C4-N9   | -8.33  | 121.00      | 126.00   |
| 20  | A     | 1167 | A    | N7-C8-N9   | 8.25   | 117.92      | 113.80   |
| 20  | A     | 509  | G    | C5-N7-C8   | -8.17  | 100.21      | 104.30   |
| 1   | a     | 183  | G    | N3-C4-N9   | -8.13  | 121.12      | 126.00   |
| 20  | A     | 1902 | G    | C8-N9-C4   | -8.11  | 103.16      | 106.40   |
| 20  | A     | 1571 | G    | N3-C2-N2   | -8.08  | 114.24      | 119.90   |
| 20  | A     | 2836 | G    | N7-C8-N9   | 7.98   | 117.09      | 113.10   |
| 20  | A     | 344  | G    | C4-N9-C1'  | 7.97   | 136.86      | 126.50   |
| 20  | A     | 1394 | G    | C4-C5-N7   | 7.96   | 113.98      | 110.80   |
| 20  | A     | 1902 | G    | O4'-C1'-N9 | 7.82   | 114.46      | 108.20   |
| 20  | A     | 208  | G    | O4'-C1'-N9 | 7.82   | 114.45      | 108.20   |
| 20  | A     | 1434 | C    | C6-N1-C2   | -7.81  | 117.18      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 2287 | A    | N1-C2-N3   | 7.81  | 133.20      | 129.30   |
| 20  | A     | 1902 | G    | N7-C8-N9   | 7.80  | 117.00      | 113.10   |
| 20  | A     | 1591 | A    | C5-C6-N6   | 7.78  | 129.92      | 123.70   |
| 20  | A     | 660  | A    | N1-C6-N6   | 7.76  | 123.26      | 118.60   |
| 20  | A     | 903  | G    | N3-C4-N9   | 7.75  | 130.65      | 126.00   |
| 20  | A     | 344  | G    | N7-C8-N9   | 7.68  | 116.94      | 113.10   |
| 1   | a     | 183  | G    | N3-C4-C5   | 7.65  | 132.43      | 128.60   |
| 21  | B     | 77   | G    | C4-C5-N7   | 7.60  | 113.84      | 110.80   |
| 1   | a     | 255  | U    | O4'-C1'-N1 | 7.57  | 114.25      | 108.20   |
| 20  | A     | 711  | C    | C6-N1-C2   | -7.56 | 117.28      | 120.30   |
| 21  | B     | 96   | G    | C4-C5-N7   | 7.54  | 113.81      | 110.80   |
| 20  | A     | 509  | G    | N7-C8-N9   | 7.48  | 116.84      | 113.10   |
| 20  | A     | 275  | A    | N1-C2-N3   | 7.48  | 133.04      | 129.30   |
| 20  | A     | 1492 | G    | C2-N3-C4   | -7.47 | 108.16      | 111.90   |
| 20  | A     | 1490 | A    | C2-N3-C4   | -7.47 | 106.86      | 110.60   |
| 20  | A     | 1497 | U    | N3-C2-O2   | -7.46 | 116.97      | 122.20   |
| 1   | a     | 488  | C    | C6-N1-C2   | 7.45  | 123.28      | 120.30   |
| 20  | A     | 586  | A    | N1-C6-N6   | -7.44 | 114.14      | 118.60   |
| 20  | A     | 769  | G    | C8-N9-C1'  | 7.38  | 136.59      | 127.00   |
| 20  | A     | 2287 | A    | O4'-C1'-N9 | 7.37  | 114.09      | 108.20   |
| 1   | a     | 113  | G    | C4-C5-N7   | 7.36  | 113.74      | 110.80   |
| 20  | A     | 992  | G    | C8-N9-C1'  | -7.34 | 117.45      | 127.00   |
| 20  | A     | 1175 | C    | C6-N1-C2   | -7.34 | 117.37      | 120.30   |
| 20  | A     | 1591 | A    | C6-C5-N7   | 7.31  | 137.42      | 132.30   |
| 20  | A     | 2044 | A    | N7-C8-N9   | 7.29  | 117.45      | 113.80   |
| 20  | A     | 1492 | G    | C4-N9-C1'  | -7.24 | 117.08      | 126.50   |
| 21  | B     | 96   | G    | C5-N7-C8   | -7.23 | 100.69      | 104.30   |
| 20  | A     | 235  | G    | N7-C8-N9   | 7.22  | 116.71      | 113.10   |
| 20  | A     | 716  | A    | C2-N3-C4   | -7.21 | 107.00      | 110.60   |
| 20  | A     | 1489 | C    | C6-N1-C2   | -7.20 | 117.42      | 120.30   |
| 20  | A     | 2406 | A    | C2-N3-C4   | -7.16 | 107.02      | 110.60   |
| 20  | A     | 344  | G    | C6-C5-N7   | -7.15 | 126.11      | 130.40   |
| 20  | A     | 2556 | A    | C8-N9-C4   | -7.14 | 102.94      | 105.80   |
| 20  | A     | 769  | G    | C4-N9-C1'  | -7.13 | 117.23      | 126.50   |
| 20  | A     | 951  | A    | O4'-C1'-N9 | 7.11  | 113.89      | 108.20   |
| 20  | A     | 2226 | A    | C5-N7-C8   | -7.08 | 100.36      | 103.90   |
| 20  | A     | 235  | G    | C8-N9-C4   | -7.07 | 103.57      | 106.40   |
| 20  | A     | 1989 | G    | N7-C8-N9   | 7.07  | 116.63      | 113.10   |
| 20  | A     | 1699 | C    | C6-N1-C2   | -7.06 | 117.47      | 120.30   |
| 20  | A     | 485  | C    | C6-N1-C2   | -7.00 | 117.50      | 120.30   |
| 21  | B     | 96   | G    | C6-C5-N7   | -6.97 | 126.22      | 130.40   |
| 20  | A     | 992  | G    | O4'-C1'-N9 | 6.97  | 113.77      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 1022 | C    | C2-N1-C1'  | 6.96  | 126.45      | 118.80   |
| 21  | B     | 77   | G    | C5-N7-C8   | -6.94 | 100.83      | 104.30   |
| 20  | A     | 2226 | A    | N7-C8-N9   | 6.93  | 117.27      | 113.80   |
| 20  | A     | 344  | G    | C8-N9-C1'  | -6.93 | 118.00      | 127.00   |
| 20  | A     | 1489 | C    | N3-C2-O2   | -6.92 | 117.05      | 121.90   |
| 20  | A     | 1994 | G    | N3-C4-C5   | -6.89 | 125.15      | 128.60   |
| 21  | B     | 77   | G    | N7-C8-N9   | 6.89  | 116.55      | 113.10   |
| 20  | A     | 1505 | C    | C6-N1-C2   | -6.89 | 117.55      | 120.30   |
| 1   | a     | 277  | A    | N7-C8-N9   | 6.85  | 117.23      | 113.80   |
| 20  | A     | 1349 | U    | C2-N1-C1'  | 6.85  | 125.92      | 117.70   |
| 20  | A     | 1394 | G    | C6-C5-N7   | -6.80 | 126.32      | 130.40   |
| 20  | A     | 1989 | G    | C4-C5-N7   | 6.79  | 113.52      | 110.80   |
| 1   | a     | 34   | U    | P-O3'-C3'  | -6.76 | 111.59      | 119.70   |
| 20  | A     | 903  | G    | C6-C5-N7   | -6.75 | 126.35      | 130.40   |
| 20  | A     | 509  | G    | C2-N3-C4   | -6.74 | 108.53      | 111.90   |
| 1   | a     | 1482 | C    | N3-C2-O2   | -6.74 | 117.18      | 121.90   |
| 21  | B     | 77   | G    | C6-C5-N7   | -6.74 | 126.36      | 130.40   |
| 20  | A     | 344  | G    | C5-N7-C8   | -6.72 | 100.94      | 104.30   |
| 20  | A     | 509  | G    | N3-C4-C5   | 6.71  | 131.96      | 128.60   |
| 20  | A     | 2441 | C    | C6-N1-C2   | -6.70 | 117.62      | 120.30   |
| 20  | A     | 903  | G    | C5-N7-C8   | -6.67 | 100.96      | 104.30   |
| 21  | B     | 96   | G    | N7-C8-N9   | 6.67  | 116.44      | 113.10   |
| 1   | a     | 1176 | C    | C2-N1-C1'  | 6.67  | 126.13      | 118.80   |
| 1   | a     | 579  | U    | N3-C2-O2   | -6.66 | 117.54      | 122.20   |
| 20  | A     | 619  | G    | N3-C4-C5   | -6.64 | 125.28      | 128.60   |
| 1   | a     | 488  | C    | N3-C4-C5   | 6.62  | 124.55      | 121.90   |
| 20  | A     | 1492 | G    | C8-N9-C1'  | 6.62  | 135.61      | 127.00   |
| 20  | A     | 298  | U    | O4'-C1'-N1 | 6.57  | 113.45      | 108.20   |
| 25  | F     | 130  | LEU  | CA-CB-CG   | 6.56  | 130.39      | 115.30   |
| 20  | A     | 1551 | U    | N1-C2-O2   | 6.54  | 127.38      | 122.80   |
| 20  | A     | 1730 | G    | N3-C4-N9   | 6.54  | 129.93      | 126.00   |
| 20  | A     | 1989 | G    | C5-N7-C8   | -6.53 | 101.03      | 104.30   |
| 20  | A     | 2044 | A    | C8-N9-C4   | -6.53 | 103.19      | 105.80   |
| 20  | A     | 2044 | A    | C5-N7-C8   | -6.53 | 100.64      | 103.90   |
| 20  | A     | 1234 | C    | C6-N1-C2   | -6.51 | 117.70      | 120.30   |
| 20  | A     | 1591 | A    | C5-C6-N1   | 6.50  | 120.95      | 117.70   |
| 20  | A     | 2606 | G    | C4-N9-C1'  | 6.50  | 134.95      | 126.50   |
| 20  | A     | 1713 | C    | C6-N1-C2   | -6.50 | 117.70      | 120.30   |
| 20  | A     | 725  | A    | C8-N9-C4   | -6.49 | 103.21      | 105.80   |
| 20  | A     | 509  | G    | N3-C4-N9   | -6.48 | 122.11      | 126.00   |
| 20  | A     | 344  | G    | C4-C5-N7   | 6.47  | 113.39      | 110.80   |
| 20  | A     | 660  | A    | C5-N7-C8   | -6.47 | 100.66      | 103.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | a     | 113  | G    | C4-N9-C1'  | 6.47  | 134.91      | 126.50   |
| 20  | A     | 953  | C    | C6-N1-C2   | -6.47 | 117.71      | 120.30   |
| 20  | A     | 1229 | G    | N3-C4-N9   | 6.45  | 129.87      | 126.00   |
| 20  | A     | 2588 | G    | C8-N9-C4   | -6.44 | 103.82      | 106.40   |
| 20  | A     | 344  | G    | O4'-C1'-N9 | 6.44  | 113.35      | 108.20   |
| 21  | B     | 77   | G    | O4'-C1'-N9 | 6.43  | 113.34      | 108.20   |
| 20  | A     | 1989 | G    | C6-C5-N7   | -6.39 | 126.56      | 130.40   |
| 20  | A     | 169  | A    | O4'-C1'-N9 | 6.39  | 113.31      | 108.20   |
| 20  | A     | 2272 | C    | C6-N1-C2   | -6.39 | 117.75      | 120.30   |
| 20  | A     | 1996 | U    | C2-N1-C1'  | 6.37  | 125.35      | 117.70   |
| 21  | B     | 68   | C    | C2-N1-C1'  | 6.37  | 125.81      | 118.80   |
| 20  | A     | 1504 | G    | O4'-C1'-N9 | 6.37  | 113.30      | 108.20   |
| 20  | A     | 1360 | G    | C8-N9-C4   | -6.37 | 103.85      | 106.40   |
| 1   | a     | 586  | U    | N3-C2-O2   | -6.36 | 117.75      | 122.20   |
| 20  | A     | 1551 | U    | C6-N1-C1'  | -6.36 | 112.30      | 121.20   |
| 1   | a     | 113  | G    | C6-C5-N7   | -6.34 | 126.60      | 130.40   |
| 20  | A     | 1388 | U    | N3-C2-O2   | -6.33 | 117.77      | 122.20   |
| 20  | A     | 275  | A    | C2-N3-C4   | -6.33 | 107.44      | 110.60   |
| 20  | A     | 583  | U    | C5-C4-O4   | -6.33 | 122.10      | 125.90   |
| 20  | A     | 776  | C    | C6-N1-C2   | -6.33 | 117.77      | 120.30   |
| 20  | A     | 331  | A    | O4'-C1'-N9 | 6.32  | 113.25      | 108.20   |
| 20  | A     | 1364 | G    | C8-N9-C4   | -6.31 | 103.88      | 106.40   |
| 1   | a     | 776  | G    | N3-C4-N9   | 6.30  | 129.78      | 126.00   |
| 20  | A     | 992  | G    | C4-N9-C1'  | 6.30  | 134.69      | 126.50   |
| 20  | A     | 2277 | C    | C6-N1-C2   | -6.29 | 117.78      | 120.30   |
| 20  | A     | 509  | G    | O4'-C1'-N9 | 6.28  | 113.22      | 108.20   |
| 20  | A     | 2365 | G    | N3-C4-N9   | 6.27  | 129.76      | 126.00   |
| 20  | A     | 1397 | G    | N3-C4-N9   | 6.25  | 129.75      | 126.00   |
| 20  | A     | 28   | G    | O4'-C1'-N9 | 6.25  | 113.20      | 108.20   |
| 20  | A     | 2241 | A    | C8-N9-C4   | -6.24 | 103.30      | 105.80   |
| 20  | A     | 905  | G    | N3-C4-C5   | -6.22 | 125.49      | 128.60   |
| 20  | A     | 1394 | G    | C5-N7-C8   | -6.22 | 101.19      | 104.30   |
| 20  | A     | 1493 | C    | C6-N1-C2   | -6.21 | 117.82      | 120.30   |
| 20  | A     | 261  | C    | C6-N1-C2   | -6.21 | 117.82      | 120.30   |
| 20  | A     | 2794 | G    | C4-N9-C1'  | 6.20  | 134.56      | 126.50   |
| 20  | A     | 367  | A    | C5-N7-C8   | -6.18 | 100.81      | 103.90   |
| 20  | A     | 2226 | A    | C8-N9-C4   | -6.17 | 103.33      | 105.80   |
| 20  | A     | 1197 | G    | C4-N9-C1'  | 6.17  | 134.53      | 126.50   |
| 20  | A     | 2039 | C    | C6-N1-C2   | -6.17 | 117.83      | 120.30   |
| 20  | A     | 235  | G    | O4'-C1'-N9 | 6.17  | 113.14      | 108.20   |
| 20  | A     | 2049 | G    | N1-C6-O6   | -6.16 | 116.20      | 119.90   |
| 20  | A     | 1902 | G    | C5-N7-C8   | -6.16 | 101.22      | 104.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 992  | G    | N3-C4-N9   | 6.15  | 129.69      | 126.00   |
| 20  | A     | 716  | A    | C5-N7-C8   | -6.12 | 100.84      | 103.90   |
| 20  | A     | 655  | G    | N7-C8-N9   | -6.11 | 110.05      | 113.10   |
| 1   | a     | 1465 | U    | C2-N1-C1'  | 6.11  | 125.03      | 117.70   |
| 20  | A     | 2628 | A    | C8-N9-C4   | -6.11 | 103.36      | 105.80   |
| 20  | A     | 1350 | C    | C2-N1-C1'  | 6.10  | 125.51      | 118.80   |
| 20  | A     | 2102 | A    | N1-C6-N6   | -6.09 | 114.95      | 118.60   |
| 20  | A     | 2296 | G    | N1-C6-O6   | -6.08 | 116.25      | 119.90   |
| 1   | a     | 277  | A    | C5-N7-C8   | -6.07 | 100.87      | 103.90   |
| 20  | A     | 1321 | G    | N1-C6-O6   | -6.06 | 116.26      | 119.90   |
| 20  | A     | 716  | A    | O4'-C1'-N9 | 6.06  | 113.05      | 108.20   |
| 20  | A     | 1708 | A    | N1-C6-N6   | -6.06 | 114.97      | 118.60   |
| 20  | A     | 2834 | A    | N1-C6-N6   | -6.05 | 114.97      | 118.60   |
| 20  | A     | 1429 | A    | O4'-C1'-N9 | 6.04  | 113.04      | 108.20   |
| 20  | A     | 1814 | C    | C6-N1-C2   | -6.04 | 117.89      | 120.30   |
| 1   | a     | 585  | G    | N3-C4-C5   | -6.04 | 125.58      | 128.60   |
| 21  | B     | 96   | G    | O4'-C1'-N9 | 6.03  | 113.03      | 108.20   |
| 20  | A     | 1195 | A    | C8-N9-C4   | -6.01 | 103.39      | 105.80   |
| 20  | A     | 1490 | A    | C5-C6-N1   | -6.00 | 114.70      | 117.70   |
| 20  | A     | 155  | U    | O4'-C1'-N1 | 6.00  | 113.00      | 108.20   |
| 1   | a     | 1294 | A    | N7-C8-N9   | 6.00  | 116.80      | 113.80   |
| 1   | a     | 35   | G    | OP1-P-OP2  | 5.99  | 128.59      | 119.60   |
| 20  | A     | 2588 | G    | N7-C8-N9   | 5.99  | 116.10      | 113.10   |
| 20  | A     | 1591 | A    | N9-C4-C5   | 5.99  | 108.19      | 105.80   |
| 20  | A     | 1487 | U    | O5'-P-OP2  | -5.99 | 100.31      | 105.70   |
| 20  | A     | 2062 | G    | N3-C4-N9   | 5.98  | 129.59      | 126.00   |
| 21  | B     | 79   | G    | N7-C8-N9   | 5.98  | 116.09      | 113.10   |
| 21  | B     | 96   | G    | C4-N9-C1'  | 5.98  | 134.27      | 126.50   |
| 20  | A     | 235  | G    | C4-N9-C1'  | 5.97  | 134.26      | 126.50   |
| 20  | A     | 2836 | G    | C8-N9-C4   | -5.97 | 104.01      | 106.40   |
| 20  | A     | 2606 | G    | C8-N9-C1'  | -5.97 | 119.24      | 127.00   |
| 20  | A     | 1800 | A    | O4'-C1'-N9 | 5.96  | 112.97      | 108.20   |
| 20  | A     | 1571 | G    | N9-C4-C5   | 5.96  | 107.78      | 105.40   |
| 20  | A     | 50   | A    | N1-C6-N6   | -5.96 | 115.03      | 118.60   |
| 20  | A     | 1506 | A    | C6-N1-C2   | 5.96  | 122.17      | 118.60   |
| 20  | A     | 2367 | G    | N3-C4-C5   | -5.96 | 125.62      | 128.60   |
| 20  | A     | 262  | G    | N3-C4-N9   | 5.95  | 129.57      | 126.00   |
| 20  | A     | 1804 | C    | C6-N1-C2   | -5.95 | 117.92      | 120.30   |
| 20  | A     | 2057 | C    | C2-N1-C1'  | 5.95  | 125.35      | 118.80   |
| 20  | A     | 1490 | A    | C6-N1-C2   | 5.95  | 122.17      | 118.60   |
| 20  | A     | 572  | G    | C2-N3-C4   | 5.94  | 114.87      | 111.90   |
| 20  | A     | 712  | C    | C6-N1-C2   | -5.94 | 117.92      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | a     | 113  | G    | C8-N9-C1'  | -5.93 | 119.29      | 127.00   |
| 20  | A     | 360  | G    | C8-N9-C4   | -5.93 | 104.03      | 106.40   |
| 20  | A     | 903  | G    | N7-C8-N9   | 5.92  | 116.06      | 113.10   |
| 20  | A     | 1337 | A    | C2-N3-C4   | -5.92 | 107.64      | 110.60   |
| 20  | A     | 2599 | U    | N3-C2-O2   | -5.92 | 118.06      | 122.20   |
| 1   | a     | 277  | A    | O4'-C1'-N9 | 5.92  | 112.93      | 108.20   |
| 1   | a     | 183  | G    | N3-C2-N2   | -5.90 | 115.77      | 119.90   |
| 20  | A     | 2602 | G    | C8-N9-C4   | -5.90 | 104.04      | 106.40   |
| 20  | A     | 1288 | A    | C5-C6-N6   | 5.89  | 128.41      | 123.70   |
| 20  | A     | 1989 | G    | O4'-C1'-N9 | 5.89  | 112.91      | 108.20   |
| 20  | A     | 370  | G    | N3-C4-C5   | -5.89 | 125.66      | 128.60   |
| 20  | A     | 703  | G    | N1-C6-O6   | -5.88 | 116.37      | 119.90   |
| 20  | A     | 2307 | C    | C6-N1-C2   | -5.88 | 117.95      | 120.30   |
| 1   | a     | 24   | G    | N3-C4-N9   | 5.87  | 129.52      | 126.00   |
| 20  | A     | 1989 | G    | C2-N3-C4   | -5.87 | 108.97      | 111.90   |
| 1   | a     | 267  | U    | C2-N1-C1'  | 5.87  | 124.74      | 117.70   |
| 20  | A     | 2809 | U    | C2-N1-C1'  | 5.87  | 124.74      | 117.70   |
| 20  | A     | 1229 | G    | N3-C4-C5   | -5.86 | 125.67      | 128.60   |
| 1   | a     | 834  | A    | C2-N3-C4   | -5.85 | 107.67      | 110.60   |
| 20  | A     | 1224 | G    | N3-C4-N9   | 5.85  | 129.51      | 126.00   |
| 1   | a     | 24   | G    | N3-C4-C5   | -5.85 | 125.67      | 128.60   |
| 20  | A     | 1011 | C    | C6-N1-C2   | -5.83 | 117.97      | 120.30   |
| 20  | A     | 654  | A    | O4'-C1'-N9 | 5.82  | 112.86      | 108.20   |
| 21  | B     | 80   | A    | O4'-C1'-N9 | 5.81  | 112.85      | 108.20   |
| 1   | a     | 976  | U    | C5-C6-N1   | -5.80 | 119.80      | 122.70   |
| 36  | T     | 24   | LEU  | CA-CB-CG   | 5.80  | 128.65      | 115.30   |
| 37  | U     | 56   | LEU  | CA-CB-CG   | 5.80  | 128.64      | 115.30   |
| 20  | A     | 509  | G    | C8-N9-C4   | -5.79 | 104.08      | 106.40   |
| 20  | A     | 2416 | U    | N3-C2-O2   | -5.79 | 118.15      | 122.20   |
| 20  | A     | 103  | A    | N7-C8-N9   | 5.79  | 116.69      | 113.80   |
| 20  | A     | 1264 | G    | N3-C4-N9   | 5.79  | 129.47      | 126.00   |
| 20  | A     | 1288 | A    | N1-C2-N3   | 5.78  | 132.19      | 129.30   |
| 20  | A     | 886  | U    | N3-C2-O2   | -5.78 | 118.16      | 122.20   |
| 20  | A     | 396  | C    | C2-N1-C1'  | 5.78  | 125.16      | 118.80   |
| 20  | A     | 990  | G    | C5-N7-C8   | -5.78 | 101.41      | 104.30   |
| 20  | A     | 2645 | G    | N1-C6-O6   | -5.77 | 116.44      | 119.90   |
| 20  | A     | 1885 | C    | N1-C2-O2   | 5.77  | 122.36      | 118.90   |
| 20  | A     | 781  | G    | C8-N9-C4   | -5.76 | 104.10      | 106.40   |
| 20  | A     | 2365 | G    | C4-N9-C1'  | 5.76  | 133.98      | 126.50   |
| 20  | A     | 1669 | G    | N1-C6-O6   | -5.75 | 116.45      | 119.90   |
| 20  | A     | 2049 | G    | C8-N9-C4   | -5.75 | 104.10      | 106.40   |
| 20  | A     | 1042 | G    | N1-C6-O6   | -5.75 | 116.45      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 2287 | A    | C6-C5-N7   | -5.73 | 128.29      | 132.30   |
| 1   | a     | 467  | A    | C5-N7-C8   | -5.73 | 101.04      | 103.90   |
| 20  | A     | 2891 | C    | C6-N1-C2   | -5.73 | 118.01      | 120.30   |
| 20  | A     | 777  | C    | C6-N1-C2   | -5.73 | 118.01      | 120.30   |
| 1   | a     | 976  | U    | N1-C2-N3   | 5.72  | 118.33      | 114.90   |
| 20  | A     | 1012 | G    | N3-C4-N9   | 5.72  | 129.44      | 126.00   |
| 20  | A     | 1471 | G    | N3-C4-N9   | 5.72  | 129.43      | 126.00   |
| 20  | A     | 367  | A    | N7-C8-N9   | 5.72  | 116.66      | 113.80   |
| 20  | A     | 2859 | G    | O4'-C1'-N9 | 5.72  | 112.77      | 108.20   |
| 20  | A     | 1379 | G    | C4-N9-C1'  | 5.71  | 133.93      | 126.50   |
| 1   | a     | 277  | A    | C8-N9-C4   | -5.71 | 103.52      | 105.80   |
| 1   | a     | 113  | G    | C5-N7-C8   | -5.71 | 101.45      | 104.30   |
| 20  | A     | 410  | G    | N3-C4-C5   | -5.71 | 125.75      | 128.60   |
| 20  | A     | 620  | G    | N3-C4-C5   | -5.71 | 125.75      | 128.60   |
| 20  | A     | 1337 | A    | N3-C4-N9   | -5.71 | 122.83      | 127.40   |
| 20  | A     | 1806 | G    | N1-C6-O6   | -5.71 | 116.48      | 119.90   |
| 21  | B     | 85   | U    | C4-C5-C6   | -5.71 | 116.28      | 119.70   |
| 27  | K     | 29   | LEU  | CA-CB-CG   | 5.71  | 128.42      | 115.30   |
| 20  | A     | 103  | A    | C5-N7-C8   | -5.70 | 101.05      | 103.90   |
| 1   | a     | 776  | G    | N3-C4-C5   | -5.69 | 125.75      | 128.60   |
| 20  | A     | 248  | G    | N3-C4-N9   | 5.69  | 129.41      | 126.00   |
| 20  | A     | 1492 | G    | O4'-C1'-N9 | 5.68  | 112.75      | 108.20   |
| 20  | A     | 654  | A    | C8-N9-C4   | 5.68  | 108.07      | 105.80   |
| 20  | A     | 817  | G    | N3-C4-C5   | -5.68 | 125.76      | 128.60   |
| 20  | A     | 823  | A    | N1-C6-N6   | -5.68 | 115.19      | 118.60   |
| 20  | A     | 367  | A    | C8-N9-C4   | -5.67 | 103.53      | 105.80   |
| 1   | a     | 539  | G    | N3-C4-C5   | -5.66 | 125.77      | 128.60   |
| 20  | A     | 2903 | G    | C2-N3-C4   | -5.66 | 109.07      | 111.90   |
| 20  | A     | 1604 | A    | P-O3'-C3'  | 5.66  | 126.49      | 119.70   |
| 20  | A     | 35   | U    | C2-N1-C1'  | 5.65  | 124.48      | 117.70   |
| 20  | A     | 18   | G    | N3-C4-N9   | 5.64  | 129.39      | 126.00   |
| 20  | A     | 1996 | U    | N1-C2-O2   | 5.64  | 126.75      | 122.80   |
| 1   | a     | 538  | A    | O4'-C1'-N9 | 5.63  | 112.71      | 108.20   |
| 20  | A     | 1434 | C    | C5-C6-N1   | 5.63  | 123.82      | 121.00   |
| 20  | A     | 1197 | G    | C8-N9-C1'  | -5.63 | 119.68      | 127.00   |
| 20  | A     | 50   | A    | C5-C6-N6   | 5.62  | 128.20      | 123.70   |
| 20  | A     | 2051 | A    | C2-N3-C4   | 5.62  | 113.41      | 110.60   |
| 20  | A     | 655  | G    | C4-N9-C1'  | -5.62 | 119.20      | 126.50   |
| 20  | A     | 1551 | U    | C5-C6-N1   | 5.61  | 125.50      | 122.70   |
| 20  | A     | 1337 | A    | N3-C4-C5   | 5.61  | 130.73      | 126.80   |
| 20  | A     | 1717 | G    | N3-C4-C5   | -5.61 | 125.80      | 128.60   |
| 20  | A     | 1591 | A    | C4-C5-N7   | -5.60 | 107.90      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 990  | G    | C4-C5-N7   | 5.60  | 113.04      | 110.80   |
| 20  | A     | 644  | U    | N3-C2-O2   | -5.60 | 118.28      | 122.20   |
| 34  | R     | 117  | LEU  | CA-CB-CG   | 5.58  | 128.12      | 115.30   |
| 20  | A     | 400  | G    | N3-C4-N9   | 5.57  | 129.34      | 126.00   |
| 1   | a     | 1294 | A    | C8-N9-C4   | -5.57 | 103.57      | 105.80   |
| 20  | A     | 904  | A    | O4'-C1'-N9 | 5.57  | 112.65      | 108.20   |
| 20  | A     | 956  | C    | C5-C6-N1   | 5.56  | 123.78      | 121.00   |
| 20  | A     | 2514 | U    | O4'-C1'-N1 | 5.56  | 112.65      | 108.20   |
| 20  | A     | 2836 | G    | N3-C2-N2   | -5.56 | 116.01      | 119.90   |
| 20  | A     | 2537 | G    | N3-C4-N9   | 5.55  | 129.33      | 126.00   |
| 20  | A     | 1717 | G    | C8-N9-C4   | -5.55 | 104.18      | 106.40   |
| 20  | A     | 1976 | C    | C6-N1-C2   | -5.54 | 118.08      | 120.30   |
| 20  | A     | 788  | G    | O4'-C1'-N9 | 5.54  | 112.63      | 108.20   |
| 20  | A     | 1658 | C    | C6-N1-C2   | -5.54 | 118.09      | 120.30   |
| 20  | A     | 235  | G    | C5-N7-C8   | -5.53 | 101.53      | 104.30   |
| 20  | A     | 2613 | G    | N3-C4-C5   | -5.53 | 125.83      | 128.60   |
| 20  | A     | 2500 | G    | C8-N9-C4   | -5.53 | 104.19      | 106.40   |
| 20  | A     | 1397 | G    | C5-C6-O6   | -5.53 | 125.28      | 128.60   |
| 20  | A     | 2044 | A    | O4'-C1'-N9 | 5.53  | 112.62      | 108.20   |
| 20  | A     | 963  | C    | C6-N1-C2   | -5.52 | 118.09      | 120.30   |
| 20  | A     | 2416 | U    | N1-C2-O2   | 5.52  | 126.66      | 122.80   |
| 1   | a     | 467  | A    | N7-C8-N9   | 5.51  | 116.56      | 113.80   |
| 20  | A     | 222  | A    | C8-N9-C4   | -5.51 | 103.60      | 105.80   |
| 20  | A     | 1288 | A    | N3-C4-N9   | -5.50 | 123.00      | 127.40   |
| 20  | A     | 1605 | C    | P-O3'-C3'  | 5.50  | 126.30      | 119.70   |
| 4   | e     | 128  | LEU  | CA-CB-CG   | 5.48  | 127.91      | 115.30   |
| 20  | A     | 905  | G    | N3-C4-N9   | 5.48  | 129.29      | 126.00   |
| 20  | A     | 2455 | C    | N3-C2-O2   | -5.48 | 118.06      | 121.90   |
| 1   | a     | 183  | G    | C5-N7-C8   | -5.48 | 101.56      | 104.30   |
| 20  | A     | 769  | G    | C5-C6-N1   | -5.47 | 108.77      | 111.50   |
| 20  | A     | 619  | G    | N3-C4-N9   | 5.47  | 129.28      | 126.00   |
| 1   | a     | 27   | C    | C2-N1-C1'  | 5.46  | 124.81      | 118.80   |
| 1   | a     | 1445 | C    | N3-C4-C5   | 5.46  | 124.09      | 121.90   |
| 20  | A     | 503  | G    | C6-C5-N7   | 5.46  | 133.68      | 130.40   |
| 20  | A     | 1536 | A    | C8-N9-C4   | -5.46 | 103.61      | 105.80   |
| 20  | A     | 1996 | U    | N3-C2-O2   | -5.46 | 118.38      | 122.20   |
| 20  | A     | 1407 | G    | N1-C6-O6   | -5.46 | 116.63      | 119.90   |
| 20  | A     | 2287 | A    | C5-C6-N1   | -5.45 | 114.97      | 117.70   |
| 20  | A     | 1841 | U    | N3-C2-O2   | -5.45 | 118.39      | 122.20   |
| 34  | R     | 79   | LEU  | CA-CB-CG   | 5.44  | 127.82      | 115.30   |
| 20  | A     | 47   | C    | C6-N1-C2   | -5.43 | 118.13      | 120.30   |
| 20  | A     | 494  | A    | N1-C6-N6   | -5.43 | 115.34      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 2365 | G    | C8-N9-C1'  | -5.42 | 119.95      | 127.00   |
| 20  | A     | 2825 | C    | C6-N1-C2   | -5.42 | 118.13      | 120.30   |
| 1   | a     | 35   | G    | C8-N9-C4   | -5.42 | 104.23      | 106.40   |
| 20  | A     | 1571 | G    | N3-C4-N9   | -5.42 | 122.75      | 126.00   |
| 20  | A     | 2416 | U    | C2-N1-C1'  | 5.40  | 124.18      | 117.70   |
| 20  | A     | 768  | G    | N3-C4-C5   | -5.40 | 125.90      | 128.60   |
| 1   | a     | 1375 | A    | N7-C8-N9   | 5.40  | 116.50      | 113.80   |
| 1   | a     | 835  | U    | O4'-C1'-N1 | -5.39 | 103.88      | 108.20   |
| 20  | A     | 494  | A    | C5-C6-N6   | 5.39  | 128.02      | 123.70   |
| 20  | A     | 2705 | C    | C6-N1-C2   | -5.39 | 118.14      | 120.30   |
| 20  | A     | 2728 | G    | C5-C6-O6   | 5.39  | 131.83      | 128.60   |
| 20  | A     | 1950 | A    | N7-C8-N9   | 5.38  | 116.49      | 113.80   |
| 20  | A     | 2903 | G    | N3-C4-C5   | 5.38  | 131.29      | 128.60   |
| 20  | A     | 1203 | G    | C5-C6-N1   | 5.38  | 114.19      | 111.50   |
| 20  | A     | 655  | G    | N3-C4-C5   | 5.38  | 131.29      | 128.60   |
| 20  | A     | 1065 | G    | C8-N9-C4   | -5.38 | 104.25      | 106.40   |
| 20  | A     | 1394 | G    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 20  | A     | 1989 | G    | C4-N9-C1'  | 5.37  | 133.48      | 126.50   |
| 20  | A     | 2359 | G    | C8-N9-C4   | -5.37 | 104.25      | 106.40   |
| 20  | A     | 2639 | G    | N1-C6-O6   | -5.37 | 116.68      | 119.90   |
| 1   | a     | 585  | G    | C4-N9-C1'  | 5.36  | 133.47      | 126.50   |
| 21  | B     | 77   | G    | C4-N9-C1'  | 5.36  | 133.47      | 126.50   |
| 20  | A     | 229  | A    | C8-N9-C4   | -5.36 | 103.66      | 105.80   |
| 20  | A     | 2637 | G    | N3-C4-C5   | -5.36 | 125.92      | 128.60   |
| 20  | A     | 721  | U    | C6-N1-C2   | -5.36 | 117.79      | 121.00   |
| 20  | A     | 781  | G    | N3-C4-C5   | -5.35 | 125.92      | 128.60   |
| 20  | A     | 2084 | G    | N3-C4-C5   | -5.35 | 125.92      | 128.60   |
| 20  | A     | 2070 | G    | N3-C4-N9   | 5.35  | 129.21      | 126.00   |
| 1   | a     | 183  | G    | C2-N3-C4   | -5.35 | 109.22      | 111.90   |
| 20  | A     | 2067 | G    | N3-C4-N9   | 5.35  | 129.21      | 126.00   |
| 20  | A     | 549  | C    | C6-N1-C2   | -5.35 | 118.16      | 120.30   |
| 21  | B     | 80   | A    | N7-C8-N9   | 5.35  | 116.47      | 113.80   |
| 20  | A     | 768  | G    | C8-N9-C4   | -5.35 | 104.26      | 106.40   |
| 21  | B     | 79   | G    | C8-N9-C4   | -5.34 | 104.26      | 106.40   |
| 20  | A     | 1994 | G    | C2-N3-C4   | 5.34  | 114.57      | 111.90   |
| 20  | A     | 1490 | A    | N3-C4-C5   | 5.33  | 130.53      | 126.80   |
| 20  | A     | 1673 | A    | N9-C4-C5   | 5.33  | 107.93      | 105.80   |
| 20  | A     | 772  | C    | C6-N1-C2   | -5.33 | 118.17      | 120.30   |
| 20  | A     | 105  | C    | C6-N1-C2   | -5.32 | 118.17      | 120.30   |
| 1   | a     | 1176 | C    | C6-N1-C1'  | -5.32 | 114.42      | 120.80   |
| 20  | A     | 400  | G    | C4-N9-C1'  | 5.32  | 133.41      | 126.50   |
| 20  | A     | 1216 | G    | C8-N9-C4   | -5.32 | 104.27      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 2345 | G    | N1-C6-O6   | -5.32 | 116.71      | 119.90   |
| 20  | A     | 1644 | G    | N3-C4-N9   | 5.31  | 129.18      | 126.00   |
| 20  | A     | 2405 | G    | O4'-C1'-N9 | 5.31  | 112.44      | 108.20   |
| 20  | A     | 509  | G    | C4-C5-N7   | 5.30  | 112.92      | 110.80   |
| 20  | A     | 1592 | G    | C2-N3-C4   | -5.30 | 109.25      | 111.90   |
| 20  | A     | 1776 | A    | O4'-C1'-N9 | 5.29  | 112.43      | 108.20   |
| 20  | A     | 539  | G    | N3-C4-N9   | -5.28 | 122.83      | 126.00   |
| 20  | A     | 2794 | G    | C6-C5-N7   | -5.28 | 127.23      | 130.40   |
| 20  | A     | 400  | G    | C8-N9-C1'  | -5.28 | 120.14      | 127.00   |
| 20  | A     | 2067 | G    | N3-C4-C5   | -5.27 | 125.96      | 128.60   |
| 20  | A     | 1730 | G    | N3-C4-C5   | -5.26 | 125.97      | 128.60   |
| 20  | A     | 1288 | A    | N3-C4-C5   | 5.25  | 130.48      | 126.80   |
| 20  | A     | 2073 | A    | O4'-C1'-N9 | 5.25  | 112.40      | 108.20   |
| 20  | A     | 2062 | G    | N3-C4-C5   | -5.25 | 125.97      | 128.60   |
| 20  | A     | 179  | A    | N7-C8-N9   | 5.24  | 116.42      | 113.80   |
| 14  | o     | 87   | LEU  | CA-CB-CG   | 5.24  | 127.36      | 115.30   |
| 20  | A     | 1978 | G    | N3-C4-C5   | -5.24 | 125.98      | 128.60   |
| 1   | a     | 376  | G    | C5-C6-O6   | -5.23 | 125.46      | 128.60   |
| 20  | A     | 807  | U    | O4'-C1'-N1 | 5.23  | 112.39      | 108.20   |
| 20  | A     | 716  | A    | N7-C8-N9   | 5.23  | 116.41      | 113.80   |
| 20  | A     | 2317 | G    | C4-N9-C1'  | 5.23  | 133.29      | 126.50   |
| 20  | A     | 13   | U    | P-O3'-C3'  | 5.22  | 125.97      | 119.70   |
| 20  | A     | 2360 | A    | N1-C6-N6   | -5.22 | 115.47      | 118.60   |
| 20  | A     | 347  | A    | O5'-P-OP1  | -5.22 | 101.00      | 105.70   |
| 20  | A     | 1491 | U    | O4'-C1'-N1 | 5.22  | 112.38      | 108.20   |
| 20  | A     | 2208 | C    | C2-N1-C1'  | 5.22  | 124.54      | 118.80   |
| 20  | A     | 367  | A    | C4-C5-N7   | 5.22  | 113.31      | 110.70   |
| 20  | A     | 1203 | G    | N1-C6-O6   | -5.21 | 116.78      | 119.90   |
| 20  | A     | 1950 | A    | O4'-C1'-N9 | 5.21  | 112.37      | 108.20   |
| 20  | A     | 1959 | G    | N3-C4-N9   | 5.21  | 129.12      | 126.00   |
| 20  | A     | 992  | G    | N9-C1'-C2' | -5.21 | 106.27      | 112.00   |
| 20  | A     | 1278 | C    | C6-N1-C2   | -5.20 | 118.22      | 120.30   |
| 20  | A     | 1431 | A    | C8-N9-C4   | -5.20 | 103.72      | 105.80   |
| 20  | A     | 660  | A    | C2-N3-C4   | -5.20 | 108.00      | 110.60   |
| 20  | A     | 521  | G    | N3-C4-C5   | -5.20 | 126.00      | 128.60   |
| 20  | A     | 2289 | C    | C6-N1-C2   | -5.20 | 118.22      | 120.30   |
| 20  | A     | 1360 | G    | O4'-C1'-N9 | 5.20  | 112.36      | 108.20   |
| 20  | A     | 2794 | G    | C4-C5-N7   | 5.19  | 112.88      | 110.80   |
| 20  | A     | 181  | G    | C2-N3-C4   | 5.19  | 114.50      | 111.90   |
| 20  | A     | 460  | G    | N3-C4-C5   | -5.18 | 126.01      | 128.60   |
| 20  | A     | 907  | A    | C6-C5-N7   | -5.18 | 128.67      | 132.30   |
| 20  | A     | 1167 | A    | C6-C5-N7   | -5.18 | 128.67      | 132.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 20  | A     | 1349 | U    | N1-C2-O2   | 5.18  | 126.43      | 122.80   |
| 20  | A     | 2592 | G    | N1-C6-O6   | -5.18 | 116.79      | 119.90   |
| 20  | A     | 660  | A    | N3-C4-C5   | 5.18  | 130.43      | 126.80   |
| 20  | A     | 2020 | C    | C6-N1-C2   | -5.18 | 118.23      | 120.30   |
| 20  | A     | 1448 | U    | C5-C6-N1   | 5.18  | 125.29      | 122.70   |
| 20  | A     | 2022 | C    | C6-N1-C2   | -5.18 | 118.23      | 120.30   |
| 20  | A     | 1193 | C    | C6-N1-C2   | -5.17 | 118.23      | 120.30   |
| 20  | A     | 1356 | G    | O4'-C1'-N9 | 5.17  | 112.33      | 108.20   |
| 20  | A     | 181  | G    | C5-C6-N1   | 5.16  | 114.08      | 111.50   |
| 20  | A     | 1397 | G    | N3-C4-C5   | -5.16 | 126.02      | 128.60   |
| 20  | A     | 1796 | C    | C6-N1-C2   | -5.16 | 118.23      | 120.30   |
| 1   | a     | 941  | G    | N3-C4-N9   | 5.16  | 129.09      | 126.00   |
| 20  | A     | 103  | A    | C8-N9-C4   | -5.16 | 103.74      | 105.80   |
| 20  | A     | 725  | A    | N9-C4-C5   | 5.16  | 107.86      | 105.80   |
| 20  | A     | 460  | G    | C8-N9-C4   | -5.15 | 104.34      | 106.40   |
| 21  | B     | 80   | A    | C5-N7-C8   | -5.15 | 101.32      | 103.90   |
| 20  | A     | 990  | G    | N7-C8-N9   | 5.15  | 115.68      | 113.10   |
| 20  | A     | 1590 | A    | P-O3'-C3'  | 5.15  | 125.88      | 119.70   |
| 20  | A     | 2728 | G    | N1-C6-O6   | -5.14 | 116.82      | 119.90   |
| 20  | A     | 2057 | C    | C6-N1-C2   | -5.13 | 118.25      | 120.30   |
| 20  | A     | 2498 | G    | N3-C4-C5   | -5.13 | 126.03      | 128.60   |
| 20  | A     | 1074 | G    | N3-C4-C5   | -5.13 | 126.03      | 128.60   |
| 20  | A     | 2575 | A    | C5-C6-N1   | 5.13  | 120.27      | 117.70   |
| 28  | L     | 91   | LYS  | C-N-CA     | -5.13 | 108.88      | 121.70   |
| 1   | a     | 590  | G    | N1-C6-O6   | -5.12 | 116.83      | 119.90   |
| 20  | A     | 2228 | C    | C6-N1-C2   | -5.12 | 118.25      | 120.30   |
| 20  | A     | 1431 | A    | N7-C8-N9   | 5.12  | 116.36      | 113.80   |
| 20  | A     | 2794 | G    | N7-C8-N9   | 5.12  | 115.66      | 113.10   |
| 20  | A     | 2794 | G    | C5-N7-C8   | -5.12 | 101.74      | 104.30   |
| 20  | A     | 1806 | G    | C5-C6-O6   | 5.11  | 131.67      | 128.60   |
| 1   | a     | 818  | G    | N3-C4-C5   | -5.11 | 126.05      | 128.60   |
| 20  | A     | 451  | G    | N3-C4-C5   | -5.11 | 126.05      | 128.60   |
| 1   | a     | 734  | C    | C6-N1-C2   | -5.11 | 118.26      | 120.30   |
| 20  | A     | 1600 | C    | P-O3'-C3'  | 5.11  | 125.83      | 119.70   |
| 20  | A     | 1730 | G    | C4-N9-C1'  | 5.10  | 133.14      | 126.50   |
| 20  | A     | 468  | A    | O5'-P-OP2  | -5.10 | 101.11      | 105.70   |
| 20  | A     | 1491 | U    | N3-C2-O2   | -5.10 | 118.63      | 122.20   |
| 20  | A     | 1584 | G    | P-O3'-C3'  | 5.10  | 125.81      | 119.70   |
| 20  | A     | 1764 | G    | N1-C6-O6   | -5.10 | 116.84      | 119.90   |
| 1   | a     | 492  | C    | C2-N1-C1'  | 5.09  | 124.40      | 118.80   |
| 20  | A     | 1011 | C    | C4-C5-C6   | 5.09  | 119.95      | 117.40   |
| 20  | A     | 1571 | G    | N1-C2-N3   | 5.09  | 126.96      | 123.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 21  | B     | 79   | G    | C5-N7-C8   | -5.09 | 101.75      | 104.30   |
| 20  | A     | 1645 | U    | O4'-C1'-N1 | 5.09  | 112.27      | 108.20   |
| 20  | A     | 2322 | G    | C5-C6-O6   | -5.09 | 125.55      | 128.60   |
| 20  | A     | 2499 | G    | N1-C6-O6   | -5.09 | 116.85      | 119.90   |
| 20  | A     | 2556 | A    | N9-C4-C5   | 5.09  | 107.83      | 105.80   |
| 1   | a     | 31   | C    | O4'-C1'-N1 | 5.08  | 112.27      | 108.20   |
| 20  | A     | 1216 | G    | N7-C8-N9   | 5.08  | 115.64      | 113.10   |
| 21  | B     | 96   | G    | C8-N9-C1'  | -5.08 | 120.40      | 127.00   |
| 20  | A     | 644  | U    | N1-C2-N3   | 5.08  | 117.94      | 114.90   |
| 20  | A     | 1645 | U    | N3-C2-O2   | -5.08 | 118.65      | 122.20   |
| 20  | A     | 568  | A    | N7-C8-N9   | 5.07  | 116.34      | 113.80   |
| 20  | A     | 2596 | G    | C4-N9-C1'  | 5.07  | 133.09      | 126.50   |
| 20  | A     | 2365 | G    | N3-C4-C5   | -5.07 | 126.06      | 128.60   |
| 20  | A     | 2521 | C    | N3-C2-O2   | -5.07 | 118.35      | 121.90   |
| 20  | A     | 2563 | G    | N3-C4-C5   | -5.06 | 126.07      | 128.60   |
| 1   | a     | 834  | A    | C5-N7-C8   | -5.06 | 101.37      | 103.90   |
| 20  | A     | 114  | U    | C2-N1-C1'  | 5.06  | 123.77      | 117.70   |
| 20  | A     | 1364 | G    | N7-C8-N9   | 5.06  | 115.63      | 113.10   |
| 20  | A     | 1605 | C    | O5'-P-OP1  | -5.06 | 101.15      | 105.70   |
| 20  | A     | 2628 | A    | N9-C4-C5   | 5.06  | 107.82      | 105.80   |
| 31  | O     | 86   | LEU  | CA-CB-CG   | 5.06  | 126.93      | 115.30   |
| 20  | A     | 1235 | G    | C2-N3-C4   | 5.05  | 114.43      | 111.90   |
| 20  | A     | 2387 | A    | N1-C6-N6   | -5.05 | 115.57      | 118.60   |
| 21  | B     | 58   | C    | C2-N1-C1'  | 5.05  | 124.36      | 118.80   |
| 20  | A     | 262  | G    | N3-C4-C5   | -5.05 | 126.07      | 128.60   |
| 20  | A     | 626  | U    | N3-C2-O2   | -5.05 | 118.67      | 122.20   |
| 20  | A     | 218  | G    | N3-C4-C5   | -5.05 | 126.08      | 128.60   |
| 20  | A     | 1022 | C    | C6-N1-C1'  | -5.05 | 114.74      | 120.80   |
| 20  | A     | 1505 | C    | N1-C2-O2   | 5.05  | 121.93      | 118.90   |
| 20  | A     | 18   | G    | N3-C4-C5   | -5.04 | 126.08      | 128.60   |
| 20  | A     | 2722 | G    | C5-C6-O6   | 5.04  | 131.62      | 128.60   |
| 20  | A     | 1167 | A    | C5-N7-C8   | -5.04 | 101.38      | 103.90   |
| 1   | a     | 35   | G    | N7-C8-N9   | 5.04  | 115.62      | 113.10   |
| 20  | A     | 25   | G    | C2-N3-C4   | 5.04  | 114.42      | 111.90   |
| 20  | A     | 1730 | G    | C6-C5-N7   | -5.04 | 127.38      | 130.40   |
| 20  | A     | 2008 | C    | C6-N1-C2   | -5.04 | 118.29      | 120.30   |
| 20  | A     | 2041 | G    | C5-C6-N1   | 5.04  | 114.02      | 111.50   |
| 20  | A     | 2317 | G    | N3-C4-N9   | 5.03  | 129.02      | 126.00   |
| 20  | A     | 2794 | G    | C8-N9-C1'  | -5.03 | 120.46      | 127.00   |
| 20  | A     | 2632 | G    | N1-C6-O6   | -5.03 | 116.88      | 119.90   |
| 20  | A     | 2664 | C    | C6-N1-C2   | -5.03 | 118.29      | 120.30   |
| 20  | A     | 1293 | G    | C4-N9-C1'  | 5.02  | 133.03      | 126.50   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 20  | A     | 1786 | G    | N1-C6-O6  | -5.02 | 116.89      | 119.90   |
| 20  | A     | 1192 | C    | N3-C2-O2  | -5.02 | 118.39      | 121.90   |
| 20  | A     | 963  | C    | C2-N1-C1' | 5.02  | 124.32      | 118.80   |
| 20  | A     | 1717 | G    | C2-N3-C4  | 5.02  | 114.41      | 111.90   |
| 20  | A     | 832  | G    | C8-N9-C4  | -5.02 | 104.39      | 106.40   |
| 20  | A     | 2444 | A    | N3-C4-N9  | -5.01 | 123.39      | 127.40   |
| 20  | A     | 1514 | G    | N1-C6-O6  | -5.01 | 116.89      | 119.90   |
| 20  | A     | 1959 | G    | N9-C4-C5  | -5.01 | 103.39      | 105.40   |
| 20  | A     | 2087 | C    | C6-N1-C2  | -5.01 | 118.30      | 120.30   |
| 27  | K     | 123  | LEU  | CA-CB-CG  | 5.01  | 126.82      | 115.30   |
| 20  | A     | 561  | G    | N3-C4-N9  | 5.01  | 129.00      | 126.00   |
| 20  | A     | 521  | G    | C5-C6-N1  | 5.00  | 114.00      | 111.50   |
| 20  | A     | 905  | G    | N7-C8-N9  | 5.00  | 115.60      | 113.10   |
| 20  | A     | 2371 | U    | C5-C6-N1  | 5.00  | 125.20      | 122.70   |

There are no chirality outliers.

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 23  | D     | 89  | GLY  | Peptide |
| 30  | N     | 16  | LYS  | Peptide |
| 30  | N     | 19  | GLY  | Peptide |
| 31  | O     | 4   | ARG  | Peptide |
| 31  | O     | 73  | VAL  | Peptide |
| 35  | S     | 50  | ALA  | Peptide |
| 36  | T     | 67  | PHE  | Peptide |
| 38  | V     | 87  | ASP  | Peptide |
| 7   | h     | 22  | HIS  | Peptide |
| 11  | l     | 37  | ASN  | Peptide |
| 18  | s     | 34  | TRP  | Peptide |

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

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

## 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 |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2   | c     | 202/204 (99%) | 174 (86%) | 28 (14%) | 0        | 100         | 100 |
| 3   | d     | 199/201 (99%) | 168 (84%) | 29 (15%) | 2 (1%)   | 15          | 45  |
| 4   | e     | 161/163 (99%) | 146 (91%) | 15 (9%)  | 0        | 100         | 100 |
| 5   | f     | 95/97 (98%)   | 82 (86%)  | 13 (14%) | 0        | 100         | 100 |
| 6   | g     | 152/154 (99%) | 138 (91%) | 14 (9%)  | 0        | 100         | 100 |
| 7   | h     | 129/131 (98%) | 115 (89%) | 14 (11%) | 0        | 100         | 100 |
| 8   | i     | 126/128 (98%) | 105 (83%) | 21 (17%) | 0        | 100         | 100 |
| 9   | j     | 97/99 (98%)   | 79 (81%)  | 18 (19%) | 0        | 100         | 100 |
| 10  | k     | 115/117 (98%) | 94 (82%)  | 21 (18%) | 0        | 100         | 100 |
| 11  | l     | 134/136 (98%) | 110 (82%) | 24 (18%) | 0        | 100         | 100 |
| 12  | m     | 108/112 (96%) | 85 (79%)  | 23 (21%) | 0        | 100         | 100 |
| 13  | n     | 58/60 (97%)   | 49 (84%)  | 9 (16%)  | 0        | 100         | 100 |
| 14  | o     | 86/88 (98%)   | 74 (86%)  | 11 (13%) | 1 (1%)   | 13          | 40  |
| 15  | p     | 87/89 (98%)   | 75 (86%)  | 12 (14%) | 0        | 100         | 100 |
| 16  | q     | 81/83 (98%)   | 69 (85%)  | 12 (15%) | 0        | 100         | 100 |
| 17  | r     | 64/66 (97%)   | 52 (81%)  | 11 (17%) | 1 (2%)   | 9           | 32  |
| 18  | s     | 76/78 (97%)   | 62 (82%)  | 13 (17%) | 1 (1%)   | 12          | 37  |
| 19  | t     | 80/82 (98%)   | 76 (95%)  | 3 (4%)   | 1 (1%)   | 12          | 37  |
| 22  | C     | 273/275 (99%) | 247 (90%) | 25 (9%)  | 1 (0%)   | 34          | 66  |
| 23  | D     | 205/207 (99%) | 188 (92%) | 16 (8%)  | 1 (0%)   | 29          | 61  |
| 24  | E     | 204/206 (99%) | 181 (89%) | 21 (10%) | 2 (1%)   | 15          | 45  |
| 25  | F     | 175/177 (99%) | 148 (85%) | 27 (15%) | 0        | 100         | 100 |
| 26  | G     | 174/176 (99%) | 145 (83%) | 27 (16%) | 2 (1%)   | 14          | 42  |
| 27  | K     | 143/145 (99%) | 133 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 28  | L     | 120/122 (98%) | 104 (87%) | 15 (12%) | 1 (1%)   | 19          | 51  |
| 29  | M     | 144/146 (99%) | 118 (82%) | 25 (17%) | 1 (1%)   | 22          | 54  |
| 30  | N     | 139/141 (99%) | 119 (86%) | 20 (14%) | 0        | 100         | 100 |
| 31  | O     | 122/124 (98%) | 102 (84%) | 20 (16%) | 0        | 100         | 100 |
| 32  | P     | 115/117 (98%) | 105 (91%) | 10 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 33  | Q     | 112/114 (98%)   | 104 (93%)  | 8 (7%)    | 0        | 100         | 100 |
| 34  | R     | 116/118 (98%)   | 113 (97%)  | 3 (3%)    | 0        | 100         | 100 |
| 35  | S     | 100/102 (98%)   | 91 (91%)   | 8 (8%)    | 1 (1%)   | 15          | 45  |
| 36  | T     | 110/112 (98%)   | 103 (94%)  | 7 (6%)    | 0        | 100         | 100 |
| 37  | U     | 87/89 (98%)     | 73 (84%)   | 14 (16%)  | 0        | 100         | 100 |
| 38  | V     | 99/101 (98%)    | 81 (82%)   | 18 (18%)  | 0        | 100         | 100 |
| 39  | X     | 74/76 (97%)     | 70 (95%)   | 4 (5%)    | 0        | 100         | 100 |
| 40  | Y     | 52/54 (96%)     | 43 (83%)   | 8 (15%)   | 1 (2%)   | 8           | 28  |
| 41  | Z     | 59/61 (97%)     | 57 (97%)   | 2 (3%)    | 0        | 100         | 100 |
| 42  | 0     | 56/58 (97%)     | 54 (96%)   | 2 (4%)    | 0        | 100         | 100 |
| 43  | 2     | 54/56 (96%)     | 46 (85%)   | 8 (15%)   | 0        | 100         | 100 |
| 44  | 3     | 47/49 (96%)     | 43 (92%)   | 4 (8%)    | 0        | 100         | 100 |
| 45  | 4     | 42/44 (96%)     | 42 (100%)  | 0         | 0        | 100         | 100 |
| 46  | 5     | 62/64 (97%)     | 59 (95%)   | 3 (5%)    | 0        | 100         | 100 |
| 47  | 6     | 36/38 (95%)     | 32 (89%)   | 4 (11%)   | 0        | 100         | 100 |
| All | All   | 4970/5060 (98%) | 4354 (88%) | 600 (12%) | 16 (0%)  | 44          | 71  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | D     | 90  | GLU  |
| 19  | t     | 67  | HIS  |
| 3   | d     | 144 | GLU  |
| 29  | M     | 16  | ARG  |
| 24  | E     | 13  | GLN  |
| 28  | L     | 25  | LEU  |
| 3   | d     | 4   | TYR  |
| 14  | o     | 25  | PRO  |
| 17  | r     | 27  | TYR  |
| 18  | s     | 6   | LYS  |
| 40  | Y     | 20  | HIS  |
| 22  | C     | 197 | ASN  |
| 26  | G     | 47  | GLY  |
| 24  | E     | 159 | GLY  |
| 26  | G     | 108 | GLY  |
| 35  | S     | 51  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | c     | 162/162 (100%) | 143 (88%) | 19 (12%) | 5           | 16 |
| 3   | d     | 175/175 (100%) | 142 (81%) | 33 (19%) | 1           | 4  |
| 4   | e     | 126/126 (100%) | 105 (83%) | 21 (17%) | 2           | 6  |
| 5   | f     | 86/86 (100%)   | 74 (86%)  | 12 (14%) | 3           | 10 |
| 6   | g     | 131/131 (100%) | 112 (86%) | 19 (14%) | 3           | 9  |
| 7   | h     | 112/112 (100%) | 93 (83%)  | 19 (17%) | 2           | 6  |
| 8   | i     | 101/101 (100%) | 94 (93%)  | 7 (7%)   | 15          | 41 |
| 9   | j     | 90/90 (100%)   | 80 (89%)  | 10 (11%) | 6           | 19 |
| 10  | k     | 91/91 (100%)   | 77 (85%)  | 14 (15%) | 2           | 8  |
| 11  | l     | 118/118 (100%) | 90 (76%)  | 28 (24%) | 1           | 2  |
| 12  | m     | 93/95 (98%)    | 79 (85%)  | 14 (15%) | 3           | 9  |
| 13  | n     | 51/51 (100%)   | 50 (98%)  | 1 (2%)   | 55          | 82 |
| 14  | o     | 78/78 (100%)   | 64 (82%)  | 14 (18%) | 2           | 5  |
| 15  | p     | 79/79 (100%)   | 68 (86%)  | 11 (14%) | 3           | 10 |
| 16  | q     | 76/76 (100%)   | 63 (83%)  | 13 (17%) | 2           | 6  |
| 17  | r     | 57/57 (100%)   | 51 (90%)  | 6 (10%)  | 7           | 21 |
| 18  | s     | 68/68 (100%)   | 55 (81%)  | 13 (19%) | 1           | 4  |
| 19  | t     | 63/63 (100%)   | 54 (86%)  | 9 (14%)  | 3           | 10 |
| 22  | C     | 225/225 (100%) | 206 (92%) | 19 (8%)  | 11          | 31 |
| 23  | D     | 170/170 (100%) | 140 (82%) | 30 (18%) | 2           | 5  |
| 24  | E     | 172/172 (100%) | 144 (84%) | 28 (16%) | 2           | 7  |
| 25  | F     | 154/154 (100%) | 129 (84%) | 25 (16%) | 2           | 7  |
| 26  | G     | 146/146 (100%) | 123 (84%) | 23 (16%) | 2           | 8  |
| 27  | K     | 122/122 (100%) | 105 (86%) | 17 (14%) | 3           | 10 |
| 28  | L     | 98/98 (100%)   | 87 (89%)  | 11 (11%) | 6           | 18 |
| 29  | M     | 112/112 (100%) | 102 (91%) | 10 (9%)  | 9           | 29 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|-----------|-------------|----|
| 30  | N     | 112/112 (100%)   | 98 (88%)   | 14 (12%)  | 4           | 14 |
| 31  | O     | 106/106 (100%)   | 92 (87%)   | 14 (13%)  | 4           | 12 |
| 32  | P     | 91/91 (100%)     | 79 (87%)   | 12 (13%)  | 4           | 12 |
| 33  | Q     | 97/97 (100%)     | 83 (86%)   | 14 (14%)  | 3           | 9  |
| 34  | R     | 94/94 (100%)     | 87 (93%)   | 7 (7%)    | 13          | 38 |
| 35  | S     | 83/83 (100%)     | 73 (88%)   | 10 (12%)  | 5           | 15 |
| 36  | T     | 95/95 (100%)     | 82 (86%)   | 13 (14%)  | 3           | 11 |
| 37  | U     | 80/80 (100%)     | 66 (82%)   | 14 (18%)  | 2           | 6  |
| 38  | V     | 85/85 (100%)     | 71 (84%)   | 14 (16%)  | 2           | 7  |
| 39  | X     | 61/61 (100%)     | 48 (79%)   | 13 (21%)  | 1           | 3  |
| 40  | Y     | 47/47 (100%)     | 38 (81%)   | 9 (19%)   | 1           | 4  |
| 41  | Z     | 55/55 (100%)     | 45 (82%)   | 10 (18%)  | 1           | 5  |
| 42  | 0     | 49/49 (100%)     | 44 (90%)   | 5 (10%)   | 7           | 22 |
| 43  | 2     | 46/46 (100%)     | 39 (85%)   | 7 (15%)   | 3           | 8  |
| 44  | 3     | 49/49 (100%)     | 46 (94%)   | 3 (6%)    | 18          | 48 |
| 45  | 4     | 39/39 (100%)     | 34 (87%)   | 5 (13%)   | 4           | 13 |
| 46  | 5     | 51/51 (100%)     | 44 (86%)   | 7 (14%)   | 3           | 11 |
| 47  | 6     | 35/35 (100%)     | 30 (86%)   | 5 (14%)   | 3           | 10 |
| All | All   | 4231/4233 (100%) | 3629 (86%) | 602 (14%) | 6           | 10 |

All (602) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | c     | 21  | LYS  |
| 2   | c     | 25  | GLU  |
| 2   | c     | 40  | LYS  |
| 2   | c     | 44  | THR  |
| 2   | c     | 45  | LYS  |
| 2   | c     | 48  | ASP  |
| 2   | c     | 51  | VAL  |
| 2   | c     | 55  | GLU  |
| 2   | c     | 67  | ILE  |
| 2   | c     | 69  | THR  |
| 2   | c     | 78  | LYS  |
| 2   | c     | 81  | SER  |
| 2   | c     | 98  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | c     | 100 | ILE  |
| 2   | c     | 171 | THR  |
| 2   | c     | 174 | LEU  |
| 2   | c     | 191 | THR  |
| 2   | c     | 199 | VAL  |
| 2   | c     | 200 | TRP  |
| 3   | d     | 3   | ARG  |
| 3   | d     | 9   | TRP  |
| 3   | d     | 14  | ARG  |
| 3   | d     | 17  | ILE  |
| 3   | d     | 22  | THR  |
| 3   | d     | 25  | GLU  |
| 3   | d     | 28  | ARG  |
| 3   | d     | 29  | ARG  |
| 3   | d     | 53  | GLU  |
| 3   | d     | 56  | LYS  |
| 3   | d     | 58  | ARG  |
| 3   | d     | 63  | MET  |
| 3   | d     | 71  | LEU  |
| 3   | d     | 74  | LYS  |
| 3   | d     | 83  | HIS  |
| 3   | d     | 94  | ARG  |
| 3   | d     | 102 | LEU  |
| 3   | d     | 104 | LEU  |
| 3   | d     | 123 | ASP  |
| 3   | d     | 125 | LYS  |
| 3   | d     | 135 | GLU  |
| 3   | d     | 139 | VAL  |
| 3   | d     | 140 | ILE  |
| 3   | d     | 143 | ARG  |
| 3   | d     | 152 | ILE  |
| 3   | d     | 159 | THR  |
| 3   | d     | 183 | ARG  |
| 3   | d     | 186 | LEU  |
| 3   | d     | 189 | GLU  |
| 3   | d     | 190 | ILE  |
| 3   | d     | 192 | GLU  |
| 3   | d     | 201 | GLN  |
| 3   | d     | 202 | LYS  |
| 4   | e     | 22  | THR  |
| 4   | e     | 24  | VAL  |
| 4   | e     | 31  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | e     | 39  | VAL  |
| 4   | e     | 43  | ASN  |
| 4   | e     | 50  | THR  |
| 4   | e     | 71  | LEU  |
| 4   | e     | 76  | MET  |
| 4   | e     | 100 | VAL  |
| 4   | e     | 101 | GLU  |
| 4   | e     | 105 | VAL  |
| 4   | e     | 111 | VAL  |
| 4   | e     | 112 | ARG  |
| 4   | e     | 116 | GLU  |
| 4   | e     | 117 | LEU  |
| 4   | e     | 123 | ILE  |
| 4   | e     | 126 | LYS  |
| 4   | e     | 128 | LEU  |
| 4   | e     | 144 | LEU  |
| 4   | e     | 147 | LEU  |
| 4   | e     | 160 | SER  |
| 5   | f     | 3   | GLN  |
| 5   | f     | 4   | ASP  |
| 5   | f     | 5   | THR  |
| 5   | f     | 33  | LEU  |
| 5   | f     | 36  | ASN  |
| 5   | f     | 41  | ILE  |
| 5   | f     | 45  | ASP  |
| 5   | f     | 65  | ILE  |
| 5   | f     | 66  | VAL  |
| 5   | f     | 77  | ILE  |
| 5   | f     | 78  | ASN  |
| 5   | f     | 88  | ASP  |
| 6   | g     | 9   | LYS  |
| 6   | g     | 10  | ARG  |
| 6   | g     | 12  | VAL  |
| 6   | g     | 13  | LEU  |
| 6   | g     | 22  | LEU  |
| 6   | g     | 52  | GLU  |
| 6   | g     | 56  | ASN  |
| 6   | g     | 64  | GLN  |
| 6   | g     | 72  | VAL  |
| 6   | g     | 85  | TYR  |
| 6   | g     | 94  | GLU  |
| 6   | g     | 95  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | g     | 115 | THR  |
| 6   | g     | 120 | LEU  |
| 6   | g     | 131 | THR  |
| 6   | g     | 141 | THR  |
| 6   | g     | 146 | ASP  |
| 6   | g     | 151 | PHE  |
| 6   | g     | 155 | ARG  |
| 7   | h     | 11  | LEU  |
| 7   | h     | 25  | LEU  |
| 7   | h     | 27  | VAL  |
| 7   | h     | 40  | LEU  |
| 7   | h     | 52  | ILE  |
| 7   | h     | 54  | ASP  |
| 7   | h     | 57  | GLN  |
| 7   | h     | 69  | ASN  |
| 7   | h     | 74  | ILE  |
| 7   | h     | 75  | THR  |
| 7   | h     | 79  | ARG  |
| 7   | h     | 86  | ARG  |
| 7   | h     | 89  | VAL  |
| 7   | h     | 92  | ASP  |
| 7   | h     | 97  | VAL  |
| 7   | h     | 101 | LEU  |
| 7   | h     | 113 | ILE  |
| 7   | h     | 114 | THR  |
| 7   | h     | 131 | VAL  |
| 8   | i     | 16  | VAL  |
| 8   | i     | 30  | VAL  |
| 8   | i     | 35  | VAL  |
| 8   | i     | 65  | VAL  |
| 8   | i     | 66  | ASN  |
| 8   | i     | 99  | LYS  |
| 8   | i     | 130 | ARG  |
| 9   | j     | 4   | GLN  |
| 9   | j     | 18  | LEU  |
| 9   | j     | 25  | ILE  |
| 9   | j     | 32  | THR  |
| 9   | j     | 51  | VAL  |
| 9   | j     | 63  | GLU  |
| 9   | j     | 72  | ARG  |
| 9   | j     | 85  | ASP  |
| 9   | j     | 87  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | j     | 91  | ASP  |
| 10  | k     | 30  | THR  |
| 10  | k     | 32  | VAL  |
| 10  | k     | 35  | THR  |
| 10  | k     | 37  | THR  |
| 10  | k     | 40  | ASN  |
| 10  | k     | 45  | SER  |
| 10  | k     | 55  | SER  |
| 10  | k     | 56  | LYS  |
| 10  | k     | 65  | MET  |
| 10  | k     | 81  | THR  |
| 10  | k     | 82  | VAL  |
| 10  | k     | 85  | THR  |
| 10  | k     | 86  | VAL  |
| 10  | k     | 126 | ARG  |
| 11  | l     | 10  | LYS  |
| 11  | l     | 18  | LYS  |
| 11  | l     | 20  | ASP  |
| 11  | l     | 24  | LEU  |
| 11  | l     | 25  | ASN  |
| 11  | l     | 28  | TYR  |
| 11  | l     | 32  | LYS  |
| 11  | l     | 33  | LYS  |
| 11  | l     | 35  | GLN  |
| 11  | l     | 36  | THR  |
| 11  | l     | 37  | ASN  |
| 11  | l     | 42  | GLN  |
| 11  | l     | 44  | ARG  |
| 11  | l     | 54  | THR  |
| 11  | l     | 63  | ARG  |
| 11  | l     | 64  | LYS  |
| 11  | l     | 72  | ASN  |
| 11  | l     | 77  | THR  |
| 11  | l     | 80  | ILE  |
| 11  | l     | 88  | GLN  |
| 11  | l     | 92  | VAL  |
| 11  | l     | 102 | ASP  |
| 11  | l     | 106 | VAL  |
| 11  | l     | 110 | ILE  |
| 11  | l     | 111 | VAL  |
| 11  | l     | 117 | THR  |
| 11  | l     | 122 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | l     | 129 | LYS  |
| 12  | m     | 14  | ARG  |
| 12  | m     | 28  | THR  |
| 12  | m     | 29  | THR  |
| 12  | m     | 34  | LEU  |
| 12  | m     | 41  | GLU  |
| 12  | m     | 66  | GLU  |
| 12  | m     | 80  | LEU  |
| 12  | m     | 83  | ILE  |
| 12  | m     | 91  | HIS  |
| 12  | m     | 98  | ARG  |
| 12  | m     | 100 | GLN  |
| 12  | m     | 102 | THR  |
| 12  | m     | 103 | LYS  |
| 12  | m     | 109 | ARG  |
| 13  | n     | 17  | SER  |
| 14  | o     | 7   | ARG  |
| 14  | o     | 12  | ILE  |
| 14  | o     | 18  | HIS  |
| 14  | o     | 22  | THR  |
| 14  | o     | 29  | ILE  |
| 14  | o     | 40  | ASN  |
| 14  | o     | 54  | ARG  |
| 14  | o     | 56  | LEU  |
| 14  | o     | 67  | LEU  |
| 14  | o     | 75  | ILE  |
| 14  | o     | 81  | LEU  |
| 14  | o     | 84  | ARG  |
| 14  | o     | 87  | LEU  |
| 14  | o     | 89  | ARG  |
| 15  | p     | 21  | VAL  |
| 15  | p     | 22  | VAL  |
| 15  | p     | 26  | ARG  |
| 15  | p     | 32  | ARG  |
| 15  | p     | 36  | THR  |
| 15  | p     | 39  | THR  |
| 15  | p     | 44  | LYS  |
| 15  | p     | 54  | ASP  |
| 15  | p     | 71  | ARG  |
| 15  | p     | 74  | LEU  |
| 15  | p     | 88  | ASN  |
| 16  | q     | 4   | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | q     | 10  | VAL  |
| 16  | q     | 14  | ARG  |
| 16  | q     | 21  | ASP  |
| 16  | q     | 28  | VAL  |
| 16  | q     | 30  | THR  |
| 16  | q     | 32  | LYS  |
| 16  | q     | 40  | ARG  |
| 16  | q     | 42  | LYS  |
| 16  | q     | 51  | ASP  |
| 16  | q     | 55  | THR  |
| 16  | q     | 62  | VAL  |
| 16  | q     | 81  | VAL  |
| 17  | r     | 20  | ASN  |
| 17  | r     | 22  | ILE  |
| 17  | r     | 27  | TYR  |
| 17  | r     | 28  | LYS  |
| 17  | r     | 63  | ILE  |
| 17  | r     | 65  | ARG  |
| 18  | s     | 6   | LYS  |
| 18  | s     | 11  | VAL  |
| 18  | s     | 22  | GLN  |
| 18  | s     | 26  | GLU  |
| 18  | s     | 27  | LYS  |
| 18  | s     | 36  | ARG  |
| 18  | s     | 39  | THR  |
| 18  | s     | 45  | VAL  |
| 18  | s     | 65  | ASP  |
| 18  | s     | 70  | LYS  |
| 18  | s     | 73  | GLU  |
| 18  | s     | 78  | ARG  |
| 18  | s     | 81  | ARG  |
| 19  | t     | 12  | ARG  |
| 19  | t     | 20  | LYS  |
| 19  | t     | 33  | LYS  |
| 19  | t     | 39  | VAL  |
| 19  | t     | 44  | ASP  |
| 19  | t     | 47  | ASP  |
| 19  | t     | 49  | LEU  |
| 19  | t     | 62  | THR  |
| 19  | t     | 81  | LEU  |
| 22  | C     | 28  | THR  |
| 22  | C     | 30  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | C     | 38  | LYS  |
| 22  | C     | 43  | ARG  |
| 22  | C     | 77  | VAL  |
| 22  | C     | 91  | ILE  |
| 22  | C     | 104 | ILE  |
| 22  | C     | 110 | LEU  |
| 22  | C     | 139 | THR  |
| 22  | C     | 167 | LYS  |
| 22  | C     | 168 | GLU  |
| 22  | C     | 177 | ASN  |
| 22  | C     | 182 | ARG  |
| 22  | C     | 191 | THR  |
| 22  | C     | 198 | GLU  |
| 22  | C     | 216 | LYS  |
| 22  | C     | 219 | THR  |
| 22  | C     | 260 | ARG  |
| 22  | C     | 261 | ASN  |
| 23  | D     | 15  | ILE  |
| 23  | D     | 21  | GLU  |
| 23  | D     | 22  | LEU  |
| 23  | D     | 23  | ILE  |
| 23  | D     | 25  | VAL  |
| 23  | D     | 43  | THR  |
| 23  | D     | 49  | ILE  |
| 23  | D     | 50  | GLN  |
| 23  | D     | 58  | GLU  |
| 23  | D     | 59  | VAL  |
| 23  | D     | 62  | ASN  |
| 23  | D     | 69  | VAL  |
| 23  | D     | 71  | LYS  |
| 23  | D     | 81  | LYS  |
| 23  | D     | 86  | VAL  |
| 23  | D     | 90  | GLU  |
| 23  | D     | 103 | GLN  |
| 23  | D     | 107 | VAL  |
| 23  | D     | 108 | VAL  |
| 23  | D     | 111 | THR  |
| 23  | D     | 119 | PHE  |
| 23  | D     | 141 | ARG  |
| 23  | D     | 145 | SER  |
| 23  | D     | 158 | LYS  |
| 23  | D     | 167 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | D     | 168 | ARG  |
| 23  | D     | 170 | THR  |
| 23  | D     | 191 | ASN  |
| 23  | D     | 199 | LEU  |
| 23  | D     | 201 | THR  |
| 24  | E     | 6   | LEU  |
| 24  | E     | 8   | LYS  |
| 24  | E     | 18  | THR  |
| 24  | E     | 20  | ASN  |
| 24  | E     | 31  | SER  |
| 24  | E     | 49  | HIS  |
| 24  | E     | 65  | TRP  |
| 24  | E     | 77  | SER  |
| 24  | E     | 79  | ARG  |
| 24  | E     | 80  | SER  |
| 24  | E     | 82  | GLN  |
| 24  | E     | 89  | VAL  |
| 24  | E     | 93  | THR  |
| 24  | E     | 94  | PRO  |
| 24  | E     | 105 | VAL  |
| 24  | E     | 113 | VAL  |
| 24  | E     | 153 | LEU  |
| 24  | E     | 157 | GLU  |
| 24  | E     | 160 | ASN  |
| 24  | E     | 165 | LEU  |
| 24  | E     | 168 | ARG  |
| 24  | E     | 176 | VAL  |
| 24  | E     | 184 | LEU  |
| 24  | E     | 190 | ASN  |
| 24  | E     | 193 | LEU  |
| 24  | E     | 195 | THR  |
| 24  | E     | 200 | THR  |
| 24  | E     | 205 | VAL  |
| 25  | F     | 6   | GLU  |
| 25  | F     | 15  | SER  |
| 25  | F     | 17  | VAL  |
| 25  | F     | 27  | GLN  |
| 25  | F     | 32  | ASP  |
| 25  | F     | 57  | LEU  |
| 25  | F     | 61  | THR  |
| 25  | F     | 66  | LEU  |
| 25  | F     | 77  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | F     | 81  | GLU  |
| 25  | F     | 88  | LYS  |
| 25  | F     | 89  | VAL  |
| 25  | F     | 110 | ARG  |
| 25  | F     | 112 | ARG  |
| 25  | F     | 114 | PHE  |
| 25  | F     | 127 | ASN  |
| 25  | F     | 130 | LEU  |
| 25  | F     | 133 | LYS  |
| 25  | F     | 137 | ILE  |
| 25  | F     | 142 | ASP  |
| 25  | F     | 143 | TYR  |
| 25  | F     | 149 | VAL  |
| 25  | F     | 152 | MET  |
| 25  | F     | 162 | THR  |
| 25  | F     | 170 | LEU  |
| 26  | G     | 8   | VAL  |
| 26  | G     | 11  | LEU  |
| 26  | G     | 25  | THR  |
| 26  | G     | 32  | GLU  |
| 26  | G     | 35  | ARG  |
| 26  | G     | 44  | ASN  |
| 26  | G     | 45  | ILE  |
| 26  | G     | 46  | GLU  |
| 26  | G     | 63  | THR  |
| 26  | G     | 67  | THR  |
| 26  | G     | 79  | VAL  |
| 26  | G     | 84  | GLN  |
| 26  | G     | 95  | ARG  |
| 26  | G     | 101 | ASN  |
| 26  | G     | 103 | LEU  |
| 26  | G     | 107 | VAL  |
| 26  | G     | 121 | VAL  |
| 26  | G     | 122 | THR  |
| 26  | G     | 136 | ILE  |
| 26  | G     | 143 | GLU  |
| 26  | G     | 152 | ARG  |
| 26  | G     | 165 | VAL  |
| 26  | G     | 171 | ARG  |
| 27  | K     | 2   | ARG  |
| 27  | K     | 14  | ARG  |
| 27  | K     | 26  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | K     | 30  | SER  |
| 27  | K     | 46  | THR  |
| 27  | K     | 58  | ILE  |
| 27  | K     | 77  | ARG  |
| 27  | K     | 80  | MET  |
| 27  | K     | 85  | LEU  |
| 27  | K     | 100 | ARG  |
| 27  | K     | 101 | LEU  |
| 27  | K     | 113 | ASN  |
| 27  | K     | 114 | THR  |
| 27  | K     | 115 | LEU  |
| 27  | K     | 118 | LYS  |
| 27  | K     | 123 | LEU  |
| 27  | K     | 145 | ASN  |
| 28  | L     | 1   | MET  |
| 28  | L     | 5   | GLU  |
| 28  | L     | 13  | ASN  |
| 28  | L     | 18  | GLU  |
| 28  | L     | 19  | ILE  |
| 28  | L     | 21  | THR  |
| 28  | L     | 42  | THR  |
| 28  | L     | 53  | LYS  |
| 28  | L     | 73  | ASP  |
| 28  | L     | 90  | ASP  |
| 28  | L     | 105 | GLU  |
| 29  | M     | 3   | LEU  |
| 29  | M     | 16  | ARG  |
| 29  | M     | 42  | SER  |
| 29  | M     | 60  | ARG  |
| 29  | M     | 76  | VAL  |
| 29  | M     | 81  | THR  |
| 29  | M     | 84  | ARG  |
| 29  | M     | 87  | ASP  |
| 29  | M     | 122 | THR  |
| 29  | M     | 131 | SER  |
| 30  | N     | 5   | LYS  |
| 30  | N     | 10  | ARG  |
| 30  | N     | 11  | ARG  |
| 30  | N     | 25  | LYS  |
| 30  | N     | 26  | GLU  |
| 30  | N     | 34  | LEU  |
| 30  | N     | 37  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | N     | 74  | TYR  |
| 30  | N     | 76  | SER  |
| 30  | N     | 85  | LYS  |
| 30  | N     | 103 | MET  |
| 30  | N     | 109 | VAL  |
| 30  | N     | 127 | VAL  |
| 30  | N     | 133 | LYS  |
| 31  | O     | 3   | TYR  |
| 31  | O     | 8   | ARG  |
| 31  | O     | 24  | LEU  |
| 31  | O     | 41  | ARG  |
| 31  | O     | 49  | THR  |
| 31  | O     | 55  | ASP  |
| 31  | O     | 56  | LEU  |
| 31  | O     | 84  | SER  |
| 31  | O     | 89  | LEU  |
| 31  | O     | 100 | ARG  |
| 31  | O     | 106 | ARG  |
| 31  | O     | 108 | LEU  |
| 31  | O     | 124 | GLU  |
| 31  | O     | 125 | PHE  |
| 32  | P     | 2   | ILE  |
| 32  | P     | 6   | ASP  |
| 32  | P     | 11  | ARG  |
| 32  | P     | 28  | CYS  |
| 32  | P     | 31  | LEU  |
| 32  | P     | 35  | ARG  |
| 32  | P     | 46  | ASP  |
| 32  | P     | 51  | VAL  |
| 32  | P     | 57  | SER  |
| 32  | P     | 67  | THR  |
| 32  | P     | 79  | VAL  |
| 32  | P     | 95  | ARG  |
| 33  | Q     | 2   | ASN  |
| 33  | Q     | 10  | GLN  |
| 33  | Q     | 11  | GLU  |
| 33  | Q     | 36  | THR  |
| 33  | Q     | 49  | LYS  |
| 33  | Q     | 55  | ILE  |
| 33  | Q     | 60  | THR  |
| 33  | Q     | 72  | ARG  |
| 33  | Q     | 76  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | Q     | 78  | THR  |
| 33  | Q     | 80  | ARG  |
| 33  | Q     | 101 | ARG  |
| 33  | Q     | 109 | ARG  |
| 33  | Q     | 114 | ARG  |
| 34  | R     | 10  | THR  |
| 34  | R     | 30  | THR  |
| 34  | R     | 51  | ARG  |
| 34  | R     | 60  | LEU  |
| 34  | R     | 79  | LEU  |
| 34  | R     | 89  | ASP  |
| 34  | R     | 92  | ARG  |
| 35  | S     | 1   | MET  |
| 35  | S     | 2   | TYR  |
| 35  | S     | 14  | VAL  |
| 35  | S     | 22  | VAL  |
| 35  | S     | 33  | VAL  |
| 35  | S     | 61  | THR  |
| 35  | S     | 73  | THR  |
| 35  | S     | 75  | GLN  |
| 35  | S     | 94  | LYS  |
| 35  | S     | 101 | ASN  |
| 36  | T     | 4   | GLN  |
| 36  | T     | 9   | LYS  |
| 36  | T     | 11  | THR  |
| 36  | T     | 14  | THR  |
| 36  | T     | 26  | ILE  |
| 36  | T     | 29  | ILE  |
| 36  | T     | 70  | ASP  |
| 36  | T     | 88  | LYS  |
| 36  | T     | 89  | ARG  |
| 36  | T     | 93  | ARG  |
| 36  | T     | 105 | THR  |
| 36  | T     | 109 | THR  |
| 36  | T     | 115 | LYS  |
| 37  | U     | 2   | GLU  |
| 37  | U     | 3   | LEU  |
| 37  | U     | 14  | GLU  |
| 37  | U     | 16  | SER  |
| 37  | U     | 29  | VAL  |
| 37  | U     | 37  | LEU  |
| 37  | U     | 47  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | U     | 49  | LYS  |
| 37  | U     | 52  | ASN  |
| 37  | U     | 56  | LEU  |
| 37  | U     | 75  | ARG  |
| 37  | U     | 76  | ARG  |
| 37  | U     | 84  | GLU  |
| 37  | U     | 87  | LYS  |
| 38  | V     | 1   | MET  |
| 38  | V     | 2   | PHE  |
| 38  | V     | 5   | LYS  |
| 38  | V     | 9   | VAL  |
| 38  | V     | 13  | THR  |
| 38  | V     | 17  | LYS  |
| 38  | V     | 29  | LYS  |
| 38  | V     | 41  | VAL  |
| 38  | V     | 58  | GLU  |
| 38  | V     | 59  | VAL  |
| 38  | V     | 68  | VAL  |
| 38  | V     | 69  | MET  |
| 38  | V     | 94  | SER  |
| 38  | V     | 99  | GLU  |
| 39  | X     | 18  | SER  |
| 39  | X     | 19  | THR  |
| 39  | X     | 20  | SER  |
| 39  | X     | 23  | ARG  |
| 39  | X     | 24  | ASP  |
| 39  | X     | 28  | LYS  |
| 39  | X     | 39  | THR  |
| 39  | X     | 40  | VAL  |
| 39  | X     | 62  | ILE  |
| 39  | X     | 67  | THR  |
| 39  | X     | 73  | ASP  |
| 39  | X     | 88  | VAL  |
| 39  | X     | 93  | VAL  |
| 40  | Y     | 12  | THR  |
| 40  | Y     | 22  | MET  |
| 40  | Y     | 24  | SER  |
| 40  | Y     | 27  | ARG  |
| 40  | Y     | 28  | THR  |
| 40  | Y     | 32  | ASN  |
| 40  | Y     | 34  | GLN  |
| 40  | Y     | 36  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | Y     | 40  | ILE  |
| 41  | Z     | 2   | LYS  |
| 41  | Z     | 3   | VAL  |
| 41  | Z     | 4   | LYS  |
| 41  | Z     | 5   | GLU  |
| 41  | Z     | 10  | THR  |
| 41  | Z     | 15  | LEU  |
| 41  | Z     | 32  | LEU  |
| 41  | Z     | 37  | LEU  |
| 41  | Z     | 38  | GLU  |
| 41  | Z     | 55  | THR  |
| 42  | 0     | 8   | LEU  |
| 42  | 0     | 16  | PRO  |
| 42  | 0     | 35  | VAL  |
| 42  | 0     | 55  | ASP  |
| 42  | 0     | 59  | VAL  |
| 43  | 2     | 3   | VAL  |
| 43  | 2     | 7   | ARG  |
| 43  | 2     | 8   | THR  |
| 43  | 2     | 18  | THR  |
| 43  | 2     | 23  | THR  |
| 43  | 2     | 32  | ASN  |
| 43  | 2     | 56  | SER  |
| 44  | 3     | 8   | GLU  |
| 44  | 3     | 10  | THR  |
| 44  | 3     | 44  | LEU  |
| 45  | 4     | 10  | ARG  |
| 45  | 4     | 20  | LYS  |
| 45  | 4     | 24  | THR  |
| 45  | 4     | 34  | ARG  |
| 45  | 4     | 43  | SER  |
| 46  | 5     | 31  | HIS  |
| 46  | 5     | 32  | ARG  |
| 46  | 5     | 41  | ARG  |
| 46  | 5     | 46  | LYS  |
| 46  | 5     | 57  | ARG  |
| 46  | 5     | 58  | ILE  |
| 46  | 5     | 65  | MET  |
| 47  | 6     | 4   | ARG  |
| 47  | 6     | 11  | CYS  |
| 47  | 6     | 15  | LYS  |
| 47  | 6     | 26  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 6     | 36  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | d     | 35  | GLN  |
| 3   | d     | 50  | GLN  |
| 3   | d     | 55  | GLN  |
| 3   | d     | 59  | HIS  |
| 3   | d     | 113 | GLN  |
| 3   | d     | 201 | GLN  |
| 4   | e     | 8   | HIS  |
| 5   | f     | 78  | ASN  |
| 6   | g     | 28  | ASN  |
| 6   | g     | 64  | GLN  |
| 6   | g     | 86  | GLN  |
| 6   | g     | 106 | ASN  |
| 7   | h     | 57  | GLN  |
| 8   | i     | 66  | ASN  |
| 8   | i     | 68  | ASN  |
| 8   | i     | 81  | HIS  |
| 10  | k     | 22  | HIS  |
| 11  | l     | 109 | HIS  |
| 11  | l     | 125 | GLN  |
| 12  | m     | 105 | ASN  |
| 14  | o     | 42  | HIS  |
| 14  | o     | 46  | HIS  |
| 14  | o     | 83  | GLN  |
| 15  | p     | 41  | ASN  |
| 15  | p     | 72  | ASN  |
| 16  | q     | 34  | HIS  |
| 18  | s     | 22  | GLN  |
| 18  | s     | 57  | HIS  |
| 18  | s     | 63  | GLN  |
| 19  | t     | 45  | ASN  |
| 22  | C     | 90  | ASN  |
| 22  | C     | 95  | HIS  |
| 22  | C     | 143 | ASN  |
| 22  | C     | 199 | GLN  |
| 23  | D     | 37  | GLN  |
| 23  | D     | 62  | ASN  |
| 23  | D     | 68  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | E     | 13  | GLN  |
| 24  | E     | 14  | ASN  |
| 24  | E     | 49  | HIS  |
| 24  | E     | 75  | GLN  |
| 24  | E     | 82  | GLN  |
| 24  | E     | 141 | GLN  |
| 24  | E     | 196 | GLN  |
| 25  | F     | 37  | ASN  |
| 25  | F     | 49  | ASN  |
| 27  | K     | 48  | HIS  |
| 27  | K     | 59  | ASN  |
| 27  | K     | 113 | ASN  |
| 27  | K     | 131 | HIS  |
| 29  | M     | 4   | HIS  |
| 29  | M     | 38  | GLN  |
| 29  | M     | 54  | GLN  |
| 29  | M     | 133 | GLN  |
| 32  | P     | 12  | GLN  |
| 32  | P     | 15  | HIS  |
| 32  | P     | 20  | ASN  |
| 32  | P     | 114 | ASN  |
| 33  | Q     | 41  | GLN  |
| 34  | R     | 101 | ASN  |
| 35  | S     | 18  | GLN  |
| 35  | S     | 83  | HIS  |
| 35  | S     | 86  | GLN  |
| 35  | S     | 88  | HIS  |
| 36  | T     | 4   | GLN  |
| 36  | T     | 46  | ASN  |
| 36  | T     | 65  | ASN  |
| 39  | X     | 49  | GLN  |
| 40  | Y     | 17  | ASN  |
| 40  | Y     | 23  | ASN  |
| 40  | Y     | 32  | ASN  |
| 40  | Y     | 34  | GLN  |
| 41  | Z     | 36  | GLN  |
| 41  | Z     | 48  | GLN  |
| 42  | 0     | 40  | ASN  |
| 43  | 2     | 40  | HIS  |
| 45  | 4     | 8   | ASN  |
| 46  | 5     | 4   | GLN  |
| 46  | 5     | 31  | HIS  |

## 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | a     | 1521/1548 (98%) | 308 (20%)         | 0               |
| 20  | A     | 2733/2908 (93%) | 536 (19%)         | 28 (1%)         |
| 21  | B     | 115/116 (99%)   | 32 (27%)          | 3 (2%)          |
| All | All   | 4369/4572 (95%) | 876 (20%)         | 31 (0%)         |

All (876) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 4   | G    |
| 1   | a     | 5   | A    |
| 1   | a     | 6   | G    |
| 1   | a     | 13  | A    |
| 1   | a     | 19  | G    |
| 1   | a     | 27  | C    |
| 1   | a     | 29  | A    |
| 1   | a     | 30  | A    |
| 1   | a     | 32  | G    |
| 1   | a     | 35  | G    |
| 1   | a     | 36  | G    |
| 1   | a     | 38  | G    |
| 1   | a     | 41  | G    |
| 1   | a     | 44  | C    |
| 1   | a     | 45  | C    |
| 1   | a     | 48  | A    |
| 1   | a     | 52  | A    |
| 1   | a     | 70  | U    |
| 1   | a     | 71  | U    |
| 1   | a     | 101 | A    |
| 1   | a     | 103 | A    |
| 1   | a     | 106 | A    |
| 1   | a     | 113 | G    |
| 1   | a     | 114 | A    |
| 1   | a     | 122 | G    |
| 1   | a     | 125 | A    |
| 1   | a     | 126 | C    |
| 1   | a     | 137 | C    |
| 1   | a     | 147 | A    |
| 1   | a     | 165 | G    |
| 1   | a     | 167 | A    |
| 1   | a     | 169 | C    |
| 1   | a     | 171 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 172 | G    |
| 1   | a     | 183 | G    |
| 1   | a     | 188 | A    |
| 1   | a     | 189 | C    |
| 1   | a     | 202 | A    |
| 1   | a     | 210 | A    |
| 1   | a     | 211 | G    |
| 1   | a     | 212 | A    |
| 1   | a     | 213 | G    |
| 1   | a     | 214 | U    |
| 1   | a     | 215 | G    |
| 1   | a     | 216 | A    |
| 1   | a     | 218 | A    |
| 1   | a     | 225 | U    |
| 1   | a     | 226 | U    |
| 1   | a     | 228 | G    |
| 1   | a     | 229 | G    |
| 1   | a     | 230 | G    |
| 1   | a     | 235 | G    |
| 1   | a     | 246 | G    |
| 1   | a     | 254 | G    |
| 1   | a     | 255 | U    |
| 1   | a     | 256 | G    |
| 1   | a     | 258 | A    |
| 1   | a     | 259 | U    |
| 1   | a     | 260 | U    |
| 1   | a     | 262 | G    |
| 1   | a     | 266 | G    |
| 1   | a     | 281 | G    |
| 1   | a     | 282 | C    |
| 1   | a     | 295 | C    |
| 1   | a     | 298 | U    |
| 1   | a     | 304 | G    |
| 1   | a     | 321 | A    |
| 1   | a     | 332 | U    |
| 1   | a     | 336 | A    |
| 1   | a     | 337 | C    |
| 1   | a     | 342 | A    |
| 1   | a     | 343 | C    |
| 1   | a     | 344 | A    |
| 1   | a     | 360 | C    |
| 1   | a     | 362 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 367 | C    |
| 1   | a     | 369 | G    |
| 1   | a     | 371 | A    |
| 1   | a     | 382 | U    |
| 1   | a     | 387 | C    |
| 1   | a     | 388 | A    |
| 1   | a     | 390 | U    |
| 1   | a     | 399 | G    |
| 1   | a     | 412 | A    |
| 1   | a     | 421 | G    |
| 1   | a     | 426 | A    |
| 1   | a     | 427 | A    |
| 1   | a     | 428 | G    |
| 1   | a     | 429 | A    |
| 1   | a     | 431 | G    |
| 1   | a     | 444 | U    |
| 1   | a     | 447 | A    |
| 1   | a     | 463 | A    |
| 1   | a     | 464 | A    |
| 1   | a     | 468 | C    |
| 1   | a     | 473 | A    |
| 1   | a     | 474 | C    |
| 1   | a     | 478 | A    |
| 1   | a     | 480 | U    |
| 1   | a     | 484 | U    |
| 1   | a     | 485 | G    |
| 1   | a     | 488 | C    |
| 1   | a     | 489 | G    |
| 1   | a     | 490 | U    |
| 1   | a     | 495 | U    |
| 1   | a     | 498 | C    |
| 1   | a     | 499 | G    |
| 1   | a     | 500 | G    |
| 1   | a     | 516 | C    |
| 1   | a     | 524 | A    |
| 1   | a     | 525 | A    |
| 1   | a     | 526 | C    |
| 1   | a     | 532 | G    |
| 1   | a     | 533 | C    |
| 1   | a     | 539 | G    |
| 1   | a     | 542 | G    |
| 1   | a     | 546 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 548 | A    |
| 1   | a     | 551 | C    |
| 1   | a     | 560 | C    |
| 1   | a     | 562 | A    |
| 1   | a     | 574 | A    |
| 1   | a     | 576 | U    |
| 1   | a     | 577 | U    |
| 1   | a     | 584 | C    |
| 1   | a     | 585 | G    |
| 1   | a     | 587 | A    |
| 1   | a     | 588 | A    |
| 1   | a     | 590 | G    |
| 1   | a     | 591 | C    |
| 1   | a     | 592 | G    |
| 1   | a     | 593 | A    |
| 1   | a     | 594 | G    |
| 1   | a     | 596 | G    |
| 1   | a     | 602 | G    |
| 1   | a     | 608 | U    |
| 1   | a     | 637 | A    |
| 1   | a     | 643 | G    |
| 1   | a     | 648 | U    |
| 1   | a     | 668 | U    |
| 1   | a     | 671 | G    |
| 1   | a     | 680 | A    |
| 1   | a     | 701 | U    |
| 1   | a     | 702 | A    |
| 1   | a     | 710 | A    |
| 1   | a     | 716 | U    |
| 1   | a     | 717 | A    |
| 1   | a     | 718 | G    |
| 1   | a     | 726 | G    |
| 1   | a     | 738 | U    |
| 1   | a     | 744 | A    |
| 1   | a     | 755 | U    |
| 1   | a     | 764 | A    |
| 1   | a     | 770 | G    |
| 1   | a     | 777 | C    |
| 1   | a     | 780 | G    |
| 1   | a     | 792 | A    |
| 1   | a     | 793 | G    |
| 1   | a     | 802 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 809  | A    |
| 1   | a     | 817  | A    |
| 1   | a     | 830  | A    |
| 1   | a     | 832  | C    |
| 1   | a     | 835  | U    |
| 1   | a     | 836  | G    |
| 1   | a     | 842  | U    |
| 1   | a     | 843  | A    |
| 1   | a     | 857  | U    |
| 1   | a     | 858  | U    |
| 1   | a     | 859  | C    |
| 1   | a     | 860  | C    |
| 1   | a     | 861  | G    |
| 1   | a     | 862  | C    |
| 1   | a     | 876  | A    |
| 1   | a     | 883  | G    |
| 1   | a     | 888  | A    |
| 1   | a     | 893  | C    |
| 1   | a     | 930  | A    |
| 1   | a     | 940  | C    |
| 1   | a     | 942  | G    |
| 1   | a     | 943  | G    |
| 1   | a     | 947  | C    |
| 1   | a     | 948  | C    |
| 1   | a     | 950  | C    |
| 1   | a     | 951  | A    |
| 1   | a     | 962  | A    |
| 1   | a     | 963  | G    |
| 1   | a     | 974  | A    |
| 1   | a     | 975  | A    |
| 1   | a     | 976  | U    |
| 1   | a     | 977  | U    |
| 1   | a     | 982  | G    |
| 1   | a     | 985  | A    |
| 1   | a     | 987  | G    |
| 1   | a     | 988  | C    |
| 1   | a     | 991  | A    |
| 1   | a     | 992  | G    |
| 1   | a     | 993  | A    |
| 1   | a     | 999  | A    |
| 1   | a     | 1003 | G    |
| 1   | a     | 1008 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1009 | G    |
| 1   | a     | 1015 | C    |
| 1   | a     | 1018 | U    |
| 1   | a     | 1020 | A    |
| 1   | a     | 1022 | C    |
| 1   | a     | 1031 | G    |
| 1   | a     | 1039 | U    |
| 1   | a     | 1040 | U    |
| 1   | a     | 1041 | U    |
| 1   | a     | 1042 | C    |
| 1   | a     | 1044 | C    |
| 1   | a     | 1045 | U    |
| 1   | a     | 1046 | U    |
| 1   | a     | 1047 | C    |
| 1   | a     | 1048 | G    |
| 1   | a     | 1049 | G    |
| 1   | a     | 1057 | G    |
| 1   | a     | 1058 | U    |
| 1   | a     | 1060 | A    |
| 1   | a     | 1061 | C    |
| 1   | a     | 1062 | A    |
| 1   | a     | 1069 | G    |
| 1   | a     | 1080 | G    |
| 1   | a     | 1081 | U    |
| 1   | a     | 1096 | A    |
| 1   | a     | 1110 | G    |
| 1   | a     | 1111 | U    |
| 1   | a     | 1117 | A    |
| 1   | a     | 1140 | G    |
| 1   | a     | 1142 | U    |
| 1   | a     | 1144 | C    |
| 1   | a     | 1146 | A    |
| 1   | a     | 1149 | A    |
| 1   | a     | 1154 | G    |
| 1   | a     | 1155 | U    |
| 1   | a     | 1156 | U    |
| 1   | a     | 1157 | G    |
| 1   | a     | 1172 | A    |
| 1   | a     | 1174 | U    |
| 1   | a     | 1183 | C    |
| 1   | a     | 1196 | G    |
| 1   | a     | 1199 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1202 | G    |
| 1   | a     | 1211 | A    |
| 1   | a     | 1212 | A    |
| 1   | a     | 1215 | C    |
| 1   | a     | 1219 | A    |
| 1   | a     | 1227 | U    |
| 1   | a     | 1229 | U    |
| 1   | a     | 1240 | A    |
| 1   | a     | 1242 | A    |
| 1   | a     | 1248 | G    |
| 1   | a     | 1253 | A    |
| 1   | a     | 1263 | A    |
| 1   | a     | 1272 | C    |
| 1   | a     | 1275 | U    |
| 1   | a     | 1276 | A    |
| 1   | a     | 1294 | A    |
| 1   | a     | 1295 | A    |
| 1   | a     | 1301 | U    |
| 1   | a     | 1302 | A    |
| 1   | a     | 1310 | U    |
| 1   | a     | 1312 | U    |
| 1   | a     | 1314 | A    |
| 1   | a     | 1317 | U    |
| 1   | a     | 1320 | G    |
| 1   | a     | 1334 | A    |
| 1   | a     | 1335 | C    |
| 1   | a     | 1353 | G    |
| 1   | a     | 1368 | G    |
| 1   | a     | 1372 | A    |
| 1   | a     | 1374 | C    |
| 1   | a     | 1378 | A    |
| 1   | a     | 1379 | C    |
| 1   | a     | 1383 | G    |
| 1   | a     | 1392 | A    |
| 1   | a     | 1393 | C    |
| 1   | a     | 1409 | A    |
| 1   | a     | 1412 | C    |
| 1   | a     | 1416 | G    |
| 1   | a     | 1438 | G    |
| 1   | a     | 1455 | U    |
| 1   | a     | 1457 | A    |
| 1   | a     | 1461 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | a     | 1466 | U    |
| 1   | a     | 1467 | U    |
| 1   | a     | 1468 | U    |
| 1   | a     | 1469 | U    |
| 1   | a     | 1470 | G    |
| 1   | a     | 1479 | C    |
| 1   | a     | 1483 | U    |
| 1   | a     | 1498 | G    |
| 1   | a     | 1503 | G    |
| 1   | a     | 1508 | A    |
| 1   | a     | 1509 | A    |
| 1   | a     | 1518 | A    |
| 1   | a     | 1519 | A    |
| 1   | a     | 1520 | G    |
| 1   | a     | 1522 | U    |
| 1   | a     | 1523 | A    |
| 1   | a     | 1524 | G    |
| 1   | a     | 1533 | G    |
| 1   | a     | 1542 | G    |
| 1   | a     | 1545 | G    |
| 1   | a     | 1546 | G    |
| 1   | a     | 1547 | A    |
| 1   | a     | 1550 | A    |
| 20  | A     | 13   | U    |
| 20  | A     | 14   | A    |
| 20  | A     | 28   | G    |
| 20  | A     | 35   | U    |
| 20  | A     | 42   | A    |
| 20  | A     | 52   | G    |
| 20  | A     | 68   | A    |
| 20  | A     | 71   | G    |
| 20  | A     | 72   | A    |
| 20  | A     | 75   | U    |
| 20  | A     | 76   | G    |
| 20  | A     | 92   | A    |
| 20  | A     | 93   | G    |
| 20  | A     | 97   | G    |
| 20  | A     | 102  | G    |
| 20  | A     | 110  | G    |
| 20  | A     | 118  | A    |
| 20  | A     | 119  | A    |
| 20  | A     | 120  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | A     | 131 | A    |
| 20  | A     | 148 | A    |
| 20  | A     | 155 | U    |
| 20  | A     | 156 | U    |
| 20  | A     | 158 | A    |
| 20  | A     | 165 | A    |
| 20  | A     | 166 | C    |
| 20  | A     | 168 | U    |
| 20  | A     | 169 | A    |
| 20  | A     | 177 | A    |
| 20  | A     | 180 | G    |
| 20  | A     | 182 | U    |
| 20  | A     | 185 | A    |
| 20  | A     | 199 | A    |
| 20  | A     | 202 | A    |
| 20  | A     | 218 | G    |
| 20  | A     | 219 | A    |
| 20  | A     | 220 | A    |
| 20  | A     | 225 | A    |
| 20  | A     | 231 | A    |
| 20  | A     | 232 | U    |
| 20  | A     | 233 | U    |
| 20  | A     | 235 | G    |
| 20  | A     | 236 | A    |
| 20  | A     | 251 | G    |
| 20  | A     | 255 | G    |
| 20  | A     | 265 | A    |
| 20  | A     | 268 | A    |
| 20  | A     | 277 | C    |
| 20  | A     | 279 | A    |
| 20  | A     | 284 | C    |
| 20  | A     | 285 | U    |
| 20  | A     | 286 | U    |
| 20  | A     | 287 | G    |
| 20  | A     | 288 | C    |
| 20  | A     | 289 | U    |
| 20  | A     | 296 | G    |
| 20  | A     | 297 | G    |
| 20  | A     | 298 | U    |
| 20  | A     | 300 | G    |
| 20  | A     | 302 | A    |
| 20  | A     | 309 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | A     | 313 | A    |
| 20  | A     | 315 | G    |
| 20  | A     | 316 | G    |
| 20  | A     | 318 | A    |
| 20  | A     | 321 | C    |
| 20  | A     | 322 | U    |
| 20  | A     | 325 | U    |
| 20  | A     | 327 | G    |
| 20  | A     | 332 | G    |
| 20  | A     | 347 | A    |
| 20  | A     | 352 | C    |
| 20  | A     | 367 | A    |
| 20  | A     | 383 | A    |
| 20  | A     | 392 | A    |
| 20  | A     | 393 | A    |
| 20  | A     | 396 | C    |
| 20  | A     | 399 | A    |
| 20  | A     | 404 | G    |
| 20  | A     | 420 | G    |
| 20  | A     | 426 | G    |
| 20  | A     | 429 | A    |
| 20  | A     | 439 | G    |
| 20  | A     | 446 | G    |
| 20  | A     | 451 | G    |
| 20  | A     | 452 | A    |
| 20  | A     | 491 | U    |
| 20  | A     | 496 | C    |
| 20  | A     | 507 | G    |
| 20  | A     | 517 | A    |
| 20  | A     | 520 | A    |
| 20  | A     | 521 | G    |
| 20  | A     | 524 | C    |
| 20  | A     | 542 | A    |
| 20  | A     | 543 | U    |
| 20  | A     | 544 | A    |
| 20  | A     | 547 | U    |
| 20  | A     | 548 | C    |
| 20  | A     | 551 | G    |
| 20  | A     | 560 | U    |
| 20  | A     | 561 | G    |
| 20  | A     | 569 | C    |
| 20  | A     | 570 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | A     | 571 | A    |
| 20  | A     | 572 | G    |
| 20  | A     | 577 | A    |
| 20  | A     | 581 | C    |
| 20  | A     | 586 | A    |
| 20  | A     | 587 | U    |
| 20  | A     | 588 | G    |
| 20  | A     | 596 | G    |
| 20  | A     | 600 | G    |
| 20  | A     | 609 | A    |
| 20  | A     | 610 | G    |
| 20  | A     | 611 | A    |
| 20  | A     | 612 | A    |
| 20  | A     | 613 | U    |
| 20  | A     | 614 | G    |
| 20  | A     | 624 | G    |
| 20  | A     | 631 | U    |
| 20  | A     | 640 | A    |
| 20  | A     | 652 | A    |
| 20  | A     | 654 | A    |
| 20  | A     | 655 | G    |
| 20  | A     | 656 | A    |
| 20  | A     | 660 | A    |
| 20  | A     | 673 | G    |
| 20  | A     | 676 | A    |
| 20  | A     | 677 | G    |
| 20  | A     | 684 | U    |
| 20  | A     | 685 | A    |
| 20  | A     | 692 | A    |
| 20  | A     | 695 | A    |
| 20  | A     | 704 | U    |
| 20  | A     | 722 | G    |
| 20  | A     | 726 | U    |
| 20  | A     | 752 | G    |
| 20  | A     | 753 | G    |
| 20  | A     | 755 | A    |
| 20  | A     | 757 | A    |
| 20  | A     | 759 | C    |
| 20  | A     | 764 | U    |
| 20  | A     | 770 | A    |
| 20  | A     | 778 | C    |
| 20  | A     | 779 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | A     | 784 | C    |
| 20  | A     | 787 | U    |
| 20  | A     | 804 | A    |
| 20  | A     | 805 | G    |
| 20  | A     | 808 | G    |
| 20  | A     | 810 | G    |
| 20  | A     | 815 | G    |
| 20  | A     | 817 | G    |
| 20  | A     | 822 | A    |
| 20  | A     | 824 | U    |
| 20  | A     | 832 | G    |
| 20  | A     | 833 | A    |
| 20  | A     | 845 | G    |
| 20  | A     | 852 | C    |
| 20  | A     | 867 | U    |
| 20  | A     | 868 | U    |
| 20  | A     | 878 | C    |
| 20  | A     | 886 | U    |
| 20  | A     | 887 | G    |
| 20  | A     | 889 | G    |
| 20  | A     | 890 | A    |
| 20  | A     | 891 | A    |
| 20  | A     | 900 | G    |
| 20  | A     | 903 | G    |
| 20  | A     | 905 | G    |
| 20  | A     | 909 | U    |
| 20  | A     | 910 | G    |
| 20  | A     | 917 | C    |
| 20  | A     | 919 | A    |
| 20  | A     | 920 | G    |
| 20  | A     | 947 | G    |
| 20  | A     | 948 | A    |
| 20  | A     | 950 | A    |
| 20  | A     | 951 | A    |
| 20  | A     | 956 | C    |
| 20  | A     | 958 | A    |
| 20  | A     | 965 | U    |
| 20  | A     | 966 | U    |
| 20  | A     | 967 | C    |
| 20  | A     | 981 | A    |
| 20  | A     | 985 | A    |
| 20  | A     | 986 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 990  | G    |
| 20  | A     | 992  | G    |
| 20  | A     | 993  | A    |
| 20  | A     | 999  | A    |
| 20  | A     | 1001 | G    |
| 20  | A     | 1014 | A    |
| 20  | A     | 1023 | A    |
| 20  | A     | 1029 | G    |
| 20  | A     | 1036 | A    |
| 20  | A     | 1045 | C    |
| 20  | A     | 1049 | A    |
| 20  | A     | 1052 | U    |
| 20  | A     | 1053 | A    |
| 20  | A     | 1057 | G    |
| 20  | A     | 1062 | G    |
| 20  | A     | 1066 | A    |
| 20  | A     | 1070 | G    |
| 20  | A     | 1073 | U    |
| 20  | A     | 1075 | U    |
| 20  | A     | 1086 | A    |
| 20  | A     | 1087 | G    |
| 20  | A     | 1088 | A    |
| 20  | A     | 1092 | C    |
| 20  | A     | 1093 | U    |
| 20  | A     | 1149 | C    |
| 20  | A     | 1150 | G    |
| 20  | A     | 1151 | A    |
| 20  | A     | 1152 | G    |
| 20  | A     | 1167 | A    |
| 20  | A     | 1168 | A    |
| 20  | A     | 1170 | U    |
| 20  | A     | 1172 | U    |
| 20  | A     | 1173 | A    |
| 20  | A     | 1174 | C    |
| 20  | A     | 1175 | C    |
| 20  | A     | 1179 | G    |
| 20  | A     | 1182 | A    |
| 20  | A     | 1188 | A    |
| 20  | A     | 1209 | A    |
| 20  | A     | 1210 | C    |
| 20  | A     | 1212 | A    |
| 20  | A     | 1215 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 1217 | G    |
| 20  | A     | 1224 | G    |
| 20  | A     | 1257 | A    |
| 20  | A     | 1275 | G    |
| 20  | A     | 1284 | A    |
| 20  | A     | 1285 | G    |
| 20  | A     | 1287 | G    |
| 20  | A     | 1290 | A    |
| 20  | A     | 1293 | G    |
| 20  | A     | 1299 | A    |
| 20  | A     | 1305 | A    |
| 20  | A     | 1308 | G    |
| 20  | A     | 1309 | A    |
| 20  | A     | 1310 | A    |
| 20  | A     | 1317 | G    |
| 20  | A     | 1320 | A    |
| 20  | A     | 1336 | U    |
| 20  | A     | 1337 | A    |
| 20  | A     | 1350 | C    |
| 20  | A     | 1365 | U    |
| 20  | A     | 1373 | G    |
| 20  | A     | 1380 | U    |
| 20  | A     | 1388 | U    |
| 20  | A     | 1397 | G    |
| 20  | A     | 1398 | C    |
| 20  | A     | 1399 | C    |
| 20  | A     | 1401 | A    |
| 20  | A     | 1404 | G    |
| 20  | A     | 1406 | C    |
| 20  | A     | 1409 | A    |
| 20  | A     | 1411 | G    |
| 20  | A     | 1415 | U    |
| 20  | A     | 1420 | A    |
| 20  | A     | 1428 | G    |
| 20  | A     | 1429 | A    |
| 20  | A     | 1431 | A    |
| 20  | A     | 1432 | U    |
| 20  | A     | 1446 | G    |
| 20  | A     | 1447 | U    |
| 20  | A     | 1452 | G    |
| 20  | A     | 1453 | U    |
| 20  | A     | 1454 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 1455 | U    |
| 20  | A     | 1456 | G    |
| 20  | A     | 1457 | A    |
| 20  | A     | 1460 | A    |
| 20  | A     | 1461 | A    |
| 20  | A     | 1462 | U    |
| 20  | A     | 1469 | A    |
| 20  | A     | 1470 | C    |
| 20  | A     | 1471 | G    |
| 20  | A     | 1475 | U    |
| 20  | A     | 1487 | U    |
| 20  | A     | 1489 | C    |
| 20  | A     | 1491 | U    |
| 20  | A     | 1492 | G    |
| 20  | A     | 1493 | C    |
| 20  | A     | 1494 | G    |
| 20  | A     | 1495 | A    |
| 20  | A     | 1497 | U    |
| 20  | A     | 1501 | A    |
| 20  | A     | 1502 | G    |
| 20  | A     | 1503 | U    |
| 20  | A     | 1504 | G    |
| 20  | A     | 1505 | C    |
| 20  | A     | 1510 | C    |
| 20  | A     | 1519 | G    |
| 20  | A     | 1521 | G    |
| 20  | A     | 1525 | U    |
| 20  | A     | 1527 | A    |
| 20  | A     | 1528 | G    |
| 20  | A     | 1532 | A    |
| 20  | A     | 1535 | U    |
| 20  | A     | 1536 | A    |
| 20  | A     | 1539 | U    |
| 20  | A     | 1548 | C    |
| 20  | A     | 1551 | U    |
| 20  | A     | 1552 | A    |
| 20  | A     | 1559 | A    |
| 20  | A     | 1560 | G    |
| 20  | A     | 1567 | C    |
| 20  | A     | 1568 | G    |
| 20  | A     | 1573 | G    |
| 20  | A     | 1577 | A    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 1578 | A    |
| 20  | A     | 1584 | G    |
| 20  | A     | 1585 | U    |
| 20  | A     | 1586 | A    |
| 20  | A     | 1591 | A    |
| 20  | A     | 1593 | U    |
| 20  | A     | 1601 | G    |
| 20  | A     | 1605 | C    |
| 20  | A     | 1606 | A    |
| 20  | A     | 1612 | A    |
| 20  | A     | 1615 | A    |
| 20  | A     | 1624 | U    |
| 20  | A     | 1629 | A    |
| 20  | A     | 1630 | G    |
| 20  | A     | 1631 | A    |
| 20  | A     | 1632 | A    |
| 20  | A     | 1634 | A    |
| 20  | A     | 1635 | C    |
| 20  | A     | 1637 | A    |
| 20  | A     | 1638 | C    |
| 20  | A     | 1651 | A    |
| 20  | A     | 1653 | A    |
| 20  | A     | 1674 | G    |
| 20  | A     | 1686 | G    |
| 20  | A     | 1689 | A    |
| 20  | A     | 1690 | G    |
| 20  | A     | 1691 | C    |
| 20  | A     | 1717 | G    |
| 20  | A     | 1730 | G    |
| 20  | A     | 1734 | C    |
| 20  | A     | 1746 | G    |
| 20  | A     | 1756 | U    |
| 20  | A     | 1757 | U    |
| 20  | A     | 1758 | C    |
| 20  | A     | 1759 | G    |
| 20  | A     | 1762 | C    |
| 20  | A     | 1770 | G    |
| 20  | A     | 1777 | G    |
| 20  | A     | 1778 | G    |
| 20  | A     | 1787 | A    |
| 20  | A     | 1790 | G    |
| 20  | A     | 1796 | C    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 1798 | A    |
| 20  | A     | 1814 | C    |
| 20  | A     | 1815 | A    |
| 20  | A     | 1824 | A    |
| 20  | A     | 1826 | A    |
| 20  | A     | 1830 | A    |
| 20  | A     | 1837 | G    |
| 20  | A     | 1843 | A    |
| 20  | A     | 1853 | G    |
| 20  | A     | 1856 | G    |
| 20  | A     | 1861 | A    |
| 20  | A     | 1862 | A    |
| 20  | A     | 1864 | G    |
| 20  | A     | 1874 | U    |
| 20  | A     | 1876 | G    |
| 20  | A     | 1877 | G    |
| 20  | A     | 1884 | U    |
| 20  | A     | 1886 | G    |
| 20  | A     | 1887 | G    |
| 20  | A     | 1890 | A    |
| 20  | A     | 1894 | U    |
| 20  | A     | 1896 | A    |
| 20  | A     | 1910 | A    |
| 20  | A     | 1920 | G    |
| 20  | A     | 1927 | A    |
| 20  | A     | 1928 | C    |
| 20  | A     | 1930 | A    |
| 20  | A     | 1934 | C    |
| 20  | A     | 1936 | G    |
| 20  | A     | 1943 | G    |
| 20  | A     | 1944 | G    |
| 20  | A     | 1950 | A    |
| 20  | A     | 1969 | U    |
| 20  | A     | 1970 | U    |
| 20  | A     | 1977 | C    |
| 20  | A     | 1981 | C    |
| 20  | A     | 1984 | A    |
| 20  | A     | 1985 | A    |
| 20  | A     | 1986 | G    |
| 20  | A     | 1996 | U    |
| 20  | A     | 2001 | G    |
| 20  | A     | 2005 | U    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 2007 | U    |
| 20  | A     | 2035 | G    |
| 20  | A     | 2037 | A    |
| 20  | A     | 2044 | A    |
| 20  | A     | 2045 | A    |
| 20  | A     | 2046 | G    |
| 20  | A     | 2047 | A    |
| 20  | A     | 2050 | C    |
| 20  | A     | 2057 | C    |
| 20  | A     | 2065 | A    |
| 20  | A     | 2069 | C    |
| 20  | A     | 2070 | G    |
| 20  | A     | 2074 | A    |
| 20  | A     | 2075 | G    |
| 20  | A     | 2076 | A    |
| 20  | A     | 2080 | C    |
| 20  | A     | 2083 | G    |
| 20  | A     | 2107 | G    |
| 20  | A     | 2109 | G    |
| 20  | A     | 2112 | U    |
| 20  | A     | 2113 | U    |
| 20  | A     | 2208 | C    |
| 20  | A     | 2211 | U    |
| 20  | A     | 2212 | A    |
| 20  | A     | 2213 | A    |
| 20  | A     | 2216 | C    |
| 20  | A     | 2217 | G    |
| 20  | A     | 2218 | C    |
| 20  | A     | 2238 | G    |
| 20  | A     | 2239 | A    |
| 20  | A     | 2252 | G    |
| 20  | A     | 2253 | G    |
| 20  | A     | 2267 | G    |
| 20  | A     | 2277 | C    |
| 20  | A     | 2283 | A    |
| 20  | A     | 2293 | G    |
| 20  | A     | 2296 | G    |
| 20  | A     | 2297 | C    |
| 20  | A     | 2301 | A    |
| 20  | A     | 2302 | A    |
| 20  | A     | 2303 | G    |
| 20  | A     | 2317 | G    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 2319 | U    |
| 20  | A     | 2323 | A    |
| 20  | A     | 2331 | C    |
| 20  | A     | 2333 | A    |
| 20  | A     | 2334 | A    |
| 20  | A     | 2335 | G    |
| 20  | A     | 2336 | A    |
| 20  | A     | 2339 | G    |
| 20  | A     | 2340 | U    |
| 20  | A     | 2343 | A    |
| 20  | A     | 2348 | G    |
| 20  | A     | 2349 | A    |
| 20  | A     | 2361 | C    |
| 20  | A     | 2364 | C    |
| 20  | A     | 2393 | G    |
| 20  | A     | 2397 | G    |
| 20  | A     | 2399 | C    |
| 20  | A     | 2402 | A    |
| 20  | A     | 2404 | U    |
| 20  | A     | 2405 | G    |
| 20  | A     | 2416 | U    |
| 20  | A     | 2417 | C    |
| 20  | A     | 2418 | C    |
| 20  | A     | 2420 | C    |
| 20  | A     | 2436 | C    |
| 20  | A     | 2437 | U    |
| 20  | A     | 2439 | A    |
| 20  | A     | 2443 | G    |
| 20  | A     | 2445 | U    |
| 20  | A     | 2449 | A    |
| 20  | A     | 2455 | C    |
| 20  | A     | 2462 | A    |
| 20  | A     | 2473 | A    |
| 20  | A     | 2488 | C    |
| 20  | A     | 2492 | A    |
| 20  | A     | 2505 | U    |
| 20  | A     | 2512 | C    |
| 20  | A     | 2517 | A    |
| 20  | A     | 2518 | U    |
| 20  | A     | 2519 | G    |
| 20  | A     | 2521 | C    |
| 20  | A     | 2522 | G    |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 2532 | A    |
| 20  | A     | 2534 | C    |
| 20  | A     | 2542 | U    |
| 20  | A     | 2543 | G    |
| 20  | A     | 2548 | C    |
| 20  | A     | 2570 | C    |
| 20  | A     | 2580 | A    |
| 20  | A     | 2581 | G    |
| 20  | A     | 2587 | C    |
| 20  | A     | 2597 | G    |
| 20  | A     | 2599 | U    |
| 20  | A     | 2600 | C    |
| 20  | A     | 2616 | A    |
| 20  | A     | 2624 | C    |
| 20  | A     | 2627 | U    |
| 20  | A     | 2629 | U    |
| 20  | A     | 2650 | U    |
| 20  | A     | 2677 | G    |
| 20  | A     | 2699 | G    |
| 20  | A     | 2703 | U    |
| 20  | A     | 2719 | A    |
| 20  | A     | 2728 | G    |
| 20  | A     | 2740 | U    |
| 20  | A     | 2747 | A    |
| 20  | A     | 2749 | G    |
| 20  | A     | 2758 | G    |
| 20  | A     | 2762 | A    |
| 20  | A     | 2766 | C    |
| 20  | A     | 2773 | G    |
| 20  | A     | 2779 | A    |
| 20  | A     | 2780 | G    |
| 20  | A     | 2789 | A    |
| 20  | A     | 2792 | A    |
| 20  | A     | 2793 | U    |
| 20  | A     | 2794 | G    |
| 20  | A     | 2795 | A    |
| 20  | A     | 2804 | A    |
| 20  | A     | 2805 | U    |
| 20  | A     | 2809 | U    |
| 20  | A     | 2810 | U    |
| 20  | A     | 2812 | A    |
| 20  | A     | 2813 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 2815 | A    |
| 20  | A     | 2831 | G    |
| 20  | A     | 2836 | G    |
| 20  | A     | 2844 | A    |
| 20  | A     | 2846 | A    |
| 20  | A     | 2847 | U    |
| 20  | A     | 2870 | G    |
| 20  | A     | 2871 | A    |
| 20  | A     | 2878 | G    |
| 20  | A     | 2883 | G    |
| 20  | A     | 2891 | C    |
| 20  | A     | 2897 | G    |
| 20  | A     | 2904 | G    |
| 21  | B     | 7    | G    |
| 21  | B     | 10   | G    |
| 21  | B     | 11   | A    |
| 21  | B     | 13   | A    |
| 21  | B     | 20   | A    |
| 21  | B     | 23   | A    |
| 21  | B     | 24   | U    |
| 21  | B     | 27   | A    |
| 21  | B     | 33   | U    |
| 21  | B     | 35   | C    |
| 21  | B     | 54   | U    |
| 21  | B     | 55   | A    |
| 21  | B     | 57   | G    |
| 21  | B     | 67   | G    |
| 21  | B     | 70   | G    |
| 21  | B     | 73   | U    |
| 21  | B     | 74   | G    |
| 21  | B     | 75   | U    |
| 21  | B     | 78   | U    |
| 21  | B     | 79   | G    |
| 21  | B     | 83   | G    |
| 21  | B     | 85   | U    |
| 21  | B     | 86   | U    |
| 21  | B     | 87   | U    |
| 21  | B     | 91   | U    |
| 21  | B     | 97   | A    |
| 21  | B     | 98   | G    |
| 21  | B     | 99   | A    |
| 21  | B     | 101  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | B     | 106 | C    |
| 21  | B     | 107 | G    |
| 21  | B     | 114 | C    |

All (31) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | A     | 13   | U    |
| 20  | A     | 29   | A    |
| 20  | A     | 179  | A    |
| 20  | A     | 427  | A    |
| 20  | A     | 519  | A    |
| 20  | A     | 545  | G    |
| 20  | A     | 655  | G    |
| 20  | A     | 725  | A    |
| 20  | A     | 890  | A    |
| 20  | A     | 947  | G    |
| 20  | A     | 949  | U    |
| 20  | A     | 974  | A    |
| 20  | A     | 1022 | C    |
| 20  | A     | 1167 | A    |
| 20  | A     | 1431 | A    |
| 20  | A     | 1486 | A    |
| 20  | A     | 1584 | G    |
| 20  | A     | 1585 | U    |
| 20  | A     | 1590 | A    |
| 20  | A     | 1600 | C    |
| 20  | A     | 1604 | A    |
| 20  | A     | 1605 | C    |
| 20  | A     | 1861 | A    |
| 20  | A     | 2419 | G    |
| 20  | A     | 2444 | A    |
| 20  | A     | 2532 | A    |
| 20  | A     | 2811 | U    |
| 20  | A     | 2812 | A    |
| 21  | B     | 32   | U    |
| 21  | B     | 90   | C    |
| 21  | B     | 97   | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 29  | M     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | M     | 60:ARG    | C      | 61:LEU    | N      | 1.18         |

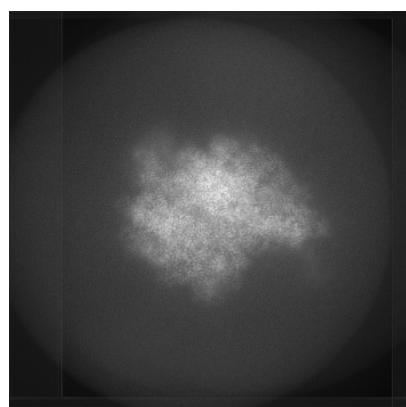
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21562. These allow visual inspection of the internal detail of the map and identification of artifacts.

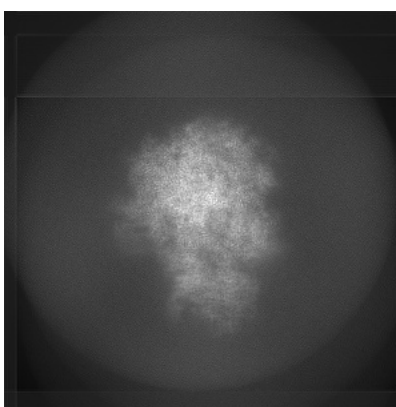
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

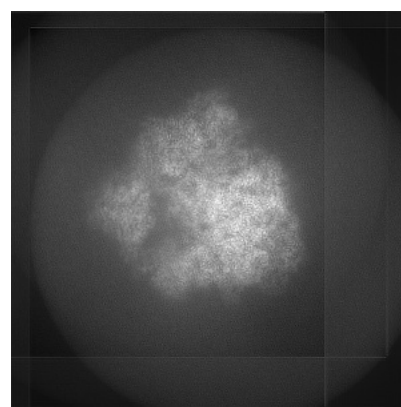
#### 6.1.1 Primary map



X



Y

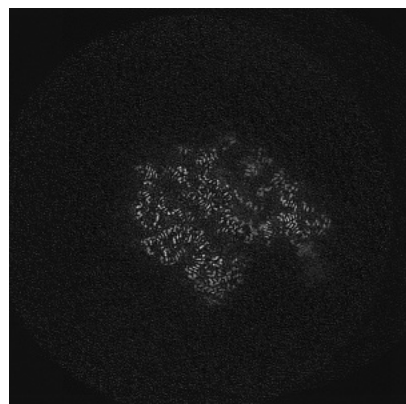


Z

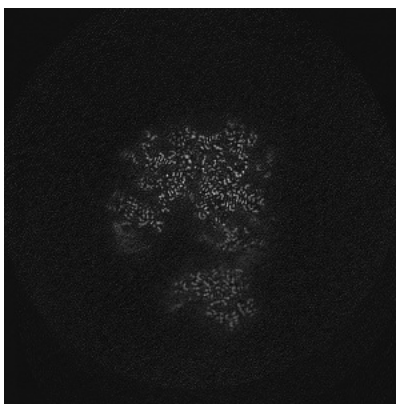
The images above show the map projected in three orthogonal directions.

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

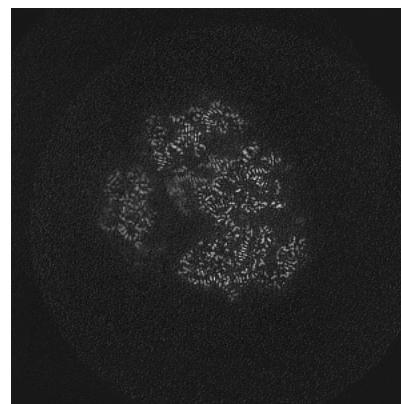
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

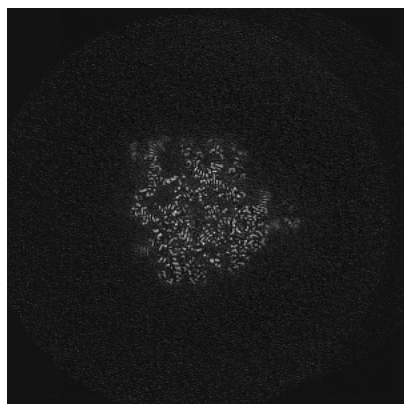


Z Index: 220

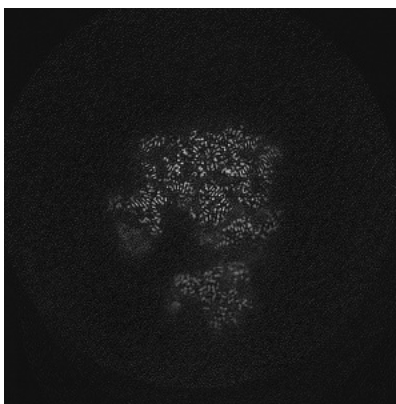
The images above show central slices of the map in three orthogonal directions.

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

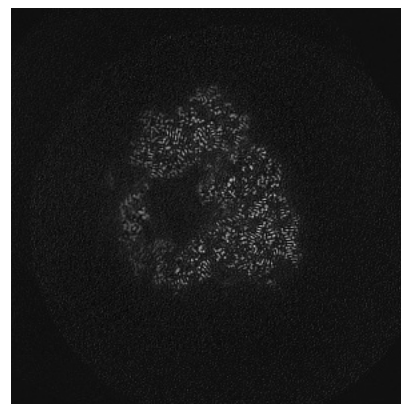
### 6.3.1 Primary map



X Index: 258



Y Index: 228



Z Index: 205

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

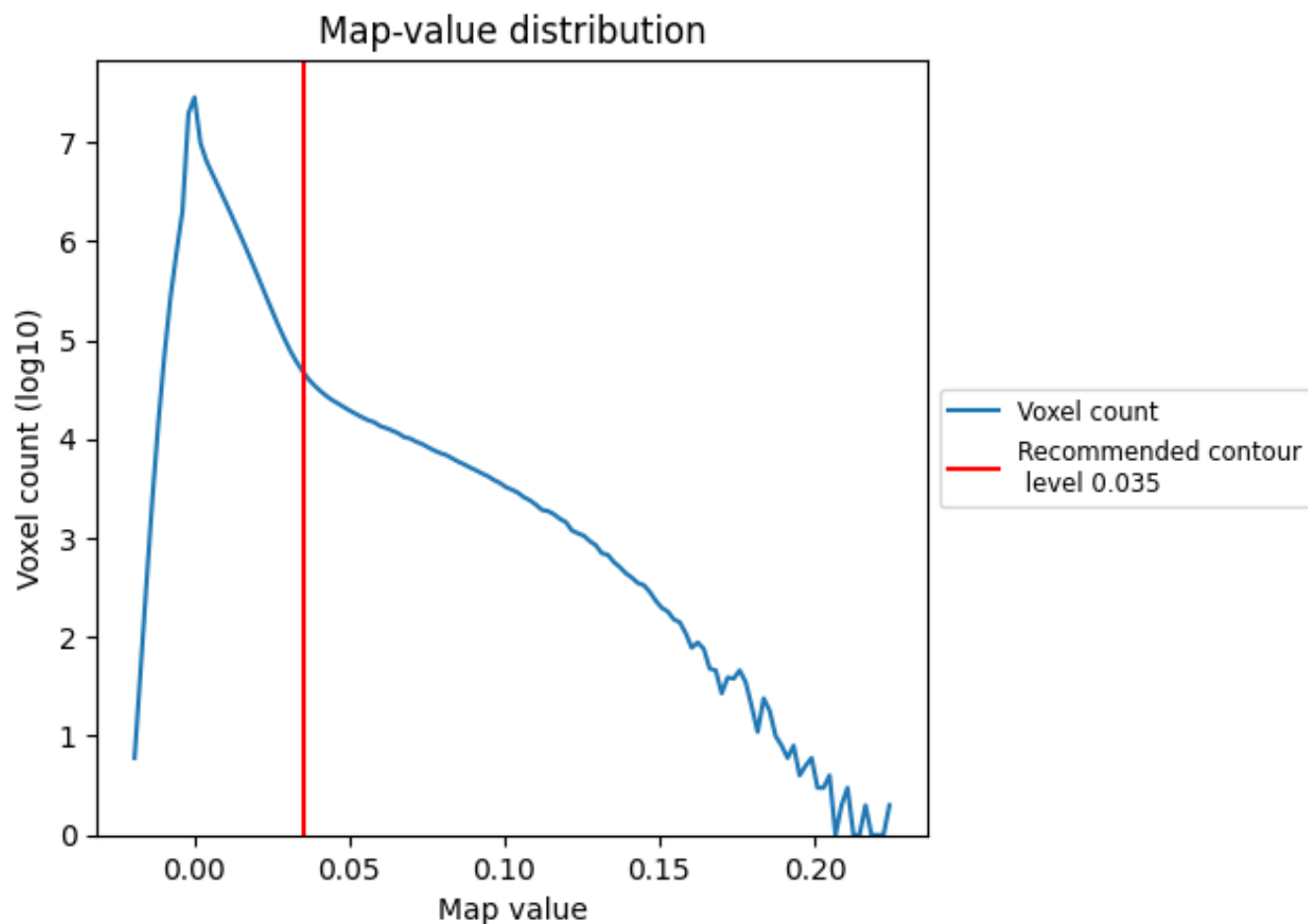
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

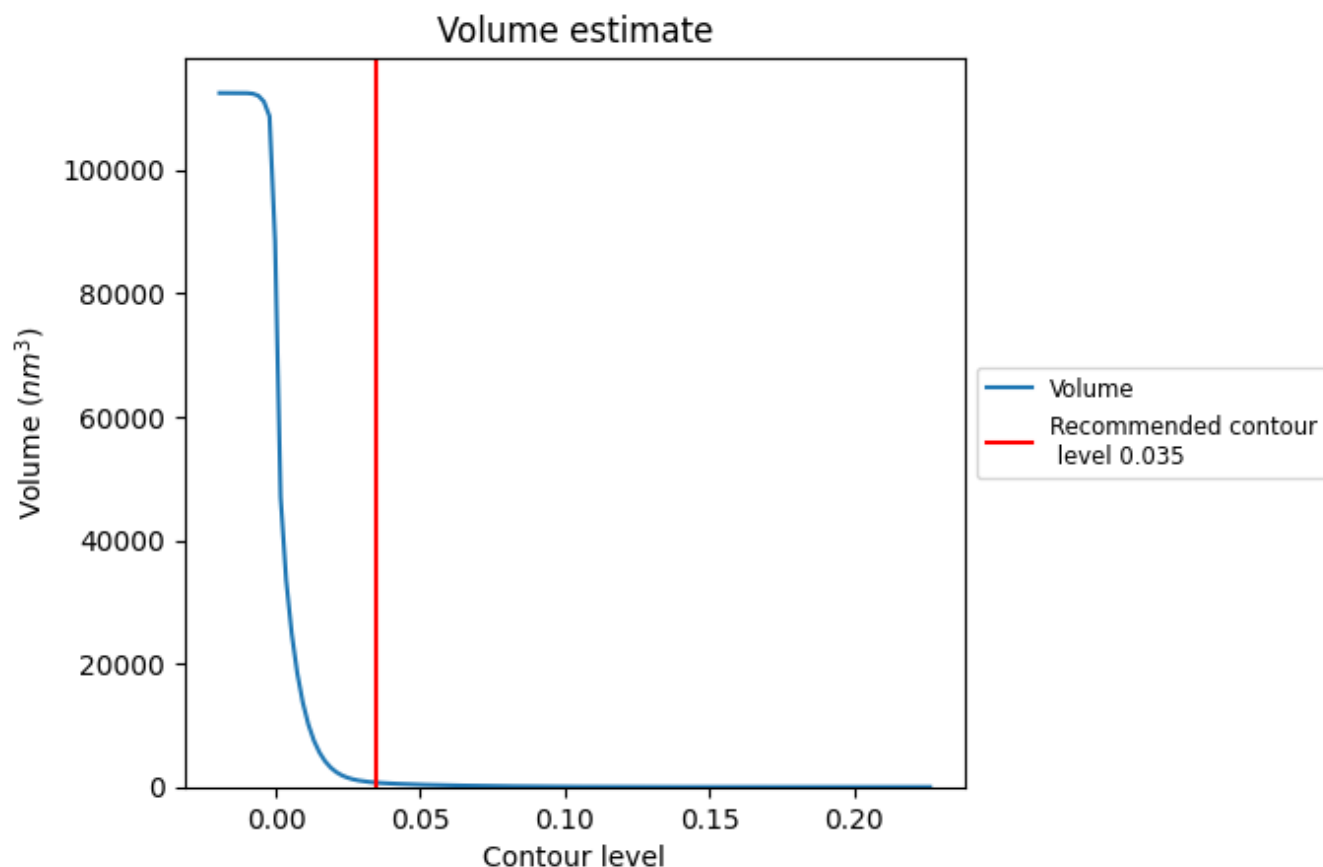
This section contains the results of statistical analysis of the map.

### 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](#)

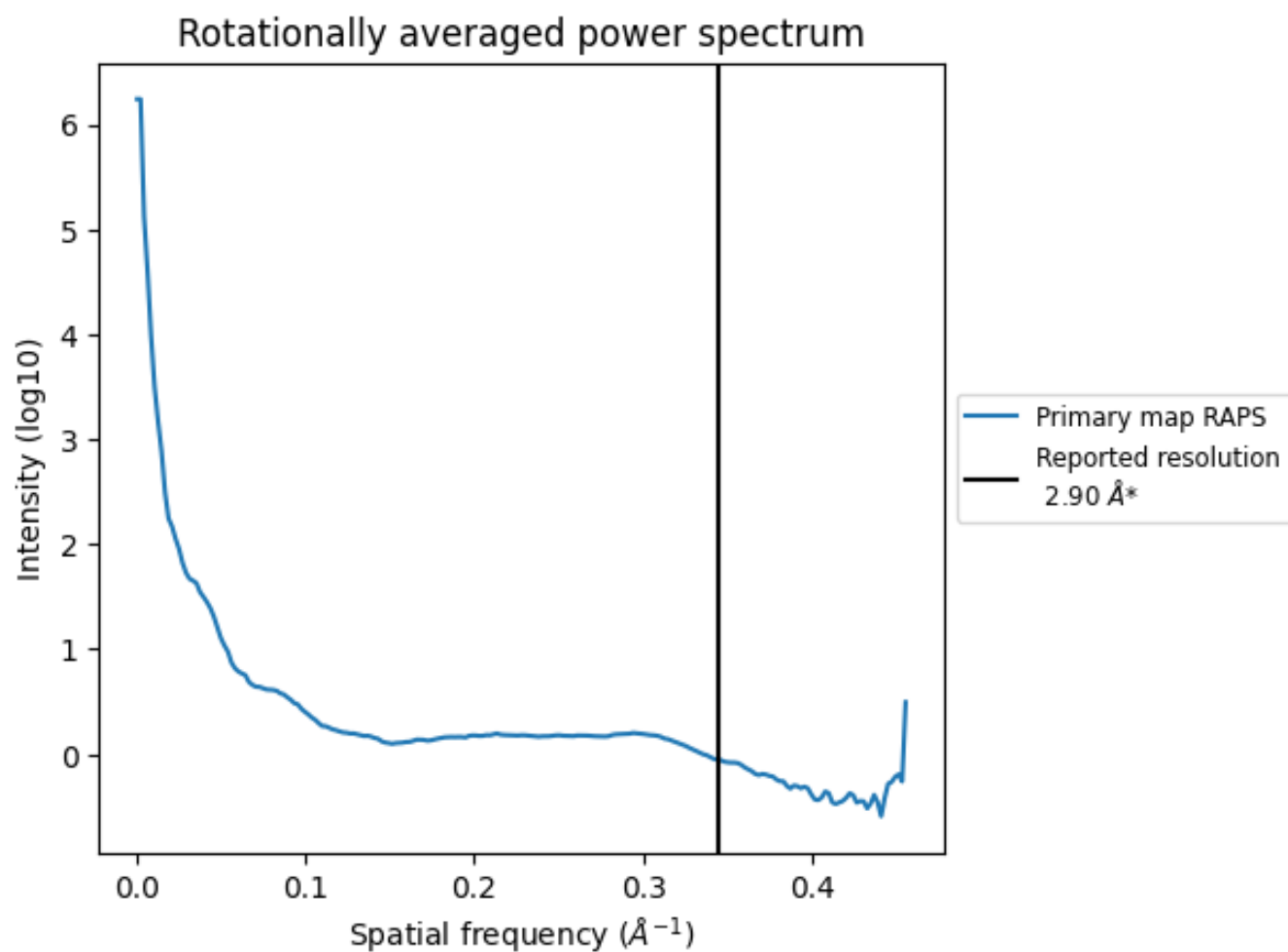


The volume at the recommended contour level is 697  $\text{nm}^3$ ; this corresponds to an approximate mass of 629 kDa.

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 0.345 Å<sup>-1</sup>

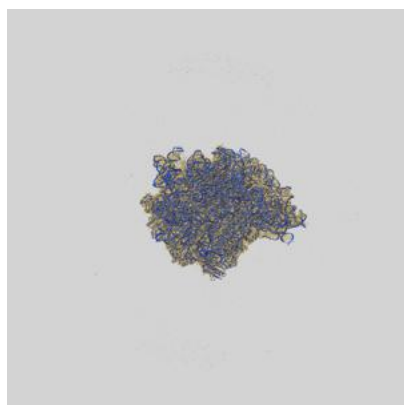
## 8 Fourier-Shell correlation

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

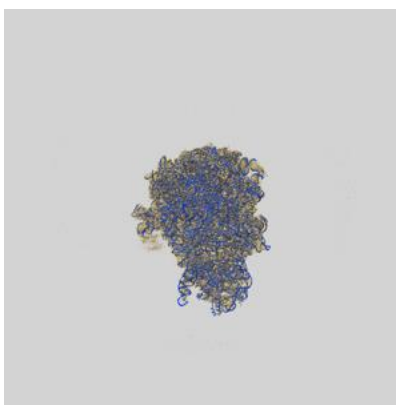
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21562 and PDB model 6W6P. Per-residue inclusion information can be found in section [3](#) on page [13](#).

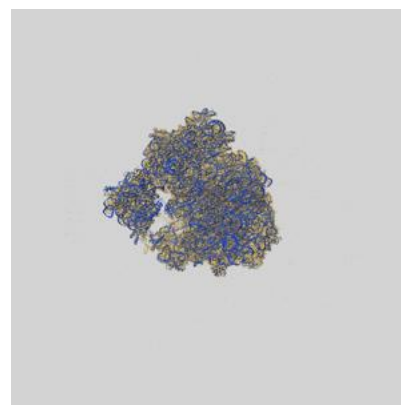
### 9.1 Map-model overlay [i](#)



X



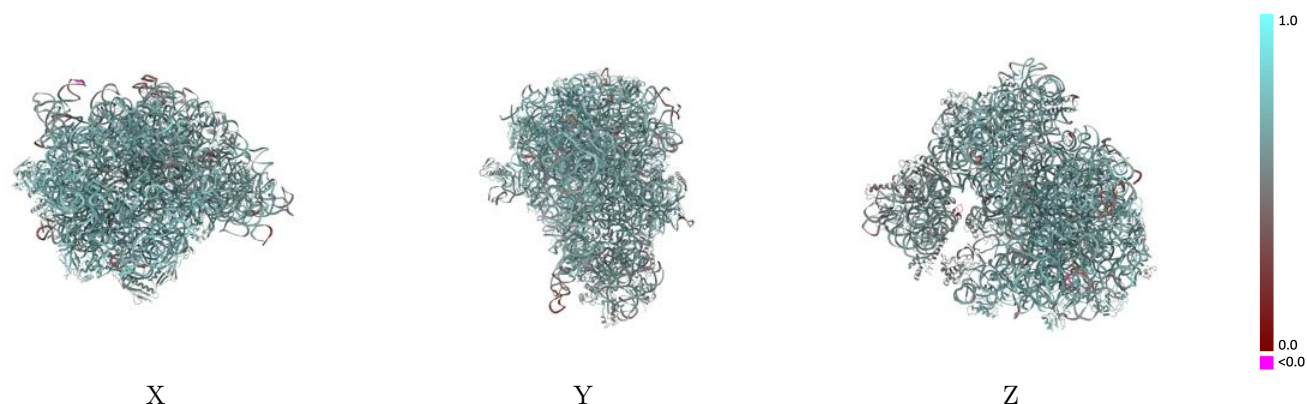
Y



Z

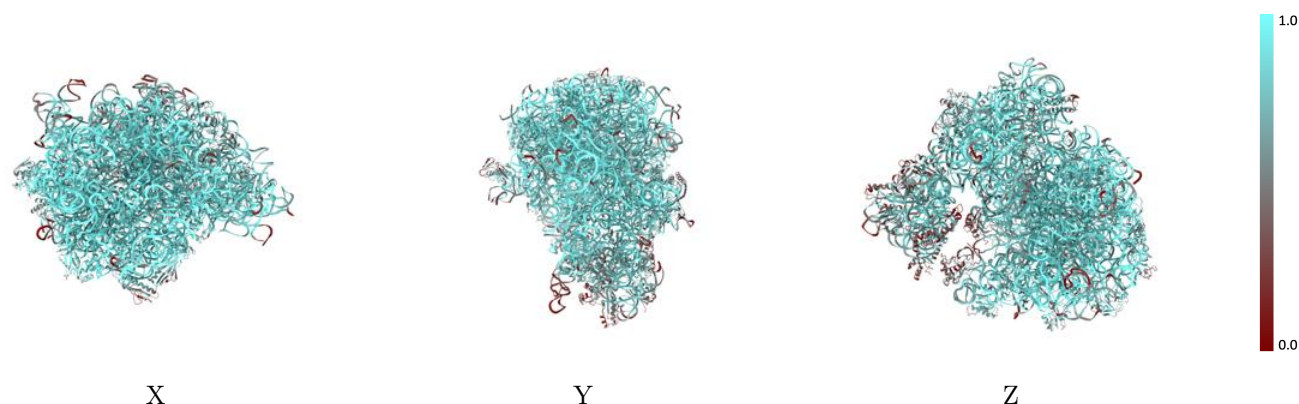
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



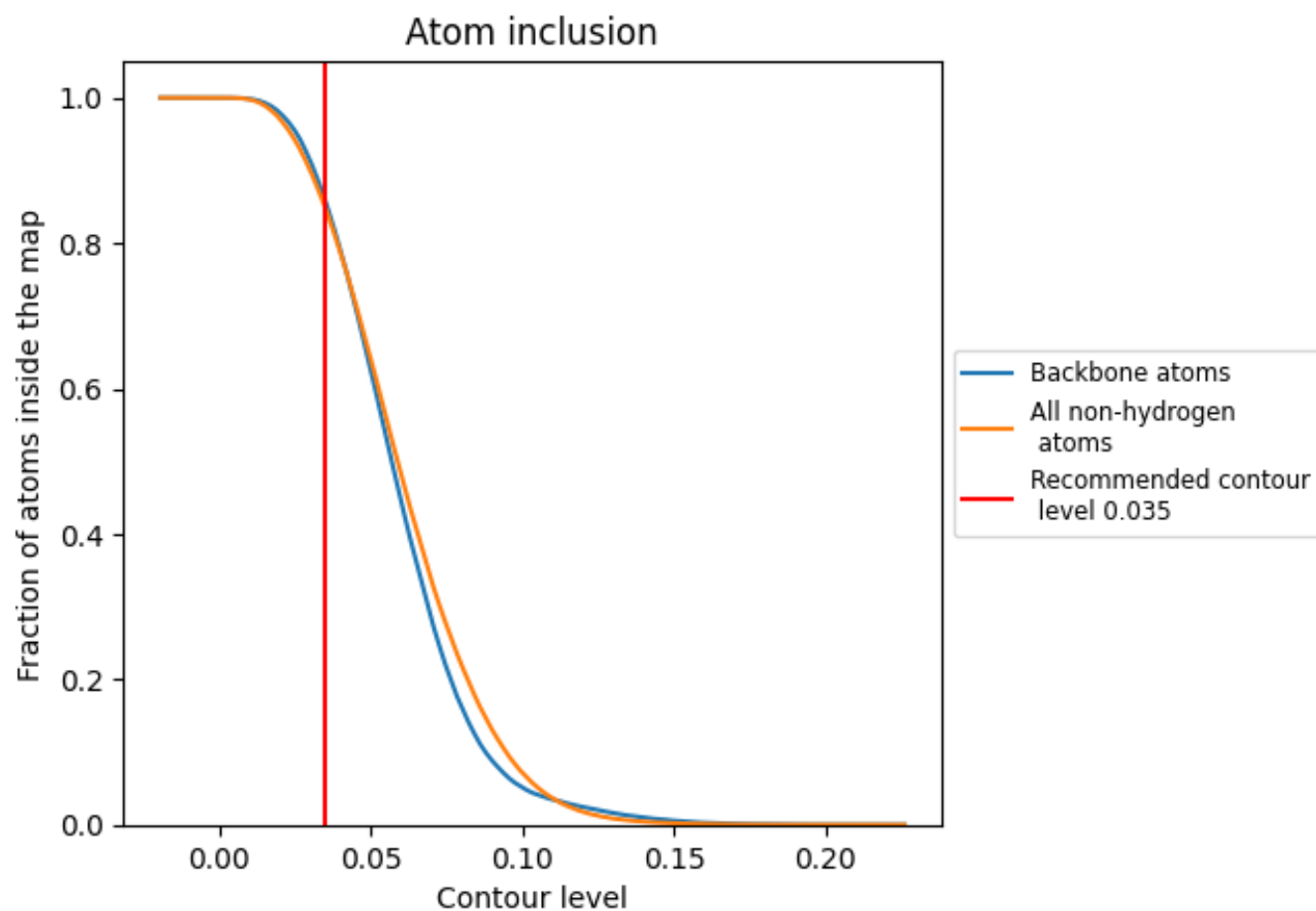
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.035) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8488   |  0.6270   |
| 0     |  0.8298   |  0.6450   |
| 2     |  0.8976   |  0.6810   |
| 3     |  0.7401   |  0.6580   |
| 4     |  0.9573   |  0.7020   |
| 5     |  0.9356   |  0.6980   |
| 6     |  0.9220   |  0.6660   |
| A     |  0.9221   |  0.6510   |
| B     |  0.8040   |  0.5900   |
| C     |  0.9159   |  0.6770   |
| D     |  0.9014   |  0.6830   |
| E     |  0.8456   |  0.6580   |
| F     |  0.3599   |  0.4980   |
| G     |  0.5632   |  0.5650   |
| K     |  0.9059  |  0.6680  |
| L     |  0.8807 |  0.6610 |
| M     |  0.8047 |  0.6510 |
| N     |  0.7924 |  0.6310 |
| O     |  0.8681 |  0.6490 |
| P     |  0.7197 |  0.6140 |
| Q     |  0.8725 |  0.6590 |
| R     |  0.9238 |  0.6850 |
| S     |  0.8119 |  0.6500 |
| T     |  0.8776 |  0.6690 |
| U     |  0.8255 |  0.6440 |
| V     |  0.6281 |  0.5900 |
| X     |  0.9099 |  0.6830 |
| Y     |  0.7651 |  0.6380 |
| Z     |  0.7114 |  0.6210 |
| a     |  0.8681 |  0.6050 |
| c     |  0.5058 |  0.5560 |
| d     |  0.6654 |  0.5800 |
| e     |  0.6689 |  0.5920 |
| f     |  0.5438 |  0.5670 |
| g     |  0.3162 |  0.5080 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| h     |  0.7451 |  0.6190 |
| i     |  0.5731 |  0.5630 |
| j     |  0.5122 |  0.5310 |
| k     |  0.4870 |  0.5420 |
| l     |  0.7490 |  0.5950 |
| m     |  0.4850 |  0.5230 |
| n     |  0.7916 |  0.6020 |
| o     |  0.7139 |  0.5900 |
| p     |  0.8046 |  0.6280 |
| q     |  0.6863 |  0.6100 |
| r     |  0.6712 |  0.5980 |
| s     |  0.6565 |  0.5550 |
| t     |  0.7442 |  0.6140 |